

Name of the Paper : Quantum Mechanics and Applications  
 Name of the Course : B.Sc. (Hons.) Physics (CBCS)  
 Semester : V  
 Duration : 3 hours  
 Maximum Marks : 75 [alllabexperiments.com](http://alllabexperiments.com)

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1. Attempt any *five* of the following:

(a) Give the expressions for Energy, Linear momentum and Angular momentum in operator form.

Ans.  $\hat{p}$  is given in the position representation by

$$\hat{p} = -i\hbar \nabla$$

Its Cartesian are

$$\hat{P}_x = -i\hbar \frac{\partial}{\partial x}, \hat{P}_y = -i\hbar \frac{\partial}{\partial y}, \hat{P}_z = -i\hbar \frac{\partial}{\partial z}.$$

• **Energy**

The total energy E for time dependant systems is associated to the operator:

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

• **Angular momentum**

In the Schrodinger Representation, use Q.M operators for x and p, etc.

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

Substituting

$$\vec{J} = -i\hbar \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \end{vmatrix}$$

$$J_x = -i\hbar \left( y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)$$

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

$$J_y = -i\hbar \left( z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right)$$

(b) Calculate the commutator  $[\hat{L}_x, \hat{p}_x]$  (given  $[\hat{x}, \hat{p}_x] = i\hbar$ )

Ans.

$$[\hat{L}_x, \hat{p}_x]$$

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y$$

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$$\text{so } [\hat{L}_x, \hat{p}_x] = [\hat{y}\hat{p}_z, \hat{p}_x] - [\hat{z}\hat{p}_y, \hat{p}_x]$$

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

$$[\hat{z}, \hat{p}_x] = 0 \text{ and } [\hat{p}_y, \hat{p}_x] = 0$$

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$$\text{so } [\hat{L}_x, \hat{p}_x] = 0$$

(c) Explain uncertainty principle with an example.

Ans. Heisenberg's uncertainty principle

In its original form, Heisenberg's uncertainty principle states that: If the x-component of the momentum of a particle is measured with an uncertainty  $\Delta p_x$ , then its x-position cannot, at the same time, be measured more accurately

than  $\Delta x \cdot \Delta p_x = \frac{h}{4\pi}$ . The three-dimensional form of the uncertainty relation for position and momentum can be written as follows:

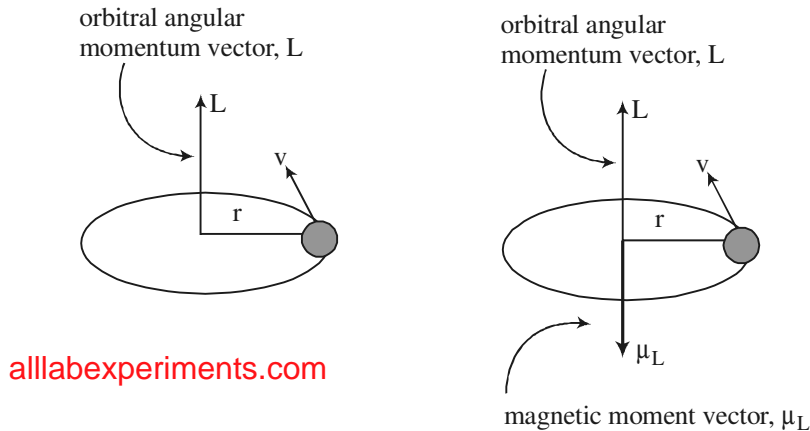
$$\Delta x \Delta p_x \geq \frac{\hbar}{2}, \Delta y \Delta p_y \geq \frac{\hbar}{2}, \Delta z \Delta p_z \geq \frac{\hbar}{2}$$

For example, electron spins around the orbital near speed of light, so for an observer if he calculates the momentum of the electron he would be uncertain about its position because by the time electron will move forward... as it takes time for the light to return and if he can fix the position of the electron he cannot specify the momentum as right the next moment the direction has changed.

(d) Derive the relation between 'magnetic' dipole moment' and 'orbital angular momentum' of an electron revolving around a nucleus.

Ans. Based on classical physics, the current,  $I$ , is nothing but charge per unit time and is expressed as

$$I = \frac{q}{t} \quad \dots(1)$$



The time is nothing but the circumference divided by the velocity of  $2\pi r / v$  electron, i.e.  $t = \frac{2\pi r}{v}$  which can be substituted in equation (1) to yield

$$I = \frac{qv}{2\pi r}$$

where  $r$  is the radius of the orbital.

Therefore, the orbital magnetic  $\mu$  moment orbit, which is a product of current,  $I$  and area,  $A = \pi r^2$  can be expressed as

$$\mu_{\text{orbit}} = A \cdot I = \pi r^2 \cdot q \cdot \frac{v}{2\pi r} = \frac{qvr}{2}$$

$$\mu_{\text{orbit}} = -\frac{e}{2m} \cdot J_{\text{orbit}} \quad \dots(2)$$

where  $q$  is the charge of electron which equals to  $-e$ ;  $v$  is velocity of electron;  $m$  is the mass of electron and  $J$  the angular momentum which is equal to  $mvr$ .

(e) Write the quantum numbers for the state represented by  $4^2F_{5/2}$ .

Ans.  $4^2F_{5/2}$ , Quantum number are given as,

$$n = 4, l = 3, j = 5/2.$$

$$m_j = -\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, +\frac{1}{2}, +\frac{3}{2}, +\frac{5}{2}$$

(f) What are symmetric and antisymmetric wave functions?

Ans. Symmetric wave function

symmetric wave function does not change its sign when I change the labeling of the particles, which means for example

$$\varphi(t, x_1, x_2, \dots, x_n) = \psi(t, x_2, x_1, \dots, x_n)$$

Such wave function belong to the particles called bosons.

### Antisymmetric wave function

An antisymmetric wave function, belonging to the particles called fermions, gets a minus when you inter change two particle labels, likewise  $\varphi(t, x_1, x_2, \dots, x_n) = -\psi(t, x_2, x_1, \dots, x_n)$ .

Only those two possibility may exist because the square of the wave function  $|\psi|^2$  must be unchanged if you only exchange particle labels, because particles.

**(g) What are free and bound states ? Explain.**

**Ans. Free state/free particle**

In the absence of an external potential, the time-dependent schrodinger equation describes the propagation of travelling waves. In one dimension, the corresponding complex wavefunction has the form

$$\Psi(x, t) = Ae^{i(kx - \omega t)}$$

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where A is the amplitude, and  $E(k) = \hbar\omega(k) = \frac{\hbar^2 k^2}{2m}$  represents the free particle energy dispersion for a nonrelativistic particle of mass,  $m$ , and wave vector  $k = 2\pi/\lambda$  with  $\lambda$  the wavelength. Each wavefunction describes a plane wave in which the particle has definite energy  $E(k)$  and, in accordance with the de Broglie relation, momentum  $p = \hbar k = \hbar/\lambda$ . The energy spectrum of a freely-moving particle is therefore continuous, extending from zero to infinity and, apart from the spatially constant state  $k = 0$ , has a two-fold degeneracy corresponding to right and left moving particles.

### Bound state

In quantum physics, a bound state is a special quantum state of a particle subject to a potential such that the particle has a tendency to remain localised in on or more regions of space. The potential may be external or it may be the results of the presence of another particle.

### Example:

A proton and an electron can move separately; when they do, the total center-of-mass energy is positive, and such a pair of particles can be described as an ionized atom. Once the electron starts to "orbit" the proton, the energy becomes negative, and a bound state- namely the hydrogen atom- is formed. Only the lowest -energy bound state, the ground state, is stable. Other excited states are unstable and will decay into stable (but not other unstable) bound states with less energy by emitting a photon.

2. Consider a particle trapped inside a one- dimensional finite square well. Solve the time independent schrodinger equation for the system and obtain state eigenfunctions. Discuss how the energy levels are obtained graphically ?

**Ans. One dimensional finite square well**

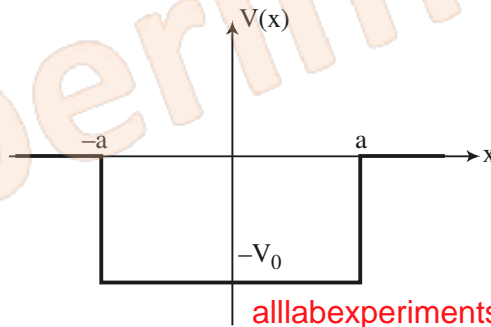
consider the finite square well

$$V(x) = \begin{cases} -V_0, & \text{for } -a < x < a, \\ 0, & \text{for } |x| > a, \end{cases} \quad \text{where } V_0 \text{ is a (positive) constant} \quad \dots(1)$$

The finite square well admits both bound states as well scattering states. We will consider the case of bound states only.

In the region  $x < -a$  the potential is zero, so the schrodinger equation reads

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi, \text{ or } \frac{d^2\psi}{dx^2} = k^2\psi.$$



where

$$k = \frac{\sqrt{-2mE}}{\hbar} \quad \dots(2)$$

is real and positive. The general solution is  $\psi(x) = A \exp(-kx) + B \exp(kx)$ , but the first term blows up (as  $x \rightarrow -\infty$ ), so the physically admissible solution (as before -see equation 2.101) is

$$\psi(x) = B e^{kx}, \quad \text{for } (x < -a) \quad \dots(3)$$

In the region  $-a < x < a$ ,  $V(x) = -V_0$ , and the schrodinger equation reads

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} - V_0\psi = E\psi, \quad \frac{d^2\psi}{dx^2} = -l^2\psi,$$

where

$$l \equiv \frac{\sqrt{2m(E + V_0)}}{\hbar} \quad \dots(4)$$

Although  $E$  is negative, for a bound state, it must be greater than  $-V_0$

$$\psi(x) = C \sin(lx) + D \cos(lx), \text{ for } (-a < x < a), \quad \dots(5)$$

where  $C$  and  $D$  are arbitrary constants. Finally, in the region  $x > a$  the potential is again zero: the general solution is  $\psi(x) = F \exp(-kx) + G \exp(kx)$ , but the second term blows up (as  $x \rightarrow \infty$ ), so we are left with

[alllabexperiments.com](http://alllabexperiments.com)  $\psi(x) = F e^{-kx}, \text{ for } (x > a) \quad \dots(6)$

The next step is to impose boundary condition:  $\psi$  and  $d\psi/dx$  continuous at  $-a$  and  $+a$ . But we can save a little time by noting that this potential is an even function, so we can assume with no loss of generality that the solution are either even or odd

The advantage is that we need only impose the boundary conditions on one side (say  $x=+a$ ), the other side is then automatic since wavefunction is symmetric. Even solutions will be worked out here. So we are looking for the solutions of the form,

$$\psi(x) = \begin{cases} F e^{-kx} & \text{for } (x > a), \\ D \cos(lx), & \text{for } (0, xa), \\ \psi(-x), & \text{for } (x < 0) \end{cases} \quad \dots(7)$$

The continuity of  $\psi(x)$ , at  $x=a$ , says

$$F e^{-ka} = D \cos(la). \quad \dots(8)$$

and the continuity of  $d\psi/dx$  says

$$-k F e^{-ka} = -D \sin(la). \quad \dots(9)$$

Dividing equation 2.135 by equation 2.134, we find that

$$k = l \tan(la). \quad \dots(10)$$

Equation 2.136 is a formula for the allowed energy, since  $k$  and  $l$  are both functions of  $E$ . To solve for  $E$ , it pays to adopt some nicer notation. Let

$$z \equiv la, \quad z_0 \equiv \frac{a}{\hbar} \sqrt{2mV_0}. \quad \dots(11)$$

According to equations 2.128 and 2.130,  $(k^2 l^2) = 2mV_0 / \hbar^2$ , so  $ka = \sqrt{z_0^2 - z^2}$ , and equation 2.136 reads

$$\tan z = r(z_0 / z)^2 - 1. \quad \dots(12)$$

This is a transcendental equation for  $z$  (and hence for  $E$ ) as a function of  $z_0$  (which is a measure of the "size" of the well). It can be solved numerically, using a calculator or a computer, or graphically, by plotting  $\tan z$  and

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$\sqrt{(z_0/z)^2 - 1}$  on the same grid, and looking for points of intersection (see figure 2.13). Two limiting cases are of special interest:

**1. Wide, deep well.** If  $z_0$  is very large, the intersections occur just slightly below  $z_n = n\pi/2$ , with  $n$  odd: it follows that

$$\text{allabexperiments.com} \quad E_n + V_0 \cong \frac{n^2 \pi^2 \hbar^2}{2m(2a)^2} \quad \dots(13)$$

Here  $(E + V_0)$  is the energy above the bottom of the well, and on the right we have precisely the infinite square well energies, for a well of width  $2a$  - or rather, half of them, since  $n$  is odd. (The other ones, of course, come from the odd wave functions, as you'll find in problem 2.28) So the finite square well goes over to the infinite square well, as  $V_0 \rightarrow \infty$ ; however, for any finite  $V_0$  there are only finitely many bound states.

**2. Shallow, narrow well.** As  $z_0$  decreases, there are fewer and fewer bound states, until finally (for  $z_0 < \pi/2$ , where the lowest odd state disappears) only one remains. It is interesting to note, however, that there is always one bound state, no matter how "weak" the well becomes.

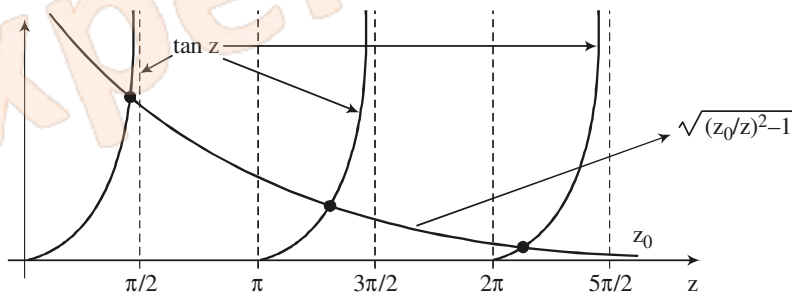


Figure: Graphical solution to equation 12, for  $z_0 =$  (even states).

**3. (a) Calculate the expectation value of the momentum for wavefunction.**

Ans. 
$$\Psi = \begin{cases} \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) & \text{for } 0 < |x| < a \\ 0 & \text{for } |x| > a \end{cases}$$

Expectation value of any observable is given as,

$$\langle \hat{Q} \rangle = \langle \psi | \hat{Q} | \psi \rangle$$

with  $|\psi\rangle$  a normalized state vector so expectation value of nomination is given by,

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$$\begin{aligned}
 \hat{p} &= \langle \psi | -i\hbar \frac{\partial}{\partial x} | \psi \rangle \\
 &= \frac{2}{a} \int_0^a \sin \frac{\pi x}{a} (-i\hbar \frac{\partial}{\partial x}) \sin \frac{\pi x}{a} \\
 &= -\frac{2}{a} i\hbar \frac{\pi}{a} \int_0^a \sin \frac{\pi x}{a} \cos \frac{\pi x}{a} \\
 &= -\frac{2i\hbar\pi}{a^2} \int_0^a \frac{1}{2} \sin \frac{2\pi x}{a} \\
 &= -\frac{i\hbar\pi}{a^2} \left[ \cos \frac{2\pi x}{a} \right]_0^a \times \frac{a}{2\pi} \\
 &= \frac{i\hbar}{2a} [\cos 2\pi - \cos 0] = 0
 \end{aligned}$$

(b) Give the theory to explain spreading of a gaussian wave packet for a free particle in one dimension.

Ans. Evolution of a free gaussian wave packet

Consider a free particle which is described at  $t=0$  by the normalized Gaussian wave function

$$\Psi(x,0) = \left(\frac{2a}{\pi}\right)^{1/4} e^{-ax^2}$$

The normalization factor is easy to contain. We wish to find its time evolution. We expand the given wave function in terms of the energy eigenfunctions and we know how individual energy eigenfunctions evolve. We then reconstruct the wave function at a later time  $t$  by superposing the parts with appropriate phase factors.

It is straight forward to find  $\Phi(k,0)$  the Fourier transform of  $\psi(x,0)$ :

$$\psi(x,0) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} \Phi(k,0) e^{ikx}$$

Recall that the Fourier transforms of a gaussian is a gaussian.

$$\phi(k) \equiv \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} \psi(x,0) e^{-ikx} \quad \text{Support by Donating} \quad \dots(1.1)$$

$$= \frac{1}{\sqrt{2\pi}} \left(\frac{2a}{\pi}\right)^{1/4} \int_{-\infty}^{\infty} dx e^{-ikx} e^{-ax^2} = \left(\frac{1}{2\pi a}\right)^{1/4} e^{-\frac{k^2}{4a}} \quad \dots(1.2)$$



What this is that the gaussian spatial wave function is a superposition of different momenta with the probability of finding the momentum between  $k_1$  and  $k_1 + dk$  being proportional to  $\exp(-k_1^2/2a) dk$ .

So the initial wave function is a superposition of different plane waves with different coefficients (usually called amplitudes). Note that  $\exp ikx$  for each real  $k$  is also an eigenfunction of the Hamiltonian with eigenvalue

$$E_k = \frac{\hbar^2 k^2}{2m}. \text{ Therefore, we know that } \exp(ikx) \text{ evolves in time with a time}$$

dependance given by  $e^{-iE_k t/\hbar}$ . So the time -evolved state.  $\psi(x, t)$ , is given by

$$\psi(x, t) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} \phi(k) e^{ikx} e^{-iE_k t/\hbar} \quad \dots(1.3)$$

$$= \left(\frac{1}{2\pi a}\right)^{1/4} \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} e^{-\frac{k^2}{4a}} e^{-iE_k t/\hbar} e^{ikx} \quad \dots(1.4)$$

where we know  $E_k$  and this integral has to be done.

The exponential has an argument given by

$$-\frac{k^2}{4a} \left[1 + \frac{2i\hbar a t}{m}\right] = -\frac{bk^2}{2} \text{ where } b = \frac{1}{2a} \left(1 + \frac{2i\hbar a t}{m}\right)$$

Thus the integral to be done is

$$\left(\frac{1}{2\pi a}\right)^{1/4} \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} e^{-bk^2/2} e^{ikx}$$

and this can be done in the usual way in spite of the fact that  $b$  is complex since the integral is well - defined, using

$$\int_{-\infty}^{\infty} dk e^{-bk^2/2} e^{ikx} = \sqrt{\frac{2\pi}{b}} e^{-\frac{x^2}{2b}} \quad \dots(1.5)$$

the result 
$$\psi(x, t) = \left(\frac{1}{2\pi a}\right)^{1/4} \sqrt{\frac{1}{b}} e^{-\frac{x^2}{2b}} \quad \dots(1.6)$$

$$= \left(\frac{2a}{\pi}\right)^{1/4} \frac{1}{\sqrt{1 + \frac{2i\hbar a t}{m}}} \exp\left[-\frac{ax^2}{(1 + \frac{2i\hbar a t}{m})}\right] \quad \dots(1.7)$$

The probability density is given by (after a wee bit of algebra)

$$|\psi(x,t)|^2 = \sqrt{\frac{2a}{\pi}} \frac{1}{\sqrt{1 + \left(\frac{2\hbar at}{m}\right)^2}} e^{-\frac{2ax^2}{1 + \left(\frac{2\hbar at}{m}\right)^2}} \quad \dots(1.8)$$

from which we can read off

$$\langle x^2 \rangle = \frac{1}{4a} \left[ 1 + \left(\frac{2\hbar at}{m}\right)^2 \right] \quad \dots(1.9)$$

Note that the initial width  $\frac{1}{4a}$  increase quadratically as a function of time.

To understand this result it is useful to rewrite it. We note that since  $\langle 0 | x^2 | 0 \rangle = 0$  we have the initial  $\langle x^2 \rangle$  is  $1/(4a)$ . Let us call this  $\sigma_0^2 = 1/(4a)$ . ub a great notational leap forward. So the width at time  $t$  is given by (chasing the factors of  $a$  and replacing them by  $\sigma_0^2/2$ )

$$\langle x^2 \rangle_t = \sigma_x^2(t) = \sigma_0^2 + \frac{\hbar^2 t^2}{4m^2 \sigma_0^2} \quad (1.10)$$

Now we note that the uncertainty in the momentum can be read off from the wave function in  $k$ -space. Since  $\phi(k)$  is gaussian we find

$$\langle k^2 \rangle = \text{and hence } \sigma_p^2 = \hbar^2 a = \frac{\hbar^2}{4\sigma_0^2} \quad \text{alllabexperiments.com}$$

where we have rewritten  $a$  in terms of  $\sigma_0$  and used the de Broglie relation.

$$\text{Therefore, } \sigma_x^2(t) = \sigma_0^2 + \frac{\sigma_p^2 t^2}{m^2} \quad (1.11)$$

So the initial uncertainty in the position increases with an extra part which can be thought of as follows:  $\sigma_p t / m$  is the distance traveled by a classical particle with momentum equal to the uncertainty  $\sigma_p$  in a time  $t$ . So for  $t \ll \sigma_0 / (\sigma_p / m)$  the width remains unchanged.

**4. (a) Solve the Schrodinger equation for a Linear Harmonic Oscillator and sine obtain first three eigenfunctions.**

**Ans.** The quantum problem is to solve the Schrodinger equation for the potential.

$$V(x) = \frac{1}{2}m\omega^2 x^2 \quad \dots(1)$$

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$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2 \psi = E\psi.$$

Things look a little cleaner if we introduce the dimensionless variable

$$\xi \equiv \frac{\sqrt{m\omega}}{\hbar} x; \quad \dots(2)$$

in terms of  $\xi$ , the Schrodinger equation reads

$$\frac{d^2\psi}{d\xi^2} = (\xi^2 - K)\psi, \quad \dots(3)$$

where  $K$  is the energy, in units of  $(1/2) \hbar\omega$ :

$$K \equiv \frac{2E}{\hbar\omega}$$

Our problem is to solve equation 2.56, and in the process obtain the allowed" values of  $K$  (and hence of  $E$ ).

To begin with, note that at very large  $\xi$  (which is to say, at very large  $x$ )  $\xi^2$  completely dominates over the constant  $K$ , so in this regime

$$\frac{d^2\psi}{d\xi^2} \approx \xi^2 \psi, \quad \text{alllabexperiments.com} \quad \dots(4)$$

which has the approximate solution (check it;)

$$\psi(\xi) \approx Ae^{-\xi^2/2} + Be^{+\xi^2/2}. \quad \dots(5)$$

The  $B$  term is clearly not normalizable (it blows up as  $|x| \rightarrow \infty$ ); the physically acceptable solutions, then, have the asymptotic form

$$\psi(\xi) \rightarrow ()e^{-\xi^2/2}, \text{ at large } \xi. \quad \dots(6)$$

This suggests that we "peel off" the exponential part,

$$\psi(\xi) = h(\xi)e^{-\xi^2/2}, \quad \dots(7)$$

in hopes that what remains  $[h \xi]$  has a simpler functional form than  $\psi(\xi)$  itself. Differentiating equation 7, we have

$$\frac{d\psi}{d\xi} = \left( \frac{dh}{d\xi} - \xi h \right) e^{-\xi^2/2},$$

and

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$$\frac{d^2\psi}{d\xi^2} = \left( \frac{d^2h}{d\xi^2} - 2\xi \frac{dh}{d\xi} + (\xi^2 - 1)h \right) e^{-\xi^2/2},$$

so the Schrodinger equation (Equation 2) becomes

$$\frac{d^2h}{d\xi^2} - 2\xi \frac{dh}{d\xi} + (K - 1)h = 0. \quad \dots(8)$$

It is proposed to look for a solution to equation 8 in the form of a power series in:

$$h(\xi) = a_0 + a_1\xi + a_2\xi^2 + \dots = \sum_{j=0}^{\infty} ja_j\xi^{j-1} \quad \dots(9)$$

Differentiating the series term by term,

$$\frac{dh}{d\xi} = a_1 + 2a_2\xi + 3a_3\xi^2 + \dots = \sum_{i=0}^{\infty} ja_j\xi^{j-1},$$

and

$$\frac{d^2h}{d\xi^2} = 2a_2 + 2.3a_3\xi + 3.4a_4\xi^2 + \dots = \sum_{i=0}^{\infty} (j+1)(j+2)a_{j+2} \xi^j.$$

Putting these into equation 8, we find

$$\sum_{j=0}^{\infty} \left[ (j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j \right] \xi^j = 0. \quad \dots(10)$$

It follows (from the uniqueness of power series expansion) that the coefficient of each power of  $\xi$  must vanish,

$$(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j = 0,$$

and hence that

$$a_{j+2} = \frac{(2j+1-K)}{(j+1)(j+2)} a_j \quad \dots(11)$$

This recursion formula is entirely equivalent to the Schrodinger equation itself given  $a_0$  it enables us(in principle) to generate  $a_2, a_4, a_6, \dots$ , and given  $a_1$  it generates  $a_3, a_5, a_7, \dots$ . Let us write

$$h(\xi) = h_{\text{even}}(\xi) + h_{\text{odd}}(\xi), \quad \dots(12)$$

where

$$h_{\text{even}}(\xi) \equiv a_0 + a_2 \xi^2 + a_4 \xi^4 + \dots$$

is an even function, of  $\xi$  (since it involves only even powers), built on  $a_0$  and

$$h_{\text{odd}}(\xi) = a_1 \xi + a_3 \xi^3 + a_5 \xi^5 + \dots$$

is an *odd* function, built on  $a_1$ . Thus equation 11 determines  $h(\xi)$  in terms of two arbitrary constants ( $a_0$  and  $a_1$ ) -which is just what we would expect, for a second order differential equation.

However, not all the solutions so obtained are normalizable. For at very large  $j$ , the recursion formula becomes (approximately)

$$a_{j+2} \approx \frac{2}{j} a_j.$$

with the (approximate) solution

$$a_j \approx \frac{c}{(j/2)!},$$

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for some constant  $C$ , and this yields (at large  $\xi$ , where the higher powers dominates)

$$h(\xi) \approx c \sum \frac{1}{(j/2)!} \xi^j \approx c \sum \frac{1}{k!} \xi^{2k} \approx C e^{\xi^2}.$$

Now, if  $h$  goes like  $(\xi^2)$  expectation, then  $\psi$  (remember  $\psi$  ?-that's we're trying to calculate) goes like  $(\xi^2 / 2) \exp$ , which is precisely the asymptotic behavior we don't want.<sup>17</sup> There is only one way to wiggle out of this : For normalizable solutions *the power series must terminate*. There must occur some "highest"  $j$  (call it  $n$ ) such that the recursion formula spits out  $a_{n+2} = 0$  (this

will truncate *either* the series  $h_{\text{even}}$  or the series  $h_{\text{odd}}$ ; the other one must be zero from the start). For physically acceptable solutions, then we must have

$$K = 2n + 1,$$

for some positive integer  $n$  which is to say that the *energy* must be of the form

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$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \text{ for } n = 0, 1, 2, \dots \quad \dots(13)$$

Thus we recover, by a completely different method, the fundamental quantization condition we found algebraically in Equation 2.50.

For the allowed values of  $K$ , the recursion formula reads

$$a_{j+2} = \frac{-2(n-j)}{(j+1)(j+2)} a_j. \quad \dots(14)$$

If  $n = 0$ , there is only one term in the series (we must pick  $a_1 = 0$  to kill  $h_{\text{odd}}$ , and  $j=0$  in Equation yields  $a_2 = 0$ ):

$$h_0(\xi) = a_0,$$

and hence

$$\psi_0(\xi) = a_0 e^{-\xi^2/2}$$

(which reproduces Equation). For  $n = 1$  we pick  $a_0 = 0$ , and Equation 2.68 with  $j = 1$  yields  $a_3 = 0$ , so

$$h_1(\xi) = a_1 \xi,$$

and hence

$$\psi_1(\xi) = a_1 \xi e^{-\xi^2/2}$$

(confirming Equation 2.51). For  $n = 2$ ,  $j = 0$  yields  $a_2 = -2a_0$ , and  $j = 2$  gives  $a_4 = 0$ , so

$$h_2(\xi) = a_0(1 - 2\xi^2)$$

and

$$\psi_2(\xi) = a_0(1 - 2\xi^2)e^{-\xi^2/2}$$

In general,  $h_n(\xi)$  will be a polynomial of degree  $n$  in  $\xi$ , involving even powers only, if  $n$  is an even integer, and odd powers only, if  $n$  is an odd integer. Apart from the overall factor ( $a_0$  or  $a_1$ ) they are the so-called **Hermite polynomials**,  $H_n(\xi)$ . The overall few of them are listed in Table 2.1. By tradition, the arbitrary multiplicative factor is chosen so that the coefficient of the highest power of  $\xi$  is  $2^n$ . With this convention, the normalized stationary states for the harmonic oscillator are

$$\Psi_n(x) = \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2}. \quad \dots(15)$$

**Table:** The first few Hermite polynomials,  $H_n(x)$

$$H_0 = 1;$$

$$H_1 = 2x,$$

$$H_2 = 4x^2 - 2,$$

$$H_3 = 8x^3 - 12x$$

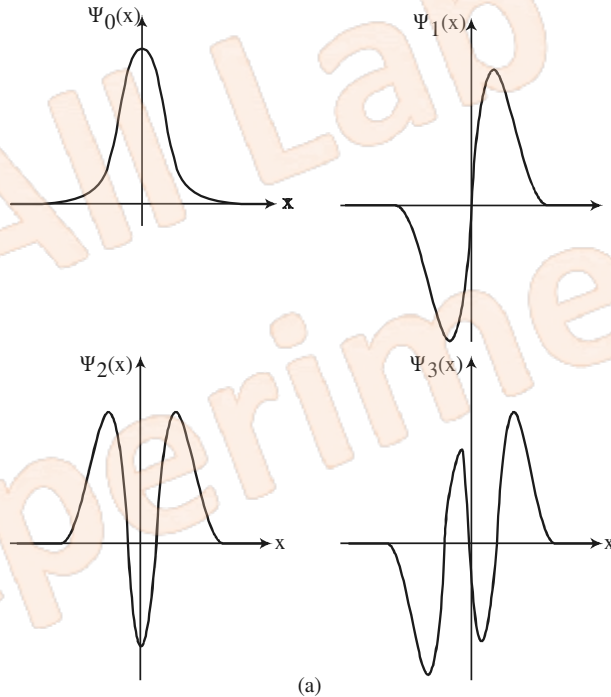
$$H_4 = 16x^4 - 48x^2 + 12,$$

$$H_5 = 32x^5 - 160x^3 + 120x.$$

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The first four stationary states of the harmonic oscillator.



**(b)** A particle of mass 1 mg is attached to a spring of spring constant

$k = 0.001 \text{ N m}^{-1}$  calculate its zero point energy.

**Ans.** Mass of the given particle,  $m = 1 \text{ mg}$  spring constant,  $k = 0.001 \text{ N/m}$  so the frequency  $\omega$ , can be calculated

as

$$\omega = \sqrt{\frac{k}{m}} = \sqrt{\frac{0.001}{10^{-3}}} = 1$$

Now the zero point energy is given as,

$$\begin{aligned} E_0 &= \frac{1}{2} \hbar \omega \\ &= \frac{1}{2} \times \frac{6.62 \times 10^{-34}}{2 \times 3.14} \times 1 \\ &= 0.527 \times 10^{-34} \text{ J} \\ &= 5.2 \times 10^{-34} \text{ J} \end{aligned}$$

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5. The 'θ' equation obtained after applying separation for variables to the Schrodinger equation for a 3D hydrogen atom in spherical polar coordinates, is given by

$$\frac{1}{\sin \theta} \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta(\theta)}{d\theta} \right) + \left( \lambda - \frac{m_l^2}{\sin^2 \theta} \right) \Theta = 0.$$

Solve the above equation for  $m_l = 0$  (or otherwise) to show that :

$$\lambda = l(l+1), l = 0, 1, 2, \dots$$

Ans. 
$$\frac{1}{\sin \theta} \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta(\theta)}{d\theta} \right) + \left( \lambda - \frac{m_l^2}{\sin^2 \theta} \right) \Theta(\theta) = 0 \dots$$

Let us introduce new variable  $\Theta = \cos \theta$ , the equation -12 becomes,

$$\frac{d}{d\Theta} \left( (1 - \omega^2) \frac{d\Theta(\omega)}{d\omega} \right) + \left( \lambda - \frac{m_l^2}{1 - \omega^2} \right) \Theta(\omega) = 0 \dots$$

The Equation -13 has similarities at  $\omega = \pm 1$ , which may be eliminated by having a solution  $\Theta$  in the form of

$$\Theta = (1 - \omega^2)^{s/2} u$$

Then Equation becomes

$$(1 - \omega^2) \frac{d^2 u}{d\omega^2} - 2\omega(s+1) \frac{du}{d\omega} + \left[ \lambda + \frac{s^2 \omega^2 - m_l^2}{1 - \omega^2} \right] u = 0$$

Which can be written as

$$(1 - \omega^2) \frac{d^2 u}{d\omega^2} - 2\omega(s+1) \frac{du}{d\omega} + \left[ \lambda - s^2 - s + \frac{s^2 - m_l^2}{1 - \omega^2} \right] u = 0 \dots$$



The last singular term in Equation-14 can be removed by taking  $s = \pm m_l \geq 0$ , and the have

$$\left( (1 - \omega^2) \frac{d^2 u}{d\omega^2} - 2\omega(m_l + 1) \frac{du}{d\omega} + [\lambda - m_l(m_l + 1)] \right) u = 0 \dots$$

Which is a regular equation and hence its series solution may be written as

$$u = \sum_{r=0}^{\infty} a_r \omega^r \quad \text{alllabexperiments.com}$$

Substituting in Equation, yields the recursion relation

$$a_{r+2} = \frac{(r + m_l)(r + m_l + 1) - \lambda}{(r + 1)(r + 2)} a_r$$

Requiring that the series be (Equation-16) be limited by a certain power  $r = q$ , *i.e.* requiring that it be a polynomial of order  $q$ , we have to introduce the condition

$$a_{r+2} = 0, a_r \neq 0 \text{ which requires } \lambda = (q + m_l)(q + m_l + 1)$$

Where  $q = 0, 1, 2, 3, \dots$

Now we introduce  $l = q + m_l = 0, 1, 2, 3, \dots$  (orbital quantum number) such that

$$l \geq m_l \quad \lambda = l(l + 1)$$

Then Equation-12 becomes

$$\frac{1}{\sin \theta} \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta(\theta)}{d\theta} \right) + \left( l(l + 1) - \frac{m_l^2}{\sin^2 \theta} \right) \Theta(\theta) = 0 \dots \text{Equation 17}$$

This is well known associated Legendre differential equation with its solution as associated Legendre polynomials

$$\Theta_{l,m_l} = C_l^{m_l} P_l^{m_l}(\omega) \quad \dots \text{Equation-18}$$

Where  $C_l^{m_l}$  is the normalization factor and  $P_l^{m_l}(\omega)$  is the associated Legendre polynomials define by

$$\begin{aligned} P_l^{m_l} &= (1 - \omega^2)^{m_l/2} \frac{d^{l+m_l}}{d\omega^{l+m_l}} \left[ \frac{(\omega^2 - 1)^2}{2^l l!} \right] \\ &= (1 - \omega^2)^{m_l/2} \frac{d^{m_l}}{d\omega^{m_l}} P_l(\omega) \end{aligned}$$

Where  $p_l(\omega)$  is the ordinary Legendre, polynomial. This expression holds for negative values of  $ml$  also

$$p_l^{ml}(\omega) = (-1)^{m_l} \frac{(l+m_l)!}{(l-m_l)!} P_l^{-m_l}(\omega)$$

From this we can establish the range of variation of the azimuthal (magnetic) quantum number  $m_l = 0, \pm 1, \pm 2, \pm 3, \dots, \pm l$

The associated Legendre polynomials satisfy the other normalization property

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$$\int_{-1}^1 p_l^{m_l}(\omega) p_l^{m_l}(\omega) d\omega = \frac{2}{2l+1} \frac{(l+m_l)!}{(l-m_l)!} \delta_{lx}$$

So,

$$C_l^{ml} = \sqrt{\frac{2l+1}{2} \frac{(l-m_l)!}{(l+m_l)!}}$$

The Equation becomes

$$\Theta_{l,m_l} = \frac{2l+1}{2} \frac{(l-m_l)!}{(l+m_l)!} P_l^{m_l}(\omega)$$

So, we have now two quantum numbers, namely. Orbital ( $l$ ) and magnetic ( $m$ )

$$l = 0, 1, 2, 3, \dots$$

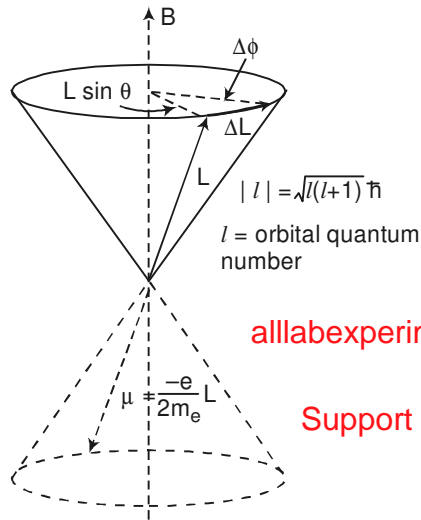
$$m_l = -l, -l+1, \dots, l-1, l$$

**6. (a) What is Larmor precession ? Drive the expression for Larmor frequency.**

**Ans. Larmor precession:** When a magnetic moment  $\mu$  is placed in magnetic field  $B$ , it experiences a torque which can be expressed in the form of a vector product

$$\tau = \mu \times B$$

For a static magnetic moment or a classical current loop, this torque to line up the magnetic moment with the magnetic field  $B$ , so this represents its lowest energy configuration. But if the magnetic moment arises from the motion of an electron in orbit around a nucleus, the magnetic moment is proportional to the angular momentum of the electron. The torque exerted then produces a change in angular momentum which is perpendicular to that angular momentum, causing the magnetic moment to precess around the direction the magnetic of the magnetic field rather settle down in the direction of the magnetic field. This is called Larmor precession.



When a torque is exerted perpendicular to the angular momentum  $L$ , it produces a change in angular momentum  $\Delta L$  which is perpendicular to  $L$ , causing it to precess about the  $z$ -axis. Labeling the precession angle as  $\phi$ , we can describe the effect of the torque as follows:

$$\tau = \frac{\Delta L}{\Delta t} = \frac{L \sin \theta \phi}{\Delta t} = \mu B \sin \theta = \frac{e}{2m_e} L B \sin \theta$$

The precession angular velocity (Larmor frequency) is

$$\omega_{Larmor} = \frac{d\phi}{dt} = \frac{e}{2m_e} B$$

**(b) Explain normal Zeeman effect with examples and energy diagram.**

**Ans. Normal Zeeman Effect**

In an experiment performed by the Dutch physicist Peter Zeeman in 1896, it was observed that each spectral line in the excitation spectrum for an atom placed in a magnetic field split into number of additional lines. Furthermore, the difference in energy between the new lines and the original line was found to be directly proportional to the strength of the external field. This effect came to be known as Zeeman effect, it should only be explained using quantum mechanics which says that the orbital angular momentum is quantized both in magnitude and direction.

For singlet states, the spin is zero and the total angular momentum  $J$  is equal to the orbital angular momentum  $L$ . When placed in an external magnetic field, the energy of the atom changes because of the energy of its magnetic moment in the field, which is given by

$$U(\theta) = -\mu \cdot B$$

The magnetic dipole moment associated with the orbital angular momentum is given by

$$\mu_{orbital} = \frac{e}{2m_e} L$$

For magnetic field in the z-direction this gives

$$U = \frac{e}{2m_e} L_z B = m_l \frac{e\hbar}{2m} B$$

Considering the quantization of angular momentum, this gives equally spaced energy levels displaced from the zero field level by

$$\Delta E = m_l \frac{e\hbar}{2m} B = m_l \mu_B B \quad \mu_B = \text{Bohr magneton}$$

$$\mu_B = \frac{e\hbar}{2m_e} = 9.2740154 \times 10^{-24} \text{ J/T} = 5.788382 \times 10^{-5} \text{ eV/T}$$

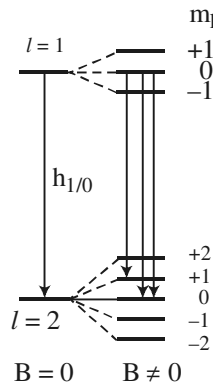
This displacement of the energy levels gives the uniformly spaced multiplet splitting of the spectral lines which is called the Zeeman effect.

**Example:** Consider transitions between two Zeeman-split atomic levels. Allowed transition frequencies are therefore.

$$h\nu = h\nu_0 + \mu_B B_z \quad \Delta m_l = -1$$

$$h\nu = h\nu_0 \quad \Delta m_l = 0$$

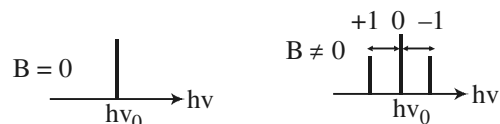
$$h\nu = h\nu_0 - \mu_B B_z \quad \Delta m_l = +1$$



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Emitted photons also have a polarization, depending on which transition they result from.



7. (a) What is spin orbit coupling ? Calculate the change in the energy levels due to this.

**Ans. Spin orbit coupling:** Imagine the electron in orbit around the nucleus; from the *electron's* point of view, the proton is circling around *it* (Figure). This orbiting positive charge sets up a magnetic field  $\mathbf{B}$  in the electron frame, which exerts a torque on the spinning electron, tending to align its magnetic moment ( $\mu$ ) along the direction of the field.

The Hamiltonian is

$$H = -\mu \cdot \mathbf{B}.$$

**The Magnetic Field of the Proton.** If we picture the proton (from the electron's perspective) as a continuous current loop (Figure), its magnetic field can be calculated from the Biot-Savart law:

$$B = \frac{\mu_0 I}{2r},$$

with an effective current  $I = e/T$ , where  $e$  is the charge of the proton and  $T$  is the period of the orbit. On the other hand, the orbital angular momentum of the *electron* (in the rest frame of the *nucleus*) is  $L = rmv = 2\pi nr^2/T$ . Moreover,  $\mathbf{B}$  and  $\mathbf{L}$  point in the same direction (up, in Figure), so

$$\mathbf{B} = \frac{1}{4\pi\epsilon_0} \frac{e-}{me^2 r^3} L.$$

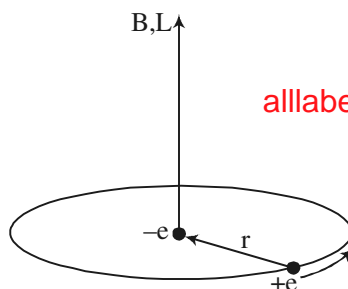


Figure: Hydrogen atom, from the electron's perspective.

**The magnetic dipole moment of electron**

The magnetic dipole moment of spinning electron is related to its spin angular momentum; the proportionality constant is geomagnetic ratio.

$$\mu_e = -\frac{e}{m} S.$$

The spin-orbit interaction. Putting all this together, we have

$$H = \left( \frac{e}{4\pi\epsilon_0} \right) \frac{1}{m^2 c^2 r^3} \text{S.L} \quad \text{J} \equiv \text{L+S}$$

$$J^2 = (\text{L+S}) \cdot (\text{L+S}) = L^2 + S^2 + 2\text{L.S}$$

so 
$$\text{L.S} = \frac{1}{2}(J^2 - L^2 - S^2).$$

and therefore the eigenvalues of L.S are

$$\frac{\hbar^2}{2}[j(j+1) - s(s+1)].$$

In this case, of source,  $s = 1/2$ . Meanwhile, the expectation value of  $1/r^3$  is

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

and we conclude that

$$E^1_{\text{so}} = \langle H^1_{\text{so}} \rangle = \frac{e^2}{8\pi\epsilon_0} \frac{1}{m^2 c^2} \frac{(\hbar^2/2)[j(j+1) - l(l+1) - 3/4]}{l(l+1/2)(l+1)n^3 a^3}$$

or, expressing it all in terms of  $E_n$  :

$$E^1_{\text{so}} = \frac{E_n^2}{mc^2} \left\{ \frac{n[j(j+1) - l(l+1) - 3/4]}{l(l+1/2)(l+1)} \right\}$$

**(b) Show the results of a JJ coupling of two non-equivalent p-electrons.**

**Ans.** The electronic configuration  $1p2p$ (non equivalent electrons)

$$l_1 = 1, s_1 = 1/2, j_1 = 3/2, 1/2 \quad l_2 = 1 \quad s_2 = 1/2, j_2 = 3/2, 1/2$$

Now, the notation for the coupling states are  $\{j_1, j_2\}$

$$\{3/2, 3/2\}_{3,2,1,0} \quad \{3/2, 1/2\}_{2,1} \quad \{1/2, 3/2\}_{2,1} \quad \{1/2, 1/2\}_{1,0}$$

The J states are degenerate in this level of consideration

Next when the electron - interaction takes place all these level will be splitted .

$$\{3/2, 3/2\}_3, \{3/2, 3/2\}_2, \{3/2, 3/2\}_1, \{3/2, 3/2\}_0$$

$$\{3/2, 1/2\}_2, \{3/2, 1/2\}_1, \{1/2, 3/2\}_2, \{1/2, 3/2\}_1$$

$$\{1/2, 1/2\}_1, \{1/2, 1/2\}_0$$