Module 2: Quantum Mechanics

Important Constant values:

Planck's Constant: h= $6.625X10^{-34}$ JS

Charge on electron (q or e) $= 1.609X10^{-19}$ J

Mass of electron m= $9.1X10^{-31}$ kg

Speed of Light in vacuum c =$3X10^{8}$ m/s

For numerical problems based on;

1. **De-Broglie wavelength.**
2. **Uncertainty Principle.**
3. **Probability of finding the particle in 1-dimenstion.**
4. **Energy Eigen value for particle in an infinite potential well (Box)**
5. **Expectation Value.**

Syllabus content:

- Wave-Particle dualism
- De Broglie hypothesis (Derivation and different forms of wavelength)
- Matter waves and its properties (Phase velocity Wave packet and Group velocity and Properties of matter waves)
- Heisenberg's Uncertainty Principle (Statement and explanation) and Application of uncertainty (electrons cannot exist inside the nucleus)
- Principle of Complementarity (Statement)
- Wave Function and Time Independent Schrödinger Wave Equation (Meaning of wave function and differential wave equation for matter in 1-dimention
- Physical significance of Wave Function: Physical Interpretation (Probability density and normalization)
- Expectation Value in quantum mechanics (Definition and example)
- Eigen values and eigen functions (Meaning and conditions for Eigen functions)
- Applications of schrödinger wave equation: Particle in one-dimensional potential well of infinite height (Applying Schrodinger wave equation and boundary conditions for particle and discussion of Eigen values and Eigen functions)
- Wave functions and the probability densities for the first three values of n for a particle in a box (Using Eigen function, for n=1, 2, and 3, probability density and discussion about the wave nodes)
- Numerical Problems: Problems on de-Broglie hypothesis, uncertainty principle, expectation value, Eigen value and Eigen functions
- Expected Model Questions: Expected questions and previous semester end exam questions.

De Broglie hypothesis:

In the year 1924 Louis de Broglie applied the concept of dual nature of radiation to the entities of matter like electron, neutron etc..

If the particle of matter has a momentum then waves associated with it. Therefore some sort of waves propagate with moving material particles called Matter waves or De-Broglie waves and the wavelength associated with matter waves is called de Broglie wavelength. Its relation is given by

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

Where **h= 6.6X10^{-34} JS** is called Planck's constant and **p =mv** is the momentum, 'm' is the mass of the moving particle and 'v' is its velocity.

De Broglie wavelength derivation by analogy and its different forms:

From Planck's quantum theory, Energy of photon is $\mathrm{E} = \mathrm{h}\nu = \mathrm{hc}/\lambda$ --------1

Where ν is its frequency, $\nu = \mathrm{c}/\lambda$ c is the speed of light and λ is the wavelength

From Mass-Energy relation $\mathrm{E} = \mathrm{mc}^2$ ---------------------------2

Where, c is the speed of light in vacuum

From the relations 1 and 2

$$\mathrm{mc}^2 = \mathrm{hc}/\lambda$$

$$\mathrm{mc} = \mathrm{h}/\lambda$$

We know that the momentum is the product of mass and speed, mc =p, which is the momentum of the photon.

The wavelength of a photon in-terms of its momentum is given by $\lambda = h/p$

Hence by analogy the de Broglie wavelength of matter waves is given by $\lambda = h/p$

- **de Broglie wavelength of particle of mass m and its velocity 'v', is given by**

$$\boldsymbol{\lambda = \frac{h}{mv} \quad ------(3)}$$

Here, momentum of the particle is, p=mv

- **de Broglie wavelength of a particle (charged or uncharged) moving with kinetic energy E is**

$$\boldsymbol{\lambda = \frac{h}{\sqrt{2mE}} \quad ----(4)}$$

Here, momentum of the particle is $p = \sqrt{2mE}$

(Since, energy of the particle is $E = \left(\frac{1}{2}\right)mv^2 = \left(\frac{1}{2}\right)\frac{m^2v^2}{m} = \left(\frac{1}{2}\right)\frac{p^2}{m} = \frac{p^2}{2m}$ then $p = \sqrt{2mE}$)

- **de Broglie wavelength of charged particle accelerated under a potential difference of *V* volt is**

$$\boldsymbol{\lambda = \frac{h}{\sqrt{2mqV}} = \frac{1.22X10^{-9}}{\sqrt{V}} \quad ----(5)}$$

Here, momentum of the particle is $p = \sqrt{2mqV}$ and

q=ne is the net charge, n =0,1,2,----- and e= $1.609X10^{-19}\,J$ is the charge on electron.

(Since, electron is accelerated under potential difference of V then energy of electron is

$$\left(\frac{1}{2}\right)mv^2 = qV$$

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

$$p = \sqrt{2mqV}$$

by substituting the constant values of h, m and q

$$\lambda = \frac{h}{\sqrt{2mqV}} = \left(\frac{6.625X10^{-34}}{\sqrt{2 * 9.1X10^{-31}X1.609X10^{-19}}}\right)\frac{1}{\sqrt{V}}$$

$$\lambda = (1.22X10^{-9})\,\frac{1}{\sqrt{V}}$$

The above equations (3), (4) and (5) are the different forms of de Broglie wavelength of particle.

Matter waves and its properties (Characteristics):

1. **Phase velocity v_p:**
   The velocity with which a wave travels is called phase velocity and is also called wave velocity. It is given by

$$v_p = \nu\lambda = \frac{\omega}{k} = \frac{c^2}{v}$$

If a point is marked on the wave representing the phase of the particle then the velocity with which the phase propagates from one point to another is called phase velocity.

Here c is the velocity of light in vacuum and v is the velocity of the matter wave.

Since, phase velocity is greater than the velocity of light. Hence there is no physical significance for phase velocity of matter waves.

2. **Wave packet and group velocity v_g:**

Since the velocity of matter waves must be equal to that of the particle velocity and since no physical meaning can be associated with phase velocity, the concept of group velocity is introduced.

Wave packet is the resultant wave of matter waves which is formed due to the superposition of two or more waves with slightly differ in their frequencies or velocities.

The velocity with which the wave packet propagates is called group velocity which is same as particle velocity. It is denoted by v_g and is as given by

$$v_g = \frac{d\omega}{dk}$$

Properties of matter waves: The following are the properties associated with the matter waves

- Waves associated with moving particles are called matter waves.
- The wave length of matter waves is given by $\lambda = h/mv$
- Matter waves are not electromagnetic waves.
- The phase velocity has no physical meaning for matter waves
- Group velocity is associated with matter waves.
- The amplitude of the matter wave at a given point is the probability of finding the particle at that point.

Heisenberg uncertainty principle (Statement and Explanation):

i) Statement: "It is impossible to determine simultaneously, the position and momentum of a moving particle accurately".

According to the principle, in any simultaneous determination of position and momentum of the particle, the product of uncertainties is equal to or greater than $\geq \frac{h}{4\pi}$

$$\Delta \boldsymbol{x}.\Delta \boldsymbol{p}_x \geq \frac{\boldsymbol{h}}{\boldsymbol{4\pi}}$$

Where, $\boldsymbol{\Delta x}$ is the uncertainty involved in the measurement of position and $\boldsymbol{\Delta p_x}$ is the uncertainty involved in the measurement of momentum. The product of the errors is of the order of Planck's constant.

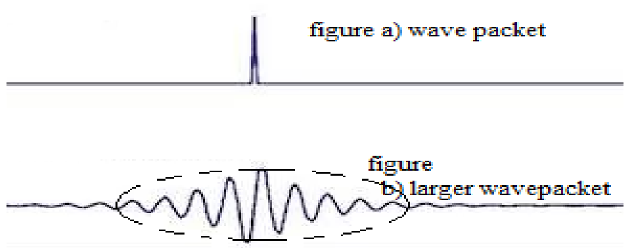
Similarly, Uncertainty Principle for

a) Energy and time is $\Delta \boldsymbol{E}.\Delta \boldsymbol{t} \geq \frac{\boldsymbol{h}}{\boldsymbol{4\pi}}$

b) Angular displacement and Angular momentum is $\Delta \boldsymbol{L}.\Delta \boldsymbol{\theta} \geq \frac{\boldsymbol{h}}{\boldsymbol{4\pi}}$

ii) Explanation:

Let us consider the wave packet of matter waves as shown in the figure (a) and (b)



If the width of the wave packet is small as shown in figure (a) then particle can be located somewhat accurately but the measurement of wavelength (momentum) introduces large error. $(if\ \Delta \boldsymbol{x} = \boldsymbol{0},\ \boldsymbol{then}\ \Delta \boldsymbol{p}_x \to \infty\ \boldsymbol{)}$

If the width of wave packet is large, then wavelength measurement is accurate, however position of the particle cannot be determined accurately. $(if\ \Delta \boldsymbol{p}_x = \boldsymbol{0},$ $\boldsymbol{then}\ \Delta \boldsymbol{x} \to \infty\ \boldsymbol{)}$

Physical significance of uncertainty principle: According to Newtonian physics the simultaneous measurement of position and momentum are exact. But the existence of matter waves induces errors due to limit of accuracy associated with the simultaneous measurement. Hence the exactness in Newtonian physics is replaced by probability in quantum mechanics.

iii) <u>Show that electrons cannot exist inside the nucleus</u>:

Beta rays are emitted by the nucleus. It was first observed that electrons exist inside the nucleus and are emitted at certain instant.

If the electron can exist inside the atomic nucleus then uncertainty in its position must not exceed the diameter of the nucleus.

The diameter of the nucleus is of the order of $\Delta x = 10^{-14}$m.

Applying Heisenberg's uncertainty principle for an electron expected to be inside the nucleus we get

$$\Delta \boldsymbol{x}.\Delta \boldsymbol{p}_x \geq \frac{\boldsymbol{h}}{\boldsymbol{4\pi}}$$

$$\Delta \boldsymbol{p}_x \geq \frac{\boldsymbol{h}}{\boldsymbol{4\pi\Delta x}} = \frac{6.625 * 10^{-34}}{4 * 3.142 ** 10^{-14}}$$

$$\Delta \boldsymbol{p}_x = 0.527 * 10^{-20} kgm/s$$

Therefore, the electron should possess momentum $p_{min} \simeq \Delta p_{min} = 0.527 * 10^{-20} kgm/s$

Non-relativistic equation of energy of the electron is given by

$$E = \frac{p^2}{2m} = \frac{(0.527 * 10^{-20})^2}{2 * 9.1X10^{-31}} \geq 1.5X10^{-11}J$$

here m is the rest mass of the electron=$9.1X10^{-31}$kg

$$E \geq \frac{1.52X10^{-11}}{1.609 * 10^{-19}}\ eV$$

$$E \geq 93MeV$$

Conclusion: According to experiments, the energy associated with the beta ray (electron) emission is around 3-4 MeV which is much lesser than the energy of the electron expected to be inside the nucleus 93 MeV. Hence electrons cannot exist inside the nucleus.

<u>Principle of Complementarity</u>: Bohr's complementarity principle:

Statement: It states that wave and particle aspects of matter are complementary, both equally essential for the full description of a physical phenomenon.

Explanation: We know that the light consists of wave and particle behaviour. In the same way particles such as electrons, neutrons, etc behave as waves. On considering the particle behaviour they require localization, on the other hand when wave extend over certain region, particle nature or wave aspects or both require to understand the physical phenomenon. We know that the consequence of the uncertainty principle is both the wave and particle nature of the matter cannot be measured simultaneously. In other words, we cannot precisely describe the dual nature of light.

So any physical situation in which a physical entity exhibits wave properties completely it is possible to attribute the particle characteristics to it. This idea is known as Bohr's complementarity principle.

Wave Function and Time Independent Schrödinger Wave Equation:

i) **Wave function**: It represents a De Broglie wave and describes the motion of particle. It can be express in complex form. A wave function that depends on space (x, y and z) and time (t) and is denoted by $\psi(r, t)$
If the wave function for a matter wave moving along +ve x-axis is given by (It is a function of only 'x' and time 't' coordinates

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

Here A is constant and ω is the angular frequency of the wave.

ii) **Time Independent Schrödinger Wave Equation:**
The wave equation which has variations only with respect to position and describes the steady state is called Time Independent Schrodinger wave equation.
Consider a particle of mass m moving with velocity v along +ve x–axis. The de Broglie wave length λ is given by relation in terms of momentum p is

$$\boldsymbol{\lambda = \frac{h}{mv}} \quad ----\mathbf{1})$$

As per classical mechanics, the wave equation for one dimensional propagation of waves is given by

$$\frac{d^2y}{dx^2} = \frac{1}{v^2}\frac{d^2y}{dt^2}$$

Where, y is the displacement and 'v' is the velocity of the wave.

By analogy, we can write the wave equation for matter wave as (1-Dimention)

$$\frac{d^2\psi}{dx^2} = \frac{1}{v^2}\frac{d^2\psi}{dt^2} \quad ---2)$$

The wave function for matter wave in one dimension is given by

$$\psi = Ae^{i(kx-\omega t)} \quad ---3)$$

Here A is constant and ω is the angular frequency of the wave

Differentiate equation (2), $\psi(x, t)$ twice w.r.t to t, then

$$\frac{d^2\psi}{dt^2} = -\omega^2\psi - - - -4)$$

Substituting equation 4) and 5) in equation 2), we can write

$$\frac{d^2\psi}{dt^2} = \frac{1}{v^2}(-\omega^2\psi\ )$$

$$\frac{d^2\psi}{dx^2} = \frac{-\omega^2}{v^2}\psi$$

Substituting for $\omega = 2\pi f$ and $v = f\lambda$, and $\psi(x,t) = \psi$ in the above equation

$$\frac{d^2\psi}{dx^2} = \frac{-(2\pi f)^2}{(f\lambda)^2}\psi$$

$$\frac{d^2\psi}{dx^2} = \frac{-4\pi^2}{\lambda^2}\psi$$

Substituting for $\lambda = \frac{\mathbf{h}}{\mathbf{p}}$ in the above equation, we can write as

$$\frac{d^2\psi}{dx^2} = \frac{-4\pi^2}{\left(\frac{h}{mv}\right)^2}\psi$$

$$\frac{d^2\psi}{dx^2} = -\left(\frac{4\pi^2(mv)^2}{h^2}\right)\psi$$

$$\frac{d^2\psi}{dx^2} = -\left(\frac{4\pi^2m^2v^2}{h^2}\right)\psi$$

Divide and multiple by 2 in the RHS term

$$\frac{d^2\psi}{dx^2} = -\left(\frac{8\pi^2 m\left(\frac{1}{2}mv^2\right)}{h^2}\right)\psi$$

$$\frac{d^2\psi}{dx^2} = -\left(\frac{8\pi^2m\ (E-V)}{h^2}\right)\psi$$

Here , $\frac{1}{2}mv^2 = E - V$, E is the total energy and V is the potential enegy of the particle

$$\boldsymbol{\frac{d^2\psi}{dx^2} + \left(\frac{8\pi^2m\ (E-V)}{h^2}\right)\psi = 0}$$

This is the time-independent Schrodinger's equation in one dimension and It can be extended to three dimension as

$$\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} + \left(\frac{8\pi^2m\ (E-V)}{h^2}\right)\psi = 0$$

Physical significance of Wave Function: Physical Interpretation

For a matter wave, wave function describes the motion of matter wave and it has no direct physical meaning. Probability in quantum mechanics is the physical significance of matter wave.

Probability of finding the particle at given location per unit volume and is called Probability Density.

Since wave function is in complex form and $\psi*$ is its complex conjugate of ψ then

$|\psi|^2 = \psi\psi^*$ is a real number which represents the probability density.

This is also referred to as Max- Born interpretation. It is given by

$$P = |\psi|^2$$

Therefore, in one dimension the probability of finding a particle in the width dx of length x is

$$P\,(x)dx = |\psi|^2 dx$$

Similarly, in three dimension, the probability of finding a particle in a given small volume dV of volume V is given by

$$P\,dV = |\psi|^2 dV$$

Here dV=dxdydz is an infinitesimal volume element surrounding point (x,y,z) and P is the Probability Density.

If particle exists, probability of finding the particle somewhere in the space must be unity $\iiint_{-\infty}^{\infty} |\psi|^2 \boldsymbol{dydz = 1}$

This condition is called normalization condition. The wave function is normalized.

Expectation Value of wave function:

In quantum mechanics, the expectation value is the probabilistic expected value of the result (measurement) of an experiment. It can be thought of as an average of all the possible outcomes of a measurement as weighted by their likelihood.

Let us consider a particle moving along the x axis and its wave function (x, t).

$|\psi(x,t)|^2$ is a probability density for the position observable and $|\psi(x,t)|^2 dx$ is the probability of finding the particle between x and $x + dx$ at time t.

Then expectation value of the possible outcomes is

$$< x >= \int_{-\infty}^{\infty} x\, |\psi(x,t)|^2 dx$$

Eigen values and Eigen functions:

The Schrodinger wave equation is a second order differential equation. While Solving the Schrodinger wave equation to a particular system we get many expressions for wave function (ψ). However, all wave functions are not acceptable. Only those wave functions which satisfy certain conditions are acceptable. Such wave functions are called Eigen functions for the system.

The energy values corresponding to the Eigen functions are called Eigen values. These Eigen values are discrete set of energy values.

The wave functions are acceptable if they satisfy the following conditions.

i) ψ must be finite everywhere (Cannot be infinite)
ii) ψ must be single valued which implies that solution is unique for a given position in space.
iii) ψ and its first derivatives with respect to its variables must be continuous everywhere.

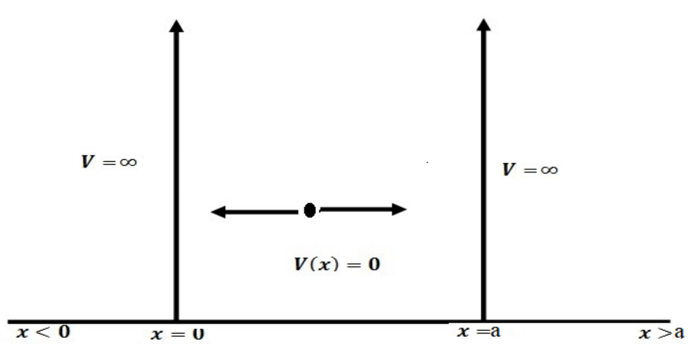
Applications of Schrödinger's wave equation:

Particle in one-dimensional potential well of infinite height:

Consider a particle of mass m bouncing back and forth between the walls of the one dimensional potential well as shown in figure 3.2. The particle is said to be under bound state.

Let the motion of the particle be confined along the x-axis in between $x = 0$ and $x = a$. Let the width of the box is 'a'

The description of the potential well is as follows. In between walls i.e. $0 < x < a$, the potential $V = 0$. Beyond the walls i.e. $x \leq 0$and $x \geq a$, the potential $V = \infty$. Such configuration of potential in space (region) is called infinite potential well.



Since the walls are infinitely hard, no energy is lost by the particle during the collision with walls and the total energy remains constant. The total energy of the particle (Eigen value) can be obtained by solving the Schrodinger wave equation.

Schrodinger wave equation is ,

$$\frac{d^2\psi}{dx^2} + \frac{8m\pi^2(E-V)\psi}{h^2} = 0$$

For outside the well, potential is considered to be infinity, $V = \infty$

$$\frac{d^2\psi}{dx^2} + \frac{8m\pi^2(E-\infty)\psi}{h^2} = 0$$

Since the potential inside the well $V = 0$, hence potential energy $U = 0$, the Schrodinger wave equation becomes

$$\frac{d^2\psi}{dx^2} + \frac{8m\pi^2(E-0)\psi}{h^2} = 0$$

$$\frac{d^2\psi}{dx^2} + \frac{8m\pi^2E\ \psi}{h^2} = 0 - - - - 1)$$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0\ - - - - - 2)$$

$$k^2 = \frac{8m\pi^2E}{h^2} - - - - 3)$$

Here k is a constant for a given value of energy E. The general solution for equation (2) is given by

$$\psi(x)\ =\ A\sin kx\ +\ B\cos kx\ - - - 4)$$

Here in the above equation A and B are arbitrary constants which can be evaluated by applying boundary conditions.

Applying Boundary Conditions:

1. The first boundary condition is, at $x = 0$, $\psi(x)\ = 0$.
   Applying this to equation 4, we get
   $0 = A\sin 0 + B\cos 0$
   $B = 0$ hence equation (4) reduces to

$$\psi(x)\ = A\sin kx \qquad - - - 5)$$

2. The second boundary condition is,at $x = a$, $\psi(x) = 0$.
   Applying this to equation 4, we get
   $0 = A\sin ka\ + B\cos ka$
   $0 = A\sin ka\ + 0$ since B=0
   $0 = A\sin ka$

   Since $A \neq 0$, then $\sin ka = 0$

$$k\,.\,a = \sin^{-1}0 = n\pi$$

$$k\,.\,a = n\pi \quad \text{-------}\rightarrow \quad k = \frac{n\pi}{a}$$

n can take integer values. Hence equation (5) could be written as

$$\psi(x) = A\sin\left(\frac{n\pi}{a}\right)x \qquad ---6)$$

Substituting the value of k in equation (3) we get

$$\left(\frac{n\pi}{a}\right)^2 = \frac{8m\pi^2 E_n}{h^2}$$

$$\boldsymbol{E_n = \frac{n^2h^2}{8ma^2}} ----\mathbf{7})$$

<u>Quantization of Energy States</u>:

Substituting for $n = 1, 2, 3, 4, ..$ in the above equation (8) Energy Eigen Values are obtained.

The lowest energy state corresponds to lowest integral value of $n = 1$ which is also called as zero Point Energy is given by

$$\boldsymbol{E_1 = \frac{h^2}{8ma^2}} ----\mathbf{8})$$

The energy values of a bound particle in one dimensional potential well are quantized (discrete) and are represented by the equation

$$\boldsymbol{E_n = n^2\left(\frac{h^2}{8ma^2}\right) = n^2E_1} \qquad ----\mathbf{9})$$

Energy states corresponding to n>1 are called excited states.

Let n=2 is called first excited state, $E_2 = 4E_1$,

n=3 is called second excited state $E_3 = 9E_1$ and so on.

<u>Normalization of wave function: Eigen function</u>:

The wave function for a particle in one dimensional potential well of infinite height is given by the equation

$$\psi(x) = A\sin\left(\frac{n\pi}{a}\right)x \qquad ---6)$$

A is an arbitrary constant and it can take any value. The process of determination of value of the arbitrary constant is called Normalization of wave function.

Probability of the finding the particle inside the potential well is given by

$$\int_0^a |\psi_n|^2\,dx = \int_0^a p\,dx = 1$$

Substituting for the wave function (6) in the integral

$$\int_0^a A^2 \sin^2\left(\frac{n\pi x}{L}\right) dx = 1 \quad ---10)$$

from trigonometry $\sin^2\theta = \frac{1}{2}(1 - \cos 2\theta)$.

Therefore the above equation (10) could be written as

$$\frac{A^2}{2}\int_0^a \left[1 - \cos 2\left(\frac{n\pi x}{L}\right)\right] dx = 1$$

$$\frac{A^2}{2}\left[\int_0^a 1\, dx - \int_0^a \cos\left(\frac{2n\pi x}{L}\right) dx\right] = 1$$

Integrating the above equation we get

$$\frac{A^2}{2}\left|x - \frac{a}{2n\pi}\sin\left(\frac{2n\pi x}{L}\right)\right|_0^a = 1$$

$$\frac{A^2}{2}|(a-0) - 0| = 1$$

Since $\sin 2n\pi = 0$

$$\frac{A^2}{2}a = 1$$

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

Which is called normalization constant.

Substituting this in equation (6) the normalized wave function or eigen function for a particle in one dimensional potential well of infinite height is given by

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}\right)x \quad -----11)$$

Waveforms and the probabilities for the first three values of *n* for a particle in a box:

Consider Eigen function for a particle in a box is given by $\psi_n = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}\right)x$

For n =1 it represents the ground state and particle is normally found in this state.

Then Eigen function is $\psi_1 = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{L}\right)x$

In the above equation, $\psi_1 = 0$ for both x =0 and x= a

But $\psi_1 = \sqrt{\frac{2}{a}}$ which is maximum when x = a/2

Thus for ground state ($n = 1$). The probability of finding the particle at the walls is zero and at the center $a/$ 2 is maximum.

For n =2 it represents the first excited state.

Then Eigen function is $\psi_2 = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi}{a}\right) x$

In the above equation, $\psi_2 = 0$ for x =0, a/2 and x= a

But $\psi_2 = \sqrt{\frac{2}{a}}$ which is maximum when x = a/4 and x= 3a/4

The first excited state has three nodes.

For n =3 it represents the second excited state.

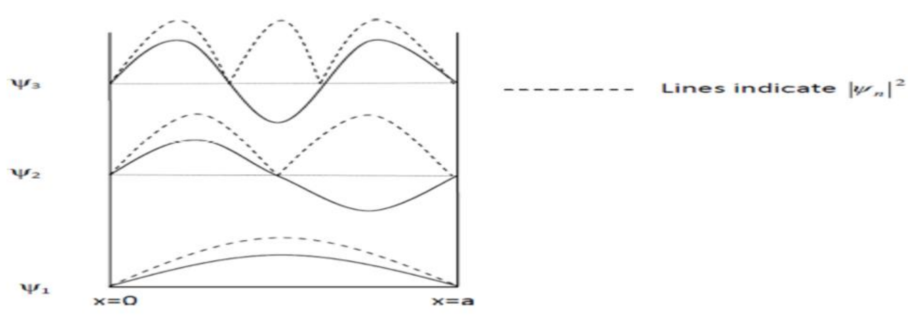
Then Eigen function is $\psi_3 = \sqrt{\frac{2}{a}} \sin\left(\frac{3\pi}{a}\right) x$

In the above equation, $\psi_2 = 0$ for x =0, a/3, 2a/3 and x= a

But $\psi_2 = \sqrt{\frac{2}{a}}$ which is maximum when x = a/6, a/2 and x= 5a/6

The second excited state has four nodes.

The wave functions and the probability densities for the first three values of n are as shown in figure below.



Numerical Problems and Model Questions:

1. What is de-Broglie wavelength of proton whose energy is 3eV. Given mass of proton is $1.675X10^{-27}$kg.
2. Calculate the de-Broglie wavelength of electron moving with one tenth part of speed of light.
3. Calculate the momentum of the particle and the de Broglie wavelength associated with an electron with a kinetic energy of $1.5keV$.
4. A particle of mass $0.65MeV/C^2$ has free energy 120eV. Find the de-Broglie wavelength of the particle.
5. Find the energy of the neutron in eV whose de Brogle wavelength is 1 Å.
6. An electron is confined to one dimensional box of length 0.1nm. Calculate the minimum uncertainty in its velocity of the electron.
7. A spectral line of wavelength 400nm has width of $80X10^{-15}$m. Evaluate the minimum time spent by the electron during excitation and de-excitation processes.
8. The position and momentum of an electron with energy $0.5keV$ are determined. What is the minimum percentage uncertainty in its momentum if the uncertainty in the measurement of position is 0.5Å.
9. An electron has speed of $4X10^5$ m/s accurate to 0.01%. With what fundamental accuracy can we locate the position of electron.
10. A particle moving in one dimension box is described by the wave function $\psi = x\sqrt{3}$ for 0<x<1 and $\psi = 0$ elsewhere. Find the probability of finding the particle within the interval (0,1/2).
11. A quantum particle confined to one–dimensional box of width a is in its first excited state. What is the probability of finding the particle over an interval of a 2 marked symmetrically at the center of the box.
12. Calculate the first three permitted energy values and de-Broglie wavelength for an electron in an infinite potential well of 0.1nm.
13. An electron is trapped in a 1-D potential well of infinite height and of width of 0.1 nm. Calculate the energy required to excite it from its ground state to fifth excited state.
14. The first excited state energy of an electron in an infinite well is $240eV$. What will be its ground state energy when the width of the potential well is doubled?
15. State de-Broglie hypothesis. Derive debroglie wavelength by analogy and mention the different forms of it.
16. What is wave packet? Give physical significance and properties of wave function. Define group velocity.
17. State and explain Heisenberg Uncertainty principle and show that the electrons do not exist inside the nucleus.
18. State and explain Complementarity Principle.
19. Define wave function and Set up one time impendent dimensional Schrödinger's wave equation.
20. Discuss physical significance of wave function and expectation value with example.
21. Discuss the solution for a particle in a box with help of Schrodinger wave equations and hence obtain the normalized wave function.

Solved problems:

1. What is de-Broglie wavelength of proton whose energy is 3eV. Given mass of proton is $1.675X10^{-27}$kg. **Ans: $1.65X10^{-11}$m**

   Solutions: Given mass of proton is m= $1.675X10^{-27}kg$ and

   Energy E= 3eV = $3\,X1.609X10^{-19}$ J

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

$$\lambda = \frac{h}{\sqrt{2mE}}$$

$$\lambda = \frac{6.625X10^{-34}}{\sqrt{2 * 1.675 * 10^{-27} * 3 * 1.609X10^{-19}}}$$

$$\lambda = 1.648 * 10^{-11}m$$

2. Calculate the de-Broglie wavelength of electron moving with one tenth part of speed of light. **Ans: $2.415X10^{-11}$m**

   Solution: Given mass of electron is m= $9.1X10^{-31}kg$

   Speed of electron v $= \frac{1}{10} * speed\ of\ light = \frac{1}{10} * 3 * 10^8 = 3 * 10^7 m/s$

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

$$\lambda = \frac{h}{m\mathrm{v}} = \frac{6.625X10^{-34}}{9.1X10^{-31} * 3 * 10^7} = 2.42 * 10^{-11}m$$

$$\lambda = 2.42 * 10^{-11}m$$

3. A particle of mass $0.65MeV/c^2$ has free energy 120eV. Find the de-Broglie wavelength of the particle. Where c is the speed of light **Ans: $9.9X10^{-11}$m**

   Solution: Given mass of particle is m =$0.65MeV/c^2$

   Here ,speed of light $c = 3X10^8$ m/s , M=10^6 and 1eV=$1.609X10^{-19}J$

$$m = \frac{0.65 * 10^6 * 1.609X10^{-19}}{(3X10^8)^2}$$

$$m = 1.16 * 10^{-30}kg$$

   Given, energy E=120eV=120*$1.609X10^{-19}$

The de-Broglie wavelength of the particle is

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

$$\lambda = \frac{h}{\sqrt{2mE}}$$

$$\lambda = \frac{6.625X10^{-34}}{\sqrt{2 * 1.16 * 10^{-30} * 120 * 1.609X10^{-19}}}$$

$$\lambda = \frac{6.63X10^{-34}}{\sqrt{2 * 1.16 * 10^{-30} * 120 * 1.609X10^{-19}}}$$

$$\lambda = 9.986X10^{-11}m$$

4. An electron is confined to one dimensional box of length $1X10^{-8}$m. Calculate the minimum uncertainty in its velocity of the electron. **Ans: 5.8km/S**

   Solution : given: Uncertainty in electron position is $\Delta x = 1 * 10^{-8}m$

   Uncertainty in its velocity is = Δv =?

   Using uncertainty principle $\Delta x * \Delta p \geq \frac{h}{4\pi}$

$$\Delta x * m\Delta \text{v} \geq \frac{h}{4\pi}$$

$$\Delta \text{v} \leq \frac{h}{4\pi * m * \Delta x}$$

$$\Delta \text{v} \leq \frac{6.625X10^{-34}}{4\pi * 9.1 * 10^{-31} * 1 * 10^{-8}}$$

Δv ≤5797.78m/s or 5.797m/s

5. Compare the momentum and the kinetic energy of an electron with a de Broglie wavelength of 40nm with that of photon with same wavelength.

   Solution:

   Given: Since the wavelength of photon and electron is same i.e

$$\lambda = 40nm = 40 * 10^{-9}m$$

   Since the value of h and λ is same for both photon and electron then

   Momentum expression is

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

$$\frac{p_e}{p_p} = 1$$

Kinetic Energy of electron is , $E_e = \frac{P^2}{2m}$

$$E_e = \frac{h^2}{2m\lambda^2}$$

$$E_e = \frac{(6.625X10^{-34})^2}{2 * 9.1 * 10^{-31} * (40 * 10^{-9})^2}$$

$$E_e = 0.001509 * 10^{-19} J$$

Energy of photon is $E_p = \frac{hc}{\lambda} = \frac{6.63X10^{-34} * 3 * 10^8}{40 * 10^{-9}}$

$$E_p = 4.95 * 10^{-18} J$$

$$\frac{E_e}{E_p} = \frac{0.001509 * 10^{-19}}{4.95 * 10^{-18}} = 0.00003048 = 3.08 * 10^{-4}$$

6. A spectral line of wavelength 400nm has width of $8X10^{-15}$m. Evaluate the minimum time spent by the electron during excitation and de-excitation processes. **Ans: 5.3nS**

   Solution: Wavelength of spectral line is λ=400nm=$400 * 10^{-9} m$

   Uncertainty in spectral line is $\Delta\lambda = 8 * 10^{-15} m$

   Uncertainty in its time is = Δt =?

   Using uncertainty principle $\Delta E * \Delta t \geq \frac{h}{4\pi}$

   But $E = \frac{hc}{\lambda}$ and $\Delta E = hc\ \frac{1}{\lambda^2} \Delta\lambda$

$$\Delta t \leq \frac{h}{4\pi(hc\ \frac{1}{\lambda^2} \Delta\lambda)}$$

$$\Delta t \leq \frac{\lambda^2}{4\pi(c\ \Delta\lambda)}$$

$$\Delta t \leq \frac{400 * 10^{-9^2}}{4\pi * 3 * 10^8 * 8 * 10^{-15}}$$

$$\Delta t \leq 5.3 * 10^{-9} S$$

$$\Delta t \leq 5.3 nS$$

7. An electron has speed of 4X10[5] m/s accurate to 0.01%. With what fundamental accuracy can we locate the position of electron. **Ans: 1.45μm**

   Solution: The electron speed is v $= 4 * 10^5 m/S$

   Uncertainty in its speed is $\Delta = 0.01\%$

   Uncertainty in its velocity is = Δv $= \frac{0.01}{100} * 4 * 10^5 = 40 m/s$

   Using uncertainty principle $\Delta x * \Delta p \geq \frac{h}{4\pi}$

$$\Delta x * m\Delta \text{v} \geq \frac{h}{4\pi}$$

$$\Delta \text{x} \leq \frac{h}{4\pi * m * \Delta v}$$

$$\Delta \text{x} \leq \frac{6.625X10^{-34}}{4\pi * 9.1 * 10^{-31} * 40}$$

$$\Delta \text{x} \leq 1.446 * 10^{-6} m$$

$$\Delta \text{x} \leq 1.446 \mu\text{m}$$

8. A particle moving in one dimension box is described by the wave function ψ = x $\sqrt{3}$ for 0<x<1 and ψ =0 elsewhere. Find the probability of finding the particle within the interval (0,1/2). **Ans: 3/8**

   The wavefunction of the particle is given by ψ = x $\sqrt{3}$ for 0<x<1

   probability of finding the particle within the interval (0,1/2) is

$$\text{P} = \int_0^{1/2} |\psi|^2 \, dx$$

$$\text{P} = \int_0^{1/2} \left| x \sqrt{3} \right|^2 dx$$

$$\text{P} = 3/8$$

9. Calculate the first two permitted energy values and de-Broglie wavelength for an electron in an infinite potential well of 0.12nm. **Ans: 26.14eV, 104.5eV, and 0.24nm, 0.12nm**

   First three permitted states means n=1, n=2 and n=3 and a=0.12nm

   The energy value for a particle in box is

$$\mathbf{E}_n = \frac{n^2 h^2}{8ma^2}$$

   And its de-Broglie wavelength is

$$\lambda = \frac{h}{\sqrt{2mE}}$$

For n=1,

$$\mathbf{E_1} = \frac{\boldsymbol{h^2}}{\boldsymbol{8ma^2}}$$

$$\mathbf{E_1} = \frac{(6.625X10^{-34})^{\mathbf{2}}}{\mathbf{8} * 9.1 * 10^{-31} * (0.12 * 10^{-9})^{\mathbf{2}}}$$

$$\mathbf{E_1} = \mathbf{4.15} * 10^{-18} J$$

$$\mathbf{E_1} = \frac{\mathbf{4.15} * 10^{-18}}{1.609X10^{-19}}$$

$$\mathbf{E_1} = \mathbf{25.82eV}$$

And its de-Broglie wavelength is

$$\lambda = \frac{h}{\sqrt{2m\mathbf{E_1}}} = \frac{6.625X10^{-34}}{\sqrt{2 * 9.1 * 10^{-31} * \mathbf{4.15} * 10^{-18}}}$$

$$\lambda = 2.42 * 10^{-10} m$$

$$\lambda = 0.242 * 10^{-9} m = 0.242 nm$$

For n=2

$$\mathbf{E_2} = \mathbf{4}\frac{\boldsymbol{h^2}}{\boldsymbol{8mL^2}} = \mathbf{4E_1} = \mathbf{4} * \mathbf{4.15} * 10^{-18} = 1.16 * 10^{-17} J$$

$$\mathbf{E_2} = \frac{\mathbf{1.16} * 10^{-17}}{1.609X10^{-19}}$$

$$\mathbf{E_2} = \mathbf{103.16eV}$$

And its de-Broglie wavelength is

$$\lambda = \frac{h}{\sqrt{2m\mathbf{E_2}}} = \frac{6.625X10^{-34}}{\sqrt{2 * 9.1 * 10^{-31} * 1.16 * 10^{-17}}}$$

$$\lambda = 1.44 * 10^{-10} m$$

$$\lambda = 0.114 * 10^{-9} m = 0.114 nm$$

10. An electron is trapped in a 1-D potential well of infinite height and of width of 0.1 nm. Calculate the energy required to excite it from its ground state to fifth excited state. **Ans:**

Solution:

The energy value for an electron trapped in a one dimension potential well is

$$\mathbf{E}_n = \frac{n^2 h^2}{8ma^2}$$

Energy required to excite it from its ground state to fifth excited state. That is from n=1 to n=6 and width of well L=0.1nm

For n=1 , $\mathbf{E_1} = \frac{h^2}{8ma^2}$

For n= 6 $\mathbf{E_6} = 36\frac{h^2}{8ma^2}$

Then energy required is $\mathbf{E_6 - E_1} = 36\frac{h^2}{8ma^2} - \frac{h^2}{8ma^2}$

$$= (36 - 1)\frac{h^2}{8ma^2}$$

$$= 35\frac{h^2}{8ma^2}$$

$$= 35 * \frac{(6.625X10^{-34})^2}{8 * 9.1 * 10^{-31} * (0.1 * 10^{-9})^2}$$

The energy required = 2.11*10^{-16}J

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