

Module – 1
Quantum Mechanics

Quantum Mechanics: de Broglie Hypothesis and Matter Waves, de Broglie wavelength and derivation of expression by analogy, Phase Velocity and Group Velocity, Heisenberg's Uncertainty Principle and its application (Nonexistence of electron inside the nucleus-Non Relativistic), Principle of Complementarity, Wave Function, Time independent Schrodinger wave equation, Physical Significance of a wave function and Born Interpretation, Expectation value, Eigen functions and Eigen Values, Particle inside one-dimensional infinite potential well, Waveforms and Probabilities.

Numerical problems.

Pre-requisite: Wave-Particle dualism

Self-learning: de Broglie Hypothesis

de Broglie hypothesis and matter waves

The origin of quantization of energy lies in the dual behavior observed in nature in particle and wave aspects. Taking for instance the case of X-ray, Compton observed in his experiment that, an X-ray radiation is scattered by an electron. Also X-rays are diffracted by a crystal. Since diffraction is a wave phenomenon, it must be said that X-rays behave as waves. While explaining the phenomenon of interference and diffraction in physical optics, light is considered purely as waves. Because of such a dual nature observed of radiation and light, Louis de Broglie of France in 1924 put forward a bold **hypothesis** that, 'since nature loves symmetry, if the radiation behaves as particle under certain circumstances and as waves under certain other circumstances, then one can even expect that, entities which ordinarily behave as particles to exhibit properties attributable to only waves under appropriate circumstances' and he termed such waves that could be associated with particles as **matter waves**.

de Broglie wavelength:

A moving body behaves in certain ways as though it has a wave nature

A photon of light of frequency ν has the momentum

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

Since $\lambda\nu=c$, the wavelength of a particle is therefore specified by its momentum according to the relation $\lambda = \frac{h}{p}$.

de Broglie went on to prove that, when a particle has a momentum p , its motion is associated with a wavelength λ , called de Broglie wavelength given by,

$\lambda = h/p$, where h is Planck's constant.

The de Broglie's predication is concerned with the wave-particle duality i.e., the particle nature of waves and wave nature of particles.

de Broglie wavelength of accelerated electron:

Consider an electron of mass 'm' charge 'e' which is accelerated under a potential difference of V volts. Then work done = kinetic energy

$$eV = \frac{1}{2}mv^2 \quad \text{-----(1)}$$

we know $p = mv$

squaring we get, $p^2 = m^2v^2$

from equation (1) we multiply and divide right hand side by m

$$\text{therefore, } eV = \frac{m^2v^2}{2m} \rightarrow eV = \frac{p^2}{2m}$$

$$\text{Or } p = \sqrt{2meV}$$

$$\text{We know } \lambda = \frac{h}{p}$$

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

where, $h = 6.625 \times 10^{-34} \text{ Js}$

$e = 1.602 \times 10^{-19} \text{ C}$

$m = 9.1 \times 10^{-31} \text{ kg}$

Substituting all these values in the above equation we get

$$\lambda = \frac{1.227 \text{ nm}}{\sqrt{V}}$$

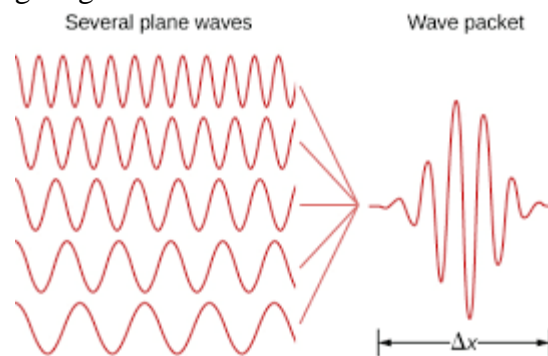
$$\text{we know } E = \frac{1}{2}mv^2$$

from (1) we can write $E = eV$

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

Wave packets

In physics, a wave packet (or wave train) is a short "burst" or "envelope" of localized wave action that travels as a unit. A wave packet can be analyzed into, or can be synthesized from, an infinite set of component sinusoidal waves of different wave numbers, with phases and amplitudes such that they interfere constructively only over a small region of space, and destructively elsewhere. Each component wave function, and hence the wave packet, are solutions of a wave equation. Depending on the wave equation, the wave packet's profile may remain constant (no dispersion, see figure) or it may change (dispersion) while propagating.



Group Velocity and Phase velocity:

Group velocity is the velocity with which the envelope enclosing a wave group called wave packet, formed due to superimposition of two or more travelling waves of slightly different wavelength, is transported. It is the velocity with which the energy transmission occurs in a wave.

$$\text{Where } V_{group} = \frac{d\omega}{dk} = v$$

If a point is imagined to be marked on a travelling wave, then it becomes a representative point for a particular phase of the wave, and the velocity with which it is transported owing to the motion of the wave, is called the **phase velocity**.

$$\text{Where, } V_{\text{phase}} = \frac{\omega}{k} = \frac{c^2}{v}$$

Heisenberg's uncertainty principle:

Heisenberg's uncertainty principle states that in the simultaneous determination of the position and momentum of a particle like electron, the product of uncertainties in the position and the momentum of a particle is equal to or greater than Planck's constant.

If Δx is the uncertainty in the position of a particle and Δp is the uncertainty in the momentum of a particle then,

$$\Delta x \Delta p \geq \frac{h}{4\pi} \text{ --- (1)}$$

Another form of the uncertainty principle concerns energy and time. We can measure the energy E emitted during the time interval given by Δt in an atomic process.

$$\Delta E \Delta t \geq \frac{h}{4\pi} \text{ --- (2)}$$

Physical significance of Heisenberg's Uncertainty principle :

The physical significance of the above argument is that, one should not think of exact position, or exact value for momentum of a particle . Instead one should think of the probability of finding the particle at a certain position or of the probable value for momentum of the particle. The estimation of such probabilities are made by means of certain mathematical functions, named probability density functions in quantum mechanics. Similar interpretation is made for the conjugate pair of ΔE and Δt .

Application of Heisenberg's uncertainty principle

Non existence/confinement of electron inside the nucleus

The energy E of a body can be expressed as,

$$E = \frac{p^2}{2m} \text{ --- (1)}$$

Where m is mass of the body and p is its momentum

Heisenberg's Uncertainty Principal states that,

$$\Delta p_x \Delta x \geq \frac{h}{4\pi}$$

This can also be written as,

$$\Delta p_x \geq \frac{h}{4\pi \Delta x} \text{ --- (2)}$$

We know that the typical value of the diameter of the nucleus is of the order of $10^{-14}m$. We can assume if the electron to exist inside the nucleus, then the uncertainty in the position Δx must not exceed this value. Allowing maximum uncertainty value we can write,

$$\Delta x \leq 10^{-14}m$$

Using this in inequality (2), we have,

$$\Delta p_x \geq \frac{6.63 \times 10^{-34}}{4\pi \times 10^{-14}}$$

$$\Delta p_x \geq 0.5 \times 10^{-20} \text{ Ns} \text{ -----(3)}$$

which is the uncertainty in the momentum of the electron. But since the momentum of the electron must at least equal to the uncertainty in the momentum

$$p_x \geq 0.5 \times 10^{-20} \text{ Ns}$$

We know, the rest mass of the electron,

$$m_0 = 9.11 \times 10^{-31} \text{ kg}$$

Now by making use of (3) we can say that, in order that the electron may exist within the nucleus, its energy E must be such that,

$$E \geq \frac{(0.5 \times 10^{-20})^2}{2 \times 9.11 \times 10^{-31}} \geq 1.372 \times 10^{-11} \text{ J}$$

Expressing in eV, we get,

$$E \geq 85 \text{ MeV}.$$

This means to say that, in order that an electron to exist inside the nucleus, its energy must be greater than or equal to 85 MeV. But, the experimental investigations on beta-decay of radioactive nuclei reveal that the kinetic energy of the beta rays is of the order of 3-4 MeV. This clearly indicates that, electrons cannot exist within the nucleus.

Principle of complementarity:

One of the milestones of quantum mechanics is Bohr's complementarity principle. It states that a single quantum can exhibit a particle-like (or) a wave-like behavior, but never both at the same time. These are mutually exclusive and complementary aspects of the quantum system. This means that we need distinct experimental arrangements in order to measure the particle or the wave nature of a physical system. One of the most known representations of this principle is the single-photon Mach-Zehnder interferometer. When the interferometer is closed an interference pattern is observed (wave aspect of the quantum) while if it is open, the quantum behaves like a particle. Using a molecular quantum information processor and employing nuclear magnetic resonant (NMR) techniques, physicists have analyzed the quantum version of this principle by means of an interferometer that is in a quantum superposition of being closed and open, and confirm that we can indeed measure both aspects of the system with the same experimental apparatus. More specifically, we observe with a single apparatus the interference between the particle and the wave aspects of a quantum system.

Wave function:

de Broglie wave in quantum mechanics is represented by a function called wave function. It is denoted by ψ . It accounts for the wave like properties of particles. Wave function is obtained by solving Schrodinger equation. To solve Schrodinger equation it is required to know

- 1) Potential energy of the particle
- 2) Initial conditions and
- 3) Boundary conditions.

There are two types of Schrodinger equations describing the behaviour of matter waves

- 1) **The time dependent Schrodinger equation:** It takes care of both the position and time variations of the wave function. It involves imaginary quantity i .

The equation is:

$$\frac{h^2}{8\pi^2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi = -\frac{ih}{2\pi} \frac{\partial \psi}{\partial t}$$

Where h is Planck's constant, m is the mass of the particle, ψ is a wave function and V is potential energy.

- 2) **The time independent Schrodinger equation:** It takes care of only position variation of the wave function.

The equation is:

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

Where h is Planck's constant, m is the mass of the particle, ψ is a wave function, V is potential energy and E is the total energy.

The time independent Schrodinger equation:

According to the de Broglie theory, for a particle of mass m , moving with a velocity v , associated with it is a wave of wavelength,

$$\lambda = h/p \quad (1)$$

Where, $p = mv$, is the momentum of the particle.

The wave function describing the de Broglie wave considered travelling in positive x -direction can be written as,

$$\Psi = Ae^{i(kx-\omega t)} \quad (2)$$

Where Ψ is the total wave function, A is a constant, and ω is the angular frequency of the wave.

The space independent part in eq (2) can be represented as a wave function,

$$\psi = Ae^{ikx}$$

Hence Eq(2) becomes

$$\Psi = \psi e^{-i\omega t} \quad (3)$$

Let us differentiate Ψ twice with respect to x . Since Ψ depends on x ,

$$\frac{\partial^2 \Psi}{\partial x^2} = e^{-i\omega t} \frac{\partial^2 \psi}{\partial x^2} \quad (4)$$

Now, again differentiating Ψ twice, but this time with respect to t , we have

$$\frac{\partial^2 \Psi}{\partial t^2} = -\omega^2 e^{-i\omega t} \psi \quad (5)$$

We have travelling wave equation as,

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 y}{\partial t^2}$$

Where, y is the displacement and v is the velocity of the wave. By analogy, we can write the wave equation for de Broglie wave for the motion of a free particle as,

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 \Psi}{\partial t^2} \quad (6)$$

The above equation represents waves propagating along x -axis with a velocity v , and Ψ is the displacement at the instant t .

Substituting equation (4) & (5) in (6), we get,

$$e^{-i\omega t} \frac{\partial^2 \psi}{\partial x^2} = \frac{1}{v^2} (-\omega^2 e^{-i\omega t} \psi)$$

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{\omega^2}{v^2} \psi$$

If λ and v are the wavelength and frequency of the wave, then $\omega = 2\pi\gamma$ and $v = \gamma\lambda$. Substituting for ω and v , the above equation becomes,

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{4\pi^2}{\lambda^2} \psi$$

$$\frac{1}{\lambda^2} = -\frac{1}{4\pi^2 \psi} \frac{\partial^2 \psi}{\partial x^2} \quad (7)$$

For a particle of mass m moving with a velocity v ,

$$\text{Kinetic energy} = \frac{1}{2}mv^2 = \frac{m^2v^2}{2m}$$

$$\text{Kinetic energy, } E = \frac{p^2}{2m} \quad (8)$$

But, we have from Eq(1), $p = \frac{h}{\lambda}$ and by substituting for p in Eq(8), we get

$$\text{Therefore we can write,} \quad E = \frac{h^2}{\lambda^2 2m} \quad (9)$$

By substituting for $\frac{1}{\lambda^2}$ from Eq(7), Eq(9) becomes,

$$\text{Kinetic energy} = -\frac{h^2}{\pi^2 8m} \frac{1}{\psi} \frac{\partial^2 \psi}{\partial x^2} \quad (10)$$

Depending on the position in the field, the particle will possess certain potential energy V. Thus, the total energy E of the particle is the sum of kinetic energy and potential energy.

Using Eq(10) we have,

$$E = -\frac{h^2}{8\pi^2 m} \frac{1}{\psi} \frac{\partial^2 \psi}{\partial x^2} + V \quad (11)$$

$$-\frac{h^2}{8\pi^2 m} \frac{1}{\psi} \frac{\partial^2 \psi}{\partial x^2} = E - V \quad (12)$$

$$\frac{\partial^2 \psi}{\partial x^2} - \frac{8\pi^2 m}{h^2} (E - V)\psi$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m}{h^2} (E - V)\psi = 0 \quad (13)$$

This is the time independent Schrodinger's equation.

Physical interpretation of wave function(ψ): The wave function ψ is a complex quantity with both real and imaginary parts. Although the wave function ψ describes a particle wave associated with a de Broglie wavelength $\lambda = \frac{h}{mv}$ in space. This does not mean that the particle itself is spread out. Therefore ψ itself has no physical meaning but the square of the wave function is always a real quantity. Max Born proposed that $|\psi|^2$ at any point as the probability that the particle will be at that point. Specifically if dv is the volume element in space located at a point whose co-ordinate are x, y, z at an instant of time 't' then $\int |\psi|^2 dv$ is the probability of finding the particle in space. The probability of finding the particle i.e. somewhere in space must be equal to unity.

i.e., $\int_{-\infty}^{+\infty} |\psi|^2 dv = 1$. This is called normalization condition.

Normalization:

If ψ is the wave function associated with a particle, then we have $|\psi|^2 d\tau$ as the probability of finding the particle in a volume $d\tau$. Further, if we are certain to the extent that the particle is definitely present in a particular region or space of volume τ , then, as per the statistical rule,

$$\int_0^{\tau} |\psi|^2 d\tau = 1 - - - (1)$$

This is based on the fact that, a value 1 for probability means, it is clearly a certainty. However, in the above case, if we are not at all certain about locating the particle in a finite volume anywhere in space, then the expectation will become limited to the extent that ‘it exists somewhere in space’.

Then the limits in Eq. (1) extend from $-\infty$ to ∞ , and the probability becomes,

$$\int_{-\infty}^{\infty} |\psi|^2 d\tau = 1 - - - (2)$$

But in most cases, the result of evaluation of $\int_{-\infty}^{\infty} |\psi|^2 d\tau$ will not be unity but involves a constant that existed in the equation for ψ . However, the actual result whatever obtained is equated to unity and the value of the constant is determined. It is then substituted in the equation for ψ which becomes the working equation for the wave function known as normalized wave function. This process is called normalization.

Born Interpretation of Ψ

The probability that a particle will be found in the infinitesimal interval dx about the point x , denoted by $P(x)dx$ is given by:

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

$$P(x) = |\Psi(x, t)|^2 \text{ (probability density function)}$$

$$P(x) = \text{probability per unit length (in 1D)}$$

- A. It follows from this definition that you cannot specify with certainty the location of a particle! You can only specify the probability!
- B. $\Psi(x, t)$ itself is NOT a measurable quantity but $|\Psi(x, t)|^2$ is measurable and equal to the probability per unit length (probability density) of finding the particle in the interval dx about the point x .
- C. $P(x) = |\Psi(x, t)|^2 = \Psi\Psi^*$ where Ψ^* is the complex conjugate of Ψ .
- D. $\Psi(x, t)$ must be single-valued and continuous function of x and t .
- E. Because the particle must be somewhere along the x -axis, the sum of the probabilities over all values of x must add up to 1:

$$\int_{-\infty}^{+\infty} P(x)dx = \int_{-\infty}^{+\infty} |\Psi(x, t)|^2 dx = 1 \quad \text{Normalization Condition}$$

F. The probability of finding the particle in any finite interval $a \leq x \leq b$ is given by:

$$P_{ab} = \int_a^b |\Psi(x, t)|^2 dx$$

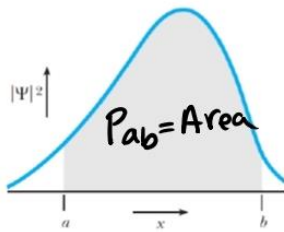


Figure 6.1 The probability for a particle to be in the interval $a \leq x \leq b$ is the area under the curve from a to b of the probability density function $|\Psi(x, t)|^2$.

G. $|\Psi(x, t)|^2 \rightarrow 0$ fast enough as $x \rightarrow \pm\infty$ so that the normalization condition holds valid.

Expectation values:

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\Psi|^2 dx$$

The expectation value for momentum cannot be calculated this way because, according to the uncertainty principles, no such function as $p(x)$ can exist. If we specify x , so that $\Delta x=0$, we cannot specify a corresponding p since $\Delta x \Delta p \geq \hbar/4\pi$. The same problem occurs for the expectation value for energy because $\Delta E \Delta t \geq \hbar/4\pi$ means that, if we specify t , the function $E(t)$ is impossible.

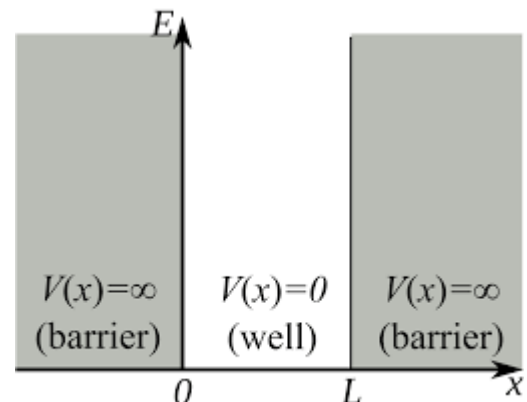
In classical physics no such limitation occurs, because the uncertainty principle can be neglected in the macroworld. When we apply the second law of motion to the motion of a body subject to various forces, we expect to get $p(x, t)$ and $E(x, t)$ from the solution as well as $x(t)$. Solving a problem in classical mechanics gives us the entire future course of the body's motion. In quantum physics, on the other hand, all we get directly by applying Schrodinger's equation to the motion of a particle is the wave function Ψ , and the future course of the particle's motion like its initial state is a matter of probabilities instead of certainties.

Application of Schrodinger's wave equation to particle in 1-D potential well of infinite depth, the energy eigen values and eigen functions

Suppose a particle of mass m is free to move in the x - direction only in the region from $x=0$ to $x=a$ (fig.1). In this region its potential V will be zero. Outside this region, it is taken to be infinite. Such a configuration of potential in space is called infinite potential well. A bound within such an infinite potential defined in 1- dimension is referred to as particle in a one dimensional box.

Outside the well, the Schrödinger equation is,

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m}{h^2} (E - \infty) \psi = 0, \text{ (since } V = \infty \text{).} \quad \text{--- (1)}$$



This equation holds good only if $\psi = 0$. The only possible solution for the above equation is that, $\psi = 0$ at the wall of the well and also everywhere outside the well. - - - condition I

Since $\psi = 0$ also means $|\psi|^2 = 0$, the particle cannot be found at all outside the well.

Inside the well, the Schrödinger's equation is given by,

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m}{h^2} (E) \psi = 0, \text{ (since } V = 0) \text{ - - - (2)}$$

Or,
$$-\frac{h^2}{8\pi^2 m} \left(\frac{d^2 \psi}{dx^2} \right) = E \psi \text{ - - - (3)}$$

This is of the form $\hat{H}\psi = E\psi$.

As per the postulate of quantum mechanics, this should be an eigenvalue equation.

In Eq(2), putting
$$\frac{8\pi^2 m}{h^2} E = k^2 \text{ - - - (4)}$$

We have,
$$\frac{d^2 \psi}{dx^2} + k^2 \psi = 0$$

The solution for the above equation is given by,

$$\psi = C \cos kx + D \sin kx \text{ - - - (5)}$$

But, $\psi = 0$ at $x = 0$, as per condition I.

\therefore Eq(5) becomes,

$$0 = C \cos 0 + D \sin 0.$$

$$\therefore C = 0. \text{ - - - (6)}$$

Again as per condition I, $\psi = 0$ at $x = a$,

For which Eq(5) becomes,

$$0 = C \cos ka + D \sin ka.$$

From Eq(6) we have $C = 0$. Hence the above equation becomes,

$$D \sin ka = 0.$$

Here, D need not be $= 0$.

$$\therefore \sin ka = 0,$$

Or,
$$ka = n\pi,$$

where, $n = 1, 2, 3 \text{ - - -}$

n is called quantum number which is either zero or a positive integer.

$$k = \frac{n\pi}{a}, \text{ - - - (7)}$$

Substituting for C and K from Eq (7) and (6), Eq (5) can now be written as,

$$\psi_n = D \sin \frac{n\pi}{a} x \text{ - - - (8)}$$

From Eq (4),

$$E = \frac{k^2 h^2}{8\pi^2 m}.$$

Using Eq(9), the above equation becomes,

$$E_n = \frac{n^2 h^2}{8ma^2}. \text{ - - - (9)}$$

As already mentioned, n can have only integer value 1,2,3 - - -the corresponding values that E takes are the energy eigen values.

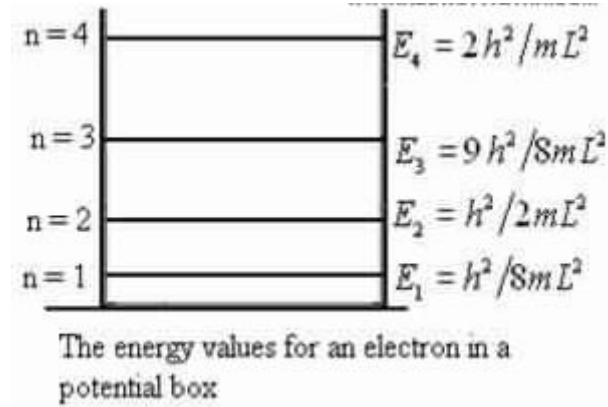
The lowest permitted state of energy is referred to as the ground state energy. Thus zero point energy is taken as the ground state energy ($n=1$). The energy states, corresponding to $n>1$ are called excited states.

In Eq (9), the values zero for n is not acceptable because, when $n = 0$, $\psi_n = 0$ by Eq (8), which means to say that the electron is not present inside the box which is not true. Hence the lowest acceptable value for

n is 1. Consequently the lowest allowed energy corresponding to n =1 which is called the zero point energy. The zero point energy of an electron of an electron in an infinite potential well is given by,

$$E_{zero\ point} = \frac{h^2}{8ma^2}.$$

The lowest permitted state of energy is referred to as the ground state energy. Thus zero point energy is taken as the ground state energy. The energy states corresponding to n > 1 are called excited states.



To evaluate D in Eq (8) one has to perform the normalization of the wave function.

Normalization: The integral of the square of the wave function over the entire space in the well must be equal to unity because, there is only one particle and at any time it is present somewhere inside the well only. Therefore,

$$\int_0^a |\psi|^2 dx = 1 \text{ --- (10)}$$

Substituting for ψ_n from Eq. (10), we have,

$$\int_0^a D^2 \sin^2 \frac{n\pi}{a} x dx = 1.$$

But, we know that,

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

$$\therefore D^2 \left[\frac{1}{2} \int_0^a dx - \frac{1}{2} \int_0^a \cos \frac{2n\pi}{a} x dx \right] = 1,$$

$$\text{Or, } \frac{D^2}{2} \left[x - \frac{a}{2n\pi} \sin\left(\frac{2n\pi x}{a}\right) \right]_0^a = 1,$$

$$\text{Or, } \frac{D^2}{2} \left[a - \frac{a}{2n\pi} \sin(2n\pi) \right] = 1,$$

$$\text{Or, } \frac{D^2 a}{2} = 1, \text{ since, } \sin(2n\pi) = 0$$

$$\therefore D = \sqrt{\frac{2}{a}}.$$

Thus the normalized wave function of a particle in a one dimensional infinite potential well is given by,

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

4.10.Eigen functions, Probability density and Energy Eigenvalues for particle in an infinite potential well

Since the particle in an infinite well is a problem under quantum mechanical conditions, the prime questions to be considered are, the most probable location of the particle in the well and its energies, both to be evaluated for the different permitted states. Let us analyze the same here.

Following Eq (11), we can write the eigen functions $\psi_1, \psi_2, \psi_3, \dots$ for particle in the well by putting $n = 1, 2, 3, \dots$ respectively in the equation.

Let us consider the first 3 cases.

Case (i), $n=1$

This is the ground state and the particle is normally found in this state.

For $n=1$, the eigenfunction is,

$$\psi_1 = D \sin \frac{\pi}{a} x, \quad \text{from eq(11)}.$$

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

But ψ_1 has a maximum value for $x=(a/2)$

A plot of $|\psi|^2$, the probability density v/s x is shown in fig(b). It indicates the probability of finding the particle at different locations inside the well. It can be seen in fig. That $|\psi|^2$ is 0 both at $x=0$ and $x=a$. It is maximum at $x=a/2$. It means to say that, in the ground state the particle cannot be found at all at the walls of the well, and the probability of finding it is maximum at the central region (prove by calculation).

Regarding the energy of the particle, using eq (4.33), the energy in the ground state is got by putting $n=1$.

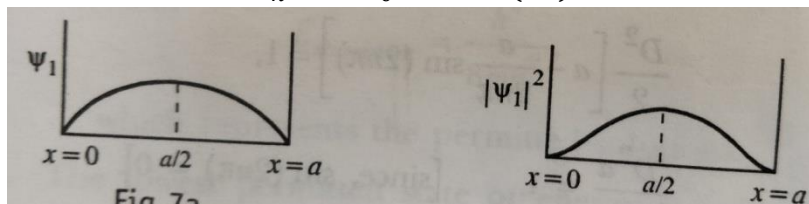
$$\therefore E_1 = \frac{h^2}{8a^2m} = E_0 \quad \text{--- (12)}$$

This is the energy eigenvalue for the ground state.

Also, $E_1 = E_0$

From eq.(9) and(11)

$$E_n = n^2 E_0 \quad \text{--- (13)}$$



Case (ii), $n=2$

This is the first excited state i.e., the next immediate higher state permitted for the particle after the ground state. The eigen function for this is,

$$\psi_2 = D \sin \frac{2\pi}{a} x. \quad \text{--- (14)}$$

Source: <http://www.adbhutvigyan.com/particle-in-one-dimensional-potential-box/>

Now, $\psi_2 = 0$ for the values $x=0, a/2$, and a . also, ψ_2 reaches maximum for $x=a/4$ and $3a/4$. These facts are seen in the plot of ψ_2 v/s x shown in above fig.

The plot of $|\psi|^2$ v/s x is shown in above fig. it is seen that $|\psi|^2 = 0$ at $x=0, a/2$ and a . It means that in the first excited state the particle cannot be observed either at the walls, and at the center.

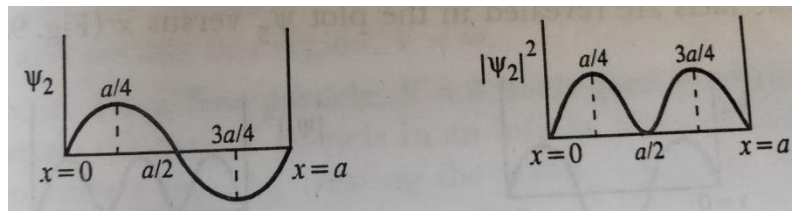
Further, for $n=2$,

$$E_2 = 4 \left(\frac{h^2}{8a^2m} \right).$$

This is the energy eigenvalues for the first excited state. Also,

$$E_2 = 4E_0 \quad \text{--- (15)}$$

Thus the energy in the first excited state is 4 times the zero point energy.



Case (iii) n=3

This is the second excited state. Following the same analysis as carried out earlier, we have the eigen function for the second excited state as,

$$\psi_3 = D \sin \frac{3\pi}{a} x. \quad \text{--- (16)}$$

$\psi_3 = 0$, for $x=0, a/3, 2a/3$ and a .

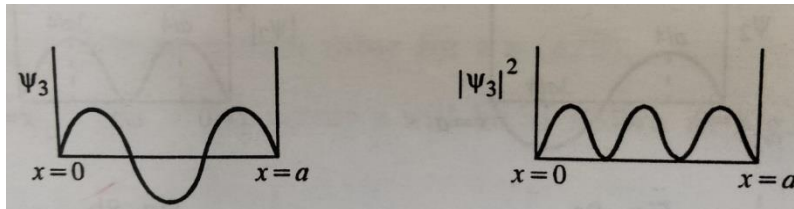
ψ_3 will have maximum value for $x = a/6, a/2$ and $5a/6$.

These facts are revealed in the plot ψ_3 v/s x . This case corresponding to second excited state.

As in the earlier case, using eq(14), the energy in this state is given by,

$$E_3 = 9 \left(\frac{h^2}{8a^2m} \right).$$

Thus $E_3 = 9E_0$. --- (19)



Questions:

1. Explain the duality of matter waves.
2. State de Broglie hypothesis.
3. Derive an expression for de Broglie wavelength
4. Show that the de Broglie wavelength for an electron accelerated by a potential difference V volts $\lambda = \frac{1.227 \text{ nm}}{\sqrt{V}}$
5. State and explain Heisenberg's uncertainty principle. Give its physical significance
6. Show that, a free electron cannot exist within the nucleus of an atom.
7. Explain eigen values and eigen functions.
8. Obtain the time- independent Schrodinger's equation for a particle in 1-d potential well of infinite height and discuss eigen values and eigen functions.
9. What is Wave function? Give its physical significance and properties.
10. What is Normalization of a wave function?
11. Derive the expression for energy eigen values for an electron in a potential well of infinite height.
12. Discuss zero- point energy.