

MODULE 2

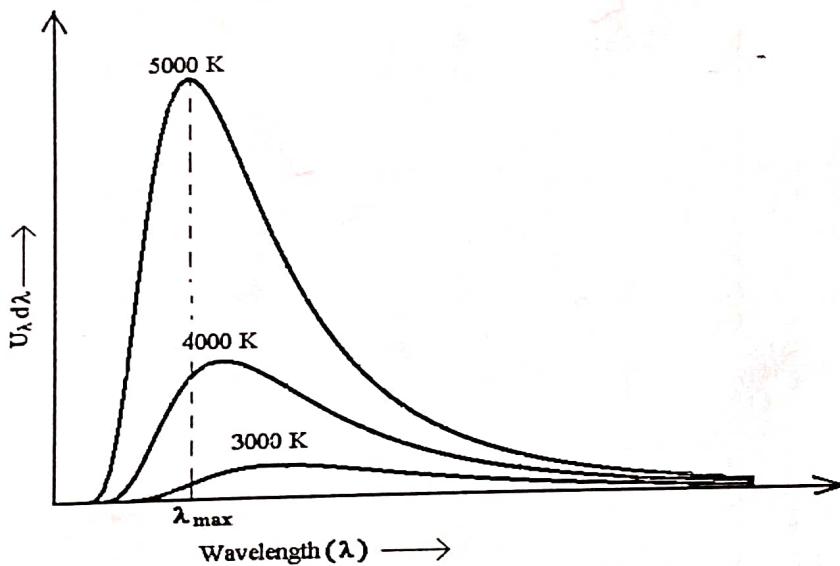
MODERN PHYSICS AND QUANTUM MECHANICS

Black body radiation spectrum:

A black body is one that will absorb all the radiations incident on it. Such a body cannot transmit or reflect any radiation and therefore it appears black. A black body can radiate energy in all possible wavelengths when it is heated to a suitable temperature. This radiation is called blackbody radiation.

A graph plotted energy density versus wavelength of emitted radiation is called black body radiation spectrum. The spectrum of the radiation emitted from the black body was studied by heating it to higher and higher temperatures. Salient features of the spectrum are:

1. There are different curves for different temperatures.
2. At a given temperature the distribution of energy is not uniform over all the wavelength.
3. At a given temperature there is a particular wavelength λ_{\max} at which the energy radiated is maximum.
4. As the temperature increases, the wavelength corresponding to maximum intensity λ_{\max} shifts towards the shorter wavelength side.



Wien's displacement law:

The wavelength corresponding to the maximum energy, λ_{\max} is inversely proportional to the absolute temperature of the emitting body.
i.e. $\lambda_{\max} \propto 1/T$ or. $\lambda_{\max} T = \text{const} = 2.898 \times 10^{-3} \text{ mK}$.
This is called Wien's displacement law.

Wien's distribution law:

Wien derived the expression for energy density U_λ using classical theory as

$$U_\lambda d\lambda = C_1 \lambda^{-5} e^{-\frac{C_2}{\lambda T}} d\lambda$$

Where $U_\lambda d\lambda$ is the energy per unit volume in the wavelength range λ and $\lambda + d\lambda$. T is the absolute temperature and C_1 and C_2 are the constants. This law is called Wien's law of energy distribution in the blackbody radiation spectrum.

Draw backs of Wien's law;

The Wien's law only suits for shorter wavelength region. It fails to explain the longer wavelength region of the blackbody radiation spectrum.

Rayleigh-Jeans law:

Rayleigh and Jeans developed an equation for the black body radiation on the basis of principle of equipartition of energy.

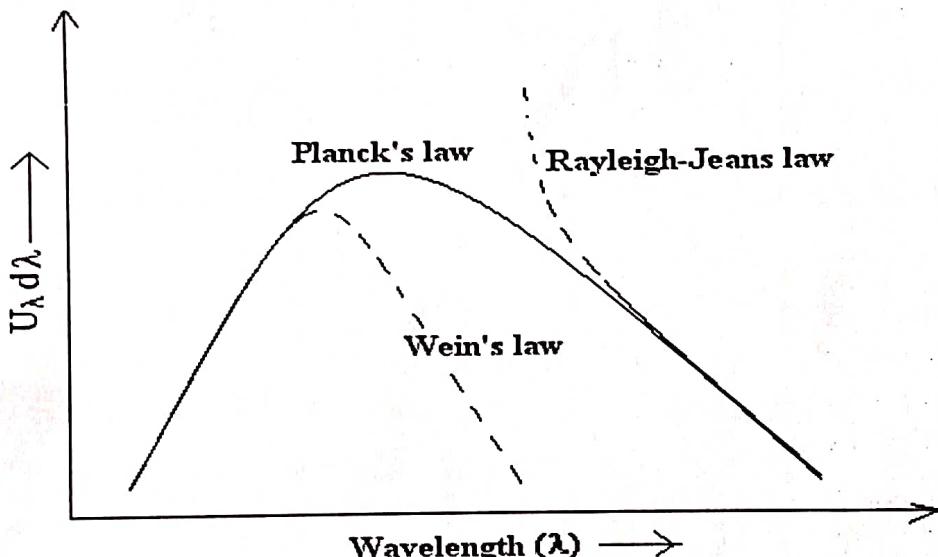
According to the principle of equipartition of energy, an average energy kT should be assigned to each mode of vibration. But the number of modes of vibration/unit volume whose wavelength are in the range λ and $\lambda+d\lambda$ is given by $8\pi\lambda^{-4}d\lambda$. Hence energy per unit volume for waves whose wavelengths are in the range λ and $\lambda+d\lambda$ is given by

$$U_\lambda d\lambda = 8\pi k T \lambda^{-4} d\lambda$$

This equation is known as Rayleigh-Jeans equation.

Draw backs of the Rayleigh-Jeans law

Rayleigh-Jeans law predicts black body to radiate all the energy at shorter wavelength side. But in actual practice, a blackbody radiates maximum energy in the infrared and visible region of the e.m. spectrum and intensity of radiation decreases down steeply for shorter wavelengths. Thus, the Rayleigh-Jeans law fails to explain the lower wavelengths side of the spectrum. The failure of the Raleigh-Jeans law to explain the spectrum beyond the violet region towards the lower wavelength region of the spectrum is particularly referred to as ***Ultra-violet catastrophe***.



Stefan-Boltzmann law:

It gives the relationship between intensity of radiation to the temperature. It states that total energy radiated by a black body per unit area per unit time is proportional to the fourth power of its absolute temperature. i.e,

$$E \propto T^4$$

$$E = \sigma T^4$$

where σ is known as Stefan's constant.

Planck's law:

Max Planck derived an equation which successfully accounted for the spectrum of black body radiation.

Assumptions of the theory are

1. The black body consists of a very large number of electrical oscillators, with each oscillator vibrating with frequency of its own.

2. Each oscillator has an energy equal to an integral multiple of $h\gamma$. Where 'h' is the Planck's constant and γ is the frequency of oscillation.

$$E = nh\gamma \text{ where } n = 1, 2, \dots \text{etc.}$$

3. An oscillator may lose or gain energy by emitting or absorbing respectively a radiation of frequency γ whose value is given by $\gamma = (\Delta E/h)$. Where ΔE is the difference in the value of the energies of the oscillator before and after the emission or absorption had taken place.

Based on the above ideas he derived the law governing the entire spectrum of black body radiation. Given by

$$U_\lambda d\lambda = \frac{8\pi hc}{\lambda^5} \left[\frac{1}{e^{\frac{h\gamma}{kT}} - 1} \right] d\lambda \quad \dots(1)$$

Where $U_\lambda d\lambda$ is the energy per unit volume in the wavelength range λ and $\lambda + d\lambda$, 'h' is Planck's constant and 'k' is Boltzmann's constant.

This is called Planck's radiation law. Wien's law and Rayleigh - Jeans law can be deduced from Planck's law.

Reduction of Planck's law to Wien's law:

For shorter wavelengths $\gamma = c/\lambda$ is large.

When γ is large $e^{\frac{h\gamma}{kT}}$ is very large

$$\therefore e^{\frac{h\gamma}{kT}} \gg 1$$

$$\therefore e^{\frac{h\gamma}{kT}} - 1 \approx e^{\frac{h\gamma}{kT}} = e^{\frac{hc}{\lambda kT}}$$

Making use of this in equation (1)

$$U_\lambda d\lambda = \frac{8\pi hc}{\lambda^5} \left[\frac{1}{e^{\frac{hc}{\lambda kT}}} \right] d\lambda$$

$$\therefore U_\lambda d\lambda = C_1 \lambda^{-5} e^{-\frac{C_2}{\lambda T}} d\lambda \quad \text{where } C_1 = 8\pi hc \text{ and } C_2 = (hc/k)$$

This equation is Wien's law of radiation.

Reduction of Planck's law to Rayleigh- Jean's law:

For larger wavelength $\gamma = \frac{c}{\lambda}$ is small. When γ is small $\frac{h\gamma}{kT}$ is very small

Expanding power series, we have

$$e^{\frac{h\gamma}{kT}} = 1 + \frac{h\gamma}{kT} + \left(\frac{h\gamma}{kT} \right)^2 + \dots$$

Since $\frac{h\gamma}{kT}$ is very small its higher power terms could be neglected.

$$\therefore e^{\frac{h\gamma}{kT}} \approx 1 + \frac{h\gamma}{kT}$$

$$\left(e^{\frac{h\gamma}{kT}} - 1 \right) = 1 + \frac{h\gamma}{kT} - 1 = \frac{h\gamma}{kT} = \frac{hc}{\lambda kT}$$

Substituting in equation (1)

$$U_\lambda d\lambda = \frac{8\pi hc}{\lambda^5 \left(\frac{hc}{\lambda kT} \right)} d\lambda$$

$$\therefore U_\lambda d\lambda = \frac{8\pi kT}{\lambda^4} d\lambda$$

This equation is Rayleigh - jeans law of radiation.

De-Broglie Concept of matter waves:

To explain photoelectric effect, Compton effect etc. light should be treated as particle. To explain the phenomena such as interference, diffraction etc. light should be treated as wave. Therefore, light some time exhibits wave nature and some other time exhibits particle nature. Thus, light has dual nature.

Louis de-Broglie proposed that if electromagnetic wave such as light has a dual nature it should also be valid for material particles such as electrons, protons, neutrons etc. His suggestion is based on the fact that nature loves symmetry. If light acts like wave as well as particle, material particles should also act as wave. The waves associated with the material particles like electrons, protons, neutrons etc. are called *matter waves*. He derived the expression for the wavelength of the matter wave and it is called de-Broglie wavelength.

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

Where 'm' is the mass of the particle, 'v' is the velocity, 'h' is the Planck's constant and 'p' is the momentum of the particle.

Relation between kinetic energy and de Broglie wavelength:

The kinetic energy can be calculated using the relation

$$E = \frac{1}{2}mv^2$$

Multiplying and dividing by m

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

Substituting for momentum $p = mv$

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

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

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

De Broglie wavelength of an accelerated electrons:

If an electron of mass m is accelerated by a potential difference V. The energy acquired by the electron is given by $eV = \frac{1}{2}mv^2$

Multiplying and dividing by m

$$eV = \frac{m^2v^2}{2m}$$

Substituting momentum $p = mv$

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

$$\therefore p = \sqrt{2meV}$$

$$\therefore \lambda = \frac{h}{p} = \frac{h}{\sqrt{2meV}} \quad \text{Substituting for electron mass } m = 9.11 \times 10^{-31} \text{ kg, Planck's constant}$$

$$h = 6.626 \times 10^{-34} \text{ J-s and electronic charge } e = 1.6 \times 10^{-19} \text{ C}$$

$$\begin{aligned} \lambda &= \frac{6.626 \times 10^{-34}}{\sqrt{V} \times \sqrt{2 \times 9.11 \times 10^{-31} \times 1.6 \times 10^{-19}}} \\ &= \frac{1.226 \times 10^{-9}}{\sqrt{V}} \text{ m} \quad = \frac{1.226}{\sqrt{V}} \text{ nm} \end{aligned}$$

Heisenberg's Uncertainty principle:

According to classical mechanics a moving particle at any instant has a fixed position in space and a definite momentum which can be determined simultaneously with any desired accuracy.

However, in wave mechanics since a moving atomic particle is described by a wave packet, there is a limit to accuracy with which we can measure its momentum and position simultaneously with any desired accuracy.

Heisenberg principle is concerned with the uncertainty in the simultaneous measurement of the members of the pair of physical variables due to the association of the matter waves. It states that it is impossible to determine precisely and simultaneously the values of members of pair of physical variables which describe the motion of the atomic system. According to Heisenberg the error in the measurement is not due to any fault in the experiment but it is due to the fundamental characteristic of nature. Since atomic particle has to be regarded as a de-Broglie wave group. The particle may be found anywhere within the wave group. If the group is considered to be narrow it is easier to locate its position but uncertainty in measuring velocity or momentum increases. On the other hand, if the group is considered to be wide its momentum can be estimated satisfactorily but there is a great uncertainty about the exact location of the particle.

Statements of the Heisenberg's Uncertainty Principle:

In any simultaneous determination of the position and momentum of a particle, the product of the corresponding uncertainties inherently present in the measurement is equal to or greater than $\frac{h}{4\pi}$

If Δx is the uncertainty in the position of the particle along the x-axis and ΔP_x is the uncertainty in the measurement of momentum

$$\text{Then } \Delta x \cdot \Delta P_x \geq h/4\pi$$

Where h is the Planck's constant.

Similarly, if ΔE and Δt are the uncertainties in the measurement of the energy and time and ΔJ and $\Delta \theta$ are the uncertainties in the measurement of the angular momentum and angle then $\Delta E \cdot \Delta t \geq h/4\pi$ and $\Delta J \cdot \Delta \theta \geq h/4\pi$.

Thus we have the uncertainty relations

$$\Delta x \cdot \Delta P_x \geq h/4\pi$$

$$\Delta E \cdot \Delta t \geq h/4\pi$$

$$\Delta J \cdot \Delta \theta \geq h/4\pi.$$

If one tries to measure one accurately other will become completely uncertain.

Physical significance:

The physical significance of the uncertainty principle is that, one should not think of the exact position or an accurate value for momentum of a particle. Instead, one should think of the probability of finding the particle at certain position or of the probable value of the momentum of the particle. The estimation of such probabilities is made by means of certain mathematical functions, named probability density functions in quantum mechanics.

Nonexistence of the electron inside the nucleus:

According to the theory of relativity, Energy E of the particle is
 $E = mc^2 = \frac{m_0 c^2}{\sqrt{1 - \frac{v^2}{c^2}}}$ where 'm₀' is the rest mass of the particle and 'm' is mass when its velocity is 'v'. squaring the both sides of the above equation

$$E^2 = \frac{m_0^2 c^4}{1 - \frac{v^2}{c^2}} = \frac{m_0^2 c^6}{c^2 - v^2} \quad \dots\dots(1)$$

If 'p' is the momentum of the particle

$$p = mv = \frac{m_0 v}{\sqrt{1 - \frac{v^2}{c^2}}}$$

Squaring the both sides of the above equation

$$p^2 = \frac{m_0^2 v^4}{1 - \frac{v^2}{c^2}} = \frac{m_0^2 v^2 c^2}{c^2 - v^2}$$

Multiplying by c²

$$p^2 c^2 = \frac{m_0^2 v^2 c^4}{c^2 - v^2} \quad \dots\dots(2)$$

Subtracting (2) from (1)

$$E^2 - p^2 c^2 = \frac{m_0^2 c^6}{c^2 - v^2} - \frac{m_0^2 v^2 c^4}{c^2 - v^2} = \frac{m_0^2 c^4 (c^2 - v^2)}{c^2 - v^2}$$

$$E^2 = p^2 c^2 + m_0^2 c^4 \quad \dots\dots(3)$$

We know that the diameter of the nucleus is of the order of 10⁻¹⁴m. If an electron is to exist inside the nucleus, the maximum uncertainty in the position of electron will be the order of the diameter of the nucleus.

$$\therefore (\Delta x)_{\max} = 10^{-14} \text{m}$$

By Heisenberg's uncertainty principle

$$(\Delta x)_{\max} \cdot (\Delta P)_{\min} = h/4\pi$$

Therefore minimum uncertainty in the momentum is

$$(\Delta P)_{\min} = \frac{h}{4\pi(\Delta x)_{\max}}$$

$$(\Delta P)_{\min} = \frac{6.63 \times 10^{-34}}{4\pi \times 10^{-14}}$$

$$(\Delta P)_{\min} = 0.5276 \times 10^{-20} \text{ kg.m/s}$$

This is the minimum uncertainty in the momentum of the electron. Then the momentum of the electron must at least be equal to the minimum uncertainty in the momentum

$$p_{\min} = (\Delta P)_{\min} = 0.5276 \times 10^{-20} \text{ kg.m/s}$$

The equation for the energy of the electron from theory of relativity from equation (3)

$$E = \sqrt{p^2 c^2 + m_0^2 c^4}$$

$$\text{Here } m_0^2 c^4 \ll p^2 c^2$$

$$\therefore E = pc$$

$$\therefore E_{\min} = (0.5276 \times 10^{-20}) (3 \times 10^8) \\ = 1.583 \times 10^{-12} \text{ J}$$

$$\therefore E_{\min} = 9.9 \text{ MeV}$$

Thus, for an electron to exist in the nucleus, its energy must be at least 9.9 MeV. Experimentally it has been observed during beta decay that the β -particles (electrons emitted by the nucleus due to neutron decay) never have energy exceeding about 4 MeV. This clearly indicates that electrons cannot exist within the nucleus.

Wave function:

Every wave is characterized by periodic variation in some physical quantities. For example, pressure varies periodically in sound waves. Similarly, the quantity whose periodic variations make up the matter waves is called wave function. The wave function is denoted by ψ . The wave function may vary with respect to both the position coordinates of the physical system and the time. Wave function ψ contains all the information about the system.

Physical significance of wave function

The wave function ψ itself does not have any direct physical significance and is not an experimentally measurable quantity. The wave function may be a complex quantity. But if we consider $\psi^* \psi$ it is a real quantity. Where ψ^* is the complex conjugate of ψ .

$|\psi|^2 = \psi^* \psi$ is called probability density.

The probability of finding the particle in a certain volume element $d\tau$ is

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

This interpretation was first given by Max Born.

Normalization:

If ψ is the wave function associated with the particle then $|\psi|^2 d\tau$ is the probability of finding the particle in a volume element $d\tau$. If it is certain that the particle is present in finite volume τ , then,

$$\int_0^\tau |\psi|^2 d\tau = 1$$

If we are not certain that the particle is present in finite volume, then

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

This condition is called normalization condition. The wave function which obeys this condition is said to be normalized wave function.

In some cases

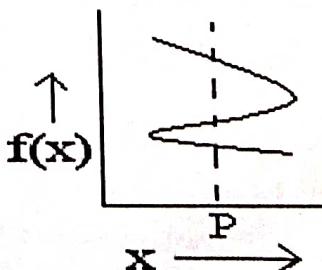
$$\int_{-\infty}^{\infty} |\psi|^2 d\tau \neq 1 \text{ and involves constant}$$

In such cases we can obtain a constant which when multiplied to the wave function will give new wave function which will satisfy the normalization condition. This is called normalization.

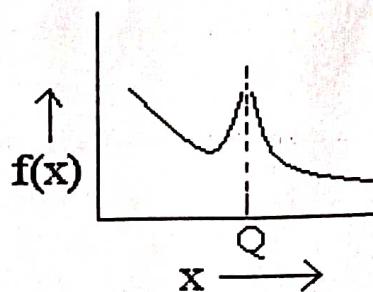
Properties of the wave function:

1. ψ must be the solution of Schrödinger's wave equation.

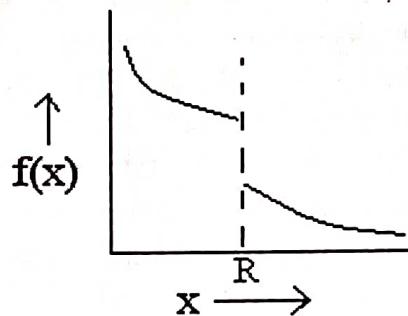
2. ψ must be single valued function at every point in space. In the figure function $f(x)$ is not single valued it has 3 different values at $x=P$.



3. ψ must be finite at each and every point in space. In the figure function $f(x)$ is not finite at $x=Q$



4. ψ must be continuous in the region where it is defined. In the figure $f(x)$ is discontinuous at $x=R$



5. $\frac{d\psi}{dx}, \frac{d\psi}{dy}, \frac{d\psi}{dz}$ must be continuous in the region where ψ is defined.

Eigen functions and Eigen values.

In order to find wave function ψ Schrödinger equation has to be solved. But it is a second order differential equation it has several solutions. All of them may not be the correct wave function which we are searching for. We have to select those wave functions which would correspond meaningfully to a given physical system. Such wave functions are said to be acceptable wave functions. They should be single valued, continuous and finite everywhere. Such acceptable wave functions are named as *Eigen functions*.

Once the Eigen functions are known quantum mechanical operators could be used to evaluate physical observables such as energy. In which case each of the Eigen functions provide one energy value. Since there are only restricted set of Eigen functions only restricted set of energy values. These values are called *Eigen values*. We can write the Eigen value equation as $\hat{A}\psi = \lambda\psi$. here differential operator \hat{A} operates on the function ψ and this gives constant λ times the function. The function ψ is called Eigen function and λ is called Eigen value.

Example if $\psi = e^{ax}$ $\hat{A} = \frac{d}{dx}$ Then $\hat{A}\psi = \frac{d}{dx}e^{ax} = ae^{ax}$ therefore Eigen value is a.

Some of the operators in quantum mechanics are

$\hat{p} = \frac{\hbar}{2\pi i} \frac{\partial}{\partial x}$ is the momentum operator

$-\frac{\hbar^2}{8\pi^2 m} \frac{\partial^2}{\partial x^2} + U$ is the total energy operator.

Schrödinger equation:

The wave function in quantum mechanics accounts for the wavelike properties of a particle. It is obtained by solving a fundamental equation called **Schrödinger equation**. The Schrödinger equation can be set in two different contexts. One which is general and takes care of the both the position and time variations of the wave function and it is called **time**

dependent Schrödinger equation. The other one which is applicable to study state conditions only in which case the wavefunction can have variation only with position but not with time. It is called **time independent Schrödinger equation** and is simpler than other. The wave functions obtained as solutions of time independent equation is not necessarily complex functions.

Setting up of one-dimensional time independent Schrödinger equation:

Based on de Broglie's idea of matter waves Schrödinger developed a mathematical theory which plays the same role as Newton's laws in classical mechanics. Consider a particle of mass 'm' moving with velocity 'v'. The de-Broglie wavelength ' λ ' is

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

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

The wave equation for a de Broglie wave considered traveling in positive x direction can be written in complex form as

$$\psi = Ae^{i(kx-wt)} \quad \dots(2)$$

Where 'A' is a constant and 'w' is the angular frequency of the wave and 'k' is wave vector.

Differentiating equation (2) twice with respect to t

$$\frac{d\psi}{dt} = Ae^{i(kx-wt)} \cdot (-iw)$$

$$\frac{d^2\psi}{dt^2} = Ae^{i(kx-wt)} \cdot (-iw) \cdot (-iw)$$

$$\frac{d^2\psi}{dt^2} = i^2 w^2 Ae^{i(kx-wt)} \quad \text{but } i^2 = -1 \text{ and } \psi = Ae^{i(kx-wt)}$$

$$\frac{d^2\psi}{dt^2} = -w^2\psi \quad \dots(3)$$

We have the equation for traveling wave as

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

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

$$\frac{d^2\psi}{dx^2} = \frac{1}{v^2} \frac{d^2\psi}{dt^2} \quad \dots(4)$$

The above equation represents wave propagating along x-axis with velocity 'v' and ' ψ ' is the displacement at the instant t.

From equations (3) and (4)

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

If ' λ ' and ' γ ' are the wavelength and frequency of the waves then $w = 2\pi\gamma$ and $v = \gamma\lambda$.

Substituting for 'w' and 'v' the above equation becomes

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

$$\text{Or } \frac{1}{\lambda^2} = -\frac{1}{4\pi^2\psi} \frac{d^2\psi}{dx^2} \quad \dots(5)$$

$$K.E = \frac{1}{2}mv^2 = \frac{m^2v^2}{2m} = \frac{p^2}{2m}$$

But $p = h/\lambda$

$$K.E = \frac{h^2}{2m\lambda^2} \quad \dots(6)$$

Using equation (5) in (6)

$$K.E = \frac{h^2}{2m} \left(-\frac{1}{4\pi^2\psi} \frac{d^2\psi}{dx^2} \right)$$

$$K.E = -\frac{\hbar^2}{8\pi^2 m \psi} \frac{d^2 \psi}{dx^2} \quad \dots \dots (7)$$

The total energy E is the sum of K.E. and Potential energy V.

$$E = K.E + V$$

Substituting for K.E. from equation (7)

$$E = -\frac{\hbar^2}{8\pi^2 m \psi} \frac{d^2 \psi}{dx^2} + V$$

$$E - V = -\frac{\hbar^2}{8\pi^2 m \psi} \frac{d^2 \psi}{dx^2}$$

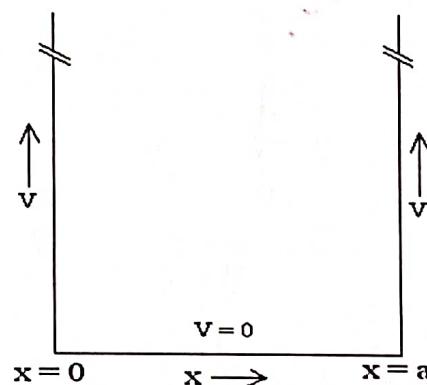
$$\frac{d^2 \psi}{dx^2} = -\frac{8\pi^2 m}{\hbar^2} (E - V) \psi$$

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

This is the time independent Schrödinger wave equation in one dimension

Application of Schrödinger wave equation to a particle inside a potential well of infinite height

Suppose a particle of mass 'm' is inside a potential well and moving in a x direction only. Let the width of the potential well is 'a'. Therefore, particle is free to move in the region $x = 0$ and $x = a$. Outside this region the potential energy V is taken to be infinite and within the region it is zero. Particle is bound within $x = 0$ to $x = a$.



$$V=0 \text{ when } 0 \leq x \leq a$$

$$V = \infty \text{ when } x < 0 \text{ and } x > a$$

Such a configuration of potential in space is called infinite potential well. It is also called particle in box. One can use Schrödinger equation to solve this. Schrödinger equation is

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

Outside the well Schrödinger equation is

$$\frac{d^2 \psi}{dx^2} + \frac{8\pi^2 m}{\hbar^2} (E - \infty) \psi = 0 \text{ since } V = \infty \text{ outside the well}$$

This equation holds good only if $\psi=0$ for all points outside the well. i.e. $|\psi|^2 = 0$ which means that the particle cannot be found at all outside the well.

Inside the well Schrödinger equation is

$$\frac{d^2 \psi}{dx^2} + \frac{8\pi^2 m}{\hbar^2} E \psi = 0 \quad \dots \dots (1) \quad \text{since } V = 0 \text{ inside the well.}$$

Let

$$\frac{8\pi^2 m}{\hbar^2} E = K^2 \quad \dots \dots (2)$$

Substituting in equation (1)

$$\frac{d^2\psi}{dx^2} + K^2\psi = 0 \quad \dots\dots(3)$$

The general solution of the above equation is given by
 $\psi = \cos Kx + D \sin Kx \quad \dots\dots(4)$

Where C and D are constants.

Applying the boundary condition $\psi = 0$ when $x = 0$ in equation (4)
 $0 = C \cos 0 + D \sin 0$

$$0 = C + 0 \text{ or } C = 0$$

$$\therefore \psi = D \sin Kx \quad \dots\dots(5)$$

Again applying the boundary condition $\psi = 0$ when $x = a$

$$0 = D \sin Ka$$

$$D \sin Ka = 0$$

$D \neq 0$ because if D is zero $\psi = 0$

$$\therefore \sin Ka = 0$$

Or $Ka = n\pi$ where $n = 0, 1, 2, \dots$ etc.

n is the quantum number which is either zero or positive number.

$$\therefore K = \frac{n\pi}{a} \quad \dots\dots(6)$$

From (5) and (6) we can write

$$\psi = D \sin \frac{n\pi}{a} x \quad \dots\dots(7)$$

This is the permitted solutions

To evaluate D , one has to perform normalization of the wave function

The particle is present somewhere inside the well. Therefore, probability of finding the particle over the entire space in the well must be equal to unity. Therefore

$$\int_0^a |\psi|^2 dx = 1$$

Substituting for Ψ from the equation (7)

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

But we know that

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

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

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

$$\text{Or } \frac{D^2}{2} \left[a - \frac{a}{2n\pi} \sin(2n\pi) - 0 \right] = 1$$

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

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

The normalized wave function of particle in one dimensional infinite potential well is given by

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

In general wave function is

$$\psi_n = \sqrt{\frac{2}{a}} \sin \left(\frac{n\pi}{a} x \right) \text{ for } n = 1, 2, \dots \text{etc. eigen functions are } \psi_1, \psi_2, \dots$$

Energy eigen values

From equations (2) and (6)

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

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

In general

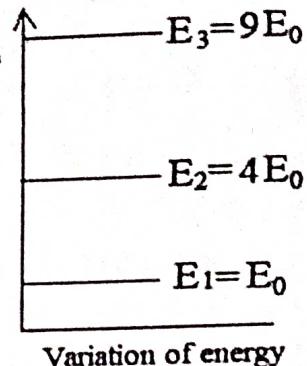
$$E_n = \frac{n^2 h^2}{8ma^2} \text{ for } n = 1, 2, \dots \text{ etc. energy eigen values are } E_1, E_2, \dots \text{ etc.}$$

If $n = 0$ in the above equation $\psi_n = 0$. Which means to say that electron does not exist in the well. Therefore $n \neq 0$.

When $n = 1$ particle is in ground state. $E_{\text{zero-point}} = E_1 = \frac{h^2}{8ma^2} = E_0$

Energy of the particle in the first excited state ($n=2$) is $E_2 = \frac{4h^2}{8ma^2} = 4E_0$

Energy of the particle in the second excited state ($n=3$) is $E_3 = \frac{9h^2}{8ma^2} = 9E_0$



Wave functions probability densities and energy levels for particle in box

Eigen functions and Eigen values for particle in one dimensional potential well are

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

$$E_n = \frac{n^2 h^2}{8ma^2}$$

Case 1

For $n = 1$ This is the ground state and particle is normally found in this state.

For $n = 1$ Eigen function is

$$\psi_1 = \sqrt{\frac{2}{a}} \sin\frac{\pi}{a}x$$

In the above equation ψ_1 is $= 0$ for both $x = 0$ and $x = a$

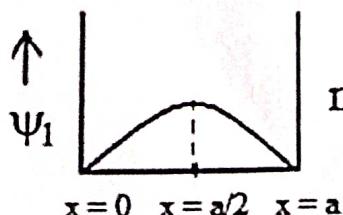
ψ_1 is maximum when $x = a/2$

Probability density $|\psi_1|^2 = 0$ for both $x = 0$ and $x = a$

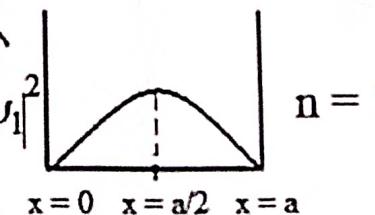
$|\psi_1|^2$ is maximum for $x = a/2$

The plot of ψ_1 versus x and $|\psi_1|^2$ versus x are shown in figure

Therefore when particle is in ground state probability of finding the particle at center will be maximum and that at the walls is zero.



$n = 1$



$n = 1$

The energy of the particle

$$E_1 = \frac{h^2}{8ma^2} = E_0$$

This is the lowest permitted energy of the particle it is also called zero point energy.

Case 2

For $n = 2$ This is the first excited state.

For $n = 2$ Eigen function is

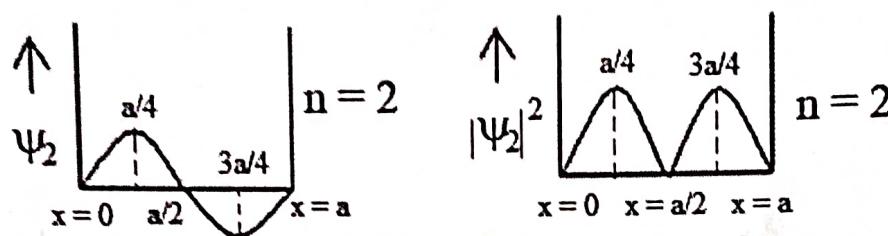
$$\psi_2 = \sqrt{\frac{2}{a}} \sin \frac{2\pi}{a} x$$

In the above equation ψ_2 is $= 0$ for $x = 0, x = a/2$ and $x = a$
 ψ_2 is maximum for $x = a/4$ and $x = 3a/4$

Probability density $|\psi_2|^2 = 0$ for $x = 0, x = a/2$ and $x = a$
 $|\psi_2|^2$ is maximum for $x = a/4$ and $x = 3a/4$

The plot of ψ_2 versus x and $|\psi_2|^2$ versus x are shown in figure

Therefore when particle is in first excited state it can not be found at walls and at the central region.



The energy of the particle

$$E_2 = \frac{4\hbar^2}{8ma^2} = 4E_0$$

Thus the energy in the first excited state is 4 times the energy at the ground state.

Case 3

For $n = 3$ This is the second excited state.

For $n = 3$ Eigen function is

$$\psi_3 = \sqrt{\frac{2}{a}} \sin \frac{3\pi}{a} x$$

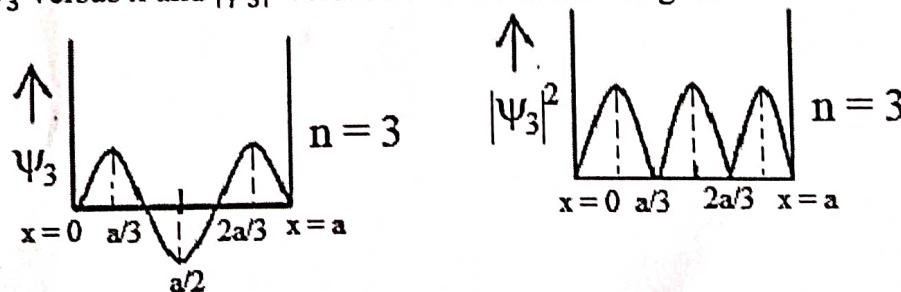
In the above equation ψ_3 is $= 0$ for $x = 0, x = a/3, x = 2a/3$ and $x = a$

ψ_3 is maximum for $x = a/6, x = a/2$ and $x = 5a/6$

Probability density $|\psi_3|^2 = 0$ for $x = 0, x = a/3, x = 2a/3$ and $x = a$

$|\psi_3|^2$ is maximum for $x = a/6, x = a/2$ and $x = 5a/6$

The plot of ψ_3 versus x and $|\psi_3|^2$ versus x are as shown in figure



The energy of the particle when it is in its second excited state is

$$E_3 = \frac{9\hbar^2}{8ma^2} = 9E_0$$

Thus, the energy in the second excited state is 9 times the energy at the ground state.

**Engineering Physics
Question Bank
Module-4**

1. Explain the energy distribution in the spectrum of a blackbody.
Give an account of attempts made through various laws to explain the spectrum.
2. What is Planck's law of radiation? Show how Wein's law and Rayleigh-Jean's laws can be derived from it
3. Explain the de-Broglie concept of matter waves. Obtain the expression for the de-Broglie wavelength of electrons accelerated by potential difference V.
4. State and explain Heisenberg Uncertainty principle. What is its physical significance?
5. Show that the electron does not pre-exist inside the nucleus using uncertainty principle
6. What is wave function? What are the properties of a wave function?
7. Give the qualitative explanation of Max Born's interpretation of wave function
8. What is the normalization of the wave function? What are Eigen functions and Eigen values?
9. Set up one dimensional time independent Schrödinger wave equation.
10. Starting from Schrodinger's time independent wave equation, derive the expression for energy Eigen value and Eigen function for a particle present in 1-D potential well of infinite depth.
11. Discuss the wave functions, probability densities and energy levels for particle in an infinite potential well by considering the ground state and first two excited states.