

**UNIT 2 – QUANTUM MECHANICS**  
**Physics of Electrical and Electronic Materials (PY21IE)**  
**EEE Stream- (2025 Scheme)**

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Content:

de Broglie Hypothesis and Matter Waves, Heisenberg's Uncertainty Principle and its application to broadening of spectral lines

Wave Mechanics: Wave function, Operators, Eigen function and Eigen values of a free particle, Expectation value and its significance, Derivation of 1-dimensional (1D) time-independent Schrodinger equation (TISE) from classical wave equation, 1D TISE for infinite well, free particle, Solution for 3-dimensional (3D) well, Concept of degeneracy, Quantum Tunneling and Finite well, Numerical problems.

### **Introduction:**

At the beginning of the 20<sup>th</sup> century, Newton's laws of motion were able to successfully describe the motion of the particles in classical mechanics (the world of large, heavy and slow bodies) and Maxwell's equations explained phenomena in classical electromagnetism. However, the classical theory does not hold in the region of atomic dimensions. It could not explain the stability of atoms, energy distribution in the black body radiation spectrum, origin of discrete spectra of atoms, etc. It also fails to explain the large number of observed phenomena like photoelectric effect, Compton Effect, Raman Effect, Quantum Hall effect, superconductivity etc. **The insufficiency of classical mechanics led to the development of quantum mechanics (QM).**

Quantum mechanics gives the description of motion and interaction of particles in the small-scale atomic system where the discrete nature of the physical world becomes important. With the application of quantum mechanics, most of the outstanding

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problems have been solved. The direct implications of QM though very subtle have dramatic effect in our day to day life. For example, QM successfully introduced the concept of discrete energy which led to the conception and advancements in quantum computing, it also paved way for efficient long distance transfer of large quantities of data electronically. By understanding the electronic spin and related atomic properties, QM has aided in realizing energy efficient materials that can be applied to consumable electronic equipment and in commercial transport vehicles like Hyper loop, Maglev trains among others.

### **Wave and particle duality of radiation**

To understand the wave and particle duality, it is necessary to know what a particle is and what a wave is.

A particle is a localized mass and it is specified by its mass, velocity, momentum, energy, etc. In contrast a wave is a spread out disturbance. A wave is characterized by its wavelength, frequency, velocity, amplitude, intensity, etc. It is hard to think mass being associated with a wave. Considering the above facts, it appears difficult to accept the conflicting ideas that radiation has a wave particle duality. However, this acceptance is essential because the radiation exhibits phenomena like interference, diffraction, polarization, etc., and shows the wave nature and it also exhibits the particle nature in the black-body radiation effect, photoelectric effect, Compton Effect etc.

**Radiation**, thus, sometimes behave as a *wave* and at some other time as a *particle*, this is the wave particle duality of radiation.

### de Broglie's concept of matter waves.

Louis de-Broglie in 1924 extended the wave particle dualism of radiation to fundamental entities, such as electrons, protons, neutrons, atoms, molecules, etc. de-Broglie put a bold suggestion that like radiation, matter also has dual characteristic, at a time when there was absolutely no experimental evidence for wave like properties of matter waves. **de-Broglie Hypothesis** of matter waves is as follows.

- In nature energy manifests itself in two forms, namely matter and radiation.
- Nature loves symmetry.
- As radiation can act like both wave and a particle, material particles (like electrons, protons, etc.) in motion should exhibit the property of waves.

These waves due to moving matter are called *matter waves or de-Broglie waves or pilot waves*.

### Wavelength of matter waves:

The concept of matter waves is well understood by combining Planck's quantum theory and Einstein's theory. Consider a photon of energy  $E$ , frequency  $\gamma$  and wavelength  $\lambda$ .

$$\text{By Planck's theory } E = h\gamma = \frac{hc}{\lambda}$$

$$\text{By Einstein's mass-energy relation } E = mc^2$$

By equating and rearranging the above equations, we get

$$mc^2 = \frac{hc}{\lambda}$$
$$\lambda = \frac{h}{mc} = \frac{h}{p}$$

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Where,  $p$  is the momentum of the photon and  $h$  is a Planck's constant.

Now consider a particle of mass  $m$  moving with a velocity  $v$  and momentum  $p$ . According to the de-Broglie hypothesis matter also has a dual nature. Hence the wavelength  $\lambda$  of matter waves is given by

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

This is the equation for the de-Broglie wavelength.

### **de Broglie wavelength of an electron**

Consider an electron of mass 'm' accelerated from rest by an electric potential  $V$ . The electrical work done (eV) is equal to the kinetic energy  $E$  gained by the electron.

$$\begin{aligned} E &= eV \\ \therefore E &= \frac{1}{2}mv^2 \\ \therefore m^2v^2 &= 2mE \\ mv &= \sqrt{2mE} \end{aligned}$$

Therefore, wavelength of electron wave

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

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

But  $E = eV$

$$\therefore \lambda = \frac{h}{\sqrt{2meV}} = \frac{\frac{h}{\sqrt{2me}}}{\sqrt{V}}$$

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Substituting the values of e, m and h, we get

$$\frac{h}{\sqrt{2me}} = 12.28 A^o$$
$$\therefore \lambda = \frac{12.28}{\sqrt{V}} A^o$$

Note: Instead of an electron, if a particle of charge ‘q’ is accelerated through a potential difference V, then

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

### Wave Packet

A **wave packet** refers to the case where two (or more) waves exist simultaneously. A wave packet is often referred to a wave group. This situation is permitted by the principle of superposition. 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 wavenumbers, 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) or it may change (dispersion) while propagating.

## Phase velocity and Group velocity

A monochromatic wave has velocity called the **phase velocity**

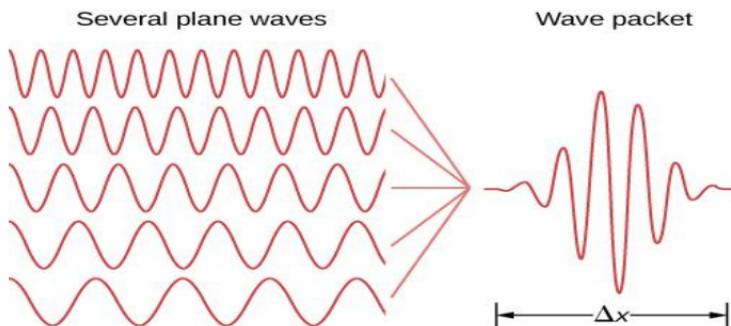
$$V_p = \frac{\omega}{k} = v\lambda$$

where  $\omega$  is the angular frequency,  $k = \frac{2\pi}{\lambda}$  is the wave number,  $v$  is the frequency.

However, if we have a compound wave (wave packet) that is composed of individual waves with a range of frequencies, each individual wave has its phase velocity, but the amplitudes of the waves add up to produce a wave packet which has a velocity all its own. This velocity is called the **group velocity** ( $v_g$ ) and is usually different from the individual phase velocities of the waves that make up the wave packet. Schrodinger postulated that moving particle (electron, proton..etc) is equivalent to a wavepacket rather than a single wave. The velocity with which the resultant envelope of the group waves travels is called group velocity ( $v_g$ ) and is equal to the particle velocity ( $v$ ).

It is given by the expression

$$V_g = \frac{d\omega}{dk} = V$$



**Fig: Schematic diagram of Wave Packet**

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The equation that describes the evolution of this wave packet is the Schrödinger equation. It can be Time independent or Time dependent.

**Properties of matter waves and how they are different from electromagnetic waves**

1. Lighter the particle, greater would be the wavelength of matter waves associated with it.
2. Smaller the velocity of the particle, greater would be the wavelength.
3. For  $p = 0$ ,  $\lambda$  is infinity ie., the wave becomes indeterminate. This means that matter waves are associated with moving particles only.
4. Matter waves are produced by charged or uncharged particles in motion. Whereas electromagnetic waves are produced only by a moving charged particle. Hence matter waves are non-electromagnetic waves.
5. In an isotropic medium the wavelength of an electromagnetic wave is a constant, whereas wavelength of a matter wave changes with the velocity of the particle. Hence matter waves are non-electromagnetic waves.
6. A particle is a localized mass and a wave is a spread-out disturbance. So, the wave nature of matter introduces a certain uncertainty in the position of the particle.
7. Matter waves are probability waves because waves represent the probability of finding a particle in space.

### **Heisenberg's uncertainty principle**

Heisenberg's uncertainty principle is a direct consequence of the dual nature of matter. In classical mechanics, a moving particle at any instant has a fixed position in space and a definite momentum which can be determined if the initial values are known (**we can know the future if we know the present**)

In wave mechanics a moving particle is described in terms of a wave group or wave packet. According to Max Born's probability interpretation the particle may be present anywhere inside the wave packet. When the wave packet is large, the momentum can be fixed, but there is a large uncertainty in its position. On the other hand, if the wave packet is small the position of the particle may be fixed, but the particle will spread rapidly and hence the momentum (or velocity) becomes indeterminate. In this way certainty in momentum involves uncertainty in position and the certainty in position involves uncertainty in momentum. Hence it is impossible to know within the wave packet where the particle is and what is its exact momentum. (**We cannot know the future because we cannot know the present**). Thus, we have Heisenberg's uncertainty principle.

According to the Heisenberg's uncertainty principle "*It is impossible to specify precisely and simultaneously certain pairs of physical quantities like position and momentum that describe the behavior of an atomic system*". Qualitatively, this principle states that in any simultaneous measurement the product of the magnitudes of the uncertainties of the pairs of physical quantities is equal to or greater than  $\hbar/4\pi$  (or of the order of  $\hbar$ )

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Considering the pair of physical quantities such as position and momentum, we have

$$\Delta p \Delta x \geq h/4\pi \quad \dots\dots 1$$

Where  $\Delta p$  and  $\Delta x$  are the uncertainties in determining the momentum and the position of the particle.

Similarly, we have other canonical forms as

$$\Delta E \Delta t \geq h/4\pi \quad \dots\dots 2$$

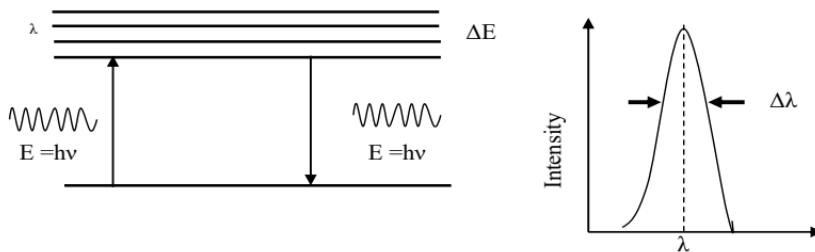
$$\Delta J \Delta \theta \geq h/4\pi \quad \dots\dots 3$$

Where  $\Delta E$  and  $\Delta t$  are uncertainties in determining energy and time while  $\Delta J$  and  $\Delta \theta$  are uncertainties in determining angular momentum and angular position.

### **Illustration of Heisenberg's uncertainty principle**

#### **Broadening of spectral lines**

When an atom absorbs a photon, it rises to the excited state and it will stay in the excited state for certain time called the lifetime. Lifetime of atoms in the excited levels is of the order of  $10^{-8}$ s. When the atom comes to the ground state it emits a photon of energy exactly equal to the energy difference between the two levels as shown in the figure.



**Fig: Line width for emitted photons**

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The energy of the emitted photon is given by

Where  $h$  is a Planck's constant,  $v$  is the frequency,  $c$  is the velocity of light and  $\lambda$  is the wavelength.

Differentiating equation (1) with respect to wavelength ( $\lambda$ ), we get

$$|\Delta E| = \frac{hc\Delta\lambda}{\lambda^2} \dots \dots \dots (2)$$

According to Heisenberg's uncertainty principle, the finite lifetime  $\Delta t$  of the excited state means there will be an uncertainty in the energy of the emitted photon is given by

$$\Delta E \geq \frac{h}{4\pi At}$$

Substituting for  $\Delta E$  from (2) and applying the condition of minimum uncertainty, we get

$$\frac{hc\Delta\lambda}{\lambda^2} = \frac{h}{4\pi\Delta t}$$

$$\text{or } \Delta\lambda \geq \frac{\lambda^2}{4\pi c \Delta t}$$

This shows that for a finite lifetime of the excited state; the measured value of the emitted photon wavelength will have a spread of wavelengths around the mean value  $\lambda$ . This uncertainty in the measured value of wavelength demands for very narrow spread, the lifetime of the excited state must be very high (of the order of  $10^{-3}$  s). Such excited levels are called **metastable states**. **This concept is adopted in the production of laser light.**

### **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 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.

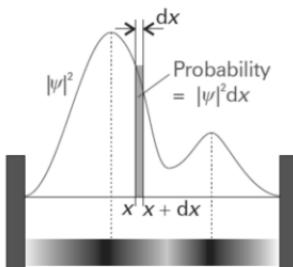
### **Physical significance of the wave function**

The wave function  $\psi(x, t)$  is the solution of Schrödinger wave equation. It gives a quantum-mechanically complete description of the behavior of a moving particle. The wave function  $\psi$  cannot be measured directly by any physical experiment. However, for a given  $\psi$ , knowledge of usual dynamic variables, such as position, momentum, angular momentum, etc., of the particle is obtained by performing suitable mathematical operations on it.

The most important property of  $\psi$  is that it gives a measure of the probability of finding a particle at a particular position.  $\psi$  is also called the **probability amplitude**. In general,  $\psi$  is a complex quantity, whereas the probability must be real and positive. Therefore, a term called probability density is defined. The **probability density  $P(x,t)$**  is a product of the wave function  $\psi$  and its complex conjugate  $\psi^*$ .

$$\therefore P(x, t) = \psi\psi^* = |\psi(x, t)|^2$$

### The Born interpretation of the wavefunction

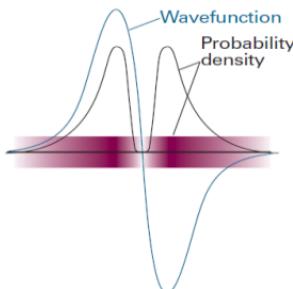


The interpretation of the wave function in terms of the location of the particle is based on a suggestion made by Max Born. He made use of an analogy with the wave theory of light, in which the square of the amplitude of an electromagnetic wave in a region is interpreted as its intensity and therefore (in quantum terms) as a measure of the probability of finding a photon present in the region. The Born interpretation of the wavefunction focuses on the square of the wavefunction (or the square modulus,  $|\psi|^2 = \psi^*\psi$ , if  $\psi$  is complex). It states that the value of  $|\psi|^2$  at a point is proportional to the probability of finding the particle in a region around that point. If the wavefunction of a particle has the value  $\psi$  at some point  $x$ , then the probability of finding the particle between  $x$  and  $x + dx$  is proportional to  $|\psi|^2 dx$ . Thus,  $|\psi|^2$  is the probability density, and to obtain the probability it must be multiplied by the length of the infinitesimal region  $dx$ . The wavefunction  $\psi$  itself is called the **probability amplitude**. The Born interpretation does away with any worry about the significance of a negative (and, in general, complex) value of  $\psi$  because  $|\psi|^2$  is real and never negative. There is no direct significance in the negative (or complex) value of a wavefunction: only the square modulus, a positive quantity, is directly physically significant, and both negative and positive

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regions of a wavefunction may correspond to a high probability of finding a particle in a region.



### **Normalization of wave function**

If  $\psi$  is a wave function associated with a particle, then  $\psi^2 d\tau$  is the probability of finding the particle in a small volume  $d\tau$ . If it is certain that the particle is present in a volume  $\tau$  then the total probability in the volume  $\tau$  is unity i.e.,  $\int_{\tau} \psi^2 d\tau = 1$ . This is the normalization condition.

**In one dimension the normalization condition is  $\int_x \psi^2 dx = 1$**

Note: When the particle is bound to a limited region the probability of finding the particle at infinity is zero i.e.,  $\psi\psi^*$  at  $x = \infty$  is zero.

### **Properties of wave function:**

The wave function  $\psi$  should satisfy the following properties to describe the characteristics of matter waves.

1.  $\psi$  must be a solution of Schrödinger wave equation.
2. The wave function  $\psi$  should be continuous and single valued everywhere. Because it is related to the probability of finding a particle at a given position at a given time, which will have only one value.

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3. The first derivative of  $\psi$  with respect to  $x$  should be continuous and single valued everywhere, since it is related to the momentum of the particle which should be finite.
4.  $\psi$  must be normalized so that  $\psi$  must go to 0 as  $x \rightarrow \pm\infty$ , so that  $\int \psi^2 d\tau$  over all the space be a finite constant.

### **Eigen functions and Eigen values**

The Schrödinger wave equation is a second order partial differential equation; it will have many mathematically possible solutions ( $\psi$ ). All mathematically possible solutions are not physically acceptable solutions. The physically acceptable solutions are called **Eigen functions ( $\psi$ )**.

The physically acceptable wave functions  $\psi$  has to satisfy the following conditions:

1.  $\psi$  is single valued.
2.  $\psi$  and its first derivative with respect to its variable are continuous everywhere.
3.  $\psi$  is finite everywhere.

Once the Eigen functions are known, they can be used in Schrödinger wave equation to evaluate the physically measurable quantities like energy, momentum, etc., these values are called **Eigen values**.

In an operator equation  $\hat{O}\psi = \lambda\psi$  where  $\hat{O}$  is an **operator** for the physical quantity and  $\psi$  is an **Eigen function** and  $\lambda$  is the **Eigen value**.

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Example:

$$\hat{H}\psi = E\psi$$

Where H is the total energy (Hamiltonian) operator,  $\psi$  is the Eigen function and E is the total energy in the system. We can have similar equations for the momentum

$$\hat{P}\psi = p\psi$$

$\hat{P}$  is the momentum operator and p denotes its momentum eigen values

### Expectation Value

**Definition:** The expectation value is a prediction of the average value measured based on infinite number of measurements were performed on a quantum system.

**Example:** For example, the expectation value of the electron's radius in the ground state of a hydrogen atom represents the average position that would be obtained, if measurements were carried out on a large number of hydrogen atoms, all in the same ground state.

In terms of operator, we can write

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

Similarly for momentum

$$\langle p \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{p} \Psi \, dx = \int_{-\infty}^{\infty} \hat{p} |\Psi|^2 \, dx$$

### Significance

1. The expectation value serves as the quantum mechanical counterpart of a classical observable.

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2. It establishes a connection between quantum theory and measurable classical quantities.
3. As expectation values represent average measurement results, they help in interpreting experimental observations.

### Schrödinger's Wave Equation:

In 1926 Schrödinger starting with **de-Broglie equation ( $\lambda = h/mv$ )** developed it into an important mathematical theory called wave mechanics which found a remarkable success in explaining the behavior of the atomic system and their interaction with electromagnetic radiation and other particles. In water waves, the quantity that varies periodically is the height of water surface. In sound waves it is pressure. In light waves, electric and magnetic fields vary. *The quantity whose variation gives matter waves is called wave function ( $\psi$ ).*

The value of wave function associated with a moving body at a particular point  $x$  in space at a time  $t$  is related to the likelihood of finding the body there at a time. A wave function  $\psi(x,t)$  that describes a particle with certain uncertainty in position, moving in a positive  $x$ -direction with precisely known momentum and kinetic energy may assume any one of the following forms:  $\sin(\omega t - kx)$ ,  $\cos(\omega t - kx)$ ,  $e^{i(\omega t - kx)}$ ,  $e^{-i(\omega t - kx)}$  or some linear combinations of them.

Schrödinger wave equation is the wave equation of which the wave functions are the solutions. **It cannot be derived from any basic principles**, but can be arrived at, by using the de-Broglie hypothesis in conjunction with the classical wave equation.

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**Time Independent 1-dimension Schrödinger wave equation (TISE)**

In many situations the potential energy of the particle does not depend on time explicitly; the force that acts on it, and hence the potential energy varies with the position of the particle only. The Schrödinger wave equation for such a particle is time independent wave equation. Let  $\Psi(x, t)$  be the wave function of the matter wave associate with a particle of mass  $m$  moving with a velocity  $v$ . The differential equation of the wave motion is as follows.

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

The solution of the Eq.(1) as a periodic displacement of time  $t$  is

$$\Psi(x, t) = \psi(x)e^{-i\omega t} \dots \dots (2)$$

Where  $\psi(x)$  is the amplitude of the matter wave.

Differentiating Eq.2 partially twice w.r.t. to  $t$ , we get

$$\begin{aligned}\frac{\partial \Psi}{\partial t} &= -i\omega \psi(x)e^{-i\omega t} \\ \frac{\partial^2 \Psi}{\partial t^2} &= i^2 \omega^2 \psi(x)e^{-i\omega t} \\ \frac{\partial^2 \Psi}{\partial t^2} &= -\omega^2 \psi(x)e^{-i\omega t} \dots \dots \dots (3)\end{aligned}$$

Differentiating eq. (2) partially twice with respect to  $x$ , we get

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

In the above equation you can note that partial differential is changed into ordinary differential because  $\psi$  is a function of  $x$  alone.  
Substituting eq. (3) and (4) in eq. (1)

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$$\frac{d^2\psi(x)}{dx^2} e^{-i\omega t} = \frac{1}{v^2} (-\omega^2 \psi(x) e^{-i\omega t}) \dots\dots (5)$$

We have  $\frac{\omega^2}{v^2} = k^2 = \left(\frac{2\pi}{\lambda}\right)^2 = \frac{4\pi^2}{\lambda^2}$

Substituting this in Eq5, we get

$$\frac{d^2\psi(x)}{dx^2} = -\frac{4\pi^2}{\lambda^2} \psi(x) \dots\dots (6)$$

$$\frac{d^2\psi(x)}{dx^2} + \frac{4\pi^2}{\lambda^2} \psi(x) = 0 \dots\dots (7)$$

Substituting the wavelength of the matter waves  $\lambda=h/mv$  in Eq.7 we get

$$\frac{d^2\psi(x)}{dx^2} + \frac{4\pi^2 m^2 v^2}{h^2} \psi(x) = 0 \dots\dots (8)$$

If E and V are the total and potential energies of the particle respectively, then the kinetic energy of the particle

$$E = \frac{1}{2} mv^2 = E - V$$
$$\therefore m^2 v^2 = 2m(E - V)$$

Substituting this in Eq.8, we get

$$\frac{d^2\psi(x)}{dx^2} + \frac{8\pi^2 m}{h^2} (E - V) \psi(x) = 0 \dots\dots (9)$$

Hence  $\psi$  is a function of  $x$  alone and is independent of time. This equation is called the one-dimensional time- independent Schrödinger wave equation.

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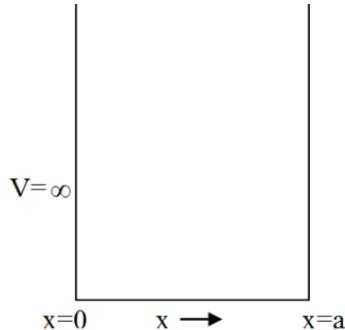
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### Applications of Schrodinger's wave equation

#### 1. Particle in a one-dimensional potential well of infinite depth (Particle in a box)

Consider a particle of mass ‘m’ moving freely in x- direction in the region from  $x=0$  to  $x=a$ . Outside this region potential energy ‘V’ is infinity and within this region  $V=0$ . Outside the box Schrodinger’s wave equation is



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

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

Inside the box  $V = 0$ , hence the Schrodinger’s equation is given by,

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

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

Equation (3) is the classical simple harmonic oscillator equation.

#### Discussion of the solution

The solution of the above equation (3) is given by

$$\psi(x) = A \cos k x + B \sin k x \dots \dots \dots (4)$$

where  $A$  and  $B$  are arbitrary constants. Typically, these constants are fixed by the boundary conditions of the problem.

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Now apply boundary conditions for this,

**Condition: I** at  $x = 0$ ,  $\psi = 0$ .

Substituting the condition I in the equation 4, we get  $A = 0$  and  $B \neq 0$ .  
(If B is also zero for all values of x,  $\psi$  is zero. This means that the particle is not present in the well.)

Now the equation 4 can be written as

$$\psi(x) = B \sin kx \dots \dots \dots \quad (5)$$

**Condition: II** at  $x = a$ ,  $\psi = 0$

Substituting the condition II in equation 5 we get

$$0 = B \sin(ka)$$

Since  $B \neq 0$ ,  $\sin ka = 0 \therefore ka = n\pi$

$$k = \frac{n\pi}{a}, k^2 = \frac{n^2\pi^2}{a^2} \quad \text{where, } n = 1, 2, 3 \dots$$

Substitute the value of  $k^2$  in equation (3).

$$\begin{aligned} \frac{8m\pi^2 E}{h^2} &= \frac{n^2\pi^2}{a^2} \\ E &= \frac{n^2 h^2}{8ma^2} \dots \dots \dots \quad (6) \end{aligned}$$

The equation (6) gives energy values or **Eigen value** of the particle in the well. When  $n=0$ ,  $\psi_n = 0$ . This means to say that the electron is not present inside the box, which is not true. Hence the lowest value of 'n' is 1.

$\therefore$  The lowest energy corresponds to ' $n=1$ ' is called the **zero-point energy or Ground state energy**.

$$E \frac{h^2}{8ma^2}_{\text{zero-point}}$$

All the states of  $n>1$  are called **excited states**.

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To evaluate B in equation (5), one has to perform normalization of wave function.

**Normalization of wave function:**

Consider the equation,  $\psi(x) = B \sin k x = B \sin \frac{n\pi}{a} x$

The integral of the wave function over the entire space in the box must be equal to unity because there is only one particle within the box, the probability of finding the particle is 1.

$$\int_0^a |\psi(x)|^2 dx = 1$$

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

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

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

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

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

$$\frac{B^2}{2} \left[ a - \frac{a}{2n\pi} \sin 2n\pi - 0 \right] = 1$$

$$\frac{B^2 a}{2} = 1 \therefore B = \sqrt{\frac{2}{a}}$$

Thus, the normalized wave function of a particle in a one-dimensional box is given by,

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin \left( \frac{n\pi}{a} x \right) \quad \text{where, } n=1,2,3\dots$$

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This equation gives the Eigen functions of the particle in the box.  
The Eigen functions for  $n=1, 2, 3\dots$  are as follows.

$$\psi_1 = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi}{a}\right) x$$

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

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

Since the particle in a box is a quantum mechanical problem, we need to evaluate the most probable location of the particle in a box and its energies at different permitted state.

### Wave functions and Probabilities

**Let us consider the three lowest energy solutions:**

**Case (1):  $n=1$**

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

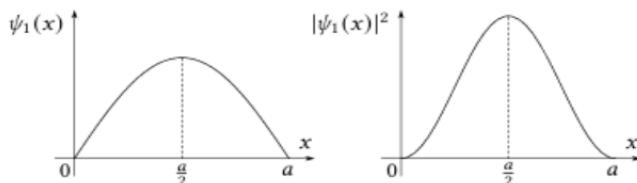
$$\psi_1 = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi}{a}\right) x$$

In the above equation  $\psi_1 = 0$  for both  $x=0$  &  $x=a$ . But  $\psi_1$  has a maximum value for  $x=a/2$ .

$$\psi_1 = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi}{a}\right) \frac{a}{2} = \sqrt{\frac{2}{a}} \quad \text{and} \quad \psi_1^2 = \frac{2}{a}$$

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A plot of  $|\psi_1|^2$  the probability density versus ‘ $x$ ’ is as shown. From the figure, it indicates the probability of finding the particle at different locations inside the box.

$\therefore |\psi_1|^2 = 0$  at  $x = 0$  and  $x = a$ , also  $|\psi_1|^2$  is maximum at  $x = (a/2)$ .

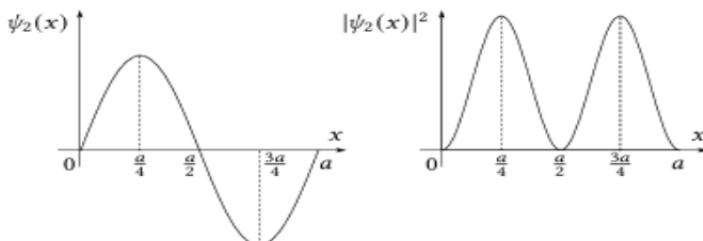
This means that in the ground state the particle cannot be found at the walls of the box and the probability of finding the particle is maximum at the central region. The Energy in the ground state is given by  $E_1 = \frac{h^2}{8ma^2}$ .

### Case (2): $n=2$

This is the first excited state. The Eigen function for this state is given

by  $\psi_2 = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi}{a}\right)x$

Now,  $\psi_2 = 0$  for the values  $x = 0, \frac{a}{2}, a$  and  $\psi_2$  reaches maximum for the values  $x = a/4, 3a/4$ . These facts are seen in the following plot.



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From the figure it can be seen that

$$|\psi_2|^2 = 0 \text{ at } x = 0, a/2, a \text{ and } |\psi_2|^2 = 2/a \text{ at } x = a/4, 3a/4$$

This means that in the first excited state the particle cannot be observed either at the walls or at the center. The energy is  $E_2 = 4E_1$ . Thus, the energy in the first excited state is four times the zero point energy.

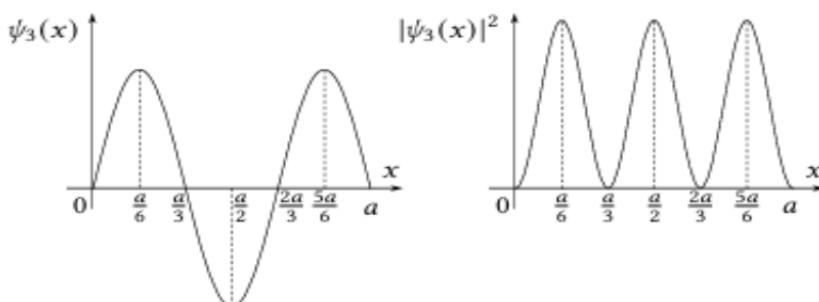
**Case 3: n = 3.**

This is the second excited state and the Eigen function for this state is given by

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

Now,  $\psi_3 = 0$  for the values  $x = 0, a/3, 2a/3, a$

and  $\psi_3$  reaches maximum  $\sqrt{\frac{2}{a}}$  at  $x = a/6, a/2, 5a/6$



$|\psi_3|^2 = 0$  for the values  $x = 0, a/3, 2a/3, a$  and  $|\psi_3|^2$  reaches maximum  $2/a$  at  $x = a/6, a/2, 5a/6$  at which the particle is most likely to be found. The energy corresponds to second excited state is given by  $E_3 = 9E_1$ .

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## 2. Free Particle:

Free particle means, it is not under the influence of any kind of field or force. Thus, it has zero potential, i.e.,  $V=0$  over the entire space. Hence Schrodinger's equation becomes,

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

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

This equation is valid for a particle for which the potential energy  $V = 0$  throughout the entire space, that is, a **free particle** with no confining boundaries. Since, for a free particle,  $V=0$  holds good everywhere, we can extend the case of particle in an infinite potential well to the free particle case, by treating the width of the well to be infinity, i.e., by allowing  $a = \infty$ .

We have the equation for energy Eigen values for a particle in an infinite potential well as,  $E = \frac{n^2 h^2}{8ma^2}$ . Where  $n=1, 2, 3, \dots$

To find the difference between two successive energy levels, we calculate:

$$\boxed{\Delta E = E_{n+1} - E_n = \frac{(2n+1)h^2}{8ma^2}}$$

This shows that the spacing between energy levels increases with increasing  $n$ , but decreases as the width ' $a$ ' of the potential well

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increases. If we take the limit as  $a \rightarrow \infty$ , the spacing between successive allowed energy levels and momentum values becomes vanishingly small. As a result, the spectrum transitions from being discrete to a continuous spectrum, just like in classical mechanics where a free particle can have any energy value. In this infinite-width limit, the wavefunctions of the infinite potential well approach the plane wave forms  $e^{ikx}$  and  $e^{-ikx}$ , which represent a free particle moving to the right and left, respectively. Hence, for a free particle, both momentum and energy can take on a continuous range of values, rather than discrete ones.

### **Solution for 2 and 3-dimensional (3D) well by analogy with 1D**

The extension of the one-dimensional infinite potential well to higher dimensions is quite straightforward. By analogy, we can write the solutions for a two-dimensional (2D) and three-dimensional (3D) infinite potential well.

In a 2D well, the quantum particle is confined within two dimensions, say  $x$  and  $y$ , while it remains free to move along the third dimension. The Schrödinger equation in two dimensions takes a similar form to the one-dimensional case but includes derivatives with respect to both  $x$  and  $y$ .

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**The Schrodinger equation in two dimensions becomes:**

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

Since confinement occurs in two directions, the quantized energy levels are now characterized by two quantum numbers,  $n_1$  and  $n_2$ , and the corresponding energy eigenvalues are given by

$$E_{n_1 n_2} = \frac{h^2}{8ma^2} (n_1^2 + n_2^2) \quad \text{where } n_1, n_2 = 1, 2, 3, \dots$$

For a two-dimensional (2D) square potential well, the wave function  $\psi(x, y)$  is expressed as:  $\psi(x, y) = \frac{2}{a} \sin\left(\frac{n_1 \pi}{a}\right) \sin\left(\frac{n_2 \pi}{a}\right)$

Here,  $a$  denote the widths of the potential well along the  $x$ - and  $y$ -directions, respectively.

**For a 3D well,** the confinement on the quantum particle is along all 3 dimensions, the Schrodinger equation is given by:

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

The quantized energies will now be labelled with three quantum numbers  $n_1, n_2, n_3$  ( $E_{n_1 n_2 n_3}$ )

$$E_{n_1 n_2 n_3} = \frac{h^2}{8ma^2} (n_1^2 + n_2^2 + n_3^2), \text{ where } n_1, n_2, n_3 = 1, 2, 3, \dots$$

The wave function for the 3D well is given by:

$$\psi(x, y, z) = \left(\frac{2}{a}\right)^{1.5} \sin\left(\frac{n_1 \pi}{a}\right) \sin\left(\frac{n_2 \pi}{a}\right) \sin\left(\frac{n_3 \pi}{a}\right)$$

**Degeneracy of energy levels:**

Degeneracy refers to the number of distinct quantum states that correspond to the same energy level. If multiple states ( $n$ ) have the same energy, the energy level is  $n$ -fold degenerate.

**Degeneracy in two-dimensional infinite square well**

In two dimensions, the energy expression becomes (by analogy)

$$E_{n_1 n_2} = \frac{\hbar^2}{8ma^2} (n_1^2 + n_2^2) \quad , \text{ where } n_1, n_2 = 1, 2, 3, \dots$$

Degeneracy occurs when different pairs of quantum numbers ( $n_1, n_2$ ) yield the same sum of squares, such as (1,2) and (2,1), or (1,3) and (3,1). This results in a two fold degeneracy for certain energy levels.

When an additional dimension is introduced, the energy levels become more closely spaced compared to those in a one-dimensional potential well. It can be observed that the spacing between adjacent energy levels tends to become nearly uniform, corresponding to a constant density of states in two dimensions.

The lowest few energy levels in a two-dimensional potential well correspond to the following pairs of quantum numbers: (1,1), {(2,1), (1,2)}, (2,2), {(3,1), (1,3)}, and {(3,2), (2,3)}.

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### **Degeneracy in three-dimensional infinite square well**

$$E_{n_1 n_2 n_3} = \frac{\hbar^2}{8ma^2} (n_1^2 + n_2^2 + n_3^2), \text{ where } n_1, n_2, n_3 = 1, 2, 3, \dots$$

Degeneracy arises when different combinations of quantum numbers ( $n_1, n_2, n_3$ ) yield the same sum of squares, such as (1,1,2), (1,2,1), and (2,1,1), or (1,1,3), (1,3,1), and (3,1,1). This results in a maximum threefold degeneracy for certain energy levels.

The introduction of a third dimension increases the number of possible energy levels compared to the two-dimensional well, thereby reducing the spacing between successive energy levels. It can be observed that as the quantum numbers ( $n_1, n_2, n_3$ ) increase, the spacing between adjacent energy levels decreases, leading to a higher density of states in three dimensions.

The lowest few energy levels of a three-dimensional potential well correspond to the following sets of quantum numbers: (1,1,1);  $\{(2,1,1), (1,2,1), (1,1,2)\}$ ;  $\{(2,2,1), (2,1,2), (1,2,2)\}$ ; and  $\{(3,1,1), (1,3,1), (1,1,3)\}$ .

### **Quantum Tunneling in 1 dimension (Finite Square Well)**

In the case of an infinite square well potential, the particle is completely confined within the well and it can never escape.

This means the probability of finding the particle at the boundaries  $x = 0$  and  $x = a$ , or outside the well, is zero.

Hence,  $V(0) = V(a) = \infty$  and  $\psi(0) = \psi(a) = 0$ .

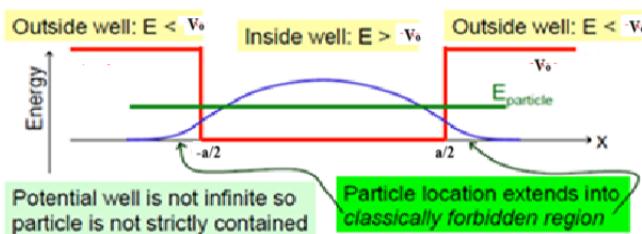
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In a realistic potential well with finite depth, the particle is not completely confined within the boundaries. There exists a small but finite probability of finding the particle outside the well. This occurs because the wave function extends slightly beyond the potential barriers instead of abruptly dropping to zero. This remarkable effect is known as **Quantum tunneling** is a purely quantum phenomenon where a particle penetrates and partially passes through a potential barrier, even when its energy is less than the height of the barrier.

### 3. Finite Potential Well

In the real world, potential energies are never infinite; however, potential wells with **finite barriers** do exist. Let us examine the **wavefunctions** and **energy levels** of a particle confined in such a potential well.



REGION I	$x < -a/2$	$V(x) = V_0$
REGION II	$-a/2 < x < a/2$	$V(x) = 0$
REGION III	$x > a/2$	$V(x) = V_0$

Figure shows a potential well with  $a$  is the width of the well and  $V_0$  is the finite potential barrier height.

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According to *classical mechanics*, a particle with energy  $E < V_0$  would be completely confined within the well and would bounce back when it hits the walls, never entering Regions I or III.

However, in *quantum mechanics*, the situation is different. The particle still oscillates within the well but has a finite probability of penetrating into the barriers (Regions I and III), even though  $E < V_0$ . This phenomenon is called **quantum tunneling**.

Let's examine, regions I and III, the potential energy is  $V(x) = V_0$ .  
The time-independent Schrödinger equation is

$$-\frac{\hbar^2}{8\pi^2 m} \frac{d^2\psi(x)}{dx^2} + V_0\psi(x) = E\psi(x) \dots (1)$$

Rearranging we get

$$\frac{d^2\psi(x)}{dx^2} = \alpha^2\psi$$

Where  $\alpha = \sqrt{\frac{8\pi^2 m(V_0 - E)}{\hbar^2}}$  is a real constant, since  $V_0 > E$

### Solutions in Regions I and III

The solution in these two regions is given by :

$$\psi_I(x) = Ee^{\alpha x} + Fe^{-\alpha x} \dots (2)$$

and  $\psi_{III}(x) = Ce^{\alpha x} + De^{-\alpha x} \dots (3)$

As  $x \rightarrow -\infty$ , the term  $e^{-\alpha x}$  diverges. To ensure the wavefunction remains finite and normalizable, we set  $F = 0$ :

$$\Psi_I(x) = Ee^{\alpha x} \dots (4)$$

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As  $x \rightarrow +\infty$ , the term  $e^{\alpha x}$  diverges, so we set  $C = 0$ :

$$\Psi_{III}(x) = De^{-\alpha x} \quad \dots\dots(5)$$

Thus, the wavefunctions in Regions I and III decay exponentially inside the barriers.

### **Region II: Inside the Well**

In Region II,  $V(x) = 0$ . The Schrödinger equation becomes

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

Where,  $k^2 = 8\pi^2mE / h^2$ , where  $k$  is a real number.

Hence, the general solution is

$$\psi_{II}(x) = A\cos(kx) + B\sin(kx) \quad \dots\dots(6)$$

In the case of infinite potential well, we found that  $A=0$  in order that  $\psi = 0$  at  $x = 0$  and  $x = a$ ,

However,  $\psi_{II} = E$  at  $x = 0$  and  $\psi_{III} = D$  at  $x = a$ , so both the sine and cosine solutions are possible.

### **Boundary Conditions**

For a physically valid wavefunction:

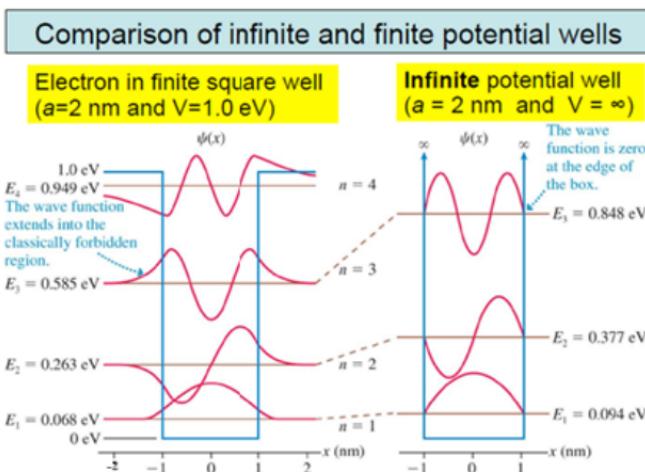
1.  $\psi(x)$  must be continuous at  $x = \pm a/2$ ,
2.  $\frac{d\psi(x)}{dx}$  must also be continuous at  $x = \pm a/2$ .

Applying these boundary conditions at both edges ensures that the wavefunctions inside and outside the well match smoothly in both value and slope. This matching is possible only for specific discrete

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energy values  $E_n$ , which correspond to the allowed bound energy levels.



The *finite potential well* demonstrates the principle of quantum tunneling — the ability of a particle to penetrate and even cross potential barriers higher than its total energy.

This concept explains several important physical phenomena, including:

- Radioactive decay (alpha particle emission),
- Scanning Tunneling Microscopy (STM) used for surface imaging,
- Chemical bonding and molecular interactions where electrons tunnel through potential barriers.

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<b>Q.No</b>	<b>Sample Questions</b>	<b>CO</b>
<b>1.</b>	State De Broglie hypothesis.	<b>1</b>
<b>2.</b>	What is wave function? Give its physical significance and properties.	<b>1</b>
<b>3.</b>	State Heisenberg's uncertainty principle. By applying Heisenberg's uncertainty principle, illustrate the broadening of spectral lines.	<b>1&amp;2</b>
<b>4.</b>	What are Eigen functions and Eigen values?	<b>1</b>
<b>5.</b>	Setup time independent one-dimensional Schrodinger's wave equation for a matter wave.	<b>1</b>
<b>6.</b>	Apply the time independent Schrodinger's wave equation to find the solutions for a particle in an infinite potential well of width 'a'. Hence obtain normalized wave function.	<b>1&amp;2</b>
<b>7</b>	Solve the Schrodinger's wave equation for a free particle.	<b>1&amp;2</b>
<b>8</b>	Set up the differential equation for a particle in a 1D well of finite depth and arrive at an Eigen Value expression.	<b>2</b>

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PNo.	Problems	CO
1.	<p>Calculate the de Broglie wavelength associated with a proton moving with a velocity equal to <math>(1/20)^{\text{th}}</math> of the velocity of light.</p> <p><b>To be found:</b> de Broglie wavelength, <math>\lambda</math></p> <p><b>Solution:</b></p> $\lambda = \frac{h}{mv} = \frac{6.625 \times 10^{-34}}{1.67 \times 10^{-27} \times (1/20) \times 3 \times 10^8}$ $= 2.64 \times 10^{-14} \text{m}$	3
2.	<p>An electron and a proton are accelerated through the same potential difference. Find the ratio of their de Broglie wavelengths.</p> <p><b>Solution:</b></p> <p><b>To be found:</b> Ratio of de Broglie wavelength, <math>\lambda</math></p> <p><b>De Broglie Wavelength, <math>\lambda</math></b></p> $\lambda = \frac{h}{\sqrt{2mE}}, \therefore \lambda \propto \frac{1}{\sqrt{m}}$ <p><b>For electron, <math>\lambda_e \propto \frac{1}{\sqrt{m_e}}</math></b>    <b>For proton, <math>\lambda_p \propto \frac{1}{\sqrt{m_p}}</math></b></p> <p><b>Ratio of De Broglie Wavelengths, <math>\therefore \frac{\lambda_e}{\lambda_p} = \frac{\sqrt{m_p}}{\sqrt{m_e}}</math></b></p>	3
3.	<p>Compare the energy of a photon with that of a neutron when both are associated with wavelength of <math>1\text{A}^{\circ}</math>.</p> <p>Given that the mass of neutron is <math>1.67 \times 10^{-27}\text{kg}</math>.</p> <p><b>Solution:</b></p> <p><b>To be found:</b> Comparison of energy of photon with that of neutron</p>	3

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	<p><b>Energy of neutron,</b></p> $E_n = \frac{P^2}{2m} = \frac{h^2}{2\lambda^2 m} = \frac{(6.625 \times 10^{-34})^2}{2 \times (1 \times 10^{-10})^2 \times 1.67 \times 10^{-27}} = 13.1 \times 10^{-21} J = 0.082 \text{ eV}$ <p><b>Energy of photon, </b><math>E_p = \frac{hc}{\lambda} = \frac{6.625 \times 10^{-34} \times 3 \times 10^8}{1 \times 10^{-10}} = 19.89 \times 10^{-16} J = 12421.9 \text{ eV}</math></p> <p><b>Ratio of energies,</b> <math>\frac{E_p}{E_n} = 1.5148 \times 10^5</math></p>	
4.	<p>An electron has a speed of <math>4.8 \times 10^5</math> m/s accurate to 0.012 %. With what accuracy with which its position can be located.</p> <p><b>To be found:</b> Uncertainty in position, <math>\Delta x</math></p> <p><b>Solution:</b></p> <p><b>Uncertainty principle</b> is given by, <math>\Delta x \Delta p \geq \frac{h}{4\pi}</math></p> <p><b>Uncertainty in speed,</b></p> $\Delta v = 4.8 \times 10^5 \times \frac{0.012}{100} = 57.6 \text{ m/s}$ <p><b>Uncertainty in position,</b> <math>\Delta x = \frac{h}{4\pi m \Delta v} = \frac{6.625 \times 10^{-34}}{4 \times 3.14 \times 9.1 \times 10^{-31} \times 57.6} = 1 \times 10^{-6} \text{ m}</math></p>	3
5.	<p>The inherent uncertainty in the measurement of time spent by Iridium-191 nuclei in the excited state is found to be <math>1.4 \times 10^{-10}</math> s. Estimate the uncertainty that results in its energy in the excited state.</p> <p><b>To be found:</b> Uncertainty in energy, <math>\Delta E</math></p>	3

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	<p><b>Solution:</b> Uncertainty principle is given by, <math>\Delta E \Delta t \geq \frac{h}{4\pi} \therefore \Delta E \geq \frac{h}{4\pi \Delta t} \geq \frac{6.625 \times 10^{-34}}{4 \times 3.14 \times 1.4 \times 10^{-10}} \geq 3.77 \times 10^{-25} J</math></p>	
6.	<p>The position and momentum of 1 keV electron are simultaneously determined and if its position is located within 1 Å. What is the percentage of uncertainty in its momentum?</p> <p><b>To be found:</b> Percentage of uncertainty in momentum of electron, <math>\Delta p</math></p> <p><b>Solution:</b> Uncertainty principle is given by, <math>\Delta x \Delta p \geq \frac{h}{4\pi}</math></p> <p><b>Uncertainty in momentum,</b></p> $\Delta p = \frac{h}{4\pi \Delta x} = \frac{6.625 \times 10^{-34}}{4 \times 3.14 \times 1 \times 10^{-10}} = 0.53 \times 10^{-24} kg.m/s$ <p><b>Momentum,</b></p> $p = \sqrt{2mE} = \sqrt{2 \times 9.1 \times 10^{-31} \times 1 \times 10^{-16}} = 1.707 \times 10^{-23} kgm/s$ <p><b>Percentage of uncertainty in momentum of electron,</b> <math>\frac{\Delta p}{p} \times 100 = 3.1</math></p>	

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7.	<p>Show that the energy Eigen value of a particle in second excited state is equal to 9 times the zero point energy.</p> <p><b>To be found:</b> Energy Eigen value for second excited state is equal to 9 times the zero point energy.</p> <p><b>Solution:</b> Energy Eigen value equation is given by,</p> $E = \frac{n^2 h^2}{8ma^2}$ <p><b>n=1, zero-point energy state,</b> <math>E_1 = \frac{h^2}{8ma^2}</math></p> <p><b>n=3, second excited state,</b> <math>E_3 = \frac{9h^2}{8ma^2} = 9E_1</math></p>	3
8.	<p>An electron is bound in a one-dimensional potential well of width 1Å, but of infinite height. Find the energy value for the electron in the ground state.</p> <p><b>To be found:</b> Energy Eigen value</p> <p><b>Solution:</b></p> <p>Energy Eigen value equation is given by,</p> $E = \frac{n^2 h^2}{8ma^2}$ <p><b>For n=1, ground state energy,</b></p> $E_1 = \frac{(6.625 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (10^{-10})^2} = 37.65eV$	

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9.	<p>An electron is bound in one dimensional potential well of infinite potential of width 0.12 nm. Find the energy values in the ground state and also the first two excited state.</p> <p><b>To be found:</b> Energy Eigen value</p> <p><b>Solution:</b></p> <p>Energy Eigen value equation is given by,</p> $E = \frac{n^2 h^2}{8ma^2}$ <p>For n=1, ground state energy, <math>E_1 = \frac{(6.625 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (0.12 \times 10^{-9})^2} = 26.16eV</math></p> <p>For n=2 and 3, first and second excited state, <math>E_2 = 4E_1 = 104.61eV</math> <math>E_3 = 9E_1 = 235.44eV</math></p>	
10.	<p>An electron is trapped in a potential well of a width 0.5nm. If a transition takes place from the first excited state to the ground state find the wavelength of the photon emitted.</p> <p><b>To be found:</b> Wavelength of the photon emitted, <math>\lambda</math></p> <p><b>Solution:</b></p> <p><b>For n=1, ground state energy,</b></p> $E_1 = \frac{(6.625 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (0.5 \times 10^{-9})^2} = 1.507eV$ <p><b>For n=2, first excited state,</b></p> $E_2 = 4E_1 = 9.64 \times 10^{-19}J = 6.025eV$ <p><b>Energy difference,</b></p>	

**UNIT 2 – QUANTUM MECHANICS**  
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	$\Delta E = E_2 - E_1 = 7.23 \times 10^{-19} J = 4.518 eV$ <p><b>Wavelength of the photon emitted ,</b></p> $\lambda = \frac{hc}{\Delta E} = \frac{6.625 \times 10^{-34} \times 3 \times 10^8}{7.23 \times 10^{-19} J} = 274.8 nm$	
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APPLY the concepts learnt above to throw light on the following issues.

1. Taking Planck's law as the starting point derive Rayleigh – Jeans law in the limit of high  $\lambda$ .
2. How can we naturally reconcile the dual Wave and Particle nature of matter?
3. Is there any connection between the position – momentum and energy-time uncertainty relationship? Discuss.
4. Is the derivation for particle in a box done above valid for highly energetic relativistic particles? Discuss.
5. With respect to the particle in a finite well, what is the change in the tunneling co-efficient as well width is increased ?
6. Derive the results of the infinite well by setting the depth of the well as infinity in the transcendental equations obtained for solving the eigen value equation in a finite well.