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Subject	Physics
Paper	Quantum Mechanics
Module No. & Title	2: A Particle in One Dimensional Potential Well.
Module Tag	DAYA_PHY_EKK_M2

Objectives:

1. To know Behaviour of a particle in One Dimensional Potential Well
2. To study the solving Schrödinger's wave equation

Outcomes:

1. Understand Behaviour of a particle in one-dimensional box.
2. Understand boundary conditions to get energy eigen values and eigen functions.

Module No. & Title	1. A Particle in One Dimensional Potential Well.
Module Tag	DAYA_PHY_EKK_M2
Contents	**1. Introduction** **2. A particle in one dimensional infinite potential well** **3. Energy eigen values** **4. Eigen functions** **5. Summary**

1. Introduction

The motion of objects having distances larger than about 1 nm can be explained on the basis of Classical Mechanics. It is based on:

1. Newton's laws of motion,
2. Law of Gravitational attraction,
3. Coulombs law of attraction or repulsion between 2 electric charges and
4. Lorentz force.

Both law of gravitational attraction and Coulombs law are inverse square laws. The Lorentz force is the force on a charged particle in motion in a magnetic field.

The phenomena like black body radiation, photoelectric effect etc. cannot be explained on the laws of classical mechanics but can be successfully explained on the basis of Quantum Mechanics. To explain distribution of energy in the spectrum, Max Plank in 1900 proposed quantum hypothesis – origin of quantum theory. By quantum hypothesis, the energy of radiation is concentrated into photons of energy, $E = h\nu$. By classical concept the energy of radiations is distributed through waves. The phenomena involving distances of the order of $10^{-10}m$ can be explained by quantum theory.

In quantum mechanics the Heisenberg's uncertainty principle plays important role. For a particle of mass m moving with velocity v the product of the uncertainty in the measurement of position Δx and the uncertainty in the measurement of velocity Δv is

$$\Delta \mathrm{m}\ \Delta \mathrm{v} \geq \frac{\hbar}{2} \qquad \dots (1)$$

For heavy particle, $\frac{\hbar}{m}$ is very small and, therefore, the ΔmΔv of the two uncertainties becomes very small. For such particles both the position x and the velocity v can be determined accurately.

For very heavy bodies, if the mass of body is such that $\frac{\hbar}{m} = 0$, the uncertainty vanishes and then all physical quantities of the heavy body can be determined with perfect accuracy. This is the limiting case of classical mechanics. Thus, classical mechanics is applicable to massive bodies, and the uncertainty are the characteristic of quantum mechanics. Quantum mechanics is applicable to light particles such as electron, proton, neutron etc.

2. A particle in one dimensional infinite potential well

Consider the one-dimensional motion along $X-$axis of a particle of mass m in a hollow rectangular box having perfectly rigid or hard or impenetrable potential walls. Let L be the distance of separation between the walls so that motion along $X-$axis is confined within the distance L or between walls at $x = 0$ to $x = L$.

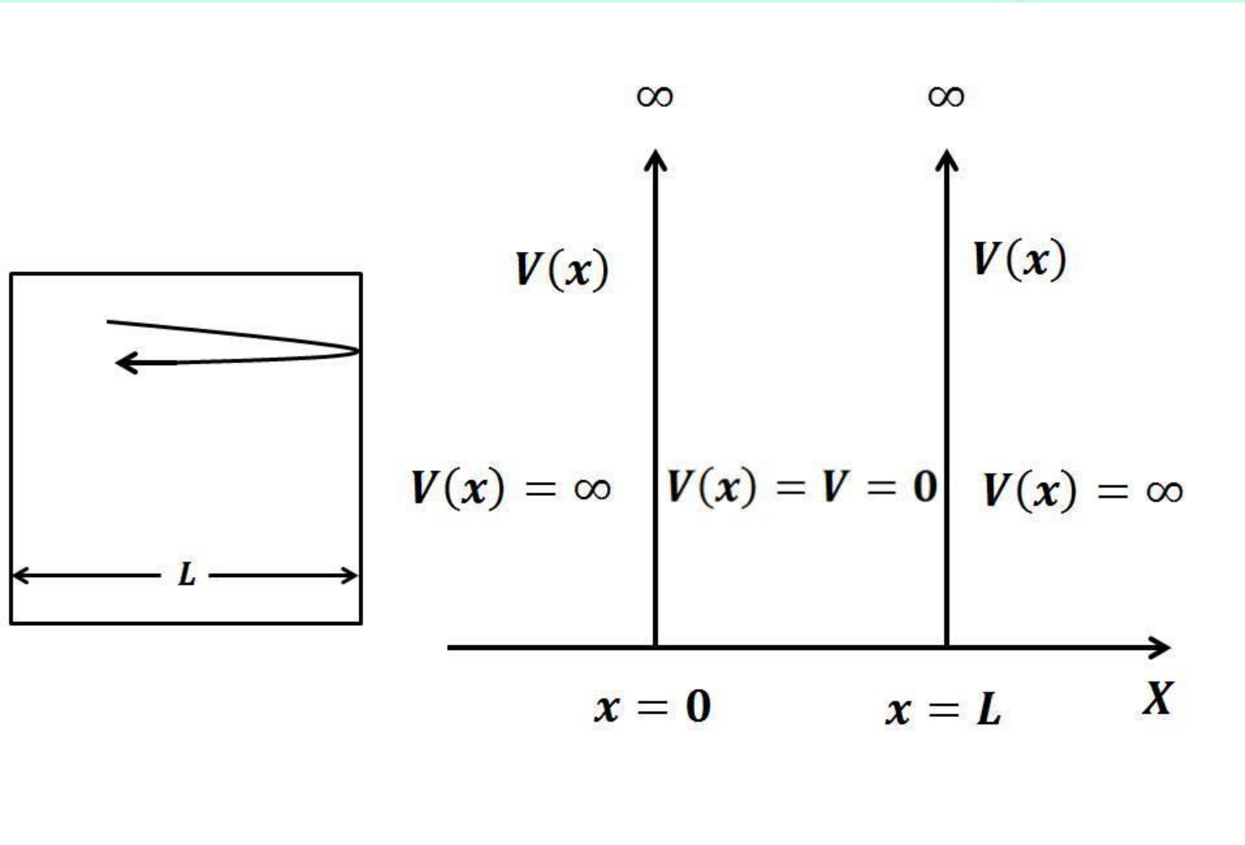

Fig. 2.1.1: One dimensional potential well

The potential V of the particle is ∞ on both sides of the box, while potential it is constant say zero for convenience on the inside. The potential energy curve for the particle is shown in figure above and, because of its appearance is called a square well potential of infinite depth. Since potential energies are never infinite in the real world, our original rigid walled box has no physical counterpart. The particle bounces back and forth between the walls of a box. As walls are rigid, particle does not loose energy when it collides with walls of one-dimensional box, so its total energy remains constant.

The particle cannot have ∞ amount of energy and hence it cannot do infinite work to come out of the box. Hence particle cannot exist outside the box and exists inside the box only. In order to leave the region, the particle will have to do an infinite amount of work and since this is not possible hence it cannot exist outside the box. Hence for $x \leq 0$ and $x \geq L$ the wave function $\psi(x) = 0$. Therefore, its wave function $\psi(x)$ do not exist outside the box and wave function exists inside the box only.

Here potential, $V(x) = 0$, is independent of time hence we use Schrödinger's time-independent or steady-state wave equation. The Schrödinger's wave equation three dimensions is

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E - V)\psi = 0 \qquad \dots (2)$$

A differential equation for the wave associated with a particle in motion cannot be derived from first principles. The first principle is the foundational proposition that stands alone and can we cannot deduce the first principle from any other proposition or assumption. The first principle is building block of true knowledge. The differential equation may be developed by any one out of many procedures. Here, it is developed by using "A complex variable quantity, called the wave function, is assumed to represent a plane simple harmonic wave associated with a free particle, and the classical expression for the total energy is used."

As potential, $V(x) = 0$, is function of single variable, we use Schrödinger's wave equation in one dimension.

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

As, inside the box,

$$V(x) = 0$$

The Schrödinger's wave equation becomes,

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2mE}{\hbar^2}\psi = 0$$

As ψ is function of single variable x, the partial derivative $\frac{\partial^2\psi}{\partial x^2}$ can be replaced by total derivative $\frac{d^2\psi}{dx^2}$.

$$Or, \quad \frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0$$

$$Let \qquad k^2 = \frac{2m}{\hbar^2}E \qquad\qquad \therefore\ k = \frac{\sqrt{2mE}}{\hbar}$$

As m and $\hbar$ are constants, for a particular value of E, k is constant.

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

Above equation is second order differential equation in variable x. Its general solution is given by:

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

Where A and B are constants to be evaluated using boundary conditions. The boundary conditions are that the wave function ψ must vanish at the boundaries.

Therefore, the boundary conditions are:

i) At $x = 0,\ \psi(x) = 0$

and

ii) At $x = L,\ \psi(x) = 0$

Using boundary condition: $\psi(x) = 0$ at $x = 0$ in the general solution, we get,

$$B = 0$$

Therefore, the general solution becomes:

$$\psi(x) = A\sin kx$$

Using boundary condition: $\psi(x) = 0$ at $x = L$ in the above equation, we get,

$$0 = A\sin kL$$

$$\Rightarrow \text{ either } \quad A = 0 \quad or \quad \sin kL = 0$$

But we cannot take, $A = 0$, because then there will be no solution. Hence,

$$\sin kL = 0$$

Why $A = 0$ is not taken? Its explained as follows:

Already, $B = 0$, and if we take $A = 0$ then the entire function, $\psi(x)$ will vanish in the well. And therefore, $A = 0$ is not taken. Therefore, surely,

$$\sin kL = 0$$

$$\Rightarrow \ kL = n\pi \quad \ where \ n = 1, 2, 3, \ldots$$

$$\therefore \ k = \frac{n\pi}{L}$$

We cannot take $n = 0$ because for $n = 0$, $k = \frac{n\pi}{L} = 0$, (and $\therefore \ E = 0$) hence $\psi(x) = 0$ everywhere in the one-dimensional box. And once the wave function vanishes, the particle does not exist in that region. Using value of, $k = \frac{n\pi}{L}$ in equation for $\psi(x)$:

$$\psi(x) = A \sin\left(\frac{n\pi}{L}\right) x$$

This is equation for $\psi(x)$ for a particle in one dimensional rigid box. Now let's obtain energy eigen values and respective eigen functions.

3. Energy eigen values

Equating equations of k:

$$\frac{\sqrt{2mE}}{\hbar} = \frac{n\pi}{L}$$

Squaring,

$$\frac{2m}{\hbar^2}E = \frac{n^2\pi^2}{L^2}$$

$$E = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

For nth state, $$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \quad where\ n = 1, 2, 3, \ldots$$

This is equation for eigen-value of energy. The wave function ψ_n corresponding to E_n are called eigen-functions of the particle. The integer n corresponds to the energy E_n is called the quantum numbers. Here $n = 0$ is not considered, means that particle with zero energy cannot exist in the box. Or, a particle in the box cannot have zero energy.

1) The lowest energy of the particle. called the ground state energy. is obtained by putting $n = 1$ in the equation of E_n.

$$E_1 = \frac{\pi^2\hbar^2}{2mL^2}$$

The value of E_n in terms of E_1, are given by

$$E_n = n^2E_1$$

2) The equation, of E_n, shows that eigen-values of energy are discrete; and not continuous. And these values are called the energy levels of the particle.
3) The spacing between the energy –levels of the particle increases with increase in n.

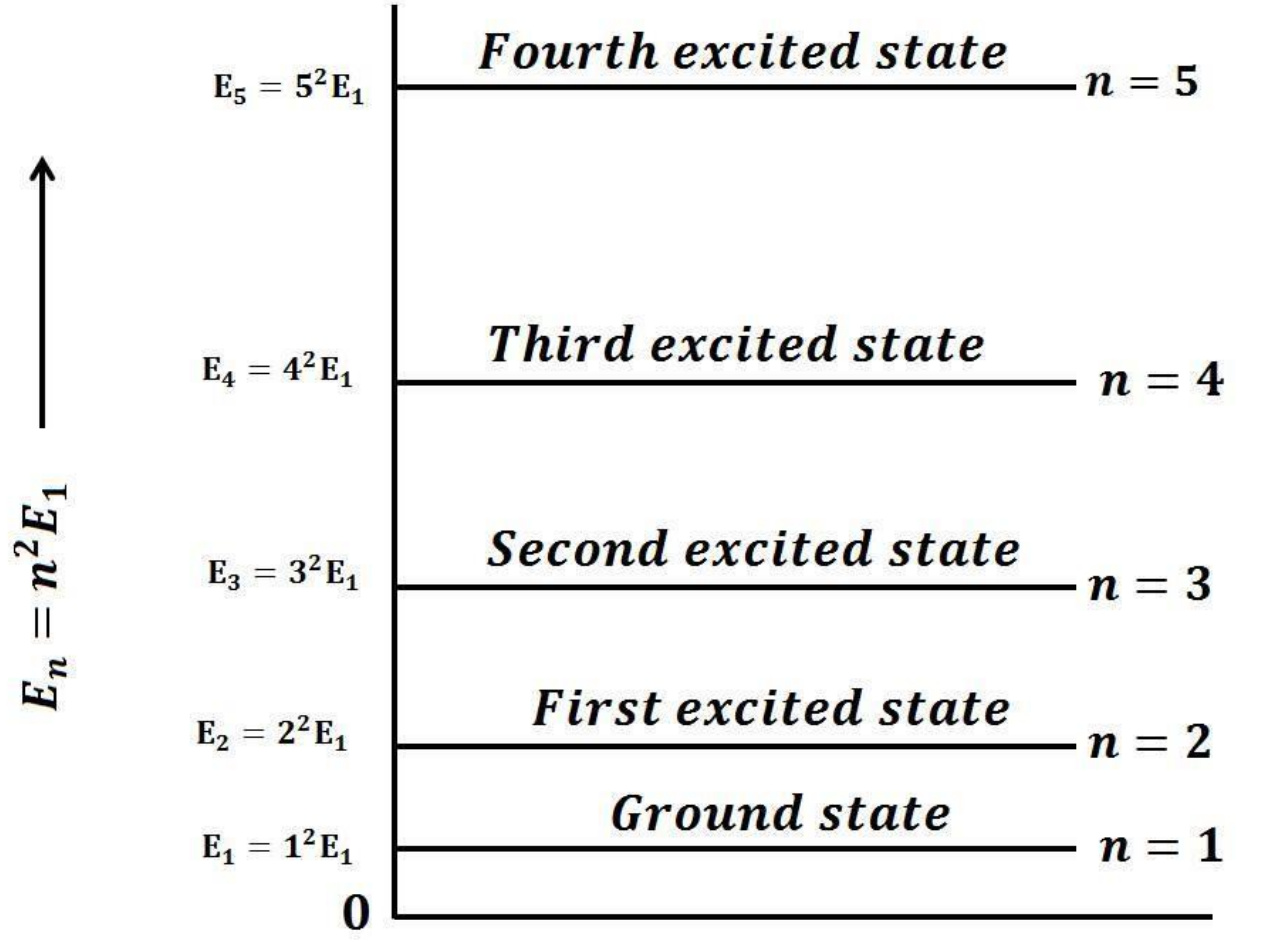

Fig. 2.1.2: Energy levels one dimensional box

4. Eigen Functions

The wave functions for the motion of the particle are:

$$\psi_n(x) = A \sin \frac{n\pi}{L} x \qquad \text{in the region } 0 < x > L$$

and

$$\psi_n(x) = 0, \text{in the region } x < 0 \;\; \& \;\; x > L$$

The total probability that the particle is somewhere in the box must be unity. Or the requirement of ψ is that it should be normalizable (normalized to unity). Therefore, we have,

$$\int_0^L |\psi_n(x)|^2 \; dx = 1$$

$$\int_0^L A^2 \sin^2 \frac{n\pi}{L} x \, dx = 1$$

$$A^2 \int_0^L \sin^2 \frac{n\pi}{L} x \, dx = 1$$

$$\because \; \sin^2 \theta = \frac{1 - \cos 2\theta}{2}$$

$$\therefore \; A^2 \int_0^L \frac{(1 - \cos 2\frac{n\pi}{L} x)}{2} dx = 1$$

$$\frac{A^2}{2} \int_0^L (1 - \cos 2 \frac{n\pi}{L} x) \; dx = 1$$

$$\frac{A^2}{2} \left[x - \frac{\sin 2 \frac{n\pi}{L} x}{2 \frac{n\pi}{L}}\right]_0^L = 1$$

$$\frac{A^2}{2}(L) = 1$$

$$A^2 = \frac{2}{L}$$

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

Every acceptable wave function can be normalized by multiplying it by an appropriate constant and this constant is known as normalization constant. Here $A = \sqrt{\frac{2}{L}}$ is normalization constant. Using value of A the equation for wave function becomes:

$$\psi_n(x) = \sqrt{\frac{2}{L}}\ \sin\frac{n\pi}{L}x$$

This is eigen function or proper function. As $\psi_n(x)$ is eigen function, it satisfies the normalization condition (normalized to unity), i.e.

$$\int_0^L \sqrt{\frac{2}{L}}\sin\frac{n\pi}{L}x\, ds = 1$$

This can be proved by substituting, $\sin^2\theta = \frac{1-\cos 2\theta}{2}$.

The wave- functions for the first three values of n are shown in figure.

It is evident that the wave function ψ_1 has two nodes: at $x = 0$ and $x = L$. The wave function ψ_2 has three nodes: at $x = 0, x = \frac{L}{2}$ and $x = L$. The wave function ψ_3 has four nodes: at $x = 0, x = \frac{L}{3}, x = \frac{2L}{3}$ and $x = L$. Thus, the wave function ψ_n will have $(n+1)$ nodes; including nodes at extremities.

For a particular energy state, characterized by the quantum number n, the number of intermediate nodes, or excluding nodes at the extremities, is $(n-1)$.

The probability of finding the particle described by the wave function ψ at the point, at the time t is proportional to the value of $|\psi|^2$ there at t. The variation of the probability densities, $|\psi|^2$, with x for 3 values of n are shown in the figure.

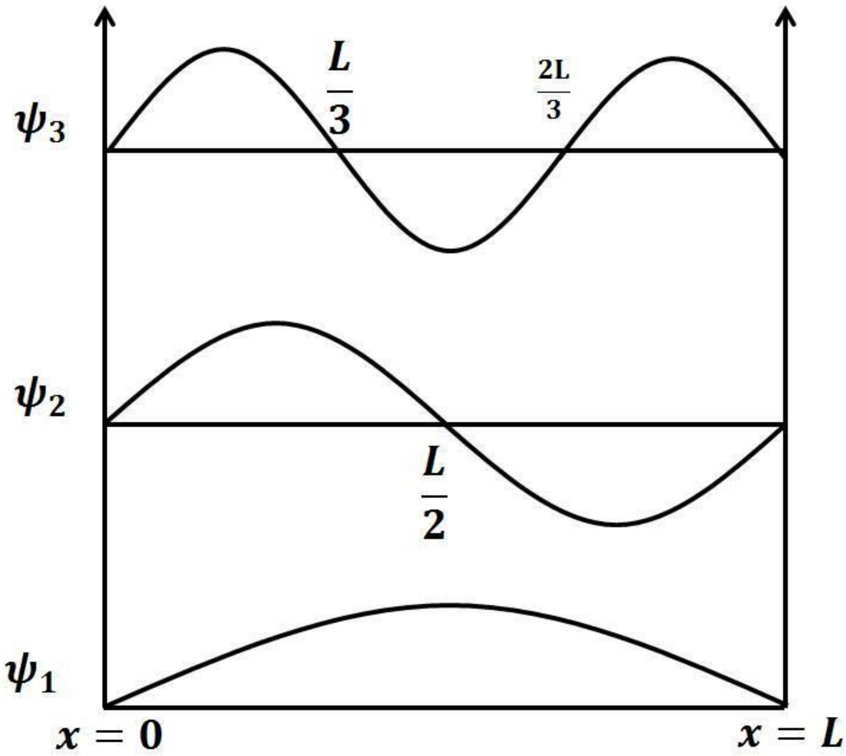

Fig. 5.1.3: Wave functions

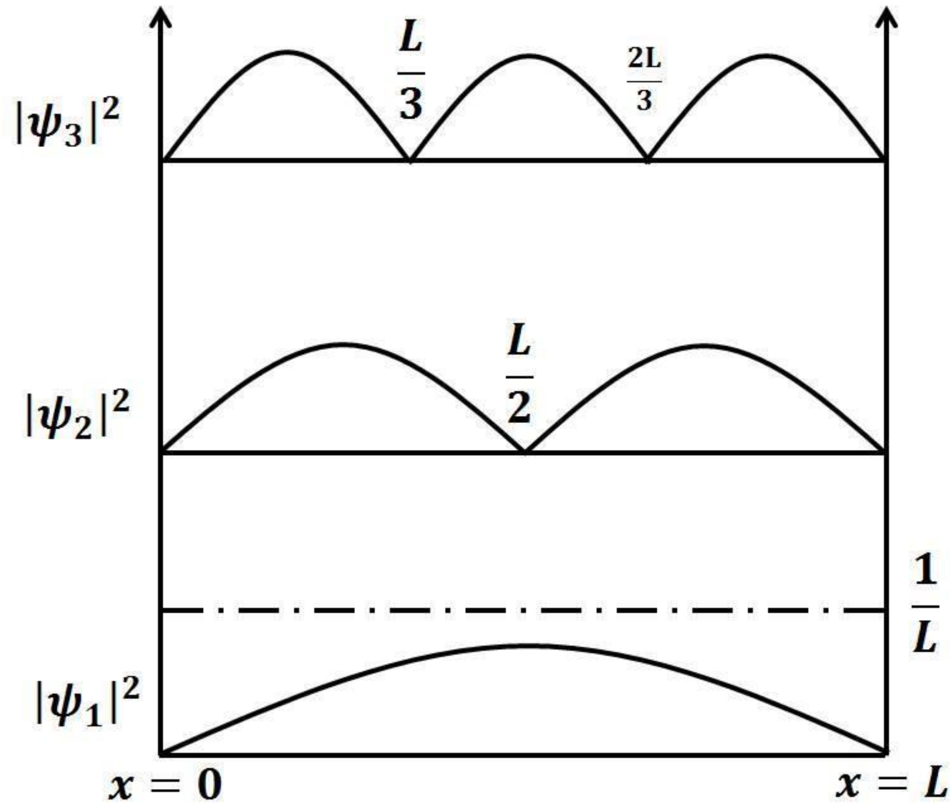

Fig. 5.1.4: Probability of finding the particle.

A particle in the lowest energy level of $n = 1$ is most likely to be in the middle of the box, which a particle in the next higher state of $n = 2$ is never there!

Classical physics, of course, predicts the same probability for the particle being anywhere in the box.

5. Summary

In this module we have obtained bound state solutions of the one-dimensional Schrödinger's wave equation. As particle cannot have infinite energy, so it cannot do infinite work, hence it cannot come out of the potential box. It bounces between the potential walls.

The solution of differential equation, is shown by a Greek letter, psi has no physical significance and experimentally it is not a measurable quantity. When a sound wave travel through the medium, there occurs pressure variations, when a light wave travels, the electromagnetic field varies in space and time. What is it whose variation constitutes de Broglie waves? It is the psi. The psi does not represent a physically measurable quantity. Modulus of square of psi is called probability density. The probability P that something be somewhere at a given time can have any values between two limits: 0 and 1, where zero corresponds to certainty of its absence while 1 corresponds to certainty of its presence.

The wave function ψ represents a solution of the Schrödinger wave equation. And the amplitude of any wave may be negative as well as positive. But the negative probability has no meaning. Hence the square of the absolute value of the wave function, i. e.$|\psi|^2$, is taken. The $|\psi|^2$; is called probability density. The probability of finding the particle described by ψ at the point(x,y.z) at the time t is proportional to the value of $|\psi|^2$ there at t. A large value of $|\psi|^2$ means the strong possibility of particles presence and a small value of $|\psi|^2$ means the slight possibility of particles presence. As long as $|\psi|^2$ is not actually zero somewhere; there is a definite chance, however small, of detecting the particle there. This interpretation was first made by Max Born in 1926 and was elaborated by Heisenberg and Bohr.

Exercise:

1. Find the lowest energy of an electron confined to move in a one-dimensional box of length 2 Å?

   Given: $m = 9.11 \times 10^{-31} kg$, $\hbar = 1.054 \times 10^{-34}\ J - s$

   Solution:

   Length of box, L= $2\ Å = 2 \times 10^{-10}\ m$

   Formula: $E = \frac{n^2\pi^2\hbar^2}{2mL^2}$

   For lowest energy, $n = 1$

$$\therefore\ E = \frac{\pi^2\hbar^2}{2mL^2}$$

$$= \frac{(3.142)^2(1.054 \times 10^{-34})^2}{2 \times 9.11 \times 10^{-31} \times (2 \times 10^{-10})^2}$$

$$E = 1.5048 \times 10^{-18}\ J$$

   As, $1\ J = 1.6 \times 10^{-19}\ eV$

$$\therefore E = \frac{1.5048 \times 10^{-18}}{1.6 \times 10^{-19}}$$

$$E = 9.405\ eV$$

2. Find the lowest energy of a neutron confined to a nucleus of size $10^{-15}\ m$. Given: mass of the neutron = $1.67 \times 10^{-27}\ kg$.

   Solution:

   Length of box, $L = 10^{-15}\ m$

   Formula: $E = \frac{n^2\pi^2\hbar^2}{2mL^2}$

   For lowest energy, $n = 1$

$$\therefore\ E = \frac{\pi^2\hbar^2}{2mL^2}$$

$$= \frac{(3.14)^2(1.054 \times 10^{-34})^2}{2(1.67 \times 10^{-27})(10^{-15})^2}$$

$$E = 3.083 \times 10^{-11}\ J$$

   As, $1\ J = 1.6 \times 10^{-19}\ eV$

$$\therefore E = \frac{3.083 \times 10^{-11}}{1.6 \times 10^{-19}}$$

$$E = 192.6875\ MeV$$

What do we understand?

Quiz on what we learned: **Multiple Choice Questions**

1) The energy spectrum of a particle in one dimensional rigid box has the nature of ….
   a) infinite sequence of discrete energy levels.
   b) infinite sequence of equidistance energy levels
   c) finite sequence of equidistance energy levels
   d) exponential increasing
2) The boundary conditions of one-dimensional square-well potential of finite depth are given by ……
   a) $V(x) = 0$ when $x \le -a$, $V(x) = V_0$ when $-a < x < a$ *and* $V(x) = V_0$ when $x \ge a$
   b) $V(x) = V_0$ when $x \le -a$, $V(x) = V_0$ when $-a < x < a$ and $V(x) = 0$ when $x \ge a$
   c) $V(x) = V_0$ when $x \le -a$, $V(x) = 0$ when $-a < x < a$ and $V(x) = 0$ when $x \ge a$
   d) $V(x) = V_0$ when $x \le -a$, $V(x) = 0$ when $-a < x < a$ and $V(x) = V_0$ when $x \ge a$
3) The energy of the lowest state in a one-dimensional potential box of length L is ……
   a) zero
   b) $\frac{3\hbar^2}{8mL^2}$
   c) $\frac{\hbar^2}{8mL^2}$
   d) $\frac{}{8mL^2}$
4) A standing wave is formed between two supports at $x = 0$ and $x = L$ with one loop, then energy possessed by a vibrating particle of mass $'m'$ which produces this standing wave is given by…...
   a) $E = \frac{\pi^2 h^2}{2mL^2}$
   b) $E = \frac{\pi^2 \hbar^2}{2mL^2}$
   c) $E = mc^2$
   d) $E = h\nu$
5) Energy of a particle which is moving in one-dimensional rigid box is proportional to …...
   a) square of length of box.
   b) reciprocal of square of length of box.

c) length of box. d) reciprocal of length of box.

6) The minimum energy of particle confined to one dimensional rigid box is obtained by substituting n equal to ……

a) one b) zero

c) half d) two

7) Which of the following is the uncertainty relation for angular momentum and angular position?

a) $\Delta L \Delta \theta \geq \hbar$ b) $\Delta p \Delta \theta \geq \hbar$

c) $\Delta L \Delta p \geq \hbar$ d) $\Delta y \Delta p \geq \hbar$

Answers to Quiz

1) a) infinite sequence of discrete energy levels.

2) d) $V(x) = V_0$ when $x \leq -a$, $V(x) = 0$ when $-a < x < a$ and $V(x) = V_0$ when $x \geq a$

3) c) $\frac{\hbar^2}{8mL^2}$

4) b) $E = \frac{\pi^2 \hbar^2}{2mL^2}$

5) b) reciprocal of square of length of box.

6) a) one

7) a) $\Delta L \Delta \theta \geq \hbar$

Feedback: (Tick mark your option)

1) How was the learning experience?

Outstanding/Excellent / Nice /Good/Fair

2) Which aspect do you like most?

Introduction/Concept/Diagrams/Exercise/Applications

3) Anything else to be added?

Applications/Problems/Illustrations/Notes/Videos

4) Which point was not up to the mark and need revision?

Introduction/Concept/Diagrams/Exercise/Applications

5) Suggestions if any:

....

....

Name of the student and class:

____

____

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Ctrl + Click Following links to Know More

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