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Paper - GE1T

Topic - One Dimensional Infinitely Rigid box

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One Dimensional Infinitely Rigid Box

Bound State :⇒

If the motion of a particle is confined to a limited region of space by potential energy so that the particle can move back and forth in the region, then the particle is in a bound state. The simplest example ~~box with~~ of all motions in bound state is the motion of a particle in a one-dimensional box with zero potential energy and the potential energy is assumed to be infinite at the walls of the box.

Particle in a One-Dimensional Box :-

We assume a particle of mass m and energy E moving in a region from $x=0$ to $x=a$ with absolutely rigid, impenetrable potential walls of infinite height Fig. 1.

$$V(x) = \begin{cases} \infty & \text{for } x=0 \text{ and } x=a \\ 0 & \text{for } 0<x<a \end{cases}$$

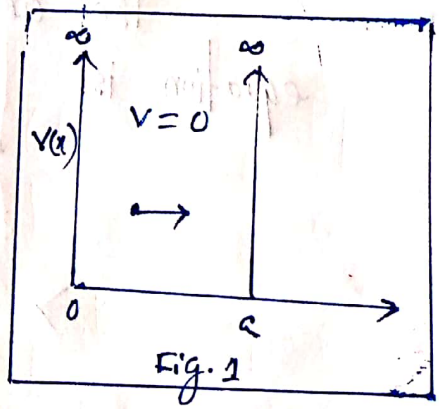

Fig. 1

The particle experiences no force in the box as $V(x)=0$. Also, the particle during its motion collides with the rigid walls with no loss of energy and as much the total energy E of the particle remains constant. As $V(x)=\infty$ at both $x=0$

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and $x = a$, the particle needs infinite work to leave the region. Since this is impossible, the particle remains confined within the box and probability of the particle to be at $x = 0$ and $x = a$ must be zero.

Since, probability is given by $|\psi|^2$, the wave function $\psi(x)$ at $x = 0$ and $x = a$ must vanish. That is

$$\psi(x)|_{x=0} = \psi(x)|_{x=a} = 0 \quad \cdots (1)$$

The potential energy curve of the appearance as shown in fig.1. is called a square well potential.

☑ The Wave Equation for the Particle :-

Since $V(x)$ is independent of time, we apply time-independent Schrödinger wave equation in the region $0 \leq x \leq a$

The one-dimensional time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m} \cdot \frac{d^2\psi}{dx^2} = E\psi \quad \cdots (2)$$

$$\Rightarrow \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E\psi = 0 \quad \cdots (3)$$

$$\Rightarrow \boxed{\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0} \quad \cdots (4)$$

where, $\alpha = \sqrt{\frac{2mE}{\hbar^2}}$

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The Solution of Equation :-

The general solution of equation (3) is given by

$$\psi(x) = A\sin\alpha x + B\cos\alpha x \quad \ldots (5)$$

where, A and B are constants of integration whose values may be found out by applying the following boundary conditions:

1. $\psi(x) = 0$ at $x = 0$
2. $\psi(x) = 0$ at $x = a$

Applying condition (1) to equation (5) we get,

$$0 = A\sin 0 + B\cos 0$$

or, $B = 0$

$$\therefore \psi(x) = A\sin\alpha x \quad \ldots (6)$$

Applying condition (2) to equation (6) we get,

$$0 = A\sin\alpha a$$

Since $A \neq 0$, $\sin\alpha a = 0$, then

$$\alpha a = n\pi, \qquad n = 1, 2, 3, \ldots$$

or, $$\alpha = \frac{n\pi}{a} \quad \ldots (7)$$

Here, $n = 0$ is not admissible because if $n = 0$, then $\alpha = 0$, $E = 0$ and hence $\psi(x) = 0$ everywhere in side of the box. In other words, a particle with zero energy can't be present in the box,

Hence, $$\psi_n(x) = A\sin\frac{n\pi x}{a} \quad [\text{for } 0 < x < a]$$

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☑ Energy Eigenvalues

From equation (7)

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

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

$$\Rightarrow \boxed{E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}} \quad \ldots\ldots (9)$$

So, we get an infinite sequence of discrete energy levels that corresponds to all integral values of n, where n is called the quantum number. As $a \to \infty$, $\Delta E_n \to 0$, i.e. the energy values are closer if the size of the box is larger, forming a continuum.

Putting $n = 1$ in equation (9) we get,

$$\boxed{E_1 = \frac{\pi^2\hbar^2}{2ma^2}} \quad \ldots\ldots (10)$$

(i) E_1 is the lowest energy of the particle in the box and is called the ground state energy level. In terms of E_1, E_n can be expressed as,

$$E_n = n^2 E_n \quad \ldots\ldots (11)$$

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(ii) The possible energy values of the particle are $E_1, E_2, E_3 \cdots E_n$ for $n = 1, 2, 3 \cdots, n$ are discrete.

(iii) Since,

$$\Delta E = E_{n+1} - E_n$$

$$= (n+1)^2 E_1 - n^2 E_1$$

$$= (2n+1) E \quad \cdots\cdots (12)$$

$$\Rightarrow \Delta E = \frac{(2n+1)}{a^2} \cdot \frac{n^2 h^2}{2m} \quad \cdots\cdots (13)$$

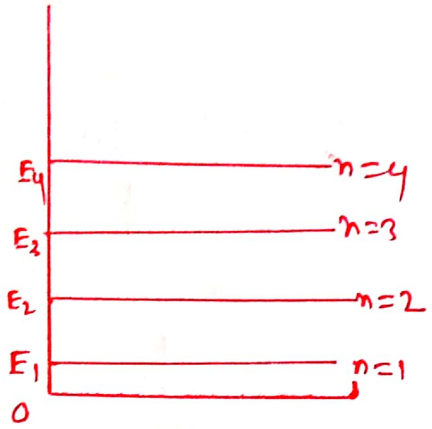

Fig. 2

Equation (13) shows that as $a \to \infty$, $\Delta E \to 0$, the energy levels leads to a continuum corresponding to a free particle.

The spacing between the energy levels increases with the the increase of n, i.e., for higher energy levels. The energy level diagram for a particle confined to mo in a one-dimensional boxis shown in Fig. 2

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