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Institute of Science and Technology

DEPARTMENT OF PHYSICS AND NANOTECHNOLOGY
SRM INSTITUTE OF SCIENCE AND TECHNOLOGY

18PYB101J-Electromagnetic Theory, Quantum Mechanics, Waves and Optics

Module 3- Lecture-9

Particle in a 1D box, Normalization

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TopicsTo be Taught:-   **Particle in a 1D box**
Normalization

Application of Schroedinger Wave Equation to a Particle (Electron) Enclosed in a One Dimensional Potential Box

Let us consider a particle (electron) of mass '*m*' moving along *x*-axis, enclosed in a one dimensional potential box as shown in Fig.6.1. and mathematical form of 1-D infinite box potential is written in Fig. 6.2

SINCE THE WALLS ARE OF INFINITE POTENTIAL THE PARTICLE DOES NOT PENETRATE OUT FROM THE BOX.

$$V(x) = \begin{cases} 0; & 0 < x < l \\ \infty; & x \leq 0 \,\&\, x \geq l \end{cases}$$

Fig. 2

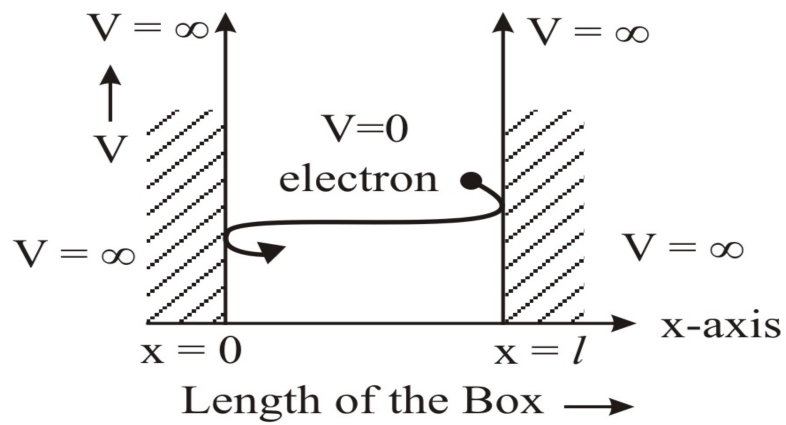

Fig. 1

ALSO, THE PARTICLE IS CONFINED BETWEEN THE LENGTH '*l*' OF THE BOX AND HAS *ELASTIC COLLISIONS* WITH THE WALLS. *THEREFORE, THE POTENTIAL ENERGY OF THE ELECTRON INSIDE THE BOX IS CONSTANT AND CAN BE TAKEN AS ZERO FOR SIMPLICITY.*

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∴ ***WE CAN SAY THAT OUTSIDE THE BOX AND ON THE WALL OF THE BOX, THE POTENTIAL ENERGY V OF THE ELECTRON IS ∞.***

INSIDE THE BOX THE POTENTIAL ENERGY (V) OF THE ELECTRON IS ZERO.

IN OTHER WORDS WE CAN WRITE THE BOUNDARY CONDITIONS **in the form of Potential function V(x) as in Fig.6.2**

SINCE THE PARTICLE CANNOT EXIST OUTSIDE THE BOX THE WAVE FUNCTION ψ = 0 WHEN $0 \geq X \geq L$.

Think This

IN QM, WAVE-FUNCTION IS DIRECTLY RELATED TO THE EXISTENCE OF A PARTICLE.

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To find the wave function of the particle within the box of length '*l*', let us consider the Schroedinger one dimensional time-independent wave equation (i.e.,)

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - V]\psi = 0 \qquad \text{------------------------------(1)}$$

Within box, V(x)=0

SINCE THE POTENTIAL ENERGY INSIDE THE BOX IS ZERO [(I.E) *V* = 0]. THE PARTICLE HAS KINETIC ENERGY ALONE AND THUS IT IS NAMED AS A FREE PARTICLE (OR) FREE ELECTRON WITHIN THE BOX

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0 \qquad \text{------------------------------(2)}$$

Let us substitute $k^2 = \frac{2mE}{\hbar^2}$, in equation(2)

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \text{------------------------------(3)}$$

EQUATION (3) IS A SECOND ORDER DIFFERENTIAL EQUATION, THEREFORE, IT SHOULD HAVE SOLUTION WITH TWO ARBITRARY CONSTANTS. AND THE SOLUTION IS GIVEN BY

$$\psi(x) = A\sin(kx) + B\cos(kx) \quad \text{------------------------------(4)}$$

where *A* and *B* are called as arbitrary constants which can be determined uniquely using BOUNDARY CONDITIONS

$$1.\ Boundary\ Condition : \psi(x=0)=0$$

From equation(4) using first Boundary Condition we have,

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

Hence, $\therefore$ **B = 0 -------------------(5)**

WAVE FUNCTION, ψ(*x*) AFTER IMPOSING FIRST BOUNDARY CONDITION IS,

$\psi(x) = A \sin k x$ ....*(6)*

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$$2.\ Boundary\ Condition : \psi(x = l) = 0$$

Imposing second Boundary Condition in equation (6)

$0 = A \sin kl$ Since A $\neq$ 0; $\sin kl = 0$

From trigonometry we can write kl = nπ, where n is an integer.

$$k = \frac{n\pi}{l} \qquad \text{.......................(7)}$$

Using equation(7) in equation (6) we have the wave function

$$\psi_n(x) = A \sin \frac{n\pi x}{l} \qquad \text{.......................(8)}$$

Where n =1,2,3,……

ENERGY (E) OF THE PARTICLE:-

$$k^2 = \frac{2mE}{\hbar^2}$$

$$= \frac{2mE}{(h^2 / 4\pi^2)} \qquad \left[\because \hbar^2 = \frac{h^2}{4\pi^2}\right]$$

$$k^2 = \frac{8\pi^2 mE}{h^2}$$

Using equation (7) $k = \dfrac{n\pi}{l}$

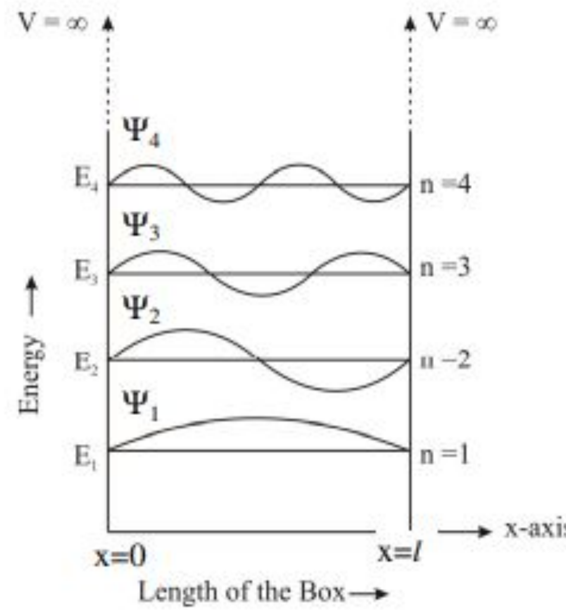
∴ Energy of the particle (electron $E_n = \dfrac{n^2 h^2}{8ml^2}$

Case1: n=1, Ground state

$$E_1 = \frac{h^2}{8ml^2}$$

Case1: n=2, First Excited state

$$E_2 = \frac{4h^2}{8ml^2} \Rightarrow 4E_1$$



Variation of eigen values and eigen function of the electron enclosed in 1 D box

Normalization Condition:

WE KNOW THAT THE TOTAL PROBABILITY (P) IS EQUAL TO 1 MEANS THEN THERE IS A PARTICLE INSIDE THE BOX.

$$P = \int_0^l |\psi|^2 \, dx = 1$$

since the particle is present inside the well between the length 0 to '*l*' the limits are chosen between 0 to *l*

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

Using equation (8) $\psi_n(x) = A \sin \frac{n\pi x}{l}$

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

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

$$A^2\left[\left[\frac{x}{2}\right]_0^l - \frac{1}{2}\left[\frac{\sin\frac{2n\pi x}{l}}{\frac{2n\pi}{l}}\right]_0^l\right] = 1 \qquad \text{-------------------(9)}$$

We know sin nπ = 0 ∴ sin 2nπ is also = 0, hence using it in equation(9) we have

$$\frac{A^2 l}{2} = 1$$

$$A = \sqrt{\frac{2}{l}} \qquad \text{------------------(10)}$$

The normalized wave function can be written using equation (10)

$$\psi_n = \sqrt{\frac{2}{l}} \sin \frac{n\pi x}{l} \quad \text{----------------------(11)}$$

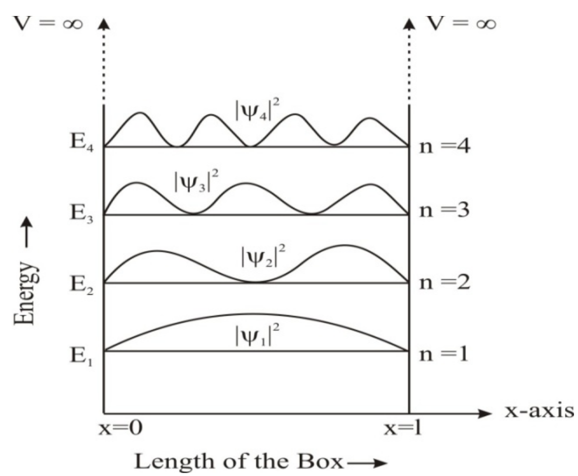


Fig.6.3