Jaipur Engineering College and Research Center

- Year & Sem. – B. Tech. I-Year, Semester - I
- Subject – Engineering Physics (1FY2-02)
- Chapter - Quantum Mechanics (Part-II)
- Department - Applied Science (Physics)

Vision and Mission

- **Vision:**

➢ To become a renowned centre of outcome based learning, and work towards academic, professional, cultural and social enrichment of the lives of individuals and communities.

- **Mission:**

➢ Focus on evaluation of learning outcomes and motivate students to inculcate research aptitude by project based learning.

➢ Identify, based on informed perception of Indian, regional and global needs, the areas of focus and provide platform to gain knowledge and solutions.

➢ Offer opportunities for interaction between academia and industry.

➢ Develop human potential to its fullest extent so that intellectually capable and imaginatively gifted leaders may emerge.

Syllabus and Course Outcome of Quantum Mechanics

Syllabus: Introduction to quantum Mechanics, Wave-particle duality, Matter waves, Wave function and basic postulates, Time dependent and time independent Schrodinger's Wave Equation, Physical interpretation of wave function and its properties, Applications of the Schrodinger's Equation: Particle in one dimensional and three dimensional boxes.

CO2: Students will be able to acquire knowledge of fundamental concepts, principles of quantum mechanics to understand numerous atomic and molecular scale phenomena.

Lecture Plan to Quantum Mechanics

S. No	Topics	Lectures required	Lect. No.
1	Introduction to Quantum Mechanics, wave particle duality and matter waves	1	10
2	Wave function and basic postulates, physical interpretation of wave function and it's properties.	1	11
3	Derivation of time dependent Schrödinger's wave equation.	1	12
4	Derivation of time independent Schrödinger's wave equation	1	13
5	Application of Schrödinger's wave equation -Particle in one dimensional box.	1	14
6	Application of Schrödinger's wave equation -Particle in three dimensional box.	1	15

Content

- Introduction to Schrodinger's Equation
- Types of Equations
- Solution of one dimensional Equation
- Solution of three dimensional Equation.
- Degeneracy of Energy Levels.
- Suggested reference books & links from NPTEL/IIT/RTU Plateforms
- Important questions.

Introduction

- The Schrödinger equation is a linear partial differential equation that describes the wave function or state of a function in a quantum-mechanical system.

- To generalizing the concept of matter waves, Schrödinger discovered the equation of propagation of the wave function associated with the particle. This equation is termed as the Schrodinger wave equation.

- The equation is named after Erwin SchrÖdinger, who postulated the equation in 1925, and published it in 1926, forming the basis for the work that resulted in his Nobel Prize in Physics in 1933.

- Time dependent Schrödinger's wave equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

OR $$H\psi = E\psi$$

- Time independent Schrödinger's wave equation

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

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

Applications of Schrödinger's Equations

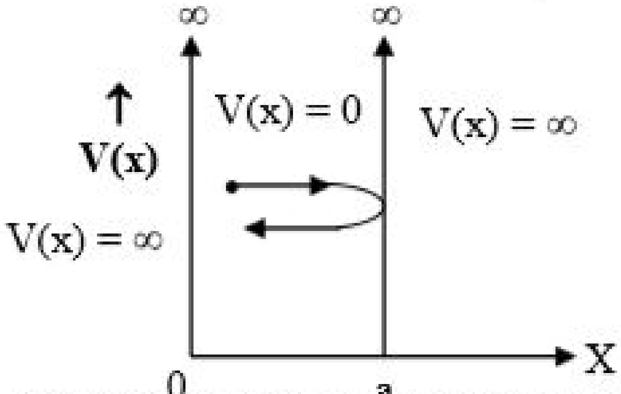
Free particle in one dimensional box

We consider the one dimensional motion along X-axis of a particle of mass m in a box having perfectly rigid walls.

Let 'a' be the distance between the walls so that the motion along the X-axis is limited between x = 0 and x = a, i.e. in the region $0 < x < a$ and there is no force acting on the particle, so that in this region the potential energy V(x) is zero, when particle collides with the perfectly rigid walls, there is no loss of energy. So that the total energy E of the particle remains constant.

In order to leave the region, the particle will have to do an infinite amount of work. So potential energy outside the box is infinite and wave function associated with the particle should be zero outside the box, i.e. $\psi(x) = 0$

$$i.e. \quad \left.\begin{aligned} V(x) &= 0 && 0 < x < a \\ V(x) &= \infty && x \le 0 \text{ and } x \ge a \end{aligned}\right\} \ldots (1)$$



Now in the region $0 < x < a$, the potential V(x) = 0, so the time independent Schrodinger wave equation of particle can be written as

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2mE}{\hbar^2}\psi = 0$$ [E $\rightarrow$ Total energy of particle]

$$\Rightarrow \quad \frac{\partial^2 \Psi}{\partial x^2} + k^2 \Psi = 0 \qquad \dots (2)$$

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

For particular value of k and E, the general solution of equation (2) is

$$\psi(x) = A \sin kx + B \cos kx \qquad \dots (3)$$

where, A and B are constants which can be determined by applying boundary conditions.

We have two boundary conditions:

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

(ii) at $x = a$, $\psi(x) = 0$

From (i) condition $B = 0$, then equation (3) is

$$\psi(x) = A \sin kx \qquad \ldots\ldots(4)$$

By (ii) condition $\psi(x) = A \sin kx = 0$, But $A \neq 0$, So

$$\sin ka = 0$$

$$\Rightarrow \quad ka = n\pi \quad \text{or} \quad k = \frac{n\pi}{a} \quad \text{where, } n = 1, 2, 3, .. \qquad \ldots\ldots.(5)$$

we cannot take $n = 0$, because for $n = 0$, $k = 0$, $E = 0$ and hence $\psi(x) = 0$ everywhere in the box.

Now from equation (4) and (5) the wave function

$$\psi_n(x) = A \sin \frac{n\pi x}{a} \qquad \ldots\ldots(6)$$

Now by normalization condition for wave function in equation (6)

$$\int_{-\infty}^{+\infty} \psi(x)\psi^*(x)dx = 1 \quad \Rightarrow \quad \int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1$$

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

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

$$\Rightarrow \quad \frac{A^2}{2}a = 1 \quad \Rightarrow \quad A^2 = \frac{2}{a} \quad \Rightarrow \quad A = \sqrt{\frac{2}{a}}$$

So wave function is

$$\boxed{\psi_n(x) = \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a}} \qquad \text{..........} (7)$$

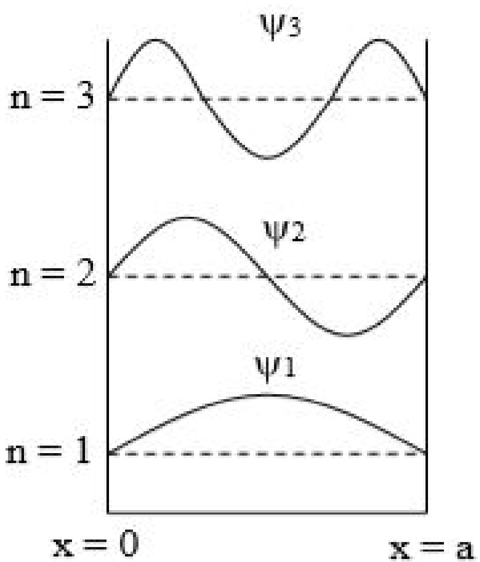
The above equation (7) shows the solution of Schrodinger's wave equation for free particle in one dimensional box.

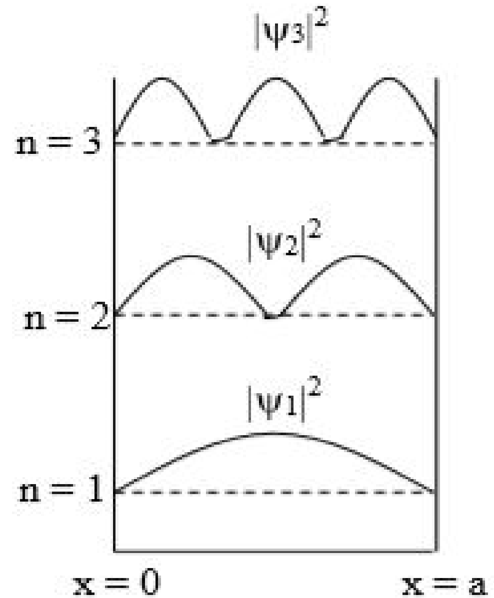
Eigen functions

The solutions of equation (2) are called Eigen functions. Therefore, the Eigen functions of a particle are

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

Eigen functions ψ_1, ψ_2 and ψ_3 and probabilities $|\psi_1|^2$, $|\psi_2|^2$ and $|\psi_3|^2$ for n = 1, 2, 3 are shown in figure as a function of x, it is evident that nodes are formed at the potential wall of the box and the number of nodes in the range $0 < x < a$ is $(n-1)$.





The wavelength of matter waves associated with the particle inside the box is:

$$\lambda = \frac{2\pi}{K} = \frac{2\pi a}{n\pi} \quad \Rightarrow \quad \boxed{\lambda = \frac{2a}{n}}$$

and the size of the box should be $\boxed{a = \frac{n\lambda}{2}}$, i.e. $\lambda/2$, λ, $3\lambda/2$, ….

Energy Eigen values

We know that

$$k = \sqrt{\frac{2mE}{\hbar^2}} \quad \text{and} \quad k = \frac{n\pi}{a}$$

$$\Rightarrow \quad \frac{n\pi}{a} = \sqrt{\frac{2mE_n}{\hbar^2}} \quad \Rightarrow \quad \frac{n^2\pi^2}{a^2} = \frac{2mE_n}{\hbar^2} \quad \Rightarrow \quad \boxed{E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}}$$

These are called eigen values of energy of a particle inside the one dimensional box.
From above equation, for n = 1

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

It is called ground state energy level or zero point energy of particle.

Similarly for n = 2, 3, 4.......

$E_2 = 4E_1$, $E_3 = 9E_1$, $E_4 = 16E_1$, ...

$\Rightarrow$ In General $E_n = n^2E_1$ where $E_1 = \dfrac{\pi^2\hbar^2}{2ma^2}$

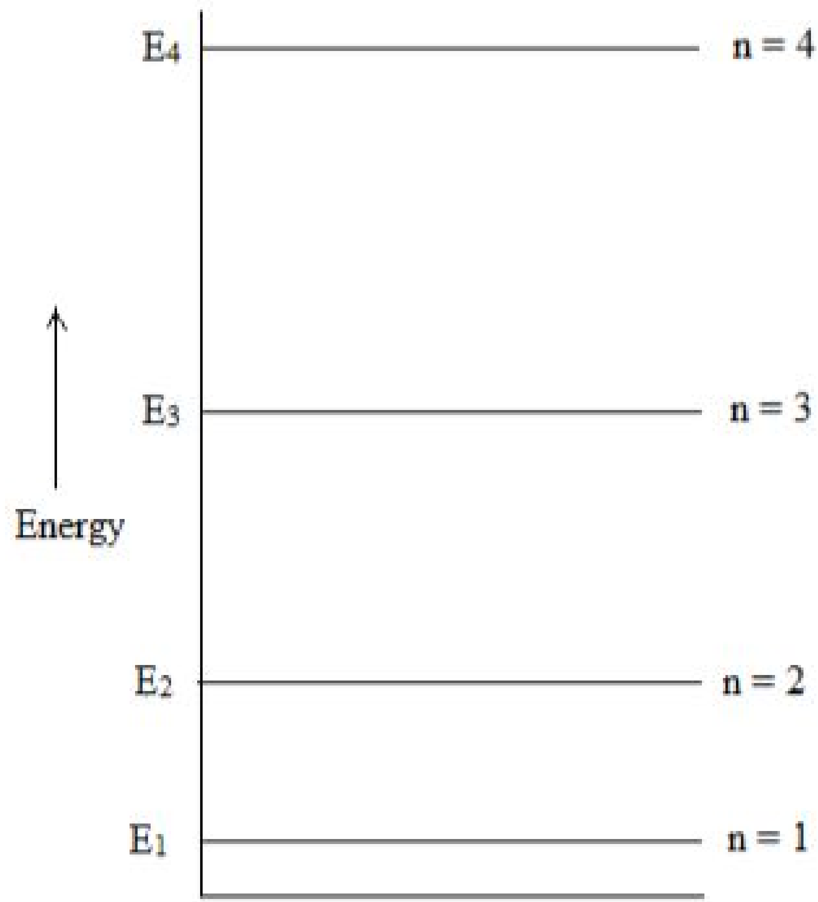


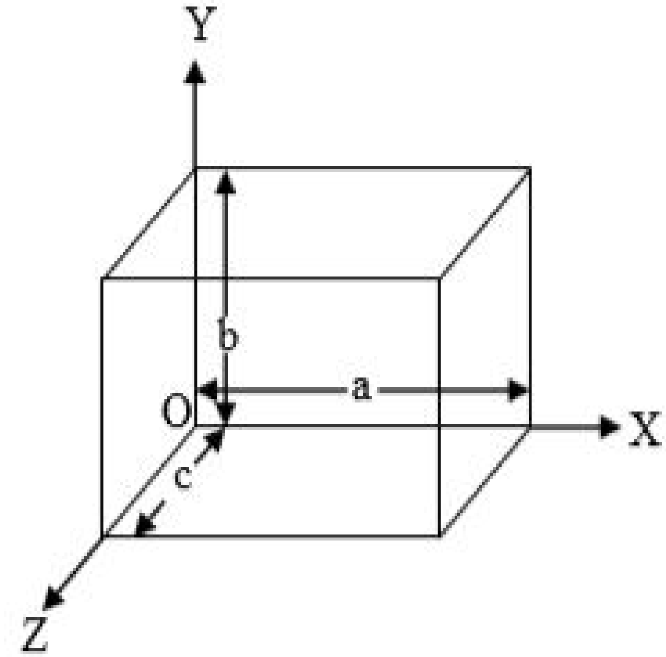
Fig. The discrete energy levels diagram for a particle in one dimensional box.

Free Particle in Three Dimensional Box

Let us consider the motion of a free particle in a three dimensional potential box of sides a, b and c parallel to X, Y and Z-axis respectively. The mass of particle is m and total energy is E. the particle can move freely inside the box because the potential inside the box is zero, because there is no force acting on the particle and in order to leave the box, the particle will have to do an infinite amount of work, so potential energy outside the box is infinite.
Thus, the potential energy can be defined as follow:

$$V(x, y, z) = 0 \; ; \qquad \text{for} \quad \begin{array}{c} 0 < x < a \\ 0 < y < b \\ 0 < z < c \end{array}$$

$$V(x, y, z) = \infty \; ; \qquad \text{for} \quad \begin{array}{c} x \le 0,\ x \ge a \\ y \le 0,\ y \ge b \\ z \le 0,\ z \ge c \end{array}$$



Now the Schrödinger's time independent wave equation for the particle in three dimensional box will be:

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}+\frac{2mE}{\hbar^2}\psi = 0 \qquad \text{... (1)}$$

To solve this equation we use method of separation of variables. Let the function ψ is product of three functions individually depending on the single variable. i.e.

$$\psi\,(x, y, z) = X(x)\,Y(y)\,Z(z)$$

OR $$\psi = XYZ \qquad \text{... (2)}$$

substituting equation (2) in equation (1) and then dividing by XYZ, we get,

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2}+\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}+\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} = -\frac{2mE}{\hbar^2} \qquad \text{... (3)}$$

All three terms on LHS are independent to each other, so that each term can be put equal to some constant. Thus, we can write:

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = -k_x^2 \qquad \frac{\partial^2 X}{\partial x^2} + k_x^2 X = 0 \qquad \text{..............(4)}$$

$$\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} = -k_y^2 \qquad \frac{\partial^2 Y}{\partial y^2} + k_y^2 Y = 0 \qquad \text{..............(5)}$$

$$\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} = -k_z^2 \qquad \frac{\partial^2 Z}{\partial z^2} + k_z^2 Z = 0 \qquad \text{..............(6)}$$

And $$k_x^2 + k_y^2 + k_z^2 = \frac{2mE}{\hbar^2} \qquad \text{..............(7)}$$

Now the solution of equation (4) is given by

$$X = A \sin k_x x + B \cos k_x x \qquad \text{.......... (8)}$$

For a box, at x = 0 and x = a, the potential V is infinite. Hence the wave function X at these positions must be zero, i.e.

$$X = 0, \text{ at } x = 0$$

So, from equation (8)

$$0 = A \sin 0 + B \cos 0 \qquad \Rightarrow \qquad \mathbf{B = 0}$$

$\Rightarrow \quad X = A \sin k_x x$ .... (9)

Also $\quad X = 0, \text{ at } x = a \quad \Rightarrow \quad 0 = A \sin k_x a$

$\Rightarrow \quad \sin k_x a = 0 \qquad (\because A \neq 0)$

$\Rightarrow \quad \sin k_x a = \sin n_1\pi \qquad$ where $n_1 = 1, 2, 3, \ldots$

$\Rightarrow \quad k_x a = n_1\pi \quad \Rightarrow \quad k_x = \frac{n_1\pi}{a}$ .... (10)

$\Rightarrow \quad X = A \sin \frac{n_1\pi}{a} x$ .... (11)

Now by normalization condition between x = 0 and x = a, we have,

$$\int_o^a XX^* dx = 1 \quad \text{OR} \quad \int_0^a A^2 \sin^2 \frac{n_1\pi}{a} x \, dx = 1$$

$$\text{OR} \quad A^2 \frac{a^2}{2} = 1 \quad \Rightarrow \quad A = \sqrt{\frac{2}{a}}$$

Therefore,

$$X = \sqrt{\frac{2}{a}} \sin\left(\frac{n_1\pi}{a}\right)x, \quad \text{and} \quad k_x = \frac{n_1\pi}{a} \qquad \text{...........} (12)$$

Similarly,

$$Y = \sqrt{\frac{2}{b}} \sin\left(\frac{n_2\pi}{b}\right)y \quad \text{and} \quad k_y = \frac{n_2\pi}{b} \qquad \text{...........} (13)$$

$$Z = \sqrt{\frac{2}{c}} \sin\left(\frac{n_3\pi}{c}\right)z \quad \text{and} \quad k_z = \frac{n_3\pi}{c} \qquad \text{...........} (14)$$

where, n_1, n_2, n_3 = 1, 2, 3 … are positive integers.

Thus, the total wave function of a free particle in three-dimensional box from equation (2):

$$\psi = XYZ$$

$$\Rightarrow \quad \boxed{\psi_{(x,y,z)} = \sqrt{\frac{8}{abc}} \sin\left(\frac{n_1\pi}{a}\right)x \sin\left(\frac{n_2\pi}{b}\right)y \sin\left(\frac{n_3\pi}{c}\right)z} \qquad \text{............} (15)$$

Eigen functions

The solutions of equation (1) are called Eigen functions. Therefore, the Eigen functions of a particle are

$$\boxed{\psi_{(x,y,z)} = \sqrt{\frac{8}{abc}} \sin\left(\frac{n_1\pi}{a}\right)x \sin\left(\frac{n_2\pi}{b}\right)y \sin\left(\frac{n_3\pi}{c}\right)z}$$

where, $n_1, n_2, n_3 = 1, 2, 3 \ldots$ are positive integers.

Energy Eigen values

The allowed value of total energy, substituting the values of k_x, k_y and k_z from equation (12), (13) and (14) in equation (7), we have

$$\left(\frac{n_1\pi}{a}\right)^2 + \left(\frac{n_2\pi}{b}\right)^2 + \left(\frac{n_3\pi}{c}\right)^2 = \frac{2mE}{\hbar^2}$$

$$\Rightarrow \quad \boxed{E = \frac{\pi^2\hbar^2}{2m}\left[\left(\frac{n_1}{a}\right)^2 + \left(\frac{n_2}{b}\right)^2 + \left(\frac{n_3}{c}\right)^2\right]} \quad \ldots\ldots\ldots\ldots (16)$$

The above equation represents the energy eigen values for particle in 3-D box.

Special Case: **If particle trapped in three dimensional cubical box.**

For cubical box, a = b = c, then, **Wave Function**

$$\boxed{\psi_{(x,y,z)} = \left(\frac{2}{a}\right)^{3/2} \sin\left(\frac{n_1\pi}{a}\right)x \sin\left(\frac{n_2\pi}{a}\right)y \sin\left(\frac{n_3\pi}{a}\right)z} \quad \text{..........} (17)$$

and Energy Eigen values

$$\boxed{E = \frac{\pi^2\hbar^2}{2ma^2}\left[n_1^2 + n_2^2 + n_3^2\right]} \quad \text{...........} (18)$$

or $$\boxed{E = E_1\left(n_1^2 + n_2^2 + n_3^2\right)}$$ where, $$E_1 = \frac{\pi^2\hbar^2}{2ma^2}$$

Degeneracy of Energy Level

- If there are more than one Eigen functions corresponding to one energy level, the state is known as degeneracy of energy level and the number of wave functions is called order of degeneracy.

- If order of degeneracy of an energy level is denoted by ‘g’ then the energy level is said to be ‘g’ times degenerate.

- If there is only one eigen function corresponding to one energy level then energy level denoted as non-degenerate.

Allowed energy levels in a three dimensional potential box is shown below:-

Energy of Energy Level	Order of degeneracy	Degeneracy	Quantum Number (n_1, n_2, n_3)
$3E_1$	Non	Non-degenerate	(1, 1, 1)
$6E_1$	3	Three-fold degenerate	(1, 1, 2), (1, 2, 1), (2, 1, 2)
$9E_1$	3	Three-fold degenerate	(2, 2, 1), (1, 2, 2), (2, 1, 2)
$11E_1$	3	Three-fold degenerate	(3, 1, 1), (1, 3, 1), (1, 1, 3)
$12E_1$	Non	Non-degenerate	(2, 2, 2)
$14E_1$	6	Six-fold degenerate	(1, 2, 3), (1, 3, 2), (2, 1, 3), (2, 3, 1), (3, 1, 2), (3, 2, 1)
$17E_1$	3	Three-fold degenerate	(3, 2, 2), (2, 3, 2), (2, 2, 3)
$18E_1$	3	Three-fold degenerate	(4, 1, 1), (1, 4, 1), (1, 1, 4)
$19E_1$	3	Three-fold degenerate	(3, 3, 1), (3, 1, 3), (1, 3, 3)
$21E_1$	6	Six-fold degenerate	(1, 2, 4), (1, 4, 2), (2, 1, 4), (2, 4, 1), (4, 1, 2), (4, 2, 1)

where $E_1 = \dfrac{\pi^2 \hbar^2}{2ma^2}$

Suggested Reference Books & links from NPTEL/IIT/RTU Plateforms

References:

1. Quantum Mechanics: Ajoy K. Ghatak and S. Loknathan (TMH)
2. Quantum Mechanics: Schiff (Tata McGraw Hill)
3. Engineering Physics: Malik and Singh (Tata McGraw Hill)
4. Engineering Physics: S. Mani Naidu (Pearson Education)
5. Concept of Modern Phyiscs: A. Baiser (Tata McGraw Hill)
6. Engineering Physics : Y. C. Bhatt (Ashirwad Publications)
7. Engineering Physics : S. K. Sharma (Genius Publication)
8. Engineering Physics: D. K. Bhattacharya (Oxford Higher Education)

Suggested Links:

1. https://nptel.ac.in/courses/115/102/115102023/
2. https://www.youtu.be/eyXoN6C6IKk (a video lecture by Prof. P. Balakrishnan IIT Madras)
3. http://youtu.be/TcmGYe39XG0 (a video lecture by Prof. P. Balakrishnan IIT Madras)
4. https://youtu.be/siM1MVvmIFA (a video lecture prepared by Prof. R. K. Mangal JECRC Jaipur)
5. https://youtu.be/7Pvb-UKPp78 (a video lecture prepared by Prof. R. K. Mangal, JECRC Jaipur)

Important Questions

1. Solve Schrödinger equation of a particle in a one-dimensional box for eigen values and eigen functions. Show that the particle takes discrete energies.
2. Solve Schrödinger equation of a particle in a three-dimensional box for eigen values and eigen functions.
3. Find the probability that a particle in a box can be found between 0.45a and 0.55a where a is the width of the box and particles in the first excited state.
4. The wave function of a particle in its ground state in one dimensional box of length L is given by Ψ= . Calculate probability of finding the particle with in an interval of 1 Å at the center of box of length L=10Å.
5. An electron confined to move in a one dimensional box of length 1Å. Find the zeropoint energy and momentum of the electron in its ground state.
6. Find the probability that a particle in a box of width 'a' can be found between x=0 and x=a/n when it is in the nth state.
7. Find the probability that a particle in a box of 25Å can be found within an interval of 5Å at the centre of the box when the particle is in ground state.
8. Answer the following questions with respect to a particle in a cubical box of side a-

   (a)What is the order of degeneracy for nx+ny+nz=4

   (b)What will happen to the degeneracy for nx+ny+nz=4 if the box is not cubical but rectangular parallelepiped with side a, b, c, such that a=b≠c ?

Thank You

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