JECRC Foundation

JAIPUR ENGINEERING COLLEGE AND RESEARCH CENTRE

Jaipur Engineering College and Research Center

Year & Sem. – B. Tech I-Year, Semester - I
Subject – Engineering Physics (1FY2-02)
Chapter - Quantum Mechanics (Part-I)
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 Quantum Mechanics
- Wave Particle duality and matter waves
- Wave function and basic postulates.
- Derivation of time independent and dependent Schrodinger's equations
- Physical Interpration of wavefunction and it's properties.
- Suggested reference books & links from NPTEL/IIT/RTU Plateforms
- Important questions.

Introduction to Quantum Mechanics

The failure of classical mechanics led to the development of quantum mechanics. This theory was developed by Max Planck in 1900, while he was trying to explain the spectral distribution of energy in black body radiation. According to Planck's quantum theory, whenever there is an interaction between matter and radiation, the exchange of energy does not occur in a continuous manner but it is discrete in nature. The minimum discrete value of energy which can be exchanged is called quantum or photon and energy of photon is proportional to the frequency of radiation i.e.

$$E \propto \nu \Rightarrow E = h\nu$$

where h is a constant called Planck's constant and its value is 6.62×10^{-34} J-S.

The photon is a quantum of radiant energy and it is indivisible when it is absorbed by matter, it is absorbed as a whole and not a part of it.

The quantum nature of light has been verified experimentally. It has been successful in explaining many effects which could not be explained by classical theories like photo-electrical effect, Compton Effect, Raman Effect etc.

Dual Nature of Light and De Broglie Hypothesis

We know that light have dual nature i.e. wave nature and particle nature. The phenomenon of interference, diffraction and polarization of light can only be explained on the basis of wave nature of light. On the other hand the phenomenon of photoelectric effect, Compton Effect, black body radiation etc. can only be explained on the basis of quantum nature of light.

According to quantum nature of light, the light is propagated in small packets or bundles of energy ($h\nu$). These packets are called photons or quanta and behave like corpuscles. This phenomenon indicates that light have corpuscular or particle nature of light. Thus we can say that light possesses dual nature.

On the basis of the concept of dual nature of light Louis de Broglie in 1924 gave the hypothesis that particles in motion should also have wave characteristics associated with them just like the radiant energy in the form of waves has particle properties associated with it. The waves associated with particles are called matter waves. The wave nature of particle (electrons) shortly explained by Davisson & Germer and G.P. Thomson experiments.
According to de Broglie hypothesis, if a particle is moving with momentum **p,** then the wavelength **λ** of wave associated with this particle is:

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

λ is also called de Broglie wavelength

If velocity of particle is very less than to velocity of light i.e. ($v << c$), and rest mass of particle is m_o, then

$$\lambda = \frac{h}{m_o v}$$

OR

$$\lambda = \frac{h}{\sqrt{2 m_o E}}$$

where $E = \frac{1}{2} m_o v^2$, kinetic energy of particle.

If $v \approx c$, then

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

where **m** relative mass of moving particle and $m = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}}$

the wavelength of wave associated with particle is decrease with increase in momentum of particle.

Wave Function (Ψ) and Basic Postulates

On the basis of wave nature of particle, the propagation of wave must be in the form of wave-packet and wave-packet behaves like amplitude of wave. This wave-packet whose variations makeup matter waves associated with the particles is called the wave functions. It denoted by ψ.

The wave function must be satisfied the following conditions:

1. The wave functions 'ψ' must obey the principle of superposition.
2. The wave function 'ψ' as well as its derivative '$\frac{d\psi}{dx}$' must be finite, continuous and single valued throughout the region considered.

SCHRODINGER'S WAVE EQUATION

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

Schrödinger's Wave Equations

(I) Time Independent Schrodinger's Wave Equation

Let us consider a system of stationary waves to be associated with a particle. Let ψ(x,y,z,t) be the wave function for matter waves at any time t. Then according to Maxwell's relation for electromagnetic waves, the differential equation of wave associated with the particle is given by:

$$\frac{\partial^2 \Psi}{\partial t^2} = v^2 \nabla^2 \Psi \qquad \ldots(1)$$

where, ∇^2 = Laplacian operator = $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

v = velocity of particle

So $$\frac{\partial^2 \Psi}{\partial t^2} = v^2 \left[\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right] \qquad \ldots(2)$$

Let us differentiate equation (3) with respect to t, then

$$\frac{\partial \psi}{\partial t} = -i\omega\psi_0 e^{-i\omega t}$$

again differentiating,

$$\frac{\partial^2 \psi}{\partial t^2} = -i\omega(-i\omega)\psi_0 e^{-i\omega t} = -\omega^2\psi$$

Substituting the value of $\frac{\partial^2 \psi}{\partial t^2}$ in equation (2), we have

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} + \frac{\omega^2}{v^2}\Psi = 0$$

$$\nabla^2\Psi + \frac{\omega^2}{v^2}\Psi = 0$$

But we know that

$$\omega = 2\pi\nu = 2\pi\frac{v}{\lambda} \qquad \text{where v velocity of particle}$$

and by de Broglie relation $\lambda = \frac{h}{mv}$

$$\Rightarrow \qquad \frac{\omega}{v} = \frac{2\pi}{\lambda} = \frac{2\pi mv}{h}$$

$$\Rightarrow \qquad \nabla^2\Psi + \frac{4\pi^2 m^2 v^2}{h^2}\Psi = 0 \qquad \ldots (4)$$

If E and V be the total and potential energies of particle respectively then it's K.E.

$$\frac{1}{2}mv^2 = E - V$$

$$\Rightarrow \qquad m^2v^2 = 2m\,(E - V) \qquad \ldots (5)$$

From equation (4) and (5), we have

$$\Rightarrow \quad \nabla^2\Psi + \frac{8\pi^2 m}{h^2}(E - V)\Psi = 0 \qquad \ldots (6)$$

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

For one dimensional problem

$$\Rightarrow \quad \frac{\partial^2\Psi}{\partial x^2} + \frac{8\pi^2 m}{h^2}(E - V)\Psi = 0 \qquad \ldots\ldots.(7)$$

But we know that

$$\hbar = \frac{h}{2\pi}$$

So equation (6)

$$\nabla^2\Psi + \frac{2m}{\hbar^2}(E - V)\Psi = 0 \qquad \ldots (8)$$

The equations (6) to (8) are known as Time Independent Schrodinger's Wave Equation.

Schrodinger's wave equation for free particle

For a field free particle, V(x, y, z) = 0. Therefore, putting V=0 in equation (8), we get Schrodinger's wave equation for a free particle as below:

$$\nabla^2 \Psi + \frac{2mE}{\hbar^2}\Psi = 0 \qquad \text{......(9)}$$

(II) Time Dependent Schrodinger's Wave Equation

To obtain the time dependent Schrodinger's wave equation, Let us consider the solution of wave equation (1)

$$\psi(\boldsymbol{r}, \boldsymbol{t}) = \psi_0(\boldsymbol{r})\, e^{-i\omega t}$$

Differentiating with respect to t, we get

$$\frac{\partial \psi}{\partial t} = -i\omega\psi_0 e^{-i\omega t}$$

$$\Rightarrow \quad \frac{\partial \Psi}{\partial t} = -i(2\pi\nu)\Psi_o e^{-i\omega t} \qquad [\omega = 2\pi\upsilon]$$

$$\Rightarrow \quad \frac{\partial \psi}{\partial t} = -2\pi i \nu \psi$$

But E = hυ $\Rightarrow \quad \nu = \frac{E}{h}$

$$\Rightarrow \quad \frac{\partial \psi}{\partial t} = -2\pi i \left(\frac{E}{h}\right)\psi$$

$$\Rightarrow \quad \frac{\partial \psi}{\partial t} = -\frac{iE}{\hbar}\psi = \frac{E}{i\hbar}\psi$$

$$or \quad i\hbar \frac{\partial \psi}{\partial t} = E\psi \quad \Rightarrow \quad E \rightarrow i\hbar \frac{\partial}{\partial t} \qquad \ldots (10)$$

Now time independent Schrodinger's wave equation is from eqn. (8)

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

Using equation (10), we have

$$\nabla^2\Psi + \frac{2m}{\hbar^2}\left(i\hbar\frac{\partial\Psi}{\partial t} - V\Psi\right) = 0$$

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

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

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = i\hbar\frac{\partial\Psi}{\partial t} \qquad \ldots (11)$$

Now equation (11) can be written as

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

OR $$H\psi = E\psi \qquad \ldots\ldots\ldots\ldots.(12)$$

where, $H = -\frac{\hbar^2}{2m}\nabla^2 + V$ is a operator and called Hamiltonian of the particle and

$E = i\hbar\frac{\partial}{\partial t}$ is energy operator.

The above eqn. (11) and (12) are represent the time dependent Schrodinger's wave equation.

Physical Significance of wavefunction (Ψ) and its properties

1. **Statistical interpretation by Max Born:**

   According to Max Born, if a particle described by a wave function ψ, then, the probability of finding of particle at point (x, y, z) and at time t is directly proportional to the $|\psi(x, y, z, t)|^2$. i.e. probability density of particle is

$$P(\boldsymbol{r}, t) = |\psi(\boldsymbol{r}, t)|^2 = \psi(\boldsymbol{r}, t)\,\psi^*(\boldsymbol{r}, t)$$

where $\psi^*(\boldsymbol{r}, t)$ is complex conjugate of wave function $\psi(\boldsymbol{r}, t)$

Similarly the probability of finding a particle in a volume element $dV = dxdydz$ at the point $\boldsymbol{r}$ at time t is given by

$$P(\boldsymbol{r}, t)dV = |\psi(\boldsymbol{r}, t)|^2 dV = \psi(\boldsymbol{r}, t)\,\psi^*(\boldsymbol{r}, t)dV$$

The wave function ψ (***r***, ***t***) is sometimes called a probability amplitude for a position of the particle.

2. Normalization of the wave function:

The probability of finding the particle in space is unity, i.e.

$$\int_{-\infty}^{\infty} P(\boldsymbol{r},\boldsymbol{t})dV = \int_{-\infty}^{\infty} |\psi(\boldsymbol{r},\boldsymbol{t})|^2 dV = \int_{-\infty}^{\infty} \psi(\boldsymbol{r},\boldsymbol{t})\ \psi^*(\boldsymbol{r},\boldsymbol{t})dV = 1$$

The above equation is called Normalization condition and wave function follows this condition is called normalized wave function.

3. Orthogonality of wave function:

For a given system if two different wave functions ψ_i and ψ_j are proper solutions of same Schrodinger equation and are such that the integral

$$\int_{-\infty}^{\infty} \psi_i(\boldsymbol{r},\boldsymbol{t})\Psi_j^*(\boldsymbol{r},\boldsymbol{t})dV = 0 \qquad \text{OR} \qquad \int_{-\infty}^{\infty} \Psi_i^*(\boldsymbol{r},\boldsymbol{t})\psi_j(\boldsymbol{r},\boldsymbol{t})dV = 0$$

Then these wave functions are called orthogonal wave functions.

4. **Expectation value of physical quantity:**
The expectation value of given physical quantity **Q** is

$$< Q > = \int_{-\infty}^{\infty} \psi \, Q \, \psi^* dV$$

5. For an acceptable wave function, ψ along its derivative $\frac{d\psi}{dx}$ must be continuous, single valued and finite throughout the region considered.

6. ψ must obey principle of superposition i.e. if ψ_1, ψ_2, …, ψ_n are solutions of Schrodinger wave equation, then ψ is also a solution given by:

$$\psi = C_1\psi_1 + C_2\psi_2 + \ldots + C_n\psi_n$$

where $C_1, C_2, \ldots C_n$ are constants.

7. **Boundary conditions:**
At a boundary separating two media the wave function as well as its derivative must be equal. i.e.

$$\psi_1 = \psi_2 \qquad and \qquad \left|\frac{d\psi}{dx}\right|_1 = \left|\frac{d\psi}{dx}\right|_2$$

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://youtu.be/R-x9KdNjQmo (a video lecture by Prof. Ajoy Ghatak IITD)
3. https://youtu.be/w7Wf3Wr0guA (a video lecture by Prof. Ajoy Ghatak IITD)
4. https://www.youtu.be/ZFUnPwNRUWA (a video lecture by Prof. P. Balakrishnan IIT Madras)
5. https://youtu.be/NfkJKIoExYo (a video lecture by Prof. Ajoy Ghatak IITD)

Important Questions

1. Explain matter waves.
2. Describe Heisenberg's uncetainity principal and apply it to explain non existance of electron in nucleus.
3. What is a wave function? Give its physical significance.
4. Explain the following terms
   - Normalized and orthogonalized wave function
   - Hamiltonian Operator
5. Derive the Schrödinger time dependent and time independent one dimensional wave equation.
6. Show that the expectatin value of the position <x> of a particle trapped in a box of width L is independent of the quantum state.
7. An electron is moving with speed 225 m/s with an accuracy of 0.001%. Calculate the uncertainity in its position.
8. Compute the de-Broglie wavelength of a proton whose kinetic energy is equal to the rest energy of an electron. Mass of a proton is 1836 times the mass of the electron.
9. Prove that the eigen functions of a particle moving in one dimenntional box are orthogonal.

Thank You

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