UNIT 4 QUANTUM MECHANICS

LECTURE 6

What we learned so far about Quantum mechanics?

1. We had a short walk down the memory lane (1900-1927)

   - ✓ Classical mechanics, relativistic mechanics, quantum mechanics and quantum field theory
   - ✓ Hertz, Planck, Einstein, Bohr, Crompton, Raman, de Broglie, Heisenberg, Schrödinger, Dirac, Pauli, Born
   - ✓ Development of quantum mechanics

2. Classical mechanics Explained

Newton's corpuscular concepts of light-particles
Maxwell’s wave concepts of light from EM theory
Reflection, refraction –explained through particle concept-ray optic
Interference, diffraction, polarization– wave nature

It was all about light!

2. How QM concept helped in overcoming classical limitation?

Black body radiation ,
Wien and Rayliegh-Jean formula,
UV catastrophe
Planck's quantum oscillator,

$$I_\nu \, d\nu = \frac{8\pi \nu^2}{c^3} kT \, d\nu$$

$$I_\nu \, d\nu = \frac{A \nu^3}{c^4} e^{-B\nu/T} \, d\nu$$

$$I_\nu \, d\nu = \frac{8\pi h}{c^3} \frac{\nu^3 d\nu}{e^{h\nu/kT} - 1}$$

Photoelectric effect,
Hertz's discovery
Einstein's photoelectric equation,
The name photon

$$E_k = h\nu - \underbrace{h\nu_0}_{\phi_m\text{-Work function}}$$

Compton effect-scattering of light by electron
Raman effect-vibration spectra of molecules upon photon irradiation

All these phenomenon were successfully explained by QM

3. Characteristic properties of a wave : **ν and λ**

4. Characteristic properties of a particle: **p and E**

5. Radiation (wave)-particle duel nature

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

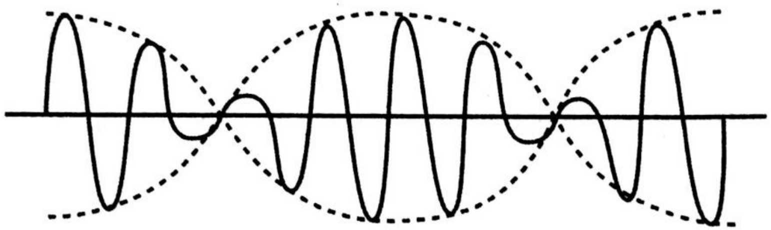
6. Matter (particle) –wave duel nature

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

De Broglie’s hypothesis; connecting the wave nature with particle nature through the Planck’s constant..

Used Einstein’s famous mass-energy relation $E=mc^2$

6.a Various relation connecting the de Broglie wavelength associated with a particle of mass m and having energy E



7. Characteristics of matter wave

8. Wave velocity, phase velocity, group velocity and particle velocity

v particle velocity

$$v_p = \frac{\omega}{k} \qquad v_g = \frac{\Delta\omega}{\Delta k} \qquad \therefore v_g = -\frac{\lambda^2}{2\pi}\frac{\partial\omega}{\partial\lambda}$$

non-dispersive- $v_p = v_g$

normal-dispersive- $v_p > v_g$

anomalous dispersive mediums- $v_p < v_g$

9. Relationship between v_g and v_p & v_g and v

$$v_g = v_p - \lambda\frac{dv_p}{d\lambda}$$

Dispersion

$$v_g = v$$

10. Heisenberg uncertainty principle

Wave-particle duality introduce the concept of uncertainty. This concept suggest that if the particle nature of the matter becomes certain, the wave nature becomes uncertain and vice versa.

Uncertainty in the measurements of physical quantities

There are three **conjugate variables** of great importance in **quantum mechanics**: position and momentum, angular orientation and angular momentum, and energy and time.

1. $\Delta p \, \Delta x \geq \hbar$ Original statement of Heisenberg uncertainty principle
2. $\Delta E \, \Delta t \geq \hbar$ Time –Energy uncertainty principle
3. $\Delta L_\theta \, \Delta\theta \geq \hbar$ Angular momentum -Angular orientation uncertainty principle

11. Applications of Heisenberg uncertainty principle are

1. Non existence of electron in the nucleus
2. Existence of proton, neutrons and α-particles in the nucleus
3. Binding energy of an electron in an atom
4. Radius of Bohr's first orbit
5. Energy of a particle in a box
6. Ground state energy of the linear harmonic oscillator
7. Radiation of light from an excited atom

12. Wave Equation and function- Classical

$$\nabla^2 u = \frac{1}{v^2}\frac{\partial^2 u}{\partial t^2}$$

$$u = a\ \sin(\omega t - kx)$$

Where 'u' is the wave function… that is the solution of the wave equation

e.g, u can be E, B or P at a position (x,y,z) at a given time t.

13. Wave function- Quantum

The characteristics of the wave functions in quantum mechanics are

- ψ must be finite, continuous and single valued everywhere
- ψ must be normalizable $\iiint_{-\infty}^{\infty} \psi^* \psi \ dV = 1$
- also $\frac{\partial \psi}{\partial x}, \frac{\partial \psi}{\partial y}, \frac{\partial \psi}{\partial z}$ must be finite, continuous and single valued

14. Schrödinger wave equation

Schrödinger time- independent wave equation for free particle

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

Schrödinger time- independent wave equation

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

Schrödinger time- dependent wave equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\psi = i\hbar\frac{\partial\psi}{\partial t}$$

$$\mathbf{H}\psi = \mathbf{E}\psi$$

15. Operators, Eigen value and Eigen function

Classical expression for total energy

$$\frac{p^2}{2m} + V = E$$

$$E = i\hbar\frac{\partial}{\partial t}$$

$$p = -i\hbar\nabla$$

When a Laplacian operator (∇^2) and Energy (E) operate on wave function (Ψ), we get the wave equation $\nabla^2\psi + \frac{2mE}{\hbar^2}\psi = 0$. What type of Schrodinger equation is this?

a) Time dependent Schrodinger equation
b) Time-independent Schrodinger equation
c) Both (a) and (b)
d) None of the above

Ans: B

The characteristics of the wave functions in quantum mechanics are

a) ψ must be finite, continuous and single valued everywhere
b) ψ must be normalizable
c) $\frac{d\Psi}{dx}$ must be finite, continuous and single valued
d) All of the above

Ans: D

Which function is considered independent of time to achieve time independent Schrodinger equation?

a) ψ

b) $\frac{d\psi}{dt}$

c) $\frac{d^2\psi}{dx^2}$

d) V, potential energy

Ans: D

What is the potential energy of a free particle having mass m ?

a) 0

b) ∞

c) $\frac{1}{2}mv^2$

d) mgh

Ans: A

The values of Energy for which Schrodinger’s equation can be solved is known as _______________

a) Eigen Vectors
b) Eigen Values
c) Eigen Functions
d) Operators

Ans: B

Which quantity is said to be degenerate when $H\Psi_n = E_n\Psi_n$?

a) Eigen Vectors
b) Eigen Values
c) Eigen Functions
d) Operators

Ans: C

Application of Schrödinger Equation

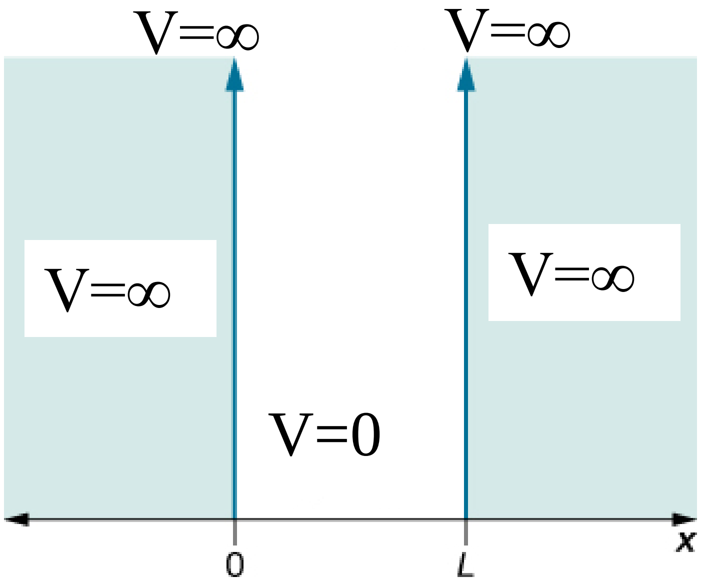
Particle in a box

- Electron confined in a potential well
- Restriction imposed by the boundary conditions on the wave function
- Exploit the characteristics of the wave function-normalization
- To find Eigen value and Eigen function

We will prove energy (Eigen value) of the particles/electrons is discrete and is quantized.

https://www.youtube.com/watch?v=LBB39u8dNw0

Particle in a box



For simplicity we consider,

1)Particle restricted to move in the x-direction only (1 dimensional) from x=0 to x=L
2)Wall is infinitely thick and hard: Particle does not loose energy upon colliding with the wall
3)Potential energy, V of the particle is 0 inside the box but rises to infinity out side

$$V = 0 \qquad\qquad 0 \leq x \leq L$$

$$V = \infty \qquad\qquad x < 0 \; and \; x > L$$

This is equivalent to the case where the particle trapped inside a infinitely deep potential well.. Let us take Schrödinger equation now

Particle in a box- Eigen value & Function

$$\nabla^2\psi + \frac{2mE}{\hbar^2}\psi = 0 \xrightarrow{\text{For 1 D}} \frac{\partial^2\psi}{\partial x^2} + \frac{2mE}{\hbar^2}\psi = 0 \quad \text{Eq.1}$$

And put $$k^2 = \frac{2mE}{\hbar^2} \quad \text{Eq.2}$$

$$\frac{\partial^2\psi}{\partial x^2} + k^2\psi = 0 \quad \text{Eq.3}$$

General solution for Eq.3 can be written as

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

Where A and B are constant. Now apply the first boundary condition. $\psi(x)=0$ at $x=0$

$$\psi(0) = A\sin 0 + B\cos 0 = 0 \Longrightarrow B=0$$

$$\psi(x) = A\sin kx \quad \text{Eq.5}$$

Now we will find k and E related to the dimensions of the well

Particle in a box- Eigen value

Now apply the 2nd boundary condition. $\psi(x)=0$ at $x=L$. Eq.5 gives

$$\psi(L) = A \sin kL = 0 \quad \Rightarrow \quad A \neq 0, \quad \sin kL = 0 \qquad \text{Eq.6}$$

Eq.6 is satisfied only when $kL = n\pi$ Where, n= 1,2,3

$$k = \frac{n\pi}{L} \quad \text{or} \quad k^2 = \frac{n^2\pi^2}{L^2} \qquad \text{Eq.7}$$

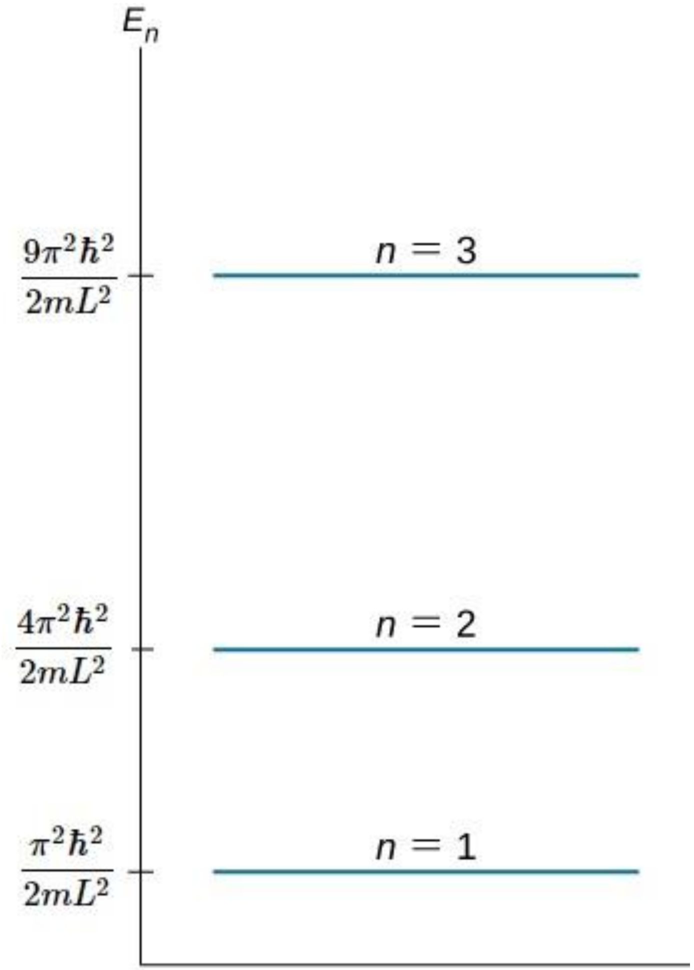
Now substitute Eq.2 in Eq.7

$$k^2 = \frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{L^2} \quad \Rightarrow \quad E = \frac{n^2\hbar^2\pi^2}{2mL^2} \qquad \text{Eq.8}$$

Energy of the particle is discrete and is quantized!!

Particle in a box- Eigen value

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



- **E** is the Eigen value of the particle in the potential well
- Constitute the energy level of the system
- ***n*** is the quantum number corresponds to the energy level $\mathbf{E_n}$

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

So we found out the energy (**Eigen value**) of the particle in a box, with the help of Schrödinger equation

Particle in a box- Eigen function

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

Now we have to find the value of **A**, and that can be obtained by the process of normalization

$$\int_{-\infty}^{\infty} \psi_n(x)^* \psi_n(x) dx = 1$$

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

$$A^2 \int_0^L \frac{\left[1 - \cos \frac{2n\pi x}{L}\right]}{2} dx = 1 \quad \Rightarrow \quad \frac{A^2}{2} \left[x - \frac{L}{2n\pi} \sin \frac{2n\pi x}{L}\right]_0^L = 1$$

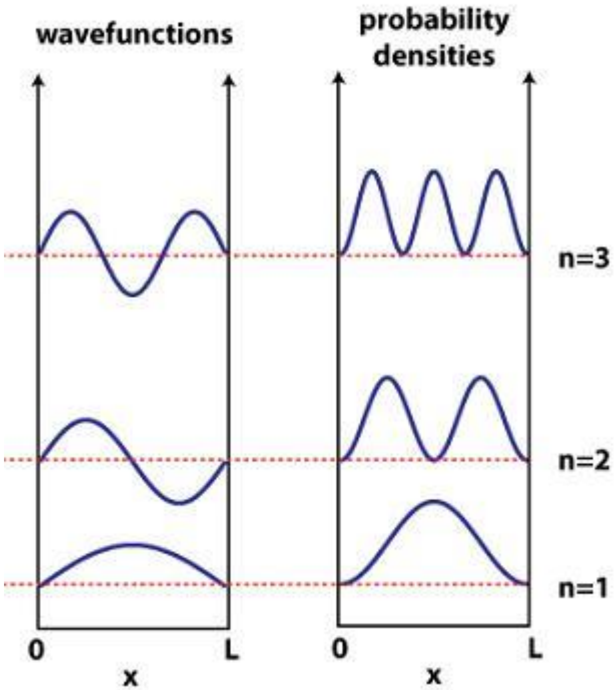
$$\frac{A^2}{2} L = 1 \qquad A = \sqrt{\frac{2}{L}}$$

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

So we found out the exact wave function for this particle

Particle in a box

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



Probability of finding the particle is

$$|\psi_n(x)|^2$$

- Classical mechanics predict the same probability to find the particle anywhere in the box
- But quantum mechanics different probability
- There are points where particle will never present
- Probability is different also with energy of the particles

The energy of a particle at a level n in infinite potential well is

(a) Proportional to n^2
(b) Proportional to n
(c) Inversely proportional to n^2
(d) Inversely proportional to n

Ans: A

The momentum of a particle in infinite potential well is

(a) Proportional to n^2
(b) Proportional to n
(c) Inversely proportional to n^2
(d) Inversely proportional to n

Ans: B

The momentum of a particle in infinite potential well of length L is

(a) Proportional to L^2
(b) Proportional to L
(c) Inversely proportional to L^2
(d) Inversely proportional to L

Ans: D

The Energy of a particle in infinite potential well of length L is

(a) Proportional to L^2
(b) Proportional to L
(c) Inversely proportional to L^2
(d) Inversely proportional to L

Ans: C

UNIT 4-Quantum Mechanics

Text Book: ENGINEERING PHYSICS by HITENDRA K MALIK AND A K SINGH, MCGRAW HILL EDUCATION, 1st Edition, (2009)

References:

- ENGINEERING PHYSICS by B K PANDEY AND S CHATURVEDI, CENGAGE LEARNING, 1st Edition, (2009).

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