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, 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!

What we learned so far about Quantum mechanics?

2. How QM concept helped in overcoming classical limitation?

Black body radiation ,
Wien and Rayleigh-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

$$E_k = h\nu - h\nu_0$$

Crompton effect-scattering of light by electron
Raman effect-vibration spectra of molecules upon photo irradiation

All these phenomenon were successfully explained by QM

What we learned so far about Quantum mechanics?

3. Characteristic properties of a wave : **ν and λ**
4. Characteristic properties of a particle: **p and E**
5. Radiation-particle duel nature
6. Matter –wave duel nature

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

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

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

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

7. Experimental verification by Davisson and Germer: wave nature of electron by diffraction experiment

What we learned so far about Quantum mechanics?

8. Characteristics of matter wave $\lambda = \frac{h}{mv} = \frac{h}{p}$

9. Wave velocity, group velocity and particle velocity

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

non-dispersive, $v_p = v_g$
normal-dispersive $v_p > v_g$
anomalous dispersive mediums $v_p < v_g$

10. Relationship between v_g and v_p & v_g and v

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

dispersion

11. Heisenberg uncertainty principle

$$\Delta p\, \Delta x \geq \hbar \qquad \Delta L_\theta\, \Delta\theta \geq \hbar$$
$$\Delta E\, \Delta t \geq \hbar$$

12. Applications of Heisenberg principle

13. Classical wave equation $\nabla^2 u = \frac{1}{v^2}\frac{\partial^2 u}{\partial t^2}$

14. Characteristics of quantum wave function ψ

15. Schrödinger time- independent wave equation $\nabla^2\psi + \frac{2m}{\hbar^2}(E - V)\,\psi = 0$

16. Schrödinger time- independent wave equation for free particle $\nabla^2\psi + \frac{2mE}{\hbar^2}\psi = 0$

17. Schrödinger time-dependant wave equation

18 Operators, Eigen value and Eigen function

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

$$\frac{p^2}{2m} + V = E \longleftarrow \mathbf{H}\psi = \mathbf{E}\psi$$

Classical expression for total energy

Quick QUIZ

Quick Quiz Response on the 10/04/2018 Lecture

No		Attempts	Right	Wrong
1	Wave nature of electron was experimentally verified by Davisson and Germer through			
2	In an anomalous dispersive medium phase velocity (v_p) and group velocity (v_g) are different. Which of the following is correct in that case			
3	Dual nature (particle and wave) of matter was proposed by:			
4	The characteristics of the wave functions in quantum mechanics are			

Wave nature of electron was experimentally verified by Davisson and Germer through

(a) Diffraction experiment
(b) Interference experiment
(c) Polarization experiments
(d) None of the above

Ans: A

In an anomalous dispersive medium phase velocity (v_p) and group velocity (v_g) are different. Which of the following is correct in that case

a) $v_g > v_p$
b) $v_g < v_p$
c) $v_g = v_p$
d) none of the above

Ans: A

Dual nature (particle and wave) of matter was proposed by:

a) de Broglie
b) Planck
c) Einstein
d) Newton

Ans: A

According to classical mechanics, if a particle of mass m is moving by the action of force then the total energy E of the particle is given by $\frac{p^2}{2m} + \mathrm{V} = \mathrm{E}$. State TRUE or FALSE

a) TRUE
b) FALSE

Ans: A

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

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 normalisable
c) ψ must be finite, continuous and single valued
d) All of the above

Ans: D

Scheduled Lectures

Lecture 1 Sept 26: Need of quantum mechanics, photoelectric effect,
Importance of quantum mechanics and quantum nature of light

Lecture 2 Sept 27 : Concept of de Broglie matter waves, wavelength of matter waves in different forms,
Wave/Dual nature of matter and relation between wavelength and momentum/energy

Lecture 3 Sept 28: properties of matter wave, Concept of phase velocity and group velocity (qualitative),

Lecture 4 Oct. 3*:*Heisenberg uncertainty principle, Application of uncertainty principle
Uncertainty principle to calculate uncertainty in the measurements of physical quantities

Lecture 5 Oct. 4 *:* Wave function and its significance, Schrodinger time dependent and independent equations
Introduction to wave functions and concept of probability, basic principle in quantum physics, Probabilistic behavior of quantum physics

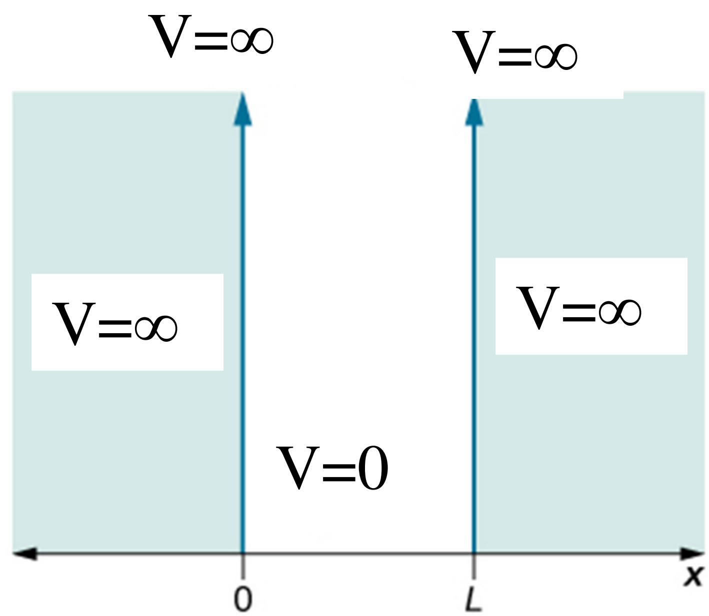
Lecture 6 Oct. 5 ***:*** Particle in a box (e.g., electron confined in a potential well)
Energy of the particles/electrons is discrete and is quantized.

Particle in a box

- Application of Schrödinger Equation
  - 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.*

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

$$\nabla^2\psi + \frac{2m\mathbf{E}}{\hbar^2}\psi = 0$$

For 1 D

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m\mathbf{E}}{\hbar^2}\psi = 0 \quad \text{Eq.1}$$

And put

$$k^2 = \frac{2m\mathbf{E}}{\hbar^2} \quad \text{Eq.2}$$

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

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

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

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

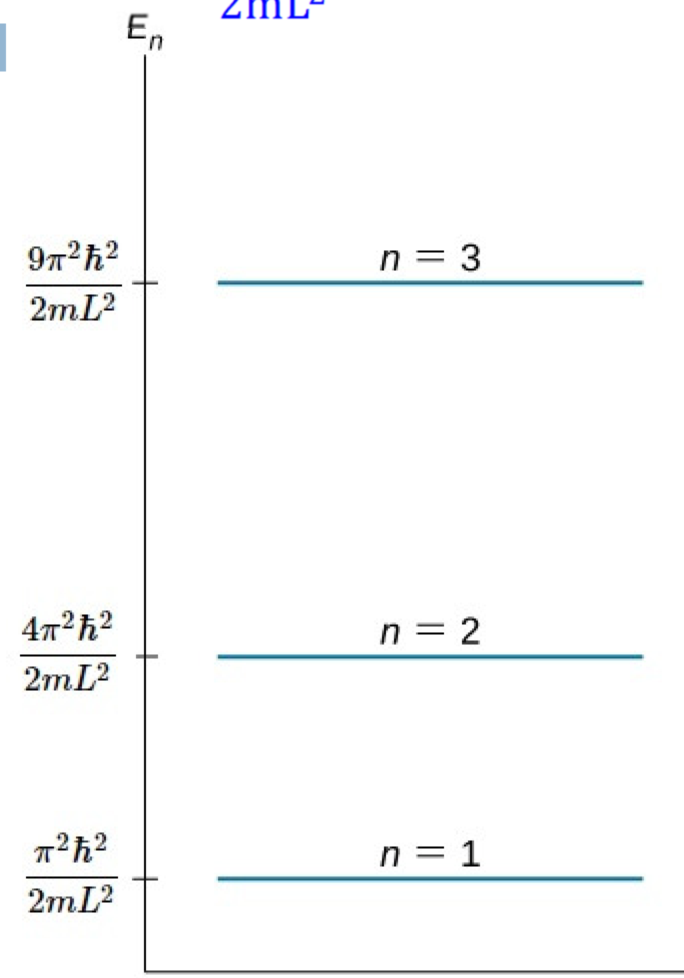
Now substitute Eq.2 in Eq.7

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

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

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

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

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

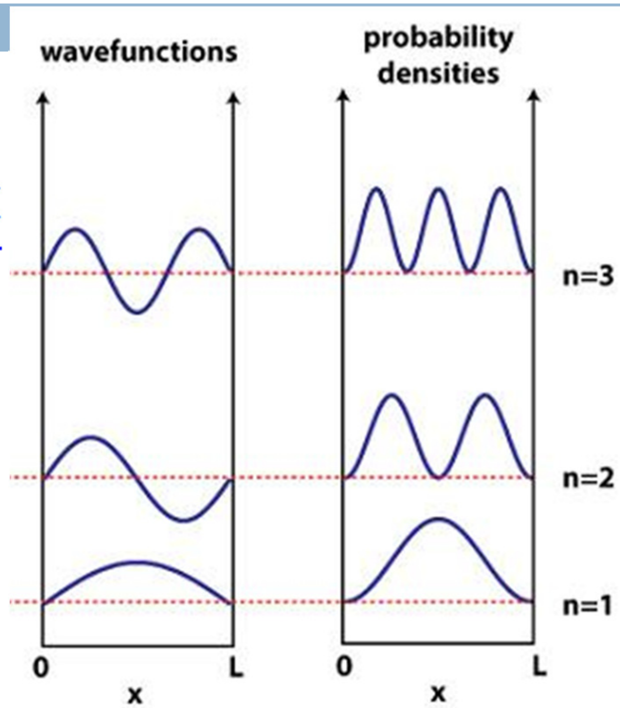
$$\frac{A^2}{2}L = 1 \qquad A = \sqrt{\frac{2}{L}}$$

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

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

Quick QUIZ

According to classical mechanics, if a particle of mass m is moving by the action of force then the total energy E of the particle is given by $\frac{p^2}{2m} + \mathrm{V} = \mathrm{E}$. State TRUE or FALSE

a) TRUE
b) FALSE

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

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

The characteristics of the wave functions in quantum mechanics are

a) ψ must be finite, continuous and single valued everywhere
b) ψ must be normalisable
c) ψ must be differentiable and finite, continuous and single valued
d) All of the above

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

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

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

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

UNIT IV: Quantum Mechanics

Syllabus

1. *Need of quantum mechanics, photoelectric effect,*
2. Concept of de Broglie matter waves, wavelength of matter waves in different forms,
3. *Heisenberg uncertainty principle,*
4. Concept of phase velocity and group velocity (qualitative)
5. *Wave function and its significance, Schrodinger time dependent and independent equation,*
6. Particle in a box

Did we uncover or just covered the syllabus?☺