UNIT 4 QUANTUM (wave) MECHANICS

LECTURE 5

https://www.youtube.com/watch?v=TQKELOE9eY4

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

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

Ans: A

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

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

ϕ_m-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

Which of the following is/are true for a photon

a) $m_0=0$

b) $E=h\nu$

c) $m = \frac{h\nu}{c^2}$

d) all of the above

Ans: D

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

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

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

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

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

Which of the following relation can be used to determine deBroglie wavelength associated with a particle of mass m and having energy E_k

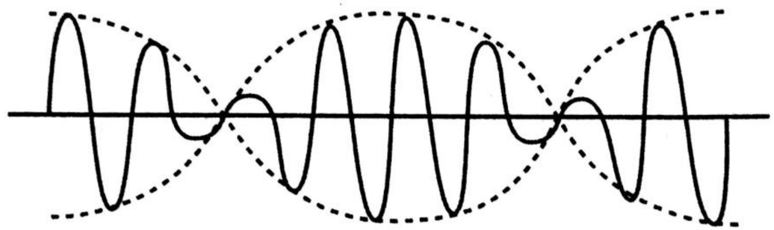
a) $\frac{h}{\sqrt{2mE_k}}$

b) $\frac{h}{\sqrt{2mqV}}$

c) $\frac{h}{\sqrt{3mkT}}$

d) All of the above

Ans: D



7. Characteristics of matter wave

8. Wave velocity, group velocity and particle velocity

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

v particle velocity

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

The original Heisenberg uncertainty principle is concerned with what two properties?

a) Mass and velocity
b) Momentum and velocity
c) Taste and smell
d) Momentum and position

Ans: D

Which of the following phenomena can not be explained by the classical theory?

a) Photoelectric effect
b) Compton effect
c) Raman effect
d) All of the above

Ans: D

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

For a non -dispersive medium derivative of the phase or wave velocity (V_p) with wavelength (λ) i.e $\frac{dV_p}{d\lambda}$ is

(a) Negative
(b) Positive
(c) Zero
(d) None of the above

Ans: C

For a normal dispersive medium derivative of the phase or wave velocity (V_p) with wavelength (λ) i.e $\frac{dV_p}{d\lambda}$ is

(a) Negative
(b) Positive
(c) Zero
(d) None of the above

Ans: B

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

For an anomalous dispersive medium derivative of the phase or wave velocity (V_p) with wavelength (λ) i.e $\frac{dV_p}{d\lambda}$ is

(a) Negative
(b) Positive
(c) Zero
(d) None of the above

Ans: A

If I know the position of a subatomic particle precisely, then

a) I know nothing about the particle's momentum.
b) I know a little about the particle's momentum
c) The particle must be at rest.
d) The particle can't be at rest.

Ans: B

Wave function- Quantum

Wave function associated with the matter wave is represented by ψ

- This ψ is not an observable quantity, unlike E and B, P we have seen in classical wave equation
- The value of ψ is related to the probability of finding the particle at a given place at a given time.
- This wave function ψ is a complex quantity
- ψ exists, its complex conjugate (ψ *) also exists

$$\iiint_{-\infty}^{\infty} \psi^{*}\psi \ \mathrm{dV} = 1; \text{where } dV = dxdydz$$

This is the probability of finding the particle over all space is unity. This the normalization condition. Wave function obeys this called normalisable or normalized.

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

Physical significance of wave function

By analogy with waves such as those of sound, a wave function, **Ψ**, may be thought of as an expression for the amplitude of the particle wave (de Broglie wave), although for such waves amplitude has no physical significance.

However, the square of the wave function, **Ψ**, does have physical significance: the probability of finding the particle described by a specific **wave function Ψ** at a given point and time is proportional to the value of $\boldsymbol{\Psi^2}$

Ψ as such has no physical significance, but it is operated with an operator that 'operation' gives us a significant physical quantity..

Matter Wave Equation- Quantum

Schrödinger derived a wave equation for **matter** that would give **wave**-like propagation when the wavelength becomes comparatively small.

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 the sum of **KE** and **PE**,

$$KE + PE = \frac{1}{2} m\mathrm{v}^2 + \mathrm{V} = \mathrm{E}$$

$$= \frac{1}{2m} m^2\mathrm{v}^2 + \mathrm{V} = \mathrm{E}$$

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

Schrödinger just changed this classical equation, and we got the so called quantum wave equation ☺.. We will see that

Schrodinger's magic with de Broglie's matter wave

In quantum physics, the wavefunction is the king!. It provides a mathematical description of the quantum state of a particle or system. What can the square of the magnitude of a particle's wavefunction tell us?

a) The probability that the particle will decay at a given time
b) Whether a Higgs boson is present
c) The mass of the particle
d) The probability that the particle is in a certain place at a given time

Ans: D

Wave function- Quantum

Schrodinger time-independent wave equation

Let us assume a wave associated with a moving particle with velocity ‘v,

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = \frac{1}{v^2}\frac{\partial^2 \psi}{\partial t^2}$$ Eq.1

v is the velocity of that wave

$$\psi(x,y,z,t) = \psi_0(x,y,z)e^{-i\omega t}$$ Eq.2

ψ-is the solution of the equation 1

$$r = x\hat{\imath} + y\hat{\jmath} + z\hat{k}$$ Eq.3

$$\psi(r,t) = \psi_0(r)e^{-i\omega t}$$ Eq.4

Differentiate Eq.4 twice with time

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

$$\frac{\partial^2 \psi}{\partial t^2} = -\omega^2 \psi$$ Eq.5

Substitute Eq.5 in Eq.1, we get

$$\frac{d^2 \psi}{dx^2} + \frac{d^2 \psi}{dy^2} + \frac{d^2 \psi}{dz^2} = -\frac{\omega^2}{v^2}\psi$$ Eq.6

But we know that, the angular frequency of the wave is related to the wave frequency

$$\omega = 2\pi\nu = \frac{2\pi \mathrm{v}}{\lambda} \quad \Longrightarrow \quad \frac{\omega}{\mathrm{v}} = \frac{2\pi}{\lambda} \qquad \text{Eq.7}$$

Also we know

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = \nabla^2\psi \qquad \text{Eq.8}$$

Substitute Eq.7 and Eq.8 in Eq.6

$$\nabla^2\psi + \frac{4\pi^2}{\lambda^2}\,\psi = 0 \qquad \text{Eq.9}$$

Half of the job done, now we go back to the de Broglie wave, the expression for wavelength (λ) in terms of momentum of the particle (p) having mass m and velocity v

deBroglie wavelength is given by $\lambda = \frac{h}{p}$

$$\lambda = \frac{\mathrm{h}}{\mathrm{mv}} \qquad \text{Eq.10}$$

And substitute for λ in Eq.9

$$\nabla^2\psi + \frac{4\pi^2 m^2 v^2}{h^2}\,\psi = 0 \qquad \text{Eq.11}$$

Total energy (E) of the particle is the sum of potential energy (V) and kinetic energy ($\frac{1}{2}mv^2$), so we can write

$$\frac{1}{2}mv^2 = E - V \quad \Rightarrow \quad m^2v^2 = 2m(E - V) \qquad \text{Eq.12}$$

By using Eq.12 in Eq.11, we get

$$\nabla^2\psi + \frac{8\pi^2 m}{h^2}(E - V)\,\psi = 0$$

But we know $\hbar = \dfrac{h}{2\pi}$

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E - V)\,\psi = 0 \qquad \text{Eq.13}$$

This is the time-independent Schrödinger equation, where the ψ is know as the wave function

For a freely moving or free particle V=0, so Eq.13 takes the form

$$\nabla^2\psi + \frac{2mE}{\hbar^2}\psi = 0$$ Eq.14

This is the time-independent Schrödinger equation for a free particle.

When a Laplacian and E operate on wave function, we get the wave equation

- The potential energy ‘V ‘ of a particle is considered to not depend on time explicitly, the forces that act on it, and hence V, vary with the position only in the case of time independent Schrödinger equation…. Equation 13
- The potential energy ‘V’is zero a free particle…. Eqn.14

✓ we derived the single-particle time-independent Schrödinger equation starting from the classical wave equation and the de Broglie relation

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

Wave function- Quantum

Schrodinger time-dependent wave equation

If we eliminate E from the time-independent Schrödinger equation we get time-dependent Schrödinger equation?.. For that that we go back to the wave function **ψ(r,t)** and differentiate it twice with respect to time

$$\psi(r,t) = \psi_0(r)e^{-i\omega t} \quad \text{Eq.4}$$

and differentiate it with respect to time

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

$$E = h\nu$$

$$\frac{\partial\psi}{\partial t} = \frac{E\psi}{i\hbar} \quad \text{Eq.15}$$

$$E\psi = i\hbar\frac{\partial\psi}{\partial t} \quad \text{Eq.16}$$

Substitute this equation in the time independent Schrödinger equation we derived before Eq.13

$$E = h\nu$$

$$\nabla^2\psi + \frac{2m}{\hbar^2}\left[i\hbar\frac{\partial\psi}{\partial t} - V\psi\right] = 0 \Rightarrow \nabla^2\psi = -\frac{2m}{\hbar^2}\left[i\hbar\frac{\partial\psi}{\partial t} - V\psi\right]$$

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

This is the time-dependent Schrödinger equation

And in terms of the operators

$$H\psi = E\psi$$

Where Hamiltonian(**H**) and energy (**E**) operators are defined as

$$H = \left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]$$

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

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

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

p momentum operator

Eigen values are the value of Energy for which Schrodinger's equation can be solved. The corresponding wave function is called Eigen Function.

https://www.youtube.com/watch?v=hce_Vq8gvfM

Operator, Eigen value and Eigen function

In quantum mechanics each measurable parameter/observable quantity is associated with an 'Operator'

In Quantum mechanics we deal with waves and wave function for very small particles rather than discrete particles

Operator is capable to do 'something' to the wave function

But if operates on the wave function it gives us the measurable quantity times the wave function. Important condition to be satisfied

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

Where H is **the operator**.. In this case, Hamiltonian operator, **E** is the **Eigen value**, Energy in this case .. The wave function,$\boldsymbol{\psi}$ that satisfy the equation is the **Eigen function**

when there is only one Eigen function corresponding to each Eigen value, the Eigen function is known as degenerate.

$$\mathrm{H}\psi_n = E_n\psi_n$$

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

UNIT 4-Quantum Mechanics

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

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