UNIT 4 QUANTUM MECHANICS

LECTURE 5

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?

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

Black body radiation ,
Wien and Rayliegh-Jean formula,

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

UV catastrophe
Planck's quantum oscillator,

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

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

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

6. Matter –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 $E=mc^2$

What we learned so far about Quantum mechanics?

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

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

dispersion

What we learned so far about Quantum mechanics?

10. Heisenberg uncertainty principle
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

What we learned so far about Quantum mechanics?

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

Quick QUIZ

Quick Quiz Response on the 10/03/2018 Lecture

No		Attempts	Right	Wrong
1	If I know the position of a subatomic particle precisely, then	49	12	37
2	Electrons show diffraction effects with crystals because their de Broglie wavelength is	49	14	35
3	Most energetic photons are	49	25	24

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

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

Ans: B

Electrons show diffraction effects with crystals because their de Broglie wavelength is

a) Similar to the spacing between atomic planes
b) Equal to the no. of atomic layers
c) Is very high compared to the spacing of atomic planes
d) None of the above

Ans: A

Most energetic photons are

a) alpha
b) beta
c) gamma
d) x-rays

Ans: C

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)
Energy of the particles/electrons is discrete and is quantized.

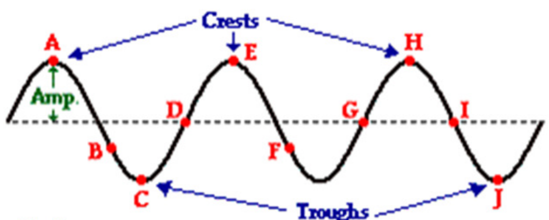
Wave function- classical

There is a mathematical relationship between the speed or velocity (v) of a wave to the second order partial derivative of physical quantity (u) with respect to position and time.

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

u= E or B for light waves

u= p, pressure for sound waves



In the equation u= **F**(x,y,z,t) is the wave function and that changes periodically..

$$v = f\,\lambda$$

Sound waves, electromagnetic waves or water waves satisfy this equation ..

$f = \nu = 1/T$

$$\nabla^2 \vec{B} = \mu_0 \varepsilon_0 \frac{\partial^2 B}{\partial t^2}$$

$v = 3 \times 10^8$ m/s

$$\nabla^2 \vec{E} = \mu_0 \varepsilon_0 \frac{\partial^2 \vec{E}}{\partial t^2}$$

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

$v = 330$ m/s

Wave function- classical

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

is the wave function… that is the solution of the wave equation

Give value of the physical quantity, E, B or P at a position (x,y,z) at a given time t.

The uncertainty is only for the microscopic particles -atomic or subatomic particles. So classical wave equation is not valid for very small particles, like electron, proton, neutron etc..

So we have to modify the wave equation for matter wave.

Before that we have to define our wave function and its properties

And we will have quantum wave equation as a result…

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

Wave function- Quantum

Schrödinger derived a wave equation for **matter/wave** that would give **wave/particle**-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 deBroglie's matter wave

Wave function- Quantum

Schrodinger time-independent wave equation

Let us assume a wave associated with a moving particle

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = \frac{1}{\mathrm{v}^2}\frac{\partial^2 \psi}{\partial t^2}$$ 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 $$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = -\frac{\omega^2}{u^2}\psi$$ Eq.6

Wave function- Quantum

Schrodinger time-independent wave equation

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

$$\omega = 2\pi\nu = \frac{2\pi v}{\lambda} \quad \Rightarrow \quad \frac{\omega}{v} = \frac{2\pi}{\lambda}$$ Eq.7

Also we know $$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = \nabla^2\psi$$ Eq.8

Substitute Eq.7 and Eq.8 in Eq.6 $$\nabla^2\psi + \frac{4\pi^2}{\lambda^2}\psi = 0$$ Eq.9

Half of the job done, now we go back to the de Broglie wave

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

And substitute for λ in Eq.9

Wave function- Quantum

Schrodinger time-independent wave equation

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

Total energy (E) of the particle is the sum of potential energy (V) and kinetic energy (½ 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 $\hbar = \dfrac{h}{2\pi}$

Wave function- Quantum

Schrodinger time-independent wave equation

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

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

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

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

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

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

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

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

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

Wave function- Quantum

Schrodinger time-dependent wave equation

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

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

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 (deBroglie 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 **Ψ^2**

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

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, ψ that satisfy the equation is the **Eigen function**

Quick QUIZ

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

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

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

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

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