Quantum Physics

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April 4, 2021

Unit 01 : Quantum Physics

Prerequisites :

(Photoelectric effect, Dual nature of radiation, Matter waves-wave nature of particles, de-Broglie relation, Davisson-Germer experiment).

Contents :

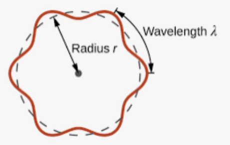
- de Broglie hypothesis of matter waves
- Properties of matter waves, wave packet
- Phase velocity and Group velocity
- Wave function and it's Physical interpretation
- Heisenberg uncertainty principle
- Schrodinger's time dependent and time independent wave equation
- Particle trapped in one dimensional infinite potential well

de Broglie Hypothesis

- *All moving objects are associated with waves.*
- These waves are known as *matter waves*.
- de Broglie wavelength $\lambda = \frac{h}{p}$
  Here h →Planck's constant, $6.63x10^{-34}$J.s.
  and $p = mv$ → momentum of the particle.
- de Broglie wavelength thus relates the particle nature with the wave nature of matter.
- de Broglie wavelength for
  1. An accelerated charge particle $\lambda = \frac{h}{\sqrt{2mq\mathcal{V}}}$
     q → charge, $\mathcal{V}$ → potential difference.
  2. A particle in thermal equilibrium $\lambda = \frac{h}{\sqrt{3mK_BT}}$
     K_B →Boltzman constant; T →temperature in absolute scale.
  3. A particle with kinetic energy $K.E$ $\lambda = \frac{h}{\sqrt{2m(K.E)}}$

The Bohr Atom

Bohr's postulate of angular momentum quantization in hydrogen atom model was a natural consequence of de Broglie hypothesis.

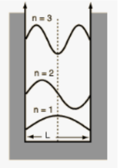


- A moving electron in its circular orbit behaves like a particle wave.
- An electron can circle a nucleus only if its orbit contains an integral number of de Broglie wavelengths.

- *Condition for orbit stability* $n\lambda = 2\pi r_n \quad n = 1, 2, 3, ...$
  $r_n \rightarrow$ the radius of the orbit containing n wavelengths,
  $n \rightarrow$ the quantum number of the orbit.
- Now $\lambda = \frac{h}{p}$
  Therefore angular momentum $L_n = r_n p = \frac{nh}{2\pi}$

Particle in a box

- Consider a particle that bounces back and forth between two infinitely hard walls separated by a distance L.
- The particle does not loose energy each time it strikes a wall.
- The situation is like a standing wave in a string stretched between the walls.



- de Broglie wavelength of trapped particle
  $\lambda_n = \frac{2L}{n} \quad n = 1, 2, 3, \ldots$
- The kinetic energy $(K.E)$ of the particle is thus restricted.
  $K.E = \frac{(mv)^2}{2m} = \frac{h^2}{2m\lambda^2}$
- The potential energy is taken to be zero within the walls.

Thus the total energy of the trapped particle is quantized.

$$E_n = \frac{n^2h^2}{8mL^2}$$

Three general conclusions

1. *A trapped particle cannot have an arbitrary energy as a free particle can.*
   The confinement leads to restrictions on the wave function which in turn allow only certain specific values of the energy.
2. *A trapped particle cannot have zero energy.*
   The situation correspond to infinite wavelength in a finite length, so not possible.
3. *This quantization of energy is conspicuous only when m and L are also small.*
   This happens because of the presence of h the Planck's constant.

Waves of probability

- Wave means some dimentioned physical quantity that varies periodically in space and time.
- The quantity whose variation makes the matter wave is the *wave function* Ψ.
- Ψ mathematically describes the wave characteristics of a particle.
- The wave function Ψ itself has no physical significance, not an observable quantity.
- The value of the wave function associated with a moving particle at a particular point(x, y, z) in space at time t is related to the likelihood of finding the particle there at that time.
- The wave function Ψ is thus a complex-valued probability amplitude.
- The probabilities of the results of measurements made on the particle can be derived from Ψ.

Probability Density

- To comprehend the dual nature of light, Einstein interpreted the square of the optical wave amplitude to be the probability density for the occurrence of photons.
- Max Born extended this idea to the Ψ function.
- $|\Psi|^2$ must represent the probability density for particles.
- *The probability of experimentally finding the particle described by the wave function Ψ at the point(x, y, z) at the time t is proportional to the value of $|\Psi|^2$ there at time t.*
- Born's development of quantum theory of atomic scattering processes verified this concept.
- A large value of $|\Psi|^2$ means the strong possibility of the particle's presence.
- As long as $|\Psi|^2$ is not actually zero somewhere there is a definite chance, however small, of detecting it there.

Describing a wave

- A wave is described mathematically by the wave formula
$$y = A\cos(\omega t - kx)$$
Here $\omega = 2\pi\nu$ is the angular frequency and
$k = \frac{2\pi}{\lambda}$ is the wave number.
- This formula describes an indefinite series of waves all with same amplitude A.
- The amplitude of the de Broglie wave reflects the probability that the particle will be found at a particular point in space at a particular time.
- Therefore the wave representation of a moving particle should correspond to a wave packet or wave group.
- The interference of individual waves of different wavelengths in the group will result in the variation of the amplitude that defines the group shape.

Interference of two waves

- Consider two waves having same amplitude but slightly differing in the angular frequency and wave number, to interfere.

$$y_1 = A\cos(\omega t - kx)$$
$$y_2 = A\cos[(\omega + \Delta\omega)t - (k + \Delta k)x]$$

- Since $\Delta\omega$ and Δk are small compared with ω and k respectively, we have

$$2\omega + \Delta\omega \approx 2\omega$$
$$2k + \Delta k \approx 2k$$

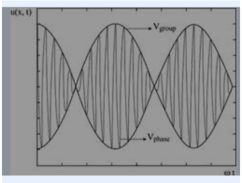
- The resultant displacement is therefore

$$y = 2Acos(\omega t - kx)cos(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x)$$

- The resultant wave represents a wave of angular frequency ω and wave number k that has superimposed upon it a modulation of angular frequency $\frac{\Delta\omega}{2}$ and wave number $\frac{\Delta k}{2}$.

Phase velocity and Group velocity

- The *phase velocity* v_p of a wave is the rate at which the plane of constant phase of the wave propagates in space.
- The *group velocity* v_g of a wave is the rate at which the overall shape(envelope) of the waves amplitude propagates in space.



- A wave of frequency ω, wave number k moves with phase velocity v_p
  $v_p = \frac{\omega}{k} = \frac{2\pi\nu}{2\pi/\lambda} = \nu\lambda$
- Another wave of frequency $\frac{\Delta\omega}{2}$, wave number $\frac{\Delta k}{2}$ moves with group velocity v_g
  $v_g = \frac{\Delta\omega}{\Delta k} \approx \frac{d\omega}{dk} = \frac{d(2\pi\nu)}{d(2\pi/\lambda)} = -\frac{\lambda^2}{2\pi}\frac{d\omega}{d\lambda}$

Relation between v_p and v_g: $$v_g = \frac{d\omega}{dk} = \frac{d}{dk}(v_p k) = v_p - \lambda\frac{dv_p}{d\lambda}$$

- The group velocity v_g is less than the phase velocity v_p in a dispersive medium(where v_p is a function of λ).
- The group velocity v_g is equal to the phase velocity v_p in a non-dispersive medium(where v_p is independent of λ).

Phase velocity and Group velocity for matter wave

- Consider a particle of rest mass m_0 moving with velocity v.
- The de Broglie wavelength is $\lambda = \frac{h}{mv}$; $k = \frac{2\pi}{\lambda}$ and
  the frequency is $\nu = \frac{mc^2}{h}$; $\omega = 2\pi\nu$
- Here mass $m = \frac{m_0}{\sqrt{1-v^2/c^2}}$ and $E = mc^2$
- de Broglie group velocity: $v_g = \frac{d\omega}{dk} = \frac{d\omega/dv}{dk/dv} = v$
- The group velocity v_g of de Broglie waves associated with a moving particle is same as the velocity of the particle.
- de Broglie phase velocity: $v_p = \nu\lambda = \frac{c^2}{v}$
- The phase velocity v_p of de Broglie waves exceeds the velocity of light c.
- v_p has no physical significance.
- It is the motion of the wave group(v_g) that corresponds to the motion of the particle or the body.

Uncertainty Principle

- **Heisenberg's uncertainty principle** states that *It is impossible to measure simultaneously and precisely the position and momentum of an object.*
- Same conclusion of uncertainty principle can be arrived at from particle properties of waves or from the wave properties of the particle.
- The relation between the uncertainties in the linear position $(\triangle x)$ and linear momentum $(\triangle p)$ is given by:
$$\triangle x \triangle p \geq \frac{h}{4\pi}$$
- The variable pairs(angular position - angular momentum) and (energy - time) also follow the same principle.
$$\triangle \theta \triangle L_\theta \geq \frac{h}{4\pi}$$
$$\triangle E \triangle t \geq \frac{h}{4\pi}$$

Applications of Uncertainty Principle

- The limitation in the measurement process becomes significant only on the atomic scale because of the presence of h, Planck's constant.
- Some important applications of this principle :

1. Energy of a particle in a box:

- Consider a particle of mass m in a one-dimensional box of length L.
- The uncertainty in its position is $\triangle x = L$.
- From the uncertainty principle, we get $\triangle p = \frac{h}{4\pi\triangle x} = \frac{h}{4\pi L}$.
- Kinetic energy is therefore:

$$K.E. = \frac{p^2}{2m} = \frac{\hbar^2}{8mL^2}$$

- This is the minimum kinetic energy of the particle in the box.

Applications contd.

2. Non-existence of Electrons in the nucleus:

- The radius of an atomic nucleus is $\sim 10^{-14}$m.
- The uncertainty in the position of the electron to be confined within the nucleus is $\triangle x = 2 \times 10^{-14}$m.
- The uncertainty in the momentum of the electron will be then $\triangle p = \frac{h}{4\pi\triangle x} = 2.6375 \times 10^{-21}$ kg-m/sec.
- This is the minimum value of the momentum the electron can posses inside the nucleus.
- The kinetic energy of the electron thus becomes $K.E = \frac{p^2}{2m} = \frac{(2.6375 \times 10^{-21})^2}{2 \times 9.1 \times 10^{-31}}$J $=23.89 \times 10^6 ev \approx 24 Mev$
- Electron can not posses this large amount of energy, hence nuclei do not contain electrons.

Wave Function

- The quantity with which the quantum mechanics deals is the wave function Ψ of an object.
- While Ψ has no physical meaning, $|\Psi|^2$ evaluated at a particular place and time gives the probability of the presence of that object then and there.
- The quantities like the linear momentum, angular momentum, energy of the object can be derived from Ψ.
- Quantum mechanics gives the most probable values of these quantities.
- The problem of quantum mechanics is therefore to determine Ψ when external forces control the motion of the object.
- The mathematical form of wave functions is in general complex with both real and imaginary parts.
- The probability density $|\Psi|^2$ is therefore the product of Ψ and its complex conjugate Ψ^*.

Acceptability of the Wave Function

- The wave function Ψ which is to mathematically represent a real moving object, must satisfy certain criteria.
- This is known as well-behaved behavior of Ψ.

1. Ψ must be finite, single-valued, continuous everywhere.
2. $\frac{\partial \Psi}{\partial x}, \frac{\partial \Psi}{\partial y}, \frac{\partial \Psi}{\partial z}$ must be finite, single-valued, continuous everywhere.
3. Ψ must be normalizable meaning Ψ must go to 0 as $x \to \pm\infty, y \to \pm\infty, z \to \pm\infty$ in order that $\int |\Psi|^2 dV$ over all space be a finite constant.
   Thus the normalization condition gives us:
   $$\int_{-\infty}^{+\infty} |\Psi|^2 dV = 1$$
   A wave function that obeys all the three above mentioned criteria is an acceptable mathematical solution.

The Wave Equation

- The standard wave equation is : $\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2}$
  Here y is the wave variable that propagates in the x direction with speed v.
- The solution must be of the form : $y = F(t \pm \frac{x}{v})$
- Consider the wave equivalent of a free particle moving in a straight path with constant speed along $+x$ direction.
- The general solution in this case for undamped monochromatic harmonic waves is : $y = Ae^{-i\omega(t-x/v)}$
- This solution y is a complex quantity with real and imaginary parts.
- The real part of the solution becomes relevant when we consider the real physical wave.

Schrödinger's Equation

- It is the fundamental differential equation of quantum mechanics to determine Ψ.
- Here the wave function Ψ correspond to the wave variable y of the wave equation.
- Since Ψ is not a measurable quantity itself, hence it can be a complex quantity.
- Consider a free particle moving in the +ve x direction.
- The wave equivalent Ψ of this particle is therefore
$$\Psi = Ae^{-i\omega(t-x/v)}$$
- Total energy $E = h\nu = 2\pi\hbar\nu = \hbar\omega$ and
Wavelength $\lambda = \frac{h}{p} = \frac{2\pi\hbar}{p}$
- Therefore $\omega t = \frac{Et}{\hbar}$ and $\omega x/v = 2\pi x/\lambda = \frac{xp}{\hbar}$
- Hence for free particle $\Psi = Ae^{(-i/\hbar)(Et-xp)}$

Derivation Contd.

- Differentiate the expression of Ψ with respect to x twice :
  $\frac{\partial^2 \Psi}{\partial x^2} = -\frac{p^2}{\hbar^2}\Psi \implies p^2\Psi = -\hbar^2 \frac{\partial^2 \Psi}{\partial x^2}$
- Differentiate same Ψ with respect to t once :
  $\frac{\partial \Psi}{\partial t} = -\frac{iE}{\hbar}\Psi \implies E\Psi = -\frac{\hbar}{i}\frac{\partial \Psi}{\partial t}$
- Total energy $E = \frac{p^2}{2m} + U(x,t)$ where the function $U(x,t)$is the potential energy.
- Multiplying both sides of the energy expression by the wave function Ψ and substituting $E\Psi$ and $p^2\Psi$ we obtain :
  Time-Dependent One-Dimensional Schrödinger Equation

$$\boxed{i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + U(x,t)\Psi}$$

Steady State Form

- Consider an environment which does not change with time i.e. potential energy $U(x,t) \rightarrow U(x)$.
- Let $\Psi(x,t) = \psi(x)e^{-i\omega t}$, $\psi(x)$is the space part.
- Then $\frac{\partial^2 \Psi}{\partial x^2} = \frac{\partial^2 \psi}{\partial x^2} e^{-i\omega t}$ and $\frac{\partial \Psi}{\partial t} = -i\omega\psi(x)e^{-i\omega t}$
- Substituting these in the time-dependent equation we get Steady State Schrödinger equation in one dimension

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + U(x) = E\psi}$$

- This differential equation can have more than one solutions.
- Each solution or wave function will correspond to a specific value of energy.
- These are known as *Eigenfunctions* and *Eigenvalues*.

Application: Particle in a well

- Consider again a particle confined to one-dimensional potential well with infinitely high barriers at the ends.
- The potential energy inside the well is taken to be zero while outside the well it is infinity.
- Here the aim is to find the wave-function ψ_n that correspond to each energy level.
- The limit of existence of the particle and correspondingly ψ is between $x = 0$ to $x = L$.
- Inside the well, Schrödinger equation becomes $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E\psi = 0$
- Let $k^2 = \frac{2m}{\hbar^2} E$ Therefore $\frac{d^2\psi}{dx^2} + k^2\psi = 0$
- The solution of this differential equation is $\psi = A \sin kx + B \cos kx$ A, B are constants

Particle in a well contd.

- Apply the boundary condition that $\psi = 0$ at $x = 0$.
- It demands B to be equal to zero thereby making the wave function $\psi = A \sin kx$.
- Next the condition $\psi = 0$ at $x = L$ demands $kL = n\pi$ or $k^2L^2 = n^2\pi^2$.
- Thus the energy becomes $E = \frac{n^2h^2}{8mL^2}$.
- The unknown constant A in the wave function is to be determined from normalization condition
  $\int_0^L |\psi|^2 dx = 1 \quad \Longrightarrow \quad A^2 \int_0^L \sin^2(kx) dx = 1$
- Solving we get $A = \sqrt{\frac{2}{L}}$
- Thus the wave function representing a particle bouncing back and forth between two hard walls is given by

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

Numerical problems - 1

1. Find the de Broglie wavelength of the 40KeV electrons used in a certain electron microscope.
2. Find the kinetic energy of an electron whose de Broglie wavelength is same as that of a 100KeV X-ray photon.
3. Green light has a wavelength of 550nm. Through what potential difference must an electron be accelerated to have this wavelength?
4. A proton and a deuteron have the same kinetic energy. Which has a longer wavelength?
5. Find de Broglie wavelength of an electron in the first Bohr's orbit of hydrogen atom.
6. Identify the particle which, when accelerated through a potential difference of 200V, has a de Broglie wavelength 0.716pm. Given mass of the particle 6.68×10^{-27}kg.

Numerical problems - 2

7. An electron has a speed of $1.0m/s$ with an accuracy of 0.05%. Calculate the uncertainty with which the position of the electron can be located.
8. Life time of a nucleus in the excited state is 10^{-12}s. Calculate the probable uncertainty in the energy and frequency of a γ-ray photon emitted by it.
9. The position and momentum of $0.5KeV$ electron are simultaneously determined. If its position is located within $0.2nm$, what is the percentage uncertainty in its momentum?
10. Compare the uncertainties in the velocities of an electron and a proton confined in a $1.0nm$ box.
11. A measurement establishes the position of a proton with an accuracy of $1.0 \times 10^{-11}m$. Find the uncertainty in the proton's position 1.0s later.

Numerical problems - 3

12. The energy of an electron constrained to move in a one dimensional box of length $4A^{\circ}$is $9.664 \times 10^{-17} J$. Find the order of excited state and the momentum of the electron in that state.
13. Obtain the minimum value of energy (in MeV) of a neutron confined to a one-dimensional box $1.0 \times 10^{-14} m$ wide.
14. A proton in a one-dimensional box has an energy of $400 KeV$ in its first excited state. How wide is the box?
15. The wave function of a certain particle is $\psi = A cos^2 x$ for $-\frac{\pi}{2} < x < \frac{\pi}{2}$. Find the value of A.
16. A particle limited to the x-axis has the wave function $\Psi = ax$ between $x = 0$ and $x = 1$; $\Psi = 0$ elsewhere. Find the probability that the particle can be found between $x = 0.45$ and $x = 0.55$.