Unit-1

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Wave Mechanics

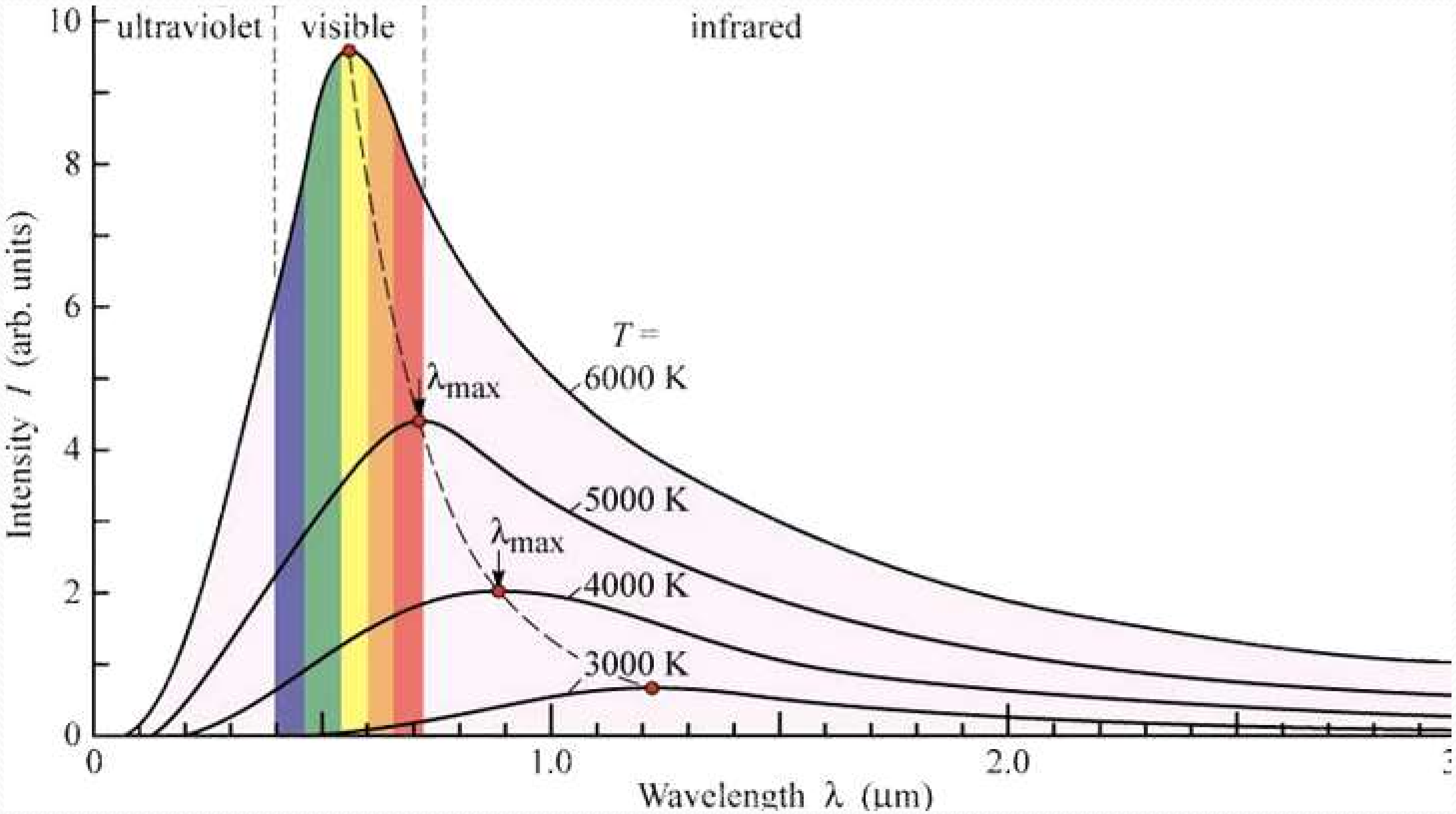
Matter Waves, De-Broglie's concept of mattar waves, Properties of Mattar Waves, Schrodinger's time dependent and Time Independent wave equations, Operators, Eigen Values and Eigen Functions, Expectation values, Physical significance of wave function.

“Unexplained” Experimental phenomenon around the year 1900:

- Blackbody Radiation

  defn, continuous radiation,
  wavelength inverse to temp :
  peak wavelength shifting to shorter wavelengths as the temp increases
- Discreate nature of atomic and molecular spectra
- Crompton Scattering
- Photoelectric effect

Blackbody Radiation



Classical Mechanics

- particle is a point object having mass and definite position at any instant of time
- Instantaneous position of particle, its velocity, momentum energy are called dynamical variables
- Governed by Newtons laws of motion
- In Classical mechanics, if state of particle is known at any instant of time T_o , the state of particle can be determined at any other time .
- Macroscopic objects move and interact according to Newtons Laws
- Physical quantities such as particle energy vary continously and take any possible value. Eg freely falling object---energy changes continously from mgh to zero

Wave Particle Duality

Photoelectric effect established that light behaves as flux of photons

Phenomenon like interference diffraction and polarization can be explained when light is treated as wave PEE and Compton effect implies particle nature of light

EMW resembles both the particle nature as well as wave nature.

Light behaves as stream of particles in some phenomenon and wave in other phenomenon. so light acts as both particle and wave and exhibits wave particle duality.

Mattar Waves

De Broglie Hypothesis

“ Mattar like radiation has dual nature” ie mattar might exhibit both wave and particle nature under appropriate conditions.

“ The waves associated with moving particles are called Mattar waves”

Energy of photon of frequency ν is given by

$E=h\nu$----------(1)

If m is the mass of photon in motion and c is speed then its energy is given by

$E= mc^2$ ....(2)

From equation (1) and (2)

$h\nu=mc^2$ ....(3)

if photon is travelling with speed c in free space then its momentum

$p=mc$

$p=mc^2/c =h\nu/c$

$P=h/\lambda$

$\lambda=h/p$-------------(4)

According to De broglies hypothesis eq (4) can be applied to moving particles also.

If particle of mass m and velocity v,

$\lambda = h/p = h/mv$

Properties of mattar waves

- Lighter is particle, greater is wavelength associated with it
- Smaller is velocity, larger is wavelength
- When v=o, $\lambda=\infty$, ie wave becomes indeterminant
- If $v=\infty$ then $\lambda=o$ ie mattar waves are generated by moving particles
- Wave and particle aspect of moving bodies are not observes together in single experiment
- Wave nature of mattar introduces uncertainty in the location of the position of particle.

Properties of mattar waves

- Let u be the velocity of mattar waves associated with the moving particle

  $u = \nu\lambda$

- $u = \nu h/mv$
- $u = h\nu/mv = mc^2/mv$
- $u = c^2 / v$

Two different velocities are associated with the mattar wave:

1) Mechanical velocity of moving particle (v)
2) Velocity of mattar wave (u)

As $v < c$

Velocity of propagation of mattar wave is greater than velocity of light

Problems

Question 1

Calculate the wavelength associated with the particle of mass 2 gm moving with velocitty 3312.5 m/sec

Answer: 10^{-34}m

Question 2

Calculate the de Broglie wavelength of an electron moving with speed $1/10^{th}$ of the velocity of light.

Answer: 0.234A

De-Broglie wavelength associated with an accelerated charge particle

- If Charge particle are accelerated by a potential difference of V volts, then

$$eV = \frac{1}{2}mv^2$$

- $$v = \sqrt{\frac{2eV}{m}}$$

- $$\lambda = \frac{h}{mv} = \frac{h}{m}\sqrt{\frac{m}{2eV}} = \frac{h}{\sqrt{2emV}}$$

Problems

Question 1

Calculate de Broglie wavelength associated with an electron accelerated through 100V and 54 V.

Question 2

Find de Broglie wavelength of neutron whose energy is 1 eV. Mass of neutron=1.676×10^{-27} kg

WaveFunction (Ψ)

Postulates of Quantum mehanics

Physical system consisting of a particle, there is an associated wavefunction Ψ ,

Wavefunction Ψ, is a mathematical equation which describes any physical system.

- Contains all the measurable information about particle.
- is continous
- Establishes the probability distribution
- Wavefunction determines everything that can be known about the system
- It can be positive, negative or complex

Probability Interpretation of wave function

- Square of magnitude of wave function $|\Psi|^2$ evaluated in particular region represents the probability of finding the particle in that region.
- Probability P of finding particle in an infinitesimally small volume dV (=dx dy dz) is proportional to $|\Psi|^2$
- $|\Psi|^2$ is called probability density.
- Since particle is certainly somewhere, total probability is equal to 1

$$\int_{-\infty}^{\infty} \Psi\Psi^* dv = 1 \longrightarrow \text{Normalization equation}$$

Normalization Constant

If Ψ is not normalized ie if $\int \Psi\Psi^* dv$ is finite but not equal to unity then the wave function is not normalized.

- if Ψ is not normalized, multiply it with some constant A such that

$$\int (A\Psi)(A\Psi)^* dv = 1$$

$$AA^* \int (\Psi)(\Psi)^* dv = 1$$

$$|A|^2 \int (\Psi)(\Psi)^* dv = 1$$

$$|A|^2 = \frac{1}{\int \Psi\Psi^* dv}$$

Constraints on well behaved wavefunction

- Finite
- Continous function of x
- Single valued
- Normalizable
- First derivative must exist
- First derivative must also be finite, continuous and single valued.

Wave function, well behaved wave function(Finite)

- Ψ must be finite:-

If x$\rightarrow$ infinity, y$\rightarrow$ infinity, z$\rightarrow$ infinity.

Ψ, Must remain finite, if Ψ is infinite it would imply an infinite large probability of finding the particle at that point (violate uncertainty principle)

So Function

Ψ=**ax** (cannot be a valid wave function)

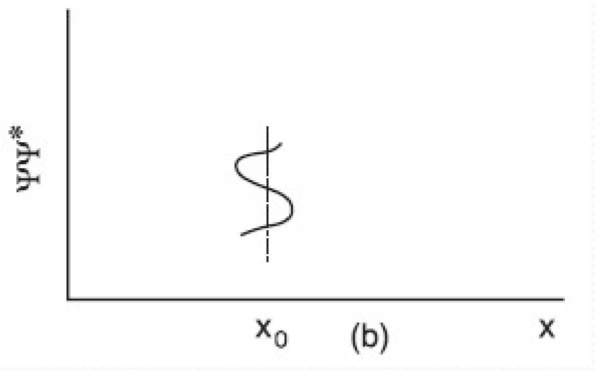
Because as x$\rightarrow$ infinity, $\Psi \rightarrow$ infinity

Valid wave function

Ψ=?????

Single Valued

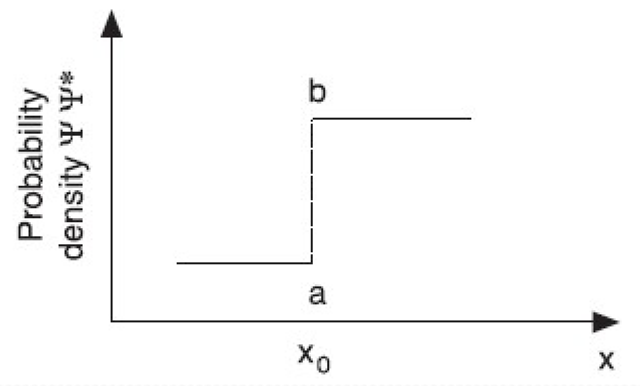
- Ψ must be single valued, if Ψ is not single valued then ????????
- There is more than one probability of finding the particle at that point



Wave function (Continous)

- Ψ must be continous

If function has discontinuity, this can be limiting case of a very rapid change in a function. In limit of step function, it would imply infinite derivative.



Well behaved wave function

First order derivatives must also be finite continous and single valued

Problem

Q-1 Normalize the wave function

$\Psi = Ae^{ix}$ $\quad -a/2 \leq x \leq a/2$

Q-2 Normalize the wave function

$\Psi = A(1-x/a)$ $\quad a/2 \leq x \leq a$

Q-3 Normalize wave function

$$\Psi = A\sin\frac{n\pi x}{L} \qquad 0 \leq x \leq L$$

Problems

Q-1 Find the relative population of two states of laser that produces a light beam of wavelength 6943A.

Q-2 Find the De broglie wavelength of neutron whose K.E. is 10eV.

Find the De broglie wavelength of neutron whose K.E. is 10eV.

Given: mass of neutron = 1.676×10^{-27}kg

k.E. of neutron = 10ev

k.E. of neutron = $10 \times 1.6 \times 10^{-19}$ J

$(½)\ mv^2 = 16 \times 10^{-19}$ J

$V^2 = (2 \times 1.6 \times 10^{-19}\ J) / m = 1.9093 \times 10^8$

$V = 13.8 \times 10^4$ m/s

$\lambda = h / mv$ = ???????

Problems

- An electron is confined to a box of length 1nm. Calculate the minimum uncertainty in its velocity.

Fiven: $m = 9 \times 10^{-31}$ kg and $h = 6.6 \times 10^{-34}$ J-s

Soln: $\Delta x \ \Delta p = h$

$\Delta p = h / \Delta x = 6.6 \times 10^{-25}$ kg m/s

$\Delta p = m \times \Delta v$

$\Delta v = \Delta p / m$

$\Delta v = 7.3 \times 10^{5}$ m/s

Schrodinger Wave Equation

Time Dependent Schrondinger Wave equation

The **Schrödinger equation** is a partial differential equation that describes the dynamics of quantum mechanical systems via the wave function. The trajectory, the positioning, and the energy of these systems can be retrieved by solving the Schrödinger equation.

Schrodinger equation plays the role of Newtons laws and conservation of energy in quantum mechanics ie it predicts the future behavior of a dynamic system. Its an equation in terms of wave function which predicts the probability of outcomes

Total Energy E of particle is sum of Kinetic energy and potential energy

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

Multiply Ψ on both sides

$$E\Psi = \frac{p^2}{2m}\Psi + V\Psi \quad \text{------------(1)}$$

Consider a wave function Ψ of particle moving along positive x axis

$$\Psi = Ae^{i(kx-\omega t)} \quad \text{----------(2)}$$

$$\lambda = \frac{h}{p} \qquad E = h\nu$$

$$p = \frac{h}{\lambda} = \frac{h}{2\pi}\frac{2\pi}{\lambda} = \hbar k \longrightarrow k = \frac{p}{\hbar}$$

$$E = h\nu = \frac{h}{2\pi}2\pi\nu = \hbar\omega \longrightarrow \omega = \frac{E}{\hbar}$$

Substituting k and ω in equation (2)

$$\Psi = Ae^{i\left(\frac{p}{\hbar}x - \frac{E}{\hbar}t\right)}$$

$$\Psi = Ae^{\frac{i}{\hbar}(px-Et)} \text{----------}(2)$$

Differentiate equation (2) wrt x

$$\frac{\partial \Psi}{\partial x} = \frac{ip}{\hbar} Ae^{\frac{i}{\hbar}(px-Et)}$$

$$\frac{\partial^2 \Psi}{\partial x^2} = -\frac{p^2}{\hbar^2} Ae^{\frac{i}{\hbar}(px-Et)}$$

$$\frac{\partial^2 \Psi}{\partial x^2} = -\frac{p^2}{h^2} \Psi$$

$$-\hbar^2 \frac{\partial^2 \Psi}{\partial x^2} = p^2 \Psi \quad \text{-----}(3)$$

Differentiate wrt to t

$$\frac{\partial \Psi}{\partial t} = -\frac{iE}{\hbar} \Psi$$

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

$$E\Psi = i\hbar \frac{\partial \Psi}{\partial t} \quad \text{------}(4)$$

Substitute expressions of $p^2\Psi$ and $E\Psi$ in equation (1)

$$-\frac{\hbar}{i}\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi$$ (Schrodinger one dimentional time dependent wave equation)

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi$$

<u>Three Dimentional Schrodinger wave equation</u>

$$\Psi = \Psi(x, y, z, t)$$

$$-\frac{\hbar}{i}\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2}\right) + V\Psi$$

Time Independent Schrodinger wave equation

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi \text{ ----------(1)}$$

$$\boldsymbol{\Psi} = \boldsymbol{\Psi}(x,t)$$

This equation can be solved by seperation of variable method

$$\boldsymbol{\Psi}(\boldsymbol{x},\boldsymbol{t}) = \Psi(x)\varphi(t)$$

Substitute Ψ(x,t) in equation (1)

$$i\hbar\frac{\partial \Psi\varphi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi\varphi}{\partial x^2} + V\Psi\varphi$$

$$i\hbar\Psi\frac{\partial \varphi}{\partial t} = -\frac{\hbar^2}{2m}\varphi\frac{\partial^2 \Psi}{\partial x^2} + V\Psi\varphi$$

Continued...........

$$i\hbar\Psi\frac{\partial\varphi}{\partial t} = -\frac{\hbar^2}{2m}\,\varphi\frac{\partial^2\Psi}{\partial x^2} + V\Psi\varphi$$

Dividing above equation by Ψφ throughout

$$i\hbar\frac{1}{\varphi}\frac{\partial\varphi}{\partial t} = -\frac{\hbar^2}{2m}\frac{1}{\Psi}\frac{\partial^2\Psi}{\partial x^2} + V$$

The right hand side of above equation is function of t and left hand side is function of x. this is possible only if both sides are equal to some constant E.

$$-\frac{\hbar^2}{2m}\frac{1}{\Psi}\frac{\partial^2\Psi}{\partial x^2} + V = E$$

$$i\hbar\frac{1}{\varphi}\frac{\partial\varphi}{\partial t} = E$$

Schrodingers Time independent wave equation

$$-\frac{\hbar^2}{2m}\frac{1}{\Psi}\frac{\partial^2\Psi}{\partial x^2}+V=E$$

$$\frac{\partial^2\Psi}{\partial x^2}+\frac{2m}{\hbar^2}(E-V)\Psi=0$$ (Schrodinger one dimensional time independent wave eqution)

$$\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}+\frac{\partial^2\Psi}{\partial z^2}+\frac{2m}{\hbar^2}(E-V)\Psi=0$$ (Schrodinger three dimensional time independent wave eqution)

Solution of Time dependent part

Time dependent part

$$i\hbar\frac{1}{\varphi}\frac{\partial\varphi}{\partial t} = E$$

$$\frac{1}{\varphi}\frac{\partial\varphi}{\partial t} = -\frac{i}{\hbar}E$$

$$\frac{1}{\varphi}\partial\varphi = -\frac{i}{\hbar}E\partial t$$

Integrate and solve this equation

Continued……

$$\ln(\varphi) = -\frac{i}{\hbar}Et$$

$$\varphi = e^{-\frac{iE}{\hbar}t}$$

$$\boldsymbol{\Psi}(\boldsymbol{x},\boldsymbol{t}) = \Psi(x)e^{-\frac{iE}{\hbar}t}$$

Definition of Operators

An operator ô is a mathematical operation which may be applied to function f(x) which changes the function f(x) to another function g(x).

$\hat{O}\, f(x)=g(x)$

For example

$$\frac{d}{dx}(4x^2 + 2x) = 8x + 2$$

Operators in Quantum Mechanics

momentum operator $\hat{p}$

Wave Function is given by

$$\Psi = Ae^{\frac{i}{\hbar}(px-Et)}$$

Differentiating wrt x

$$\frac{\partial \Psi}{\partial x} = \frac{ip}{\hbar} Ae^{\frac{i}{\hbar}(px-Et)}$$

$$\frac{\partial \Psi}{\partial x} = \frac{ip}{\hbar}\Psi$$

$$-i\hbar\frac{\partial \Psi}{\partial x} = p\Psi$$

There is an association between the dynamical quantity p and the differential operator $-i\hbar\frac{\partial}{\partial x}$

This differential operator is called momentum operator

$$-i\hbar\frac{\partial}{\partial x} \qquad -i\hbar\frac{\partial}{\partial y} \qquad -i\hbar\frac{\partial}{\partial z}$$

Energy Operator $\hat{E}$

Wave function is given by

$$\Psi = Ae^{\frac{i}{\hbar}(px - Et)}$$

Differentiate wrt t

$$\frac{\partial \Psi}{\partial t} = -\frac{iE}{\hbar}\Psi$$

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

Energy Operator $\hat{E}$

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}$$

Eigen Value, Eigen Function

If Ψ is well behaved wave function of the state of the system and an operator $\hat{A}$ operates on this function such that it satisfies the equation

$\hat{A}\Psi(x) = a\,\Psi(x)$

Then we say

a is an eigen value of operator $\hat{A}$ and

$\Psi(x)$ is called eigen function of $\hat{A}$

Example: $f(x)=e^{4x}$

$d^2/dx^2\,(e^{4x}) = 16e^{4x}$

is eigen function of operator(d^2/dx^2) and 16 is its eigen value

Expectation Value

- To relate a quantum mechanical calculation to experimental observation in the laboratory, the "expectation value" of the measurable parameter is calculated.
- Expectation value gives us average value of what is expected experimental outcome.

Expectation Value

- In general, the expectation value for any observable quantity can be calculated as

$$\langle f \rangle = \frac{\int \Psi^* \hat{f}\, \Psi\, dx}{\int \Psi^* \Psi\, dx}$$

- $\hat{f}$ is an operator corresponding to dynamical variable f.

If Ψ is normalized

<u>Expectation Value of Momentum</u>

$$\langle p \rangle = \int \Psi^* \hat{p}\, \Psi\, dx$$

$$\langle p \rangle = \int \Psi^* \left(-i\hbar \frac{\partial}{\partial x}\right) \Psi\, dx$$

$$\langle p \rangle = -i\hbar \int \Psi^* \frac{\partial \Psi}{\partial x}\, dx$$

Expectation value of Energy

$$\langle E \rangle = \int \Psi^* \, \hat{E} \, \Psi dx$$

$$\langle E \rangle = \int \Psi^* \left(i\hbar \frac{\partial}{\partial t} \right) \Psi dx$$

$$\langle E \rangle = i\hbar \int \Psi^* \frac{\partial \Psi}{\partial t} dt$$

Expectation value of position

- In measurement of position of particle in a system described by wavefunction there is certain finite probability that a particle will be found at any particular position x within the range x and x+dx.
- The expectation value of x over whole range is given by

$$\langle x \rangle = \frac{\int \Psi^* x \Psi dx}{\int \Psi^* \Psi dx}$$

$$\int \Psi^* \Psi dx = 1$$

$$\langle x \rangle = \int \Psi^* x \Psi dx$$

Problems

Q-1 Find eigen value of operator d^2/dx^2 for eigen function $e^{-i\alpha x}$.

Q-2 Eigen function for momentum operator is e^{ikx} , Find eigen value of momentum.

Q-3 A particle is limited to move on x-axis has the normalized wavefunction

$\Psi = ax \qquad 0 \leq x \leq 1$

$\Psi = 0 \qquad$ elsewhere

a) Determine the probability that it can be found between $x=0.45$ and $x=0.55$

b) determine expectation value of position between 0 and 1.

Q4 Consider the wave function of a particle

$\Psi = A(1 - x/a) \qquad a/2 \leq x \leq a$

Obtain expectation value of $< x >$.