



1. SCHRODINGER EQUATION

At the turn of twentieth century ,classical physics which had been quite unstable ,was seriously challenged by two major fronts such as relativistic domain and microscopic domain. In 1905 Einstein's theory of relativity showed that the validity of the Newtonian mechanics ceases at high speeds.As soon as the new experimental technique was developed to the point of probing atomic and sub atomic stuctures it turns out that classical physics fails miserably in providing proper explanantion of several newly discovered phenomena like blackbody radiation,photoelectric effect ,atomic stability and atomic spectroscopy.

The first real break through came in 1900 when Max Plank introduced the concept of the quatm of energy postulating that the energy exchange between radiation and surroundings takes place in descrete or quantized amounts .Which gives accurate explanation to blackbody,photoelectric effect etc.In 1905 Einstein provided poerful consolidation to Plank's quantum concept. In trying to understand photoelectric effect ,Einstein recognized that Plank's idea of quandization of the electromagnetic waves must be valid for light as well.The series of breakthrough due to Plank, Einstein,Bohr and compton gave both theoretical foubdation as well as the conclusive experimental confirmation for the particle aspects of the waves.That is ,the cocepts that waves exhibits particle behaviour at the microscopic level.

In 1923 another new powerful concept that classical physics could not reconcile:He postulated that not only does radiation exhibits particle like behaviour but conversly ,material particle themselves display wave like behaviour.

Quantum mechanichs is the theory that describes the dynamics of matter at the microscopic level.There are two independent formulation of quantum mechanics.The first called matrix mechanics developed by Heisenberg to desribe atomic structure starting from observed spectral lines.The second formulation called wave mechanics was due to Schrodinger ;it is a generalization of the debroglie postulates.

1.1 Wave Particle Duality

According to classical physics ,a particle is characterized by an energy E and a momentum P ,whereas a wave characterized by an amplitude and and a wavevector $\vec{k}(\vec{k} = 2\pi/\lambda)$ that specifies the direction of the propagation of the wave.Particle and waves exhibits entirely different behaviours;for instance the particle and wave properties are mutually exslusive.We should note that waves can exchange any amount energy with particles.

1.2 PARTICLE ASPECTS of RADIATION

In this section we are going to find how classical physics led to its failure in explaining number of microscopic phenomena such as blackbody radiation ,the photoelectric effect and the compton effect .As it turns out these

phenomena could only be explained by by abandoning the concepts of classical physics and introducing a new concept:the particle aspects of radiation.

1.2.1 Blackbody Radiation

Blackbody:

A black body, by definition, is an object which absorbs all radiation that falls on it. Since it does not reflect any light, it appears black. In a laboratory, one could approximate a blackbody by a cavity with highly polished walls. If the walls of the cavity has a small hole, any radiation that enters through the hole gets trapped in it. Stars may also be approximated as black bodies as any radiation directed at them gets absorbed.

Every body at constant temperature will emit radiation with a frequency depends up on the temperature of the body. At room temperature most of the radiation is in the infrared part of the spectrum and hence invisible. A hot metal piece will emit visible light an its colour changes from red to yellow to white as it become hotter and hotter. To study the radiation emitted by a hot body , it is convenient to consider an ideal body which absorbs all the radiation , of any frequency incident on it. Such a body is called blackbody ,which reflect nothing at all. We introduced the ideal black body to study the thermal radiation is that we can now disregard the precise nature of the radiation, since all black bodies behaves identically.

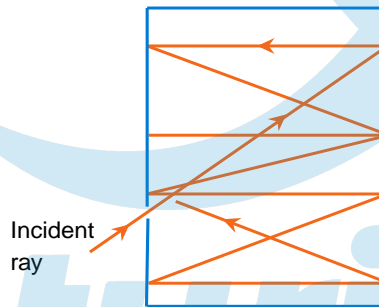


Figure 1.1: Black body radiation

If we consider a cavity with a hole as in figure.1.1, Any light entering through the hole is trapped in the cavity undergoes continuous reflection and absorption until it is finally absorbed. So the cavity wall is constantly emitting and absorbing radiation. This radiation is called blackbody radiation. Experimentally we study the blackbody radiation by examining the radiation coming through the hole in the cavity. The results agree with the observed one.

The Ultraviolet Catastrophe

The observed spectrum of a black body radiation is given below.

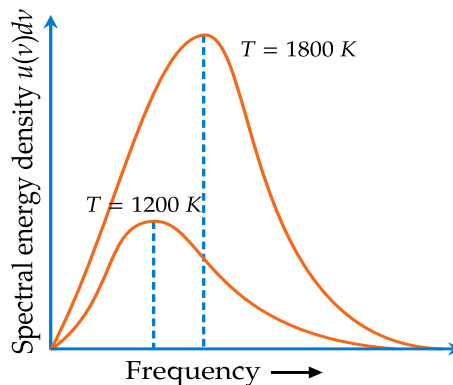


Figure 1.2: Ultraviolet Catastrophe

First theoretical expression for energy density is given by Rayleigh and Jean. They assumed that the light in

the cavity forms standing waves with node occurs at each reflecting surface. The no. of standing waves per unit volume, that is density of standing waves $G(\nu)d\nu$ is given by,

$$G(\nu)d\nu = \frac{8\pi\nu^2 d\nu}{c^3}$$

Where ν is the frequency, c the speed of light. Thus density of standing wave is directly proportional to the square of frequency according to them. The expression for energy density is given by multiplying $G(\nu)d\nu$ with average energy per standing wave ($\bar{\epsilon}$), so,

$$u(\nu)d\nu = G(\nu)d\nu \times \bar{\epsilon}.$$

We already know that the EM waves are produced by oscillating electric charge in the cavity. For a body at constant temperature the average energy per degree of freedom is given by,

$$\frac{1}{2}KT - \text{Equipartition theorem.}$$

A one-dimensional harmonic oscillator has two degrees of freedom, one that corresponds to its kinetic energy and one that corresponds to its potential energy. Because each standing wave in a cavity originates in an oscillating electric charge in the cavity wall, two degrees of freedom are associated with the wave and it should have an average energy of $2\left(\frac{1}{2}\right)kT$.

$$\text{So average energy } \bar{\epsilon} = 2 \times \frac{1}{2}KT = KT$$

\therefore Energy density,

$$u(\nu)d\nu = G(\nu)d\nu \times KT$$

$$u(\nu)d\nu = \frac{8\pi KT \nu^2}{c^3} d\nu \Rightarrow \text{Rayleigh-Jean formula}$$

That is, $u(\nu)d\nu$ is proportional to ν^2

If we plot we will get,

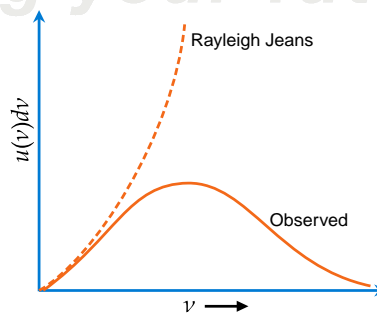


Figure 1.3

This discrepancy of Rayleigh Jeans formula with the observed spectrum is called ultraviolet catastrophe. When the frequency increases towards ultraviolet end of the spectrum energy density should increase as ν^2 according to Rayleigh - Jeans formula. But actually energy density is decreasing towards 0, When frequency increases to ∞ .

Plank Radiation Formula

The problem of ultraviolet catastrophe is solved by Maxplank by considering that the average energy per standing wave or the energy of a harmonic oscillator is not a continuous value as KT but a discrete value.

$$\epsilon_n = nh\nu \quad n = 1, 2, 3, \dots$$

So average energy per standing wave,

$$\bar{\varepsilon} = h\nu \times \frac{1}{e^{\frac{h\nu}{KT}} - 1}$$

Where $\frac{1}{e^{\frac{h\nu}{KT}} - 1}$ is the Bose- Einstein distribution function, which gives the average number of particle in each state of energy ε . Therefore energy density of radiation,

$$\begin{aligned} u(\nu)d\nu &= \frac{8\pi\nu^2}{c^3}d\nu \times \frac{h\nu}{e^{\frac{h\nu}{KT}} - 1} \\ &= \frac{8\pi h}{c^3} \frac{\nu^3 d\nu}{e^{\frac{h\nu}{KT}} - 1} \quad \Rightarrow \text{Plank radiation formula} \end{aligned}$$

This result agree with the observed spectrum ie,

- At high frequencies $h\nu \gg KT$, $\frac{h\nu}{KT} \rightarrow \infty$

Then, $u(\nu)d\nu \rightarrow 0$ as observed.

- At low frequencies

$$h\nu \ll KT, \frac{h\nu}{KT} \ll 1$$

$$\text{Then, } e^{\frac{h\nu}{KT}} = 1 + \frac{h\nu}{KT} \quad \because \left[e^x = 1 + x + \frac{x^2}{0!} + \frac{x^3}{3!} + \dots \right]$$

$$\frac{1}{e^{\frac{h\nu}{KT}} - 1} = \frac{1}{1 + \frac{h\nu}{KT} - 1}$$

$$= \frac{KT}{h\nu}$$

$$u(\nu)d\nu = \frac{8\pi h}{c^3} \nu^3 \left(\frac{KT}{h\nu} \right) d\nu$$

$$= \frac{8\pi KT}{c^3} \nu^2 d\nu$$

$$u_\nu(\nu) = \frac{8\pi h\nu^3}{c^3} \cdot \frac{1}{\exp\left(\frac{h\nu}{KT}\right) - 1}$$

At low frequencies plank radiation formula reduces to Reyleigh-Jeans formula. No discrepancy at low frequencies.

Note

1. $u(\nu)$ is called spectral energy density and has a dimension: $ML^{-1}T^{-1}$
2. The spectral frequency in terms of angular frequency ω .

$$u(\omega) = \frac{\hbar\omega^3}{\pi^2 c^3} \cdot \frac{1}{e^{\left(\frac{\hbar\omega}{KT}\right)} - 1}$$

3. The spectral frequency in terms of wave length λ

$$u(\lambda) = \frac{8\pi hc}{\lambda^5} \cdot \frac{1}{e^{\left(\frac{hc}{\lambda KT}\right)} - 1}$$

Photon

Planck's explanation of black body radiation was revolutionary as it suggested that atoms could exchange energy only in multiples of quantum of energy. In this concept light consist of particles known as **photon** with energy equal to $h\nu$. So it's total energy is quantized ($h\nu$) in terms of each quanta photon ($h\nu$) which is discrete. But according to wave theory, light waves leave a source with their energy spread out continuously through the wave pattern. That is the difference from quantum theory.

- **Energy of Photon**

$$E = h\nu,$$

ν is the frequency and h is called the Plancks constant

$$h = 6.626 \times 10^{-34} \text{J} \cdot \text{S}$$

$$\text{Dimension of } h = ML^2T^{-2} \times T$$

$$= ML^2T^{-1} \quad (h \text{ has a dimension of angular momentum.})$$

Now we can define a new quantity, $\hbar = \frac{h}{2\pi}$

$$\omega = 2\pi f$$

$$\therefore E = \hbar\omega$$

- **Momentum of Photon**

The momentum associated with photon is expressed in terms of wave number , $k = \frac{2\pi}{\lambda}$

$$p = \hbar k \Rightarrow p = \frac{h}{\lambda}$$

In relativity total energy can be expressed in terms of momentum and restmass energy as

$$E^2 = P^2c^2 + (m_0c^2)^2$$

For a photon, rest mass m_0 is zero.

$$\therefore E = Pc$$

Then momentum,

$$p = \frac{E}{c} = \frac{h\nu}{c}$$

- **Mass of a photon**

Although a photon have no restmass if it interact with an electron, it acquires a mass, m

$$\begin{aligned} p &= \frac{E}{c} \\ mc &= \frac{E}{c} \\ m &= \frac{E}{c^2} = \frac{h\nu}{c^2} \end{aligned}$$

Exercise 1.1 Find the wave length and frequency of a 1 kev photon.

Solution:

$$\begin{aligned}
 E &= 1 \times 10^3 \text{ eV} \\
 E &= 10^3 \times 1.6 \times 10^{-19} \text{ J} \\
 E &= \frac{hc}{\lambda} \\
 \lambda &= \frac{hc}{E} = \frac{6.6 \times 10^{-34} \times 3 \times 10^8}{10^3 \times 1.6 \times 10^{-19}} \\
 &= 12.4 \text{ \AA} \\
 \nu &= \frac{c}{\lambda} = \frac{3 \times 10^8}{12.4 \times 10^{-10}} \\
 &= 2.42 \times 10^{17} \text{ Hz}
 \end{aligned}$$

Wien's Displacement Law

There is an interesting relationship between the peak wavelength and the temperature at which a blackbody radiates. For a given temperature, the spectrum of emitted radiation has maximum intensity for a wavelength λ_{max} .

We will get the maximum wavelength by differentiating $u(\lambda)$ with respect to λ ,

$$\frac{du(\lambda)}{d\lambda} = 0 \text{ at } \lambda = \lambda_{max}$$

At maximas and minimas the first derivative of a function must vanish. After differentiation we will obtain $u(\lambda)$ as,

$$\begin{aligned}
 \frac{hc}{KT\lambda_{max}} &= 4.965 \\
 \lambda_{max}T &= \frac{hc}{4.965} = 2.898 \times 10^{-3} \text{ m} \cdot \text{K} \\
 \lambda_{max}T &= 2.898 \times 10^{-3} \text{ m} \cdot \text{K} \Rightarrow \text{Wien's displacement law}
 \end{aligned}$$

Which expresses the empirical fact that the peak in the blackbody spectrum shift to progressively shorter wavelength (higher frequencies) as the temperature increases.

The shift of that peak is a direct consequence of the plank radiation law. Which describes the spectral brightness of black body radiation as a function of wavelength at a given temperature. However it had been discovered by Wilhelm Wien several years before Max Plank developed that more general equation, and describes the entire shift of the spectrum of blackbody radiation towards shorter wavelength as temperature increases.

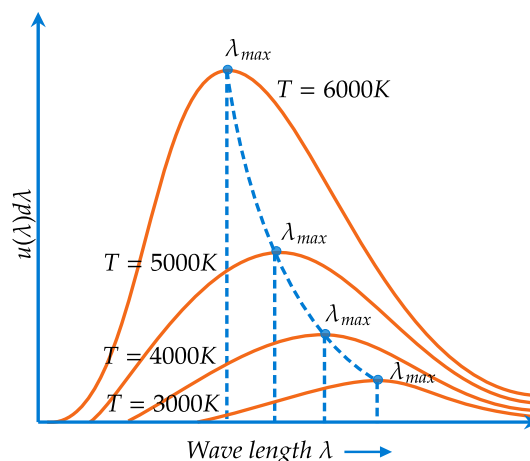


Figure 1.4

Exercise 1.2 Find the peak wave length in the spectrum of radiation from a blackbody at a temperature of 500 Å. In what part of the em spectrum is this wavelength

Solution:

$$\begin{aligned}\lambda_{max}T &= 2.898 \times 10^{-3} \\ T &= 500 + 273 = 773K \\ \lambda_{max} &= \frac{2.898 \times 10^{-3}}{773} \\ 3.7 \times 10^{-3} \times 10^{-3} &= 3.7\mu m \quad (\text{Mid-infrared region})\end{aligned}$$

Stefan-Boltzman Law

The total energy density u of the radiation in the cavity is given by,

$$\begin{aligned}u &= \int u(\nu)dx \\ &= \frac{8\pi^5 k^4}{15c^3 h^3} T^4 \\ &= aT^4\end{aligned}$$

a is a universal constant, $a = 7.56 \times 10^{-16}$ Since u (Energy density) is proportional to T^4 , the energy R (Radiation per second per unit area) is also proportional to T^4 . So ,

$$\begin{aligned}R &\propto T^4, \\ R &= e\sigma T^4 \Rightarrow \text{Stefan-Boltzmann law}\end{aligned}$$

σ is called Stefan's constant

$$\sigma = \frac{ac}{4} = 5.670 \times 10^{-8} \text{W/m}^2 \cdot \text{K}^4$$

e is the emissivity, depends on the nature of the body radiating

Note

- $e = 0$ For a perfect reflector.
 - $e = 1$ (Maximum) For a blackbody (zero reflection).
 - $e = .07$ For polished steel.
 - $e = 0.6$ For oxidized copper and brass.
 - $e = 0.97$ For black paint.
- R is the energy radiated per unit time per unit area. So R can be written as ,

$$R = \frac{\text{Power output}}{\text{Surface Area}}$$

Exercise 1.3 A copper sphere 5cm in diameter whose emissivity is 0.3 is heated in a furnace to 400°C. At what rate it radiate?

Solution:

$$R = \frac{\text{Power}}{\text{Surface area}}$$

$$R = \sigma e T^4$$

$$\therefore \text{Power} = \sigma e T^4 \times 4\pi r^2$$

$$T = 400 + 273 = 673K$$

$$e = 0.3$$

$$\sigma = 5.67 \times 10^{-8}$$

$$r = 5 \times 10^{-2}m$$

$$\text{Power rate} = 27.39W$$

1.2.2 Photo Electric Effect

When light certain minimum frequency falls on certain metals, electrons are emitted in all directions from the surface of the metal , this phenomenon is called photo-electric effect. These electrons are called photoelectrons.

This was first observed by Hertz during his experiment on em waves. But he did not follow up this observation. The correct explanation of photoelectric effect is given by Einstein using Planck's quantum hypothesis. Einstein put forward a theory of photoelectric effect which suggested that the quantum of energy was not a property associated with the radiation emitted by atoms but is a property of radiation itself. He assumed that light consist of small packets called photons having energy equal to $h\nu$ (ν is the frequency).

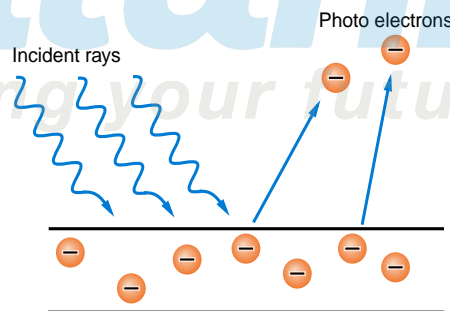


Figure 1.5: Photo Electric Effect

Experimental setup

In the arrangement shown in the figure. 1.6 , the wire marked anode is held at positive potential with respect to the curved plate marked cathode. When light of certain minimum frequency falls on the cathode, electrons are emitted in all directions. These electrons are called photoelectrons. Some of these electrons reach the anode wire which provides a path to the electrons to give rise to a mesurable photo-current . By making the anode more positive with respect to the cathode, more electrons are attracted towards the anode and the photo-current increases. When the anode potential is such that all the emitted electrons reach the anode, any further increase in the anode voltage does not increase current any further.

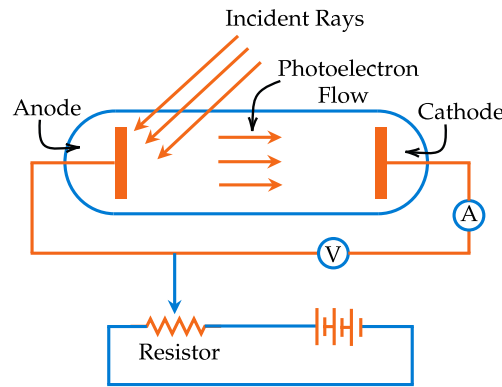


Figure 1.6: Experimental setup for Photoelectric effect

Einstein explained the three experimental observations using his hypothesis.

- (1) Because wave energy is concentrated in photon it's not spread out in space (as in classical wave). **There should be no delay in the emission of photoelectrons.**
- (2) All photons of frequency ν have the same energy, so changing the intensity of monochromatic light beam will change the no. of photoelectrons but not their energies. A bright light yields more photoelectrons than a dim one of the same frequency.

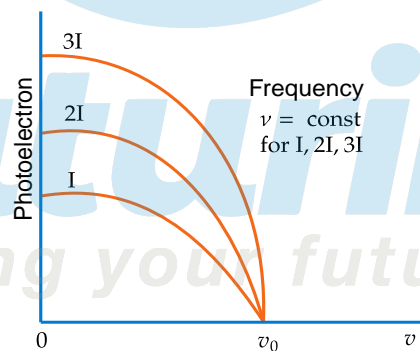


Figure 1.7

Where V_0 is called **retarding potential** or **stopping potential**. Which refers to the voltage difference required to stop electrons from moving between plates during a photoelectric experiment. In order to stop an electron the energy we applied (eV_0) must be equal to the maximum kinetic energy of the photoelectron emitted.

$$\therefore eV_0 = \frac{1}{2}mV^2 = KE_{max}$$

Here in this figure. 1.7, all the three lights ($I, 2I, 3I$) have the same frequency. So KE of photoelectron depends only on the energy of incident photon and work function of the metal. So retarding potential is also the same for all the three lights.

- (3) The higher the frequency ν , the greater the photon energy $h\nu$ and the more energy the photoelectrons have.

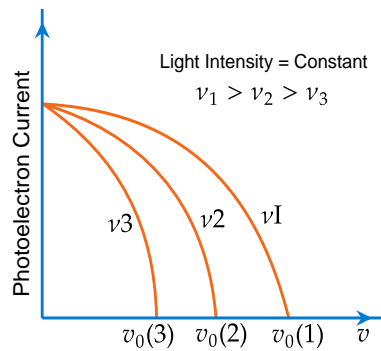


Figure 1.8

Here, $\nu_1 > \nu_2 > \nu_3 \rightarrow KE_1 > KE_2 > KE_3 \rightarrow \nu_0(1) > \nu_0(2) > \nu_0(3)$

Einstein's Photoelectric Equation

According to Einstein's explanation, photoelectric effect occurs due to absorption of a single photon by an electron in the atom. When radiation falls on a metal surface, an electron may absorb one quantum of energy and increase its energy by $h\nu$. Some of the absorbed energy, ϕ , will be used to separate the electron from the metal surface. The surplus energy appears as the kinetic energy of the emitted electron.

$$K.E. = h\nu - \phi$$

The electrons which are more tightly bound to the metal (e.g. electrons which lie two or three atomic layers below the surface) require more energy to be removed. We define **Work Function** ϕ of a metal as the minimum energy that must be supplied to an electron at the metal surface to dislodge it from the metal. Such electrons are emitted with maximum possible kinetic energy. Thus Einstein's equation becomes,

$$KE_{\max} = \frac{1}{2}mv_{\max}^2 = h\nu - \phi$$

Since kinetic energy cannot be negative, the above equation implies the existence of a minimum frequency ν_0 for photoemission to take place

$$h\nu_0 = \phi \Rightarrow \nu_0 = \frac{\phi}{h}$$

Using this, we can rewrite Einstein's equation as,

$$KE_{\max} = h(\nu - \nu_0)$$

Work Function:

The minimum energy ϕ of an electron to escape from a particular metal surface is called work function of the metal

$$\phi = h\nu_0$$

Where ν_0 is the critical frequency below which no photoelectrons are emitted. The greater the work function of a metal, the more energy is needed for an electron to leave its surface, and the higher the critical frequency for photoelectric emission to occur.

Exercise 1.4 The minimum frequency for photoelectric emission in copper is $1.1 \times 10^{15} \text{ Hz}$. Find the maximum energy of the photoelectron (electron volts) when light of frequency $1.5 \times 10^{15} \text{ Hz}$ is directed on a copper surface.

Solution:

$$KE_{\max} = h(\nu - \nu_0)$$

$$\nu = 1.5 \times 10^{15} \text{ Hz}$$

$$\begin{aligned}
 \nu_0 &= 1.1 \times 10^{15} \text{ Hz} \\
 KE_{\max} &= 6.6 \times 10^{-34} (1.5 \times 10^{15} - 1.1 \times 10^{15}) \\
 &= 6.6 \times 10^{-34} \times 0.4 \times 10^{15} \\
 &= 2.64 \times 10^{-19} \text{ J} \\
 KE_{\max} &= \frac{2.64 \times 10^{-19}}{1.6 \times 10^{-19}} \\
 &= 1.65 \text{ eV}
 \end{aligned}$$

1.2.3 X-rays and Compton effect.

X-rays were discovered accidentally by German scientist Rontgen in 1895. The first Nobel Prize was awarded to Rontgen in 1901. Within a few years it became clear that x-rays are another form of electromagnetic radiation of wavelengths typically some tens or hundreds of picometers ($1 \text{ pm} = 10^{-12} \text{ m}$). These are highly penetrating electromagnetic radiation and it has proved to be a very powerful tool to study the crystal structure, in material research and in various other fields of science and technology. X-rays are highly energetic radiations with very short wavelengths.

Properties

- X-rays do not require any medium for propagation and they cannot be refracted.
- Electric and magnetic fields do not have any effect on these rays.
- These radiations ionize the surrounding air by discharging electrified bodies.
- X-rays have short wavelength varying between 0.1 \AA to 1 \AA .
- X-rays are produced when a metal anode is bombarded by very high energy electrons.

X-ray - Diffraction.

X - ray diffraction is one of the earliest methods for studying the structure of solids. In the process of diffraction, electromagnetic waves of a given frequency but different phases interact to produce constructive interference (bright spots on the film exposed to the light) and destructive interference (dark spots). By a careful analysis of the diffraction patterns, very accurate values of the lattice parameters (unit cell dimensions) can be inferred. The x - rays only for a particular angle of incidence, such that x-ray beams reflected from successive planes of atoms have their electric and magnetic fields in phase. The atomic planes of a crystal cause an incident beam of X-rays to interfere with one another as they leave the crystal. The phenomenon is called X-ray diffraction. Diffraction occurs only when Bragg's Law is satisfied the condition for constructive interference from planes with spacing d .

Bragg's law

Bragg's law plays a central role in the analysis of diffraction data. This law relates the angle θ (at which there is a maximum in diffracted intensity) to the wavelength λ of X -rays and the inter-layer distance d between the planes of atoms , ions or molecules in the lattice. Mathematically the condition can be written as,

$$2d \sin \theta = n\lambda \quad n = 1, 2, 3, \dots \quad \text{Bragg's law.} \quad (1.1)$$

1.2.4 Compton Effect

Photoelectric effect provides evidence that energy is quantized. In order to establish the particle nature of radiation, it is necessary that photons must carry momentum. In 1922, Arthur Compton studied the scattering of x -rays of known frequency from graphite and looked at the recoil electrons and the scattered x -rays. The hypothesis proposed by Arthur Compton suggested that when an X-ray quantum is scattered it spends all of its energy and momentum upon some particular electron. This electron in turn scatters the ray in some definite direction. The change in momentum of the X-ray quantum due to the change in its direction of propagation results in a recoil of the scattering electron. The energy in the scattered quantum is thus less than the energy in the primary quantum by the kinetic energy of the recoil of the electron.

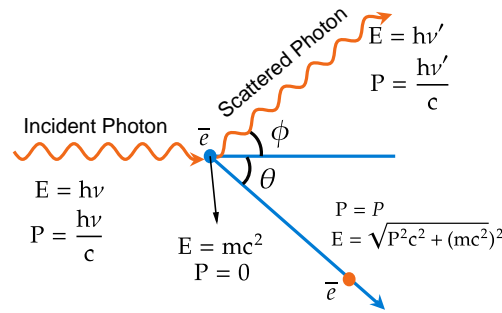


Figure 1.9: Compton effect

$h\nu =$ The energy of incident photon

$\frac{h\nu}{c} =$ Momentum of incident photon $[E = Pc \therefore P = \frac{E}{c}]$

$h\nu' =$ The energy of scattered photon

$\frac{h\nu'}{c} =$ Momentum of scattered photon

$h\nu > h\nu'$

KE of electron $= h\nu - h\nu'$

$E = mc^2$ is the rest energy of electrons.

$E = \sqrt{P^2c^2 + (mc^2)^2}$ is the total energy of scattered electron.

$\phi =$ The scattering angle for incident photon.

$\theta =$ The angle between the direction of initial photon and the recoil electron.

If we treat the incident radiation as a stream of particles which are named as photons-colliding elastically with individual electrons. In that scattering process we use the laws of elastic collisions the conservation of energy and momentum.

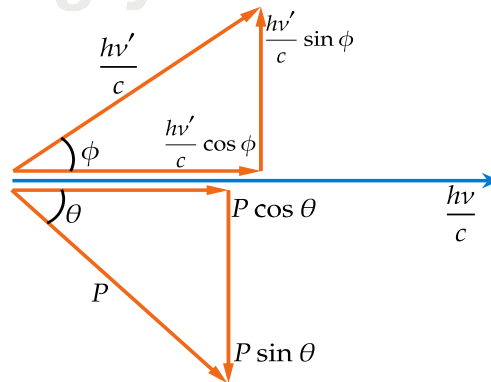


Figure 1.10

By using momentum conservation,

Initial momentum = final momentum

$$\frac{h\nu}{c} + 0 = \frac{h\nu'}{c} \cos \phi + p \cos \theta \quad (1.2)$$

$$pc \cos \theta = h\nu - h\nu' \cos \phi \quad (1.3)$$

In perpendicular to this direction,

$$0 = \frac{h\nu'}{c} \sin \phi - p \sin \theta \quad (1.4)$$

$$pc \sin \theta = h\nu' \sin \phi \quad (1.5)$$

By squaring equations 1.3 and 1.5 and adding the new ones together, the angle θ is eliminated, leaving

$$p^2 c^2 = (h\nu)^2 - 2(h\nu)(h\nu') \cos \phi + (h\nu')^2 \quad (1.6)$$

The total energy of scattered particle can be written as,

$$E = \text{KE} + mc^2 \quad \text{And} \quad E = \sqrt{m^2 c^4 + p^2 c^2} \quad (1.7)$$

Equating both of them we get,

$$(\text{KE} + mc^2)^2 = m^2 c^4 + p^2 c^2 \quad (1.8)$$

$$p^2 c^2 = \text{KE}^2 + 2mc^2 \text{KE} \quad (1.9)$$

$$\therefore \text{KE} = h\nu - h\nu' \quad (1.10)$$

$$p^2 c^2 = (h\nu)^2 - 2(h\nu)(h\nu') + (h\nu')^2 + 2mc^2 (h\nu - h\nu') \quad (1.11)$$

Substituting the value of $P^2 c^2$ in equation. 1.6, we get

$$2mc^2 (h\nu - h\nu') = 2(h\nu)(h\nu') (1 - \cos \phi) \quad (1.12)$$

In terms of wavelength, equation. 1.12 becomes,

$$\frac{mc}{h} \left(\frac{\nu}{c} - \frac{\nu'}{c} \right) = \frac{\nu \nu'}{c} (1 - \cos \phi) \quad (1.13)$$

And so, since $\nu/c = 1/\lambda$ and $\nu'/c = 1/\lambda'$,

$$\frac{mc}{h} \left(\frac{1}{\lambda} - \frac{1}{\lambda'} \right) = \frac{1 - \cos \phi}{\lambda \lambda'} \quad (1.14)$$

$$\lambda' - \lambda = \frac{h}{mc} (1 - \cos \phi) \quad (1.15)$$

Equation 1.15 gives the change in wavelength expected for a photon that is scattered through the angle ϕ by a particle of rest mass m . This change is independent of the wavelength λ of the incident photon.

$$\Delta \lambda = \lambda' - \lambda = \lambda_c (1 - \cos \phi)$$

$$\lambda_c = \frac{h}{mc}$$

λ_c is called Compton wavelength of the scattered particle. For electron

$$\lambda_c = 2.426 \times 10^{-12} \text{m}$$

$$\lambda_c = 2.426 \text{pm}$$

- Note** 1) The shift is independent of the wavelength λ of incident photon. Which depends only on the scattering angle ϕ , and the constant parameters h, c and mass of the particle scattered.
- 2) The shift is maximum when $\phi = 180$ ie when it scattered back in the incident direction.
- 3) The maximum KE of the recoil electron occurs when $\phi = 180$

$$KE_{max} = \frac{2h^2\nu^2}{mc^2} \frac{1}{\left(1 + \frac{2h\nu}{mc^2}\right)}$$

Exercise 1.5 How much energy must a photon have . If it is to have the momentum of a 10MeV proton. ■

Solution:

$$\begin{aligned} KE &= \frac{P^2}{2m} \\ P &= \sqrt{2mKE} \\ &= \sqrt{2 \times 1.67 \times 10^{-27} \times 10 \times 10^6 \times 1.6 \times 10^{-19}} \\ &= 7.31 \times 10^{-20} \text{ kgm/s} \\ \text{For photon } E &= Pc \\ E &= 7.31 \times 10^{-20} \times 3 \times 10^8 \\ E &= 21.93 \times 10^{-12} \text{ J} \\ E &= \frac{21.93 \times 10^{-12}}{1.6 \times 10^{-19}} \text{ eV} \\ &= 13.706 \times 10^7 \\ &= 137 \text{ MeV} \end{aligned}$$

Exercise 1.6 A monochromatic X-ray beam whose wavelength is 55.8pm is scattered through 46° . Find the wavelength of the scattered beam. ■

Solution:

$$\begin{aligned} \lambda' - \lambda &= \lambda_c (1 - \cos \phi) \\ \lambda &= 55.8 \times 10^{-12} \text{ m} \\ \lambda_c &= 2.426 \times 10^{-12} \text{ m} \\ \phi &= 46^\circ \\ \lambda' &= \lambda + \lambda_c (1 - \cos \phi) \\ &= 55.8 \text{ pm} + 0.742 \text{ pm} \\ &= 56.54 \text{ pm} \end{aligned}$$

1.2.5 Pair production

Unlike Photoelectric effect and Compton effect, the photon, passing near the nucleus of an atom, subjected to strong field effects from the nucleus may disappear as a photon and reappear as a positive and negative electron pair. This process is called the pair production. In pair production, electromagnetic energy is converted into matter. No conservation principles are violated when an electron positron pair is created.

the photon must have a minimum energy to pair production take place, The rest energy mc^2 of an electron or positron is 0.51MeV, hence pair production requires a photon energy of at least 1.02MeV. Any additional photon energy becomes kinetic energy of the electron and positron. The corresponding maximum photon wavelength is

1.2pm. Electromagnetic waves with such wavelengths are called gamma rays, symbol γ , and are found in nature as one of the emissions from radioactive nuclei and in cosmic rays.

The kinetic energy of the electrons produced will be the difference between the energy of the incoming photon and the energy equivalent of two electron masses (1.022MeV).

$$E_{e+} + E_{e-} = h\nu - 1.022(\text{MeV})$$

The inverse of pair production occurs when a positron is near an electron and the two come together under the influence of their opposite electric charges. Both particles vanish simultaneously, with the lost mass becoming energy in the form of two gamma-ray photons:

$$e^+ + e^- \rightarrow \gamma + \gamma$$

And this process is called pair annihilation.

1.3 Wave Aspects of Particles

1.3.1 De Broglie's Hypothesis: matter Waves

As discussed above-in the photoelectric effect, the Compton effect, and the pair production effect-radiation exhibits particle-like characteristics in addition to its wave nature. In 1923 de Broglie took things even further by suggesting that this wave-particle duality is not restricted to radiation, but must be universal: all material particles should also display a dual wave-particle behavior. That is, the wave-particle duality present in light must also occur in matter.

So, starting from the momentum of a photon $p = h\nu/c = h/\lambda$, we can generalize this relation to any material particle with nonzero rest mass: each material particle of momentum \vec{p} behaves as a group of waves (matter waves) whose wavelength λ and wave vector \vec{k} are governed by the speed and mass of the particle

$$\lambda = \frac{h}{p}, \quad \vec{k} = \frac{\vec{p}}{\hbar}$$

where $\hbar = h/2\pi$. The expression known as the de Broglie relation, connects the momentum of a particle with the wavelength and wave vector of the wave corresponding to this particle.

Exercise 1.7 Calculate the wavelength associated with a cricket ball of mass 0.2 kg moving with a speed of 30 m/s.

Solution:

$$\begin{aligned} p &= mv = 0.2 \times 30 \\ &= 6 \text{ kg m/s} \\ \lambda &= \frac{h}{p} \\ &= \frac{6.63 \times 10^{-34}}{6} \\ &= 1.1 \times 10^{-34} \text{ m} \end{aligned}$$

Exercise 1.8 What is the speed of an electron if its de Broglie wavelength equals its Compton wavelength ?

Solution:

$$\lambda_{\text{Rel}} = \frac{h}{p} = \frac{hc}{pc}$$

$$\begin{aligned}
 &= \frac{hc}{\sqrt{E^2 - E_0^2}} && \text{But } E = \gamma E_0 \\
 &= \frac{hc}{\sqrt{\gamma E_0^2 - E_0^2}} = \frac{hc}{\sqrt{E_0^2(\gamma^2 - 1)}} \\
 &= \frac{hc}{m_0 c \sqrt{(\gamma^2 - 1)}} = \frac{hc}{m_0 c^2 \sqrt{(\gamma^2 - 1)}} \\
 &= \frac{\lambda_C}{\sqrt{(\gamma^2 - 1)}} && \gamma = \sqrt{1 - \frac{v^2}{c^2}}
 \end{aligned}$$

Then if de Broglie wavelength equals Compton wavelength then,

$$\begin{aligned}
 \lambda_{Rel} &= \lambda_C \\
 1 &= \frac{1}{\sqrt{(\gamma^2 - 1)}} \\
 \gamma^2 &= 2 \Rightarrow \gamma = \sqrt{2} \\
 \sqrt{2} &= \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} \\
 \text{On solving we get, } v &= \frac{c}{\sqrt{2}}.
 \end{aligned}$$

1.3.2 Velocity of a Matterwave

We know that every material particle in motion is associated with a wave called matterwave.

According to the mass energy relation,

$$E = mc^2 \quad (1.16)$$

$$\text{For a matterwave, } E = h\nu \quad (1.17)$$

$$\text{Then, } h\nu = mc^2 \Rightarrow v = \frac{mc^2}{h} \quad (1.18)$$

$$\text{Velocity of a wave, } v = v\lambda \quad (1.19)$$

$$v_{mw} = \frac{mc^2}{h} \times \frac{h}{mv} \quad \lambda = \frac{h}{p} = \frac{h}{mv} \quad (1.20)$$

$$v_{mw} = \frac{c^2}{v} \gg \gg c \quad (1.21)$$

That is the velocity of de-Broglie wave associated with a moving material is greater than the velocity of light. But according to the special theory of relativity, no energy can be transmitted with velocity greater than c . So we need to explain the behaviour of matterwave.

1.3.3 Phase Velocity

The phase velocity v_p of a wave is the rate at which the phase of the wave propagates in space. It is also the velocity of a monochromatic wave with which crest or trough of the wave travels in a medium. A plane wave propagating along the $+ve$ x -direction can be represented as,

$$\psi(x, t) = A e^{i(kx - \omega t)} \quad (1.22)$$

ω = The angular frequency.

v = The velocity.

A = The amplitude of the wave.

The phase ϕ of the wave at any time ' t ' at a distance ' x ' from the origin is ,

$$\phi(x, t) = (kx - \omega t) \quad (1.23)$$

We know that the phase of a wave is a constant quantity, then,

$$kx - \omega t = \text{constant} \quad (1.24)$$

$$kdx - \omega dt = 0 \quad (1.25)$$

$$kdx = \omega dt$$

$$\frac{dx}{dt} = \frac{\omega}{k} \quad (1.26)$$

$$v_p = \frac{\omega}{k} \quad (1.27)$$

Multiplying numerator and denominator by \hbar we get,

$$v_p = \frac{\hbar\omega}{\hbar k} \quad (1.28)$$

$$v_p = \frac{E}{p} \quad \text{Since, } E = \hbar\omega \text{ and } p = \hbar k \quad (1.29)$$

Phase velocity

$$v_p = \frac{\omega}{k} \quad ; \quad v_p = \frac{E}{p}$$

The phase velocity of a matter wave can be obtained as,

From the relativistic mass energy relation,

$$v_p = \frac{E}{p} \quad (1.30)$$

$$= \frac{\gamma m_0 c^2}{\gamma m_0 v} \quad m_0 = \text{Rest mass of the particle} \quad ; \quad \gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} \quad (1.31)$$

$$v_p = \frac{c^2}{v} \quad (1.32)$$

The phase velocity of a de-Broglie wave is always greater than the velocity of light in freespace. But according to the special theory of relativity, no energy can be transmitted with velocity greater than c . This suggests that the phase velocity has no physical significance and we can not represent the wave nature of a moving particle by a single plane wave. Thus what we have derived in section.1.3.2 is the phase velocity of the matterwave.

1.3.4 Group Velocity

A moving particle is not associated with a single wave but a group of waves called wavepacket. A wave packet therefore consists of a group of waves of slightly different wavelengths, with phases and amplitudes so chosen that they interfere constructively over a small region of space and destructively elsewhere. Let, the wave group is formed by the superposition of two monochromatic waves having same amplitude but differing in angular frequency by an amount ' $\Delta\omega$ ' and in wave number ' Δk ' i.e

$$\psi_1(x, t) = A \sin(\omega t - kx)$$

$$\psi_2(x, t) = A \sin[(\omega + \Delta\omega)t - (k + \Delta k)x]$$

The resultant wave i.e. wave packet can be written as,

$$\psi(x, t) = 2A \cos \left[\frac{1}{2}(\Delta\omega t - \Delta kx) \right] \sin(\omega t - kx)$$

Now, group velocity is the velocity with which maximum amplitude or the envelope of the wave packet moves and it is given as:

$$v_g = \frac{d\omega}{dk} = \frac{dE}{dp}$$

. From the relativistic mass-energy relation :

$$E^2 = p^2 c^2 + m_0^2 c^4 \Rightarrow 2E \frac{dE}{dp} = 2pc^2 \quad (1.33)$$

$$v_g = \frac{dE}{dp} = \frac{pc^2}{E} \quad (1.34)$$

$$= \frac{\gamma m_0 v c^2}{\gamma m_0 c^2} \quad (1.35)$$

$$v_g = v < c \quad (1.36)$$

Group velocity

$$v_g = \frac{d\omega}{dk} \quad ; \quad v_g = \frac{dE}{dp}$$

Note

Other useful expressions for Group velocity

$$\begin{aligned} v_g &= \frac{d\omega}{dk} \\ &= \frac{d(\hbar\omega)}{d(\hbar k)} \\ &= \frac{1}{\hbar} \frac{d(\hbar\omega)}{dk} \\ v_g &= \frac{1}{\hbar} \frac{dE}{dk} \end{aligned} \quad \begin{aligned} v_g &= \frac{d\omega}{dk} \\ &= \frac{d(2\pi\nu)}{d(2\pi/\lambda)} \\ &= \frac{2\pi}{d(2\pi/\lambda)} \cdot \frac{d(2\pi\nu)}{d(2\pi/\lambda)} \\ v_g &= \frac{-1}{\lambda^2} \frac{d\nu}{d\lambda} \end{aligned}$$

1.3.5 Group and Phase Velocities

When we superimpose many waves of different amplitudes and frequencies, we can obtain a wave packet or pulse which travels at the group velocity v_g ; the individual waves that constitute the packet, however, move with different speeds; each wave moves with its own phase velocity v_{ph} . Figure .1.11 gives a qualitative illustration: the group velocity represents the velocity with which the wave packet propagates as a whole, where the individual waves (located inside the packet's envelope) that add up to make the packet move with different phase velocities.

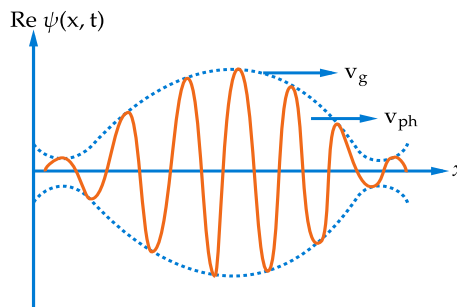


Figure 1.11: Phase and group velocity

1.3.6 De-Broglie's Dispersion Relation

The dispersion relation for de Broglie waves

$$v_p = \frac{\omega}{k} \quad \text{And} \quad v_g = \frac{d\omega}{dk} \quad (1.37)$$

$$\begin{aligned} V_g &= \frac{d}{dk}(v_p k) = v_p \cdot 1 + k \frac{dv_p}{dk} \\ &= v_p + k \frac{dv_p}{dk} \end{aligned} \quad \begin{aligned} k &= \frac{2\pi}{\lambda} \\ dk &= \frac{-2\pi}{\lambda^2} d\lambda \end{aligned} \quad (1.38)$$

$$\begin{aligned} &= v_p + \frac{2\pi}{\lambda} dv_p \cdot \frac{-\lambda^2}{2\pi d\lambda} \\ v_g &= v_p - \lambda \frac{dv_p}{d\lambda} \rightarrow (\text{Dispersion relation.}) \end{aligned} \quad (1.39)$$

$$\begin{aligned} v_g &= v_p + k \frac{dv_p}{dk} \\ v_g &= v_p - \lambda \frac{dv_p}{d\lambda} \end{aligned}$$

Dispersive medium are of two types:

- Normal dispersive medium: $\frac{dv_p}{d\lambda} = +ve \Rightarrow v_g < v_p$.
- Anamolous dispersive medium: $\frac{dv_p}{d\lambda} = -ve \Rightarrow v_g > v_p$.

For, non-dispersive medium, all waves travel with same phase velocity: $\frac{dv_p}{d\lambda} = 0 \Rightarrow v_g = v_p$.

1.3.7 Phase and Group Velocity Relation for a Free Particle

For a free particle the potential energy is zero . Then,

$$E = \text{K.E} = \frac{p^2}{2m} \quad (1.40)$$

$$v_p = \frac{E}{p} \quad (1.41)$$

Puttting equation. 1.40 in 1.41 , we get,

$$\begin{aligned} v_p &= \frac{p}{2m} \\ v_g &= \frac{dE}{dp} \end{aligned} \quad (1.42)$$

$$= \frac{2p}{2m} = \frac{p}{m} \quad (1.43)$$

$$v_g = 2v_p \quad (1.44)$$

Free particle

$$v_g = 2v_p$$

1.3.8 Phase and group velocity Relation for a relativistic particle

For a relativistic particle, The energy E is given by,

$$E^2 = p^2 c^2 + m_0^2 c^4 \quad (1.45)$$

$$E = \sqrt{p^2 c^2 + m_0^2 c^4}$$

$$v_p = \frac{E}{p} \quad (1.46)$$

$$= \sqrt{\frac{p^2 c^2 + m_0^2 c^4}{p^2}}$$

$$v_g = \frac{dE}{dp} \quad (1.47)$$

$$= \frac{2pc^2}{2\sqrt{p^2 c^2 + m_0^2 c^4}}$$

$$= \frac{pc^2}{\sqrt{p^2 c^2 + m_0^2 c^4}} \quad (1.48)$$

$$v_p \cdot v_g = \sqrt{\frac{p^2 c^2 + m_0^2 c^4}{p^2}} \cdot \frac{pc^2}{\sqrt{p^2 c^2 + m_0^2 c^4}} \quad (1.49)$$

$$v_p \cdot v_g = c^2 \quad (1.50)$$

Relativistic particle

$$v_p \cdot v_g = c^2$$

	Group Velocity v_g	Relation between v_p and v_g
Phase Velocity v_p	$v_g = \frac{d\omega}{dk}$ $v_g = \frac{dE}{dp}$ $v_g = \frac{1}{\hbar} \frac{dE}{dk}$ $v_g = \frac{-1}{\lambda^2} \frac{dv}{d\lambda}$	$v_g = v_p + k \frac{dv_p}{dk}$ $v_g = v_p - \lambda \frac{dv_p}{d\lambda}$ $v_g = 2v_p \rightarrow \text{Free particle}$ $v_p \cdot v_g = c^2 \rightarrow \text{Relativistic particle}$
$v_p = \frac{\omega}{k}$ $v_p = \frac{E}{p}$		

1.4 The Wave equation

The wave equation governs many physical phenomenon in nature. It is important to understand the properties of wave propagation. Here we are discussing the one dimensional wave equation, like the one in a stretched string. The results are however readily transferable or modified for sound waves any and other types of waves. The standard form of wave equation is ,

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 y}{\partial t^2} \quad (1.51)$$

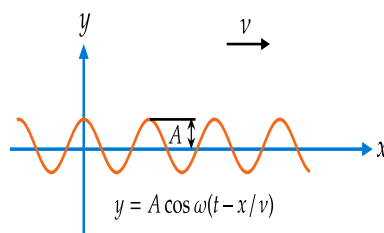


Figure 1.12: Waves in the xy plane traveling in the $+x$ direction

where, it's a wave whose variable quantity is y that propagates in the x direction with the speed v . In the case of a wave in a stretched string, y is the displacement of the string from the x axis; in the case of a sound wave, y is the pressure difference. The properties of wave propagation is derived from the solutions of the wave equation. The solution is obtained by the method of separation of variables. All solutions must be of the form,

$$y = F\left(t \pm \frac{x}{v}\right) \quad (1.52)$$

Where F is any function that can be differentiated. The solutions $F\left(t - \frac{x}{v}\right)$ represent waves traveling in the $+x$ direction, and the solutions $F\left(t + \frac{x}{v}\right)$ represent waves traveling in the $-x$ direction. The wave equivalent of a "free particle," which is a particle that is not under the influence of any forces and therefore pursues a straight path at constant speed. This wave is described by the general solution of Equation.1.51 for undamped (constant amplitude A), monochromatic (constant angular frequency ω) harmonic waves in the $+x$ direction. The solution is of the form,

$$y = Ae^{-i\omega(t-x/v)} \quad (1.53)$$

$$y = A \cos \omega\left(t - \frac{x}{v}\right) - iA \sin \omega\left(t - \frac{x}{v}\right) \quad (1.54)$$

1.5 Schrödinger equation: Time-dependant form

It was observed that the wave function of a particle of fixed energy E could be written as a linear combination of wave functions of the form,

$$\psi = Ae^{-i\omega(t-x/v)} \quad (1.55)$$

The above equation.1.55, represents a wave travelling in the positive x direction. The physical quantity, ψ is the 'wave function' corresponds to the wave variable y of wave motion in general.

$$\text{We know that, } \omega = 2\pi\nu \quad (1.56)$$

$$\nu = \frac{v}{\lambda} \quad (1.57)$$

Replacing ω and ν in the above formula we get,

$$\psi = Ae^{-2\pi i(\nu t - x/\lambda)} \quad (1.58)$$

But we know that,

$$E = h\nu = 2\pi\hbar\nu \quad \text{Since, } \hbar = \frac{h}{2\pi} \quad (1.59)$$

$$\text{And } \lambda = \frac{h}{p} = \frac{2\pi\hbar}{p} \quad (1.60)$$

Then the solution of the free particle becomes,

$$\psi = Ae^{-(i/\hbar)(Et - px)} \quad (1.61)$$

The Schrödinger equation is not a one which can be derived from any basic principles, since itself the Schrödinger equation is a basic principle. But we can be arrived at the equation in various ways. Differentiating the equation . 1.61 twice with respect to x , we get,

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{p^2}{\hbar^2} \psi \quad (1.62)$$

$$p^2 \psi = -\hbar^2 \frac{\partial^2 \psi}{\partial x^2} \quad (1.63)$$

Differentiating the equation . 1.61 twice with respect to t , we get,

$$\frac{\partial \psi}{\partial t} = -\frac{iE}{\hbar} \psi \quad (1.64)$$

$$E\psi = -\frac{\hbar}{i} \frac{\partial \psi}{\partial t} \quad (1.65)$$

A particle of mass 'm' moving along x axis, under the potential field $V(x)$ which is independent of time. The total energy of the system can be written as,

$$E = E_k + E_p = \frac{p_x^2}{2m} + V(x, t) \quad (1.66)$$

Multiplying both sides of Equation. 1.66 by the wave function ψ gives,

$$E\psi = \frac{p(x)^2 \psi}{2m} + V(x, t) \psi \quad (1.67)$$

Substituting for $E\psi$ and $p^2\psi$ from Equations.1.62 and 1.65 to obtain the time-dependent form of Schrödinger's equation,

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x, t) \psi \quad (1.68)$$

In 3-D, the Schrödinger's equation becomes,

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + V(x, y, z, t) \psi \quad (1.69)$$

Schrödinger's equation

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

1.6 Schrödinger equation: Time-independant form

In a great many situations the potential energy of a particle does not depend on time explicitly; the forces that act on it, and hence U , vary with the position of the particle only. When this is true, Schrödinger's equation may be simplified by removing all reference to t .

We begin by noting that the one-dimensional wave function Ψ of an unrestricted particle may be written

$$\begin{aligned} \Psi &= Ae^{-(i/\hbar)(Et - px)} \\ &= Ae^{-(iE/\hbar)t} e^{+(ip/\hbar)x} \\ &= \psi e^{-(iE/\hbar)t} \end{aligned}$$

Evidently Ψ is the product of a time-dependent function $e^{-(iE/\hbar)t}$ and a positiondependent function ψ . Substituting the Ψ into the time-dependent form of Schrödinger's equation, we find that

$$E\psi e^{-(iE/\hbar)t} = -\frac{\hbar^2}{2m} e^{-(iE/\hbar)t} \frac{\partial^2 \psi}{\partial x^2} + U\psi e^{-(iE/\hbar)t}$$

Dividing through by the common exponential factor gives

Steady-state Schrödinger equation in one dimension

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} (E - U) \psi = 0$$

Steady-state Schrodinger equation in three dimension

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{2m}{\hbar^2} (E - U) \psi = 0$$

An important property of Schrödinger's steady-state equation is that, if it has one or more solutions for a given system, each of these wave functions corresponds to a specific value of the energy E . Thus energy quantization appears in wave mechanics as a natural element of the theory, and energy quantization in the physical world is revealed as a universal phenomenon characteristic of all stable systems.

1.7 Postulates of quantum mechanics

1.7.1 First Postulate

"The configuration or state of a quantum mechanical system is completely specified by the wavefunction $\Psi(x, t)$ associated with it . "

We are not familiar with what is a wavefunction , how it is associated with a particle and how the whole information about a particle or a system is embedded in it. Let us see what is really a Wave function is.

1.7.2 Wavefunction

Imagine a particle of mass m , constrained to move along the x -axis, subject to some specified force $F(x, t)$. The program of classical mechanics is to determine the position of the particle at any given time: $x(t)$. We apply Newton's second law ($F = ma$) for this purpose. Once we know that, we can figure out the velocity, the momentum, the kinetic energy , or any other dynamical variable of interest. In concise , It's the position of an object that we are interested in classical mechanics. **When we deal the same problem in quantum mechanics what we are looking for is the wavefunction $\Psi(x, t)$ of the particle and we get it by solving the Schrödinger equation .** (We will deal with Schrödinger equation later in this section).

- The wave function of a localised particle is spread out in the space as a function of x for any given time t .
- The wave function Ψ does not give any information about the state of the particle. It is given by the Born's statistical interpretation of wave function.
- A particle simply does not have a precise position prior to measurement. It is the measurement process that insists on one particular number, and thereby in a sense creates the specific result. The wavefunction collapse at a particular point immediately after the measurement . Any immediate measurement will give the same results since the wavefunction is already collapsed. If you give enough time for the wavefunction to evolve in time through Schrodinger equation then the results may or may not be the same.
- If $\Psi_1(x, t)$ and $\Psi_2(x, t)$ are two possible states of a system, then the linear combination

$$\Psi(x, t) = a_1 \Psi_1(x, t) + a_2 \Psi_2(x, t)$$

is also a possible state. Where a_1 and a_2 are complex numbers. (This property follows directly from the linearity of the Schrödinger Equation)

Born's statistical interpretation

Born's statistical interpretation of the wave function says that $|\Psi(x, t)|^2$ gives the probability of finding the particle at point x , at time t — or, more precisely,

$$\int_a^b |\Psi(x, t)|^2 dx = \left\{ \begin{array}{l} \text{Probability of finding the particle} \\ \text{between } a \text{ and } b, \text{ at time } t. \end{array} \right\}$$

$$\text{Where, } |\Psi(x, t)|^2 = \Psi^*(x, t) \Psi(x, t)$$

For 3-D wave functions,

$$\int_a^b |\Psi(r,t)|^2 d\tau = \left\{ \begin{array}{l} \text{Probability of finding the particle} \\ \text{between } a \text{ and } b, \text{ at time } t. \end{array} \right\}$$

Properties of wavefunction

- The wavefunction Ψ can be a real function or imaginary function.
- Ψ must be finite. i.e. as $x \rightarrow \pm\infty$, $\Psi \rightarrow 0$. That is the wavefunction should be converging.
- Ψ must be single valued. If multiple values exist the particle will have multiple probabilities which is not practically possible.
- $\frac{\partial \Psi}{\partial x}$ must be single valued and continuous. i.e. it should be represented using a smooth curve.
- The wavefunction should be square integrable.

Square integrable functions

A Square integrable function is a real or complex valued function for which, the integral of the square of the absolute value of the function is finite. i.e.

$$\int_{-\infty}^{\infty} |\Psi|^2 < \infty$$

Normalization

The wavefunction of a particle or a system should be chosen such that the probability of finding the particle in the entire space as 1. It's obvious that if a wave function exist, then it should be found somewhere between $-\infty$ and ∞ . Then,

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1 \quad (1.70)$$

Or,

$$\int_{-\infty}^{\infty} |\Psi(r,t)|^2 d\tau = 1 \quad (1.71)$$

Every wave functions associated with a particle should obey this. If not we have to normalize it according to the condition in equation 1.70 or equation 1.71. Let us find how to normalize an un-normalised wavefunction.

Method of Normalization

Let us consider an unnormalized wave function $\phi(x,t)$. We can construct a normalized wave function as $\Psi(x,t) = A\phi(x,t)$ where A is the normalization constant. Therefore,

$$\int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(x,t)dx = |A|^2 \int_{-\infty}^{\infty} \phi^*(x,t)\phi(x,t)dx = 1$$

Exercise 1.9 Normalize the wave function given by $\Psi(x) = Ae^{-ax^2}$. ■

Solution:

$$\begin{aligned} \int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx &= A^2 \int_{-\infty}^{\infty} (e^{-ax^2})^2 dx \\ &= A^2 \int_{-\infty}^{\infty} e^{-2ax^2} dx \\ &= A^2 \sqrt{\frac{\pi}{2a}} \end{aligned} \quad \because \int_{-\infty}^{\infty} e^{-2ax^2} dx = \sqrt{\frac{\pi}{2a}}$$

$$A = \left(\frac{2a}{\pi} \right)^{1/4}$$

Exercise 1.10 Hydrogen atom:

Normalize the ground state function of hydrogen atom given by, $\Psi(r) = Ae^{-r/a_0}$.

Solution:

$$\begin{aligned}\int_{-\infty}^{\infty} |\Psi(r,t)|^2 d\tau &= A^2 \int_{-\infty}^{\infty} (e^{-r/a_0})^2 d\tau \\ &= A^2 \int_{-\infty}^{\infty} \int_0^\pi \int_0^{2\pi} (e^{-r/a_0})^2 r^2 dr \sin\theta d\theta d\phi \\ &= 4\pi A^2 \int_{-\infty}^{\infty} (e^{-r/a_0})^2 r^2 dr \quad \because \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi = 4\pi\end{aligned}$$

since the radius of an atom doesn't have a negative value, we eliminate the negative limit

$$\begin{aligned}\int_{-\infty}^{\infty} |\Psi(r,t)|^2 d\tau &= 4\pi A^2 \int_0^{\infty} r^2 (e^{-r/a_0})^2 dr \\ &= 4\pi A^2 \frac{2}{(2/a_0)^3} \quad \because \int_0^{\infty} x^n (e^{-ax}) = \frac{n!}{a^{n+1}} \\ A &= \left(\frac{1}{\pi a_0^3} \right)^{1/2}\end{aligned}$$

Exercise 1.11 Consider the wave function of a particle in 1-D potential $\Psi = \frac{1}{\sqrt{a}} e^{-|x|/a}$ Find the probability from $-a$ to a .

Solution:

$$\begin{aligned}P_{-a \text{ to } a} &= \int_{-a}^a \left(\frac{1}{\sqrt{a}} e^{-|x|/a} \right)^2 dx \\ &= \frac{1}{a} \int_{-a}^a e^{-2|x|/a} dx \\ &= \frac{1}{a} \times 2 \int_0^a e^{-2|x|/a} dx \quad \because |x| \text{ is an even function.} \\ &= \frac{2}{a} \left[\frac{e^{-2|x|/a}}{-2/a} \right]_0^a \\ &= \frac{2}{a} \times \frac{-a}{2} [e^{-2} - 1] \\ &= [1 - e^{-2}]\end{aligned}$$

1.7.3 Second Postulate

"Corresponding to every observable physical quantity, there exists a Hermitian operator."

Every classically obtained dynamical variables such as energy, angular momentum, etc. can be replaced by a Hermitian operator that acts on the wavefunction. And the result of the operation is the desired quantity. The operator can be a matrix operator, a differential operator, an integral operator etc.

In general an operator is represented as, \hat{A} .

Operators corresponding to some dynamical variables

Position $= x$

Potential energy $= V(x)$

$$\begin{aligned}
 \text{Momentum } p_x &= -i\hbar \frac{\partial}{\partial x} \\
 \text{Kinetic energy} &= -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \\
 \text{Total energy} &= i\hbar \frac{\partial}{\partial t} \\
 \text{Hamiltonian} &= -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x)
 \end{aligned}$$

1.7.4 Third Postulate

The only measurable values of a physical observable A are the various eigenvalues of the corresponding operator \hat{A} .

Eigen values and Eigen function

The effect of an operator acting on an operand (Wavefunction) is such that the operand is only modified by a scalar constant. **The operand is the Eigen function of the operator, and the scalar constant is the eigen value.**

$$\hat{A}\phi_k = a_k\phi_k \quad (1.72)$$

Where $k = 1, 2, 3, \dots$ indexes the possible solutions.

ϕ_k = Eigen function.

a_k = Eigen value.

And the equation 1.72 is known as the eigen value equation.

Concisely eigenvalues and eigenfunctions of an operator are defined as the solutions of the eigenvalue problem. **If we are operating a momentum operator then the result of the operation i.e., the value of the momentum is given by the eigen value.**

Exercise 1.12 Find the eigen value corresponding to the operator, $\hat{A} = \frac{d^2}{dx^2}$ for the wavefunction $\Psi(x) = ae^{-2x}$.

Solution:

$$\begin{aligned}
 \hat{A} &= \frac{d^2}{dx^2} \quad ; \quad \Psi(x) = ae^{-2x} \\
 \hat{A}\Psi(x) &= \frac{d^2}{dx^2} (ae^{-2x}) \\
 &= 4ae^{-2x} = 4\Psi(x) \\
 \hat{A}\Psi(x) &= 4\Psi(x)
 \end{aligned}$$

Then 4 is the eigen value corresponding to the operator.

Exercise 1.13 An eigenfunction of the operator $\frac{d^2}{dx^2}$ is $\psi = e^{2x}$. Find the corresponding eigen value?

Solution:

$$\begin{aligned}
 \hat{A}\phi_k &= a_k\phi_k \\
 \hat{A}\phi_k &= \frac{d^2}{dx^2} (e^{2x}) = 4e^{2x}
 \end{aligned}$$

but $\phi_k = e^{2x}$

$$\hat{A}\phi_k = 4 \cdot \phi_k$$

Therefore eigen value of A is 4.

Properties of eigen functions

- The eigenfunctions of an operator are orthogonal functions. We will as well assume that they are normalized.
- The set of eigenfunctions forms a complete basis. This means that any other function can be written in terms of the set of eigenfunctions $\{\phi_k(\mathbf{x})\}$ of an operator A .

We have stated that set of eigenfunctions of a Hermitian operators forms a complete basis. ie every wavefunction $\Psi(x, t)$ can be written as a linear combination of the set of eigenfunctions $\{\phi_k(\mathbf{x})\}$.

$$\Psi(x) = \sum_i C_i \phi_i(\mathbf{x}) \quad (1.73)$$

Where C_i is a complex number in general.

We know that the only measurable values of a physical observable A are the various eigenvalues of the corresponding operator \hat{A} . If we operate \hat{A} on $\Psi(x)$ then the set of possible outcomes are the set of eigenvalues of \hat{A} . i.e $\{a_i\}$ Suppose we make a measurement of \hat{A} on $\Psi(x)$ and we obtain the eigenvalue a_j then it means that the wavefunction Ψ_x collapsed into $\phi_j(x)$. The probability of getting a particular eigenvalue on measurement is given by the

1.7.5 Fourth Postulate

The outcome of the measurement of an observable of a quantum mechanical system in a particular state is given by the expectation value of the corresponding operator in that state.

The expectation value of an operator \hat{A} , is defined as

$$\langle \hat{A} \rangle = \int_{-\infty}^{\infty} \Psi^*(x) \hat{A} \Psi(x) dx \quad (1.74)$$

Remember the wave function Ψ should be normalised before finding the expectation value.

1.7.6 Fifth Postulate

The wavefunction or state function of a system evolves in time according to the time-dependent Schrödinger equation

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

Where \hbar is the reduced Planck constant $\frac{h}{2\pi}$ (with h the Planck constant, allowing conversion from energy to frequency units).

$$\hbar = 1.054 \times 10^{-34} \text{ Js}$$

1.8 Uncertainty principle

Whenever we have some quantity which. can assume several values with various probabilities, it is customary to use the mean squared deviation as a measure of the 'width' of the probability distribution or in other words, the uncertainty in the value of the quantity. The uncertainty in the values of quantum mechanical observables also is defined in the same way. If A is an observable and $\langle A \rangle$ its expectation or mean value in the state ψ ,

$$\mathcal{A} \equiv A - \langle A \rangle$$

is the self-adjoint operator representing the deviation of A from its mean. The expectation value of \mathcal{A}^2 is the mean squared deviation; and the uncertainty in A (usually denoted by ΔA) is defined by

$$\begin{aligned}(\Delta A)^2 &= \langle \mathcal{A}^2 \rangle \\ &\equiv \langle (A - \langle A \rangle)^2 \rangle = \langle A^2 \rangle - \langle A \rangle^2\end{aligned}$$

The uncertainty depends on the state in which the system is. essential use of the positivity property. We apply it to the operator $\mathcal{A} - i\lambda \mathcal{B}$ where is defined by Eq. $\mathcal{A} \equiv A - \langle A \rangle$; \mathcal{B} is defined similarly as $\mathcal{B} \equiv B - \langle B \rangle$ and λ is a real parameter (not an operator). Noting that the adjoint of $(\mathcal{A} - i\lambda \mathcal{B})$ is $(\mathcal{A} + i\lambda \mathcal{B})$ since \mathcal{A} and \mathcal{B} are self-adjoint, we have

$$\langle (\mathcal{A} - i\lambda \mathcal{B})(\mathcal{A} + i\lambda \mathcal{B}) \rangle \geq 0$$

Expanding the product, keeping in mind that \mathcal{A} and \mathcal{B} may not commute. we simplify get

$$\langle \mathcal{A}^2 \rangle + \lambda^2 \langle \mathcal{B}^2 \rangle - \lambda \langle C \rangle \geq 0$$

Here C is the self-adjoint operator defined by

$$iC = [\mathcal{A}, \mathcal{B}] = [A, B]$$

The left hand side of $\langle \mathcal{A}^2 \rangle + \lambda^2 \langle \mathcal{B}^2 \rangle - \lambda \langle C \rangle \geq 0$ has its minimum value when its derivative with respect to λ is zero. This happens when

$$\lambda = \frac{\langle C \rangle}{2 \langle \mathcal{B}^2 \rangle}$$

For this value of λ

$$\begin{aligned}\langle \mathcal{A}^2 \rangle - \frac{\langle C \rangle^2}{4 \langle \mathcal{B}^2 \rangle} &\geq 0 \\ (\Delta A)^2 (\Delta B)^2 &\geq -\frac{1}{4} \langle [A, B] \rangle^2\end{aligned}$$

The equation gives the general statement of the uncertainty principle for any pair of observables A, B .

In particular, if A, B are a canonically conjugate pair of operators, which are characterized by

$$[A, B] = i\hbar$$

1.8.1 Heisenberg's Uncertainty principle

In classical physics, the future behavior of a physical system can be determined exactly if we are given the initial conditions and the forces acting on a system, then the position and velocity of the system can be uniquely determined by Newton's laws of motion. This makes Classical physics **Deterministic**. In quantum mechanical world the matterwaves associated with particle, unlike classical particles, spread over space and cannot be localized. Then classical concepts of exact position, exact momentum, and unique path of a particle therefore make no sense at the microscopic scale. This is the essence of Heisenberg's uncertainty principle.

Definition 1.8.1 Heisenberg's uncertainty principle states that: If the x -component of the momentum of a particle is measured with an uncertainty Δp_x , then its x -position cannot, at the same time, be measured more accurately than,

$$\Delta x \geq \frac{\hbar}{2(\Delta p_x)}.$$

The three-dimensional form of the uncertainty relations for position and momentum can be written as follows:

$$\Delta x \Delta p_x \geq \frac{\hbar}{2} \quad ; \quad \Delta y \Delta p_y \geq \frac{\hbar}{2} \quad ; \quad \Delta z \Delta p_z \geq \frac{\hbar}{2}.$$

This principle indicates that, **although it is possible to measure the momentum or position of a particle accurately, it is not possible to measure these two observables simultaneously to an arbitrary accuracy.** That is, we cannot localize a microscopic particle without giving to it a rather large momentum. We cannot measure the position without disturbing it; there is no way to carry out such a measurement passively as it is bound to change the momentum.

Heisenberg's uncertainty principle can be generalized to any pair of complementary, or canonically conjugate, dynamical variables.

Note Canonically conjugate variables:

Canonically conjugate variables are pair of physical variables describing a physical system such that their commutator is a nonzero constant. The x component of the position of a particle and the y component of the momentum are not canonically conjugate to each other. x with p_x , y with p_y and so on are canonically conjugate variables.

1.8.2 Time - Energy Uncertainty relation.

The time-energy uncertainty principle states that, In any simultaneous determination of time and energy of a moving particle, the product of the uncertainties is greater or equal to the Planck's constant,

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

Here, ΔE is the uncertainty in the measurement of energy of Δt , the corresponding uncertainty in the measurement of time.

1.8.3 Angular momentum- angular position Uncertainty Relation.

$$\Delta L \Delta \theta \geq \frac{\hbar}{2}$$

Where, ΔL is the uncertainty in the angular momentum of the particle and $\Delta \phi$ is the uncertainty in the angular position of the particle.

Exercise 1.14 Estimate the uncertainty in the position of (a) a neutron moving at $5 \times 10^6 \text{ m s}^{-1}$ and (b) a 50 kg person moving at 2 m s^{-1} . ■

Solution: According to the position-momentum uncertainty relation,

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

$$\begin{aligned} \text{(a.) } \Delta x &\geq \frac{\hbar}{2\Delta p} \simeq \frac{\hbar}{2m_n v} \\ &= \frac{1.05 \times 10^{-34} \text{ J s}}{2 \times 1.65 \times 10^{-27} \text{ kg} \times 5 \times 10^6 \text{ m s}^{-1}} \\ &= 6.4 \times 10^{-15} \text{ m.} \end{aligned}$$

This distance is comparable to the size of a nucleus.

$$\text{(b.) } \Delta x \geq \frac{\hbar}{2\Delta p} \simeq \frac{\hbar}{2mv}$$

$$\begin{aligned}
 &= \frac{1.05 \times 10^{-34} \text{ J s}}{2 \times 50 \text{ kg} \times 2 \text{ m s}^{-1}} \\
 &= 0.5 \times 10^{-36} \text{ m}
 \end{aligned}$$

1.9 Probability current density

As the time changes from $t = 0$, the probability of finding the particle in some region of space may increase or decrease. If the probability increases in some region, then it should decrease in some other region such that total probability of finding the particle in the entire space should be equal to one. We can assume this as a flow of probability from one region to another region, like a fluid or current. Therefore, the probability flow satisfies the equation of continuity i.e.

$$\vec{\nabla} \cdot \vec{J} + \frac{\partial \rho}{\partial t} = 0$$

where ρ = probability density
and \vec{J} = probability current density

$$J = -\frac{i\hbar}{2m} \left[\psi^* \vec{\nabla} \psi - \psi \vec{\nabla} \psi^* \right]$$

The magnitude of probability current density represents the flux of the particles i.e number of particles passing through per unit area per unit time and the direction of probability current density is along the direction of flow of the particles.

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Practice set 1

1. Let v , p and E denote the speed, the magnitude of the momentum, and the energy of a free particle of rest mass m . Then

[NET DEC 2012]

- A. $dE/dp = \text{constant}$ B. $p = mv$
 C. $v = cp/\sqrt{p^2 + m^2c^2}$ D. $E = mc^2$

2. If a particle is represented by the normalized wave function

$$\psi(x) = \begin{cases} \frac{\sqrt{15}(a^2 - x^2)}{4a^{5/2}}, & \text{or } -a < x < a \\ 0 & \text{, otherwise} \end{cases}$$

the uncertainty Δp in its momentum is

[NET DEC 2012]

- A. $2\hbar/5a$ B. $5\hbar/2a$
 C. $\sqrt{10}\hbar/a$ D. $\sqrt{5}\hbar/\sqrt{2}a$

3. The energies in the ground state and first excited state of a particle of mass $m = \frac{1}{2}$ in a potential $V(x)$ are -4 and -1 , respectively, (in units in which $\hbar = 1$). If the corresponding wavefunctions are related by $\psi_1(x) = \psi_0(x) \sinh x$, then the ground state eigenfunction is

[NET DEC 2012]

- A. $\psi_0(x) = \sqrt{\sec hx}$ B. $\psi_0(x) = \sec hx$
 C. $\psi_0(x) = \text{sech}^2 x$ D. $\psi_0(x) = \sec h^3 x$

4. If $\psi(x) = A \exp(-x^4)$ is the eigenfunction of a one dimensional Hamiltonian with eigen value $E = 0$, the potential $V(x)$ (in units where $\hbar = 2m = 1$) is

[NET DEC 2013]

- A. $12x^2$ B. $16x^6$
 C. $16x^6 + 12x^2$ D. $16x^6 - 12x^2$

5. A particle of mass m moves in one dimension under the influence of the potential $V(x) = -\alpha\delta(x)$, where α is a positive constant. The uncertainty in the product $(\Delta x)(\Delta p)$ in its ground state is

[NET JUNE 2016]

- A. $2\hbar$ B. $\frac{\hbar}{2}$
 C. $\frac{\hbar}{\sqrt{2}}$ D. $\sqrt{2}\hbar$

6. Consider the two lowest normalized energy eigenfunctions $\psi_0(x)$ and $\psi_1(x)$ of a one dimensional system. They satisfy $\psi_0(x) = \psi_0^*(x)$ and $\psi_1(x) = \alpha \frac{d\psi_0}{dx}$, where α is a real constant. The expectation value of the momentum operator in the state ψ_1 is

[NET DEC 2016]

- A. $-\frac{\hbar}{\alpha^2}$ B. 0
 C. $\frac{\hbar}{\alpha^2}$ D. $\frac{2\hbar}{\alpha^2}$

7. A particle in one dimension is in a potential $V(x) = A\delta(x-a)$. Its wavefunction $\psi(x)$ is continuous everywhere. The discontinuity in $\frac{d\psi}{dx}$ at $x = a$ is

[NET DEC 2016]

A. $\frac{2m}{\hbar^2} A \psi(a)$

B. $A(\psi(a) - \psi(-a))$

C. $\frac{\hbar^2}{2m} A$

D. 0

8. The normalized wavefunction of a particle in three dimensions is given by $\psi(r, \theta, \phi) = \frac{1}{\sqrt{8\pi a^3}} e^{-r/2a}$ where $a > 0$ is a constant. The ratio of the most probable distance from the origin to the mean distance from the origin, is [You may use $\int_0^\infty dx x^n e^{-x} = n!$]

[NET DEC 2017]

A. $\frac{1}{3}$

B. $\frac{1}{2}$

C. $\frac{3}{2}$

D. $\frac{2}{3}$

9. The normalized wavefunction in the momentum space of a particle in one dimension is $\phi(p) = \frac{\alpha}{p^2 + \beta^2}$, where α and β are real constants. The uncertainty Δx in measuring its position is

[NET DEC 2017]

A. $\sqrt{\pi} \frac{\hbar \alpha}{\beta^2}$

B. $\sqrt{\pi} \frac{\hbar \alpha}{\beta^3}$

C. $\frac{\hbar}{\sqrt{2}\beta}$

D. $\sqrt{\frac{\pi}{\beta}} \frac{\hbar \alpha}{\beta}$

10. The product $\Delta x \Delta p$ of uncertainties in the position and momentum of a simple harmonic oscillator of mass m and angular frequency ω in the ground state $|0\rangle$, is $\frac{\hbar}{2}$. The value of the product $\Delta x \Delta p$ in the state, $e^{-i\hat{p}\ell/\hbar} |0\rangle$ (where ℓ is a constant and \hat{p} is the momentum operator) is

[NET DEC 2018]

A. $\frac{\hbar}{2} \sqrt{\frac{m\omega\ell^2}{\hbar}}$

B. \hbar

C. $\frac{\hbar}{2}$

D. $\frac{\hbar^2}{m\omega\ell^2}$

Answer key

Q.No.	Answer	Q.No.	Answer
1	c	2	d
3	c	4	d
5	c	6	b
7	a	8	d
9	c	10	c

Practice set 2

1. Which of the following is an allowed wavefunction for a particle in a bound state? N is a constant and $\alpha, \beta > 0$.

[GATE 2010]

A. $\psi = N \frac{e^{-\alpha r}}{r^3}$

B. $\psi = N(1 - e^{-\alpha r})$

C. $\psi = N e^{-\alpha x} e^{-\beta(x^2+y^2+z^2)}$

D. $\psi = \begin{cases} \text{non - zero constant} & \text{if } r < R \\ 0 & \text{if } r > R \end{cases}$

Common data questions for 2 and 3

The wavefunction of particle moving in free space is given by, $\psi = (e^{ikx} + 2e^{-ikx})$

2. The energy of the particle is

[GATE 2012]

A. $\frac{5\hbar^2 k^2}{2m}$

B. $\frac{3\hbar^2 k^2}{4m}$

C. $\frac{\hbar^2 k^2}{2m}$

D. $\frac{\hbar^2 k^2}{m}$

3. The probability current density for the real part of the wavefunction is

A. 1

B. $\frac{\hbar k}{m}$

C. $\frac{\hbar k}{2m}$

D. 0

4. Consider the wave function $Ae^{ikr}(r_0/r)$, where A is the normalization constant. For $r = 2r_0$, the magnitude of probability current density up to two decimal places, in units of $(A^2 \hbar k/m)$ is

[GATE 2013]

5. The recoil momentum of an atom is p_A when it emits an infrared photon of wavelength 1500 nm, and it is p_B when it emits a photon of visible wavelength 500 nm. The ratio $\frac{p_A}{p_B}$ is

[GATE 2014]

A. 1 : 1

B. 1 : $\sqrt{3}$

C. 1 : 3

D. 3 : 2

6. The state of a system is given by $|\psi\rangle = |\phi_1\rangle + 2|\phi_2\rangle + 3|\phi_3\rangle$, where $|\phi_1\rangle$, $|\phi_2\rangle$ and $|\phi_3\rangle$ form an orthonormal set. The probability of finding the system in the state $|\phi_2\rangle$ is

[GATE 2016]

7. The Compton wavelength of a proton is fm. (up to two decimal places).

[GATE 2017]

8. Consider a one-dimensional potential well of width 3 nm. Using the uncertainty principle ($\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$), an estimate of the minimum depth of the well such that it has at least one bound state for an electron is ($m_e = 9.31 \times 10^{-31}$ kg, $h = 6.626 \times 10^{-34}$ J.s, $e = 1.602 \times 10^{-19}$ C)

[GATE 2017]

A. 1 μ eV

B. 1 meV

C. 1 eV

D. 1 MeV

9. The Hamiltonian for a quantum harmonic oscillator of mass m in three dimensions is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 r^2$$

where ω is the angular frequency. The expectation value of r^2 in the first excited state of the oscillator in units of $\frac{\hbar}{m\omega}$ (rounded off to one decimal place) is

[GATE 2018]

10. Consider the motion of a particle along the x - axis in a potential $V(x) = F|x|$. Its ground state energy E_0 is estimated using the uncertainty principle. Then E_0 is proportional to

[GATE 2019]

A. $F^{1/3}$

B. $F^{1/2}$

C. $F^{2/5}$

D. $F^{2/3}$

Answer key			
Q.No.	Answer	Q.No.	Answer
1	c	2	c
3	d	4	0.25
5	c	6	0.28
7		8	b
9	2.5	10	d

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Practice set 3

1. Consider the Gaussian probability distribution $f(x) = Ae^{-\lambda(x-a)^2}$ where $-\infty < x < \infty$ where A, a and λ are positive real constants.
- (a) Determine A such that $f(x)$ is probability density
- (b) Find $\langle x \rangle, \langle x^2 \rangle$ and $\sigma = \Delta x$

Solution: (a)

$$f(x) = Ae^{-\lambda(x-a)^2} \Rightarrow \int_{-\infty}^{\infty} f(x) dx = 1$$

$$A \int_{-\infty}^{\infty} e^{-\lambda(x-a)^2} dx = 1 \Rightarrow A \int_{-\infty}^{\infty} e^{-\lambda t^2} dt = 1 \Rightarrow A \cdot 2 \cdot \int_0^{\infty} e^{-\lambda t^2} dt = 1$$

$$A \times 2 \cdot \frac{1}{2} \frac{1}{\lambda^{1/2}} \Big|_{-\infty}^{\infty} = 1 \Rightarrow A = \left(\frac{\lambda}{\pi} \right)^{\frac{1}{2}}$$

(b)

$$\langle x \rangle = \int_{-\infty}^{\infty} x f(x) dx = \left(\frac{\lambda}{\pi} \right)^{\frac{1}{2}} \int_{-\infty}^{\infty} x e^{-\lambda(x-a)^2} dx$$

put $x-a = t \Rightarrow dx = dt$

$$\left(\frac{\lambda}{\pi} \right)^{\frac{1}{2}} \int_{-\infty}^{\infty} t e^{-\lambda t^2} dt + a \left(\frac{\lambda}{\pi} \right)^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{-\lambda t^2} dt = 0 + a$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 f(x) dx = \left(\frac{\lambda}{\pi} \right)^{\frac{1}{2}} \int_{-\infty}^{\infty} x^2 e^{-\lambda(x-a)^2} dx$$

$$\left(\frac{\lambda}{\pi} \right)^{\frac{1}{2}} \left[\int_{-\infty}^{\infty} t^2 e^{-\lambda t^2} dt + \int_{-\infty}^{\infty} 2at e^{-\lambda t^2} dt + \int_{-\infty}^{\infty} a^2 e^{-\lambda t^2} dt \right]$$

$$\langle x^2 \rangle = \frac{1}{2\lambda} + a^2$$

$$\sigma = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\frac{1}{2\lambda} + a^2 - a^2} = \frac{1}{\sqrt{2\lambda}}$$

2. Consider the function $\psi(x, t) = Ae^{-\lambda|x|}e^{-i\omega t}$ $-\infty < x < \infty$, where λ and ω are constant. Find the value of A such that $\psi(x, t)$ is normalized.

Solution:

$$\psi(x, t) = Ae^{-\lambda|x|}e^{-i\omega t}$$

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1 \Rightarrow |A|^2 \int_{-\infty}^{\infty} e^{-2\lambda|x|} dx = 1$$

$$|A|^2 2 \cdot \int_0^{\infty} e^{-2\lambda x} dx = 1 \Rightarrow A = \sqrt{\lambda}$$

3. (a) If $\phi_1(\theta, \phi) = A$ find the value of A such that $\phi_1(\theta, \phi)$ is normalized .
- (b) Prove that $\phi_2 = \sqrt{\frac{3}{4\pi}} \cos \theta$ is orthogonal to ϕ_1

Solution: The wave function $\phi_1(\theta, \phi) = A$ is defined in spherical symmetry variable is solid- angle

$$\int_0^{2\pi} \int_0^\pi \phi_1^* \phi_1 \sin \theta d\theta d\phi = 1$$

$$|A|^2 \int_0^{2\pi} \int_0^\pi \sin \theta d\theta d\phi = |A|^2 \cdot 4\pi = 1 \Rightarrow A = \frac{1}{\sqrt{4\pi}}$$

$$(b) (\phi_1, \phi_2) = \int_0^{2\pi} \int_0^\pi \phi_1^* \phi_2 \sin \theta d\theta d\phi = \int_0^{2\pi} \int_0^\pi \frac{1}{\sqrt{4\pi}} \cdot \sqrt{\frac{3}{4\pi}} \cos \theta \sin \theta d\theta d\phi = 0$$

4. A state function is given by

$$|\psi\rangle = |\phi_1\rangle + \frac{1}{\sqrt{2}} |\phi_2\rangle.$$

It is given that $\langle \phi_i | \phi_j \rangle = \delta_{ij}$

(a) write down normalized wavefunction $\langle \psi |$.

(b) It is given $H |\phi_n\rangle = (n+1)\hbar\omega |\phi_n\rangle \quad n = 0, 1, 2, 3, \dots$

If H will measured on $|\psi\rangle$, what will be measurement with what probability.

(c) Find the expectation value at H i.e., $\langle H \rangle$

(d) Find the error in the measurement in H .

Solution: (a) Now we need to find normalized $|\psi\rangle$ let A be normalization constant.

$$|\psi\rangle = A |\phi_1\rangle + \frac{1}{\sqrt{2}} |\phi_2\rangle$$

$$\langle \psi | \psi \rangle = A^2 + \frac{A^2}{2} = 1 \Rightarrow \frac{3A^2}{2} = 1 \Rightarrow A = \sqrt{\frac{2}{3}}$$

$$|\psi\rangle = \sqrt{\frac{2}{3}} |\phi_1\rangle + \frac{1}{\sqrt{3}} |\phi_2\rangle$$

$$\langle \psi | = \langle \phi_1 | \frac{2}{\sqrt{3}} + \langle \phi_2 | \frac{1}{\sqrt{2}}$$

(b) It is given that

$$H |\phi_n\rangle = (n+1)\hbar\omega \quad n = 0, 1, 2, 3, \dots$$

$$H |\phi_1\rangle = 2\hbar\omega$$

$$H |\phi_2\rangle = 3\hbar\omega$$

When H will measured $|\psi\rangle$ it will measured either $2\hbar\omega$ or $3\hbar\omega$ The probability of measured $2\hbar\omega$ is $P(2\hbar\omega)$ is given by

$$P(2\hbar\omega) = \frac{|\langle \phi_1 | \psi \rangle|^2}{\langle \psi | \psi \rangle} = \frac{2}{3}$$

$$P(3\hbar\omega) = \frac{|\langle \phi_2 | \psi \rangle|^2}{\langle \psi | \psi \rangle} = \frac{1}{3}$$

So when H will measure state $|\psi\rangle$ the following outcome will come.

Measurement of H on state : $|\phi_1\rangle \quad |\phi_2\rangle$

Measurement : $2\hbar\omega \quad 3\hbar\omega$

Probability : $2/3 \quad 1/3$

(c)

$$\begin{aligned}
 \langle H \rangle &= \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} = \sum_n P_n(a_n) a_n \\
 &= 2\hbar\omega \times \frac{2}{3} + 3\hbar\omega \times \frac{1}{3} \quad \langle H \rangle = \frac{7\hbar\omega}{3} \\
 \langle H^2 \rangle &= \frac{\langle \psi | H^2 | \psi \rangle}{\langle \psi | \psi \rangle} = \sum P_n(a_n) a_n^2 = \frac{2}{3} \times (2\hbar\omega)^2 + \frac{1}{3} \times (3\hbar\omega)^2 \\
 &= \frac{8\hbar^2\omega^2}{3} + \frac{9\hbar^2\omega^2}{3} = \frac{17\hbar^2\omega^2}{3}
 \end{aligned}$$

(d) The error in measurement in H is given as

$$\begin{aligned}
 \Delta H &= \sqrt{\langle H^2 \rangle - \langle H \rangle^2} = \frac{17\hbar^2\omega^2}{3} \\
 \langle H \rangle^2 &= \left(\frac{7\hbar\omega}{3} \right)^2 = \frac{49\hbar^2\omega^2}{9} \quad \Delta H = \sqrt{\frac{17}{3} - \frac{49}{9}} \hbar\omega \\
 \Delta H &= \sqrt{\frac{51-49}{9}} \hbar\omega = \frac{\sqrt{2}}{3} \hbar\omega
 \end{aligned}$$

5. A time $t = 0$ the state vector $|\psi(0)\rangle$

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}} (|\phi_1\rangle + |\phi_2\rangle)$$

It is given as Hamiltonian is defined as $H|\phi_n\rangle = n^2 \epsilon_0 |\phi_n\rangle$

- What is wave function $|\psi(t)\rangle$ at later time t .
- Write down expression of evolution of $|\psi(x,t)\rangle^2$
- Find ΔH
- Find the value of $\Delta H \cdot \Delta t$

Solution:

$$(a) |\psi(t)\rangle = \frac{1}{\sqrt{2}} \left[e^{\frac{-i\epsilon_0 t}{\hbar}} |\phi_1\rangle + e^{\frac{-i4\epsilon_0 t}{\hbar}} |\phi_2\rangle \right]$$

$$|\psi(t)\rangle \propto [|\phi_1\rangle + e^{-i\omega_{21}t} |\phi_2\rangle]$$

$$\text{Where } \omega_{21} = \frac{E_2 - E_1}{\hbar} = \frac{3\epsilon_0}{\hbar}$$

(b) Evolution of shape of the wave packet

$$|\psi(x,t)|^2 = \frac{1}{2} |\phi_1(x)|^2 + \frac{1}{2} |\phi_2(x)|^2 + \phi_1 \phi_2 \cos \omega_{21}t$$

(c)

$$\Delta H = (\langle H^2 \rangle - \langle H \rangle^2)^{1/2}$$

$$\langle H \rangle = \frac{1}{2} E_1 + \frac{1}{2} E_2 = \frac{5}{2} E_1 \quad \langle H^2 \rangle = \frac{1}{2} E_1^2 + \frac{1}{2} E_2^2 = \frac{17}{2} E_1^2$$

$$\Delta H = \frac{3}{2} E_1 \quad \Delta H = \frac{3}{2} \times \epsilon_0$$

$$(d) \Delta H = \frac{3}{2} \epsilon_0 \quad \Delta t = \frac{\hbar_1}{3\epsilon_0}$$

$$\Delta H \cdot \Delta t = \frac{3}{2} \epsilon_0 \times \frac{\hbar}{3\epsilon_0} = \frac{\hbar}{2}$$

