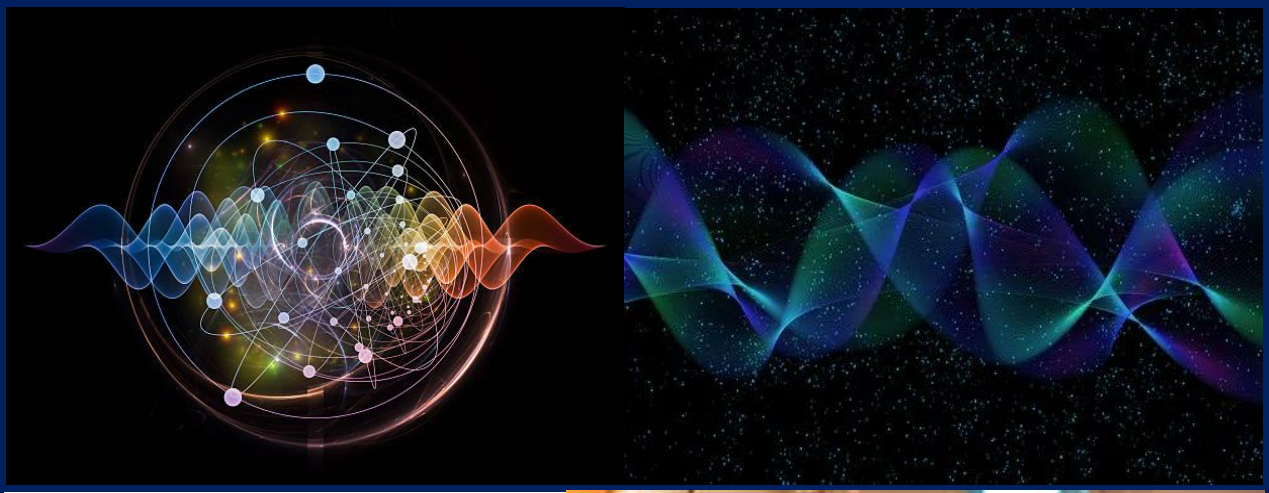
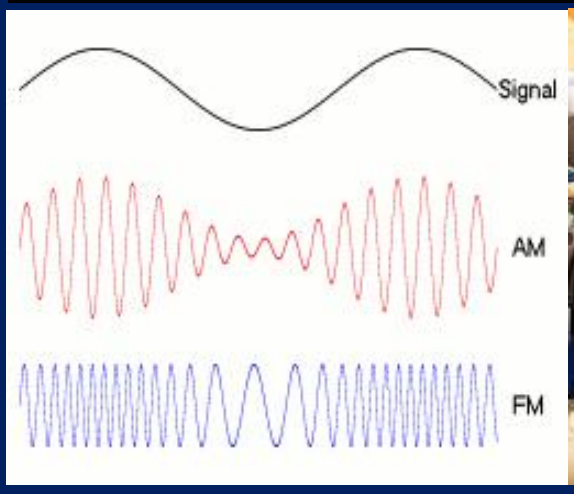
MSCPH-512

M. Sc. III SEMESTER

Advanced Quantum Mechanics





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Course Title and Code : **Advanced Quantum Mechanics (MSCPH-512)**
ISBN :
Copyright : **Uttarakhand Open University**
Edition : **2022**
Published By : **Uttarakhand Open University, Haldwani, Nainital- 263139**
Printed By :

Advanced Quantum Mechanics

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Credit: 3

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UNIT 1 SCATTERING THEORY

Structure

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1.1 INTRODUCTION

The scattering of waves and particles can be studied and understood in mathematics and physics using the scattering theory as a framework. When a wave collides and scatters with a physical object, such as sunlight reflected off of raindrops to create a rainbow, this is known as wave scattering. Billiard balls colliding on a table, alpha particle Rutherford scattering (or angle change) by gold nuclei, electron and X-ray Bragg scattering (or diffraction), and the inelastic scattering of a fission fragment as it passes through a thin foil are examples of other scattering phenomena. In more detail, the study of scattering focuses on how solutions to partial differential equations that were initially flowing freely "in the distant past" eventually congregate and interact with one another or with other objects.

Determining the distribution of scattered radiation or particle flow based on the characteristics of the scatterer is known as the "direct scattering problem." The inverse scattering problem is the problem of identifying an object's properties from measurements of radiation or particles scattered from it, such as its shape or internal composition.

Almost everything we know about nuclear and atomic physics has been discovered by scattering experiments, e.g., Rutherford's discovery of the nucleus, the discovery of sub-atomic particles (such as quarks), etc. In low energy physics, scattering phenomena provide the standard tool to explore solid state systems, e.g., neutron, electron, x-ray scattering, etc.

It therefore remains a key topic in any advanced quantum mechanics course.

1.1.1 Classical Theory of Scattering

The motion of a particle cannot be completely represented by classical orbits. In order to approach the scattering problem quantum mechanically, one must use wave packets whose average coordinates provide the classical orbits. As a result, wavefunctions, which are solutions to the Schrodinger equations, must be used to represent scattering rather than particle trajectories, which are solutions to the classical equation of motion.

If a classical description is to be applicable, one must be able without seriously altering any significant results, to obtain this classical description by scattering being determined by the magnitude of the force in the neighbourhood of the distance of closest approach, therefore the wave-packet must be narrower than this distance, otherwise there is no way of being sure that the particle experiences a definite predictable force from which deflection can be calculated in a classical way.

So, let's assume that the closest approach distance is of the same order of magnitude as the collision parameter '*b*' in order to determine the condition of validity of the classical approximation. The range of wavelengths must be $\leq b$, in order to generate a wave-packet smaller than *'b*'. From the principle of uncertainty $\Delta x \Delta p \geq \hbar/2$, the first requirement is that

the incident particle's momentum must be significantly greater than $p \approx \hbar/2b$. We will consider the momentum of the particle uncertain by a quantity much greater than $\delta p \approx \hbar/2b$ when defining the position of this packet. This uncertainty will cause the angle of deflection to be uncertain by a quantity much greater than $\delta p/p$.

In order to calculate deflection using classical methods, the uncertainty $\delta p/p$ must be far smaller than the deflection itself; else, the calculation will be meaningless. The criterion is equivalent to stating that because of momentum uncertainty, significantly less momentum must have been transferred as a result of the collision i.e.

$$\frac{\delta p}{\Delta p} \approx \frac{\hbar/2b}{\Delta p} = \frac{\hbar}{2b\,\Delta p} \leq 1 \qquad \ldots\ldots (1)$$

The classical orbital theory is applied to determine the value of Δp. The calculation is quite difficult for larger angles of scattering; however, we can apply classical perturbation theory for scattering at small angles. This theory is applicable only when the scattering angle is larger compared with quantum fluctuations but small compared with π.

1.2 *OBJECTIVES*

After studying this unit, you should be able to-

- define the scattering phenomenon
- understand differential cross section and total cross section
- define scattering amplitude
- understand partial wave analysis
- apply the optical theorem

1.3 THE SCATTERING PROBLEM

In an idealized scattering experiment, a sharp beam of particles (A) of definite momentum k are scattered from a localized target (B). As a result of collision, several outcomes are possible:

A + B $\longrightarrow$ A + B elastic

A + B$*$

A + B + C -inelastic

C - absorption

In high energy and nuclear physics, we are usually interested in deep inelastic processes. To keep our discussion simple, we will focus on elastic processes in which both the energy and particle number are conserved although many of the concepts that we will develop are general.

1.4 FORMULATION OF THE SCATTERING THEORY

The Schrodinger equation for central potential $V(r)$ is written as,

$$\left[-\frac{\hbar^2}{2m}\Delta^2 + V(r)\right]\psi = E\psi \qquad \text{….. (1)}$$

The complete time-dependent solution of above equation can be written as,

$$\begin{aligned}\psi(r,t) &= \psi(r)e^{-iEt/\hbar} \\ &= \left[e^{ik\cdot r} + \psi_s(r)\right]e^{-iEt/\hbar} \qquad \text{.....(2)} \\ \textit{where} \quad \psi_s(r) &= f(\theta,\phi)\frac{e^{ikr}}{r} + g(\theta,\phi)\frac{e^{-ikr}}{r}\end{aligned}$$

The first term in bracket of equation (2) represents the incident wave; while the second term $\psi_s(r)$, the scattered wave. The first term in $\psi_s(r)$, represents outgoing scattered wave, while the second term represents the incoming scattered wave which does not exist in most of the physical problems. The stationary slate solution of Schrodinger equation (1) is

$$\psi(r) = e^{ik.r} + \psi_s \qquad \text{….. (3)}$$

Comparing equation (1) with $(H^0 + \mathrm{H}')\cdot\psi = \mathrm{E}\psi$, we note that the perturbation operator is $V(r)$ which is very-very less than E; here H^0 is the unperturbed Hamiltonian. The unperturbed Schroedinger equation is therefore written as,

$$\left[-\frac{\hbar^2}{2m}\Delta^2 + E\right]e^{ik.r} = 0 \qquad \text{….. (4)}$$

Hence the Schrodinger equation is written as

$$\begin{aligned}\left(-\frac{\hbar^2}{2m}\nabla^2 - E\right)\psi_s &= -V(r)\left[e^{ik\cdot r} + \psi_s\right] \qquad \text{.....(5)} \\ &= -V(r)\psi(\mathbf{r}).\end{aligned}$$

This equation may be written as

$$(\nabla^2 + k^2)\psi_s = \frac{2m}{\hbar^2}V(r)\psi(r) \qquad \ldots\ldots(6)$$

Where, $k^2 = \frac{2mE}{\hbar^2}$

Further substituting,

$$(\nabla^2 + k^2)\psi_s = -4\pi\rho(r) \qquad \ldots\ldots(8)$$

$$\frac{2m}{\hbar^2}V(r)\psi(r) = -4\pi\rho(r) \qquad \ldots\ldots(7)$$

Equation (6) takes the form,

The quantity *ρ(r)* may be regarded as a source density for divergent spherical waves. Equation (8) may be solved by using principle of superposition. Accordingly, if ψ_{s1} and ψ_{s2} are solutions of equation (8) belonging to density functions $\rho_1(r)$ and $\rho_2(r)$ and satisfying,

$$\psi_{s1} = f1\frac{e^{ikr}}{r}, \psi_{s2} = f2\frac{e^{ikr}}{r} \qquad \ldots\ldots (9)$$

then the function $\psi = \psi_{s1} + \psi_{s2}$ is a solution of equation (8) belonging to

$\rho(r) = \rho_1(r) + \rho_2(r)$ such that

$$\psi_s = f\frac{e^{ikr}}{r}; \text{ where, } f = f1 + f2$$

By the principle of superposition, a solution of equation (9) can be obtained by adding solutions for simple point sources of unit strength.

The identity;

$$\rho(r) = \int \delta(r - r')\rho(r')d\mathbf{r}' \qquad \ldots\ldots(10)$$

represents the arbitrary density *ρ(r)* as a sum of point sources $\delta(\mathbf{r} - \mathbf{r}')$ at the point $\mathbf{r}'$

Now to express ψ_s as a function of *ρ(r),* we use the following theorem.

$$(\nabla^2 + k^2)G(\mathbf{r}, \mathbf{r}') = -4\pi\delta(\mathbf{r} - \mathbf{r}') \qquad \ldots\ldots(11)$$

$$G(\mathbf{r}, \mathbf{r}') = \frac{\exp(ik|\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|}$$

$G(\mathbf{r},\mathbf{r}')$ is called **Green's function**.

If $G(\mathbf{r},\mathbf{r}')$ is asymptotic to a function of r of the form (9), then solution of the scattering problem of density $\rho(\mathbf{r})$ is given by,

$$\psi_s = \int G(\mathbf{r},\mathbf{r}')\ \rho(\mathbf{r}')d\tau' \qquad \text{..... (12)}$$

The **Green's function;**

$$G(\mathbf{r},\mathbf{r}') = \frac{\exp(i\mathbf{k}|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|}$$

is a solution of the scattering problem for a source of unit strength at point $\mathbf{r}'$**.**

Hence the stationary state solution of Schrodinger equation (1) is given as

$$\psi(r) = e^{ik.r} + \int G(\mathbf{r},\mathbf{r}')\ \rho(\mathbf{r}')d\tau'$$

1.5 CROSS-SECTIONS

The scattering cross-section is a measurement that can be used to represent the probability that a particle will be scattered as it traverses through a given thickness of matter, *dx*. For doing this let us note that each molecule presents in the incident particle is coming to a target area πd^2, *d* being diameter of the molecule. This target area is just a cross-section of the area where a collision occur that can be seen along the path of incident particle beam. The idea of a **scattering cross section** comes now. The results of the collision experiments are expressed by means of cross section and directly related to the asymptotic behaviour of the stationary solutions of the Schrodinger equation.

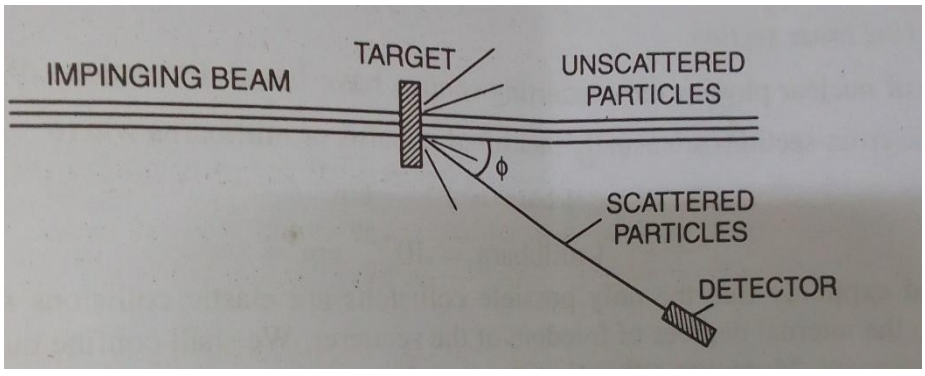

Fig. 1.1

Consider a typical experiment where a target is struck by a beam of mono-energetic particles, and the scattered particles are counted with the help of a detector. Let *J* be the magnitude of the incident flux i.e., the number of incident particles crossing per unit time a unit surface

area placed perpendicular to the direction of incident beam and at rest with respect to the target. If $\boldsymbol{\rho}$ is the number of particles per unit volume in the incident beam and **v** is the velocity of the incident particles, then $J = \boldsymbol{\rho}\,\mathbf{v}$

If ρ is small, that the mutual interaction of the incident particles can be neglected, then they undergo their collisions independently of each other. If *n* is the number of particles scattered per unit time into a solid angle $d\omega$ located in the direction (θ, ϕ)(polar coordinates), then *n* is directly proportional to the incident current *i.e.*

$$n \propto Jd\omega$$

$$\text{Or} \quad n = \sum(\omega)Jd\omega$$

where Σ(ω) is a proportionality constant which has dimension of surface area and is characteristic parameter of the collision of particle with target. It is known as *scattering cross-section of the particle and the target in the direction ω(θ, ϕ).*

1.5.1 Differential Scattering cross section

Let's now imagine that the target is made up of large number *N* of atomic or nuclear scattering centres, and that the distances between these atoms or nuclei are suitably big with respect to the incident particle's wavelength, as is seen in most real-world situations. Each scattering centre behaves as it were alone. In addition, if the target is thin enough, multiple scattering can be neglected, and in that case, *n* is directly proportional to *N* also i.e.$n \propto N$

So, in this case, $n \propto NJd\omega$

$$n = \sigma(\omega)NJd\omega$$

Here, $\sigma(\omega)$ is the constant of proportionality, has the dimension of surface area and is called the ***scattering cross-section*** of the particle by the scattering centre in the direction ω(θ,ϕ) or in brief the ***differential scattering cross-section.***

1.5.2 Total Scattering Cross-section

The total scattering cross-section is the total number of particles scattered in unit time is obtained by integrating *n* over all angles. It is equal to,

$$N_{total} = \int \sigma(\omega)NJd\omega = NJ\sigma_{total}$$

where $\sigma_{total} = \int \sigma(\omega)d\omega$

In the cases of nuclear physics, the scattering centres have linear dimensions of the order of 10^{-13} to 10^{-12} cm and the cross-sections are usually measured in barns or millibarns

1 barn =10^{-24} cm^2

And 1 millibarn $=10^{-27}$ cm^2

We have made the clear assumption that the only collisions that can occur are elastic collisions, in which no energy is transferred to the scatterer's internal degrees of freedom. For the time being, we shall confine our study to this type of collision. Additionally, we will treat the scatterer atom or nucleus by a static potential V(r) depending on the coordinate r of the particle.

1.5.3 Laboratory and centre of mass reference systems

The scattering of particles can be visualised in two kinds of coordinates:

1. Laboratory frame or system (L-system): It is that co-ordinate system in which the bombarded particle (or target) is initially at rest.
2. Centre of mass co-ordinate system (C-system): It is that coordinate system in which the centre of mass of two colliding particles is at rest (initially and always).

It is easy to calculate the result of collision experiment in the centre of mass system than the laboratory system, since there are three degrees of freedom in centre of mass system (C-system) and six degrees of freedom in laboratory system (L-system). Generally, calculations are made in C-system and observations are made in L -system. In C-system the reduced mass of two particles of masses m_1 and m_2 is;

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

So μ must remain at rest before and after collision in C- system.

1.6 SCATTERING AMPLITUDE (STATIONARY SCATTERING WAVE)

In wave mechanics, a plane wave in an incidence channel represents an incident beam of particles. Let's take into account the scattering of a particle of mass *m* by a central potential *V(***r***)* such that *V(***r***)* tends to zero more quickly than $\frac{1}{r}$ as $\mathbf{r} \to \infty$.

Let *E* be the particle's energy and $\boldsymbol{p} = \hbar \boldsymbol{k}$ starting momentum where $\boldsymbol{k}$ is the wave-vector. The Schrodinger equation central potential for *V(***r***)* is,

$$\left[-\frac{\hbar^2}{2m}\Delta^2 + V(\mathbf{r})\right]\psi_k(\mathbf{r}) = E\psi_k(\mathbf{r}) \qquad \ldots\ldots (1)$$

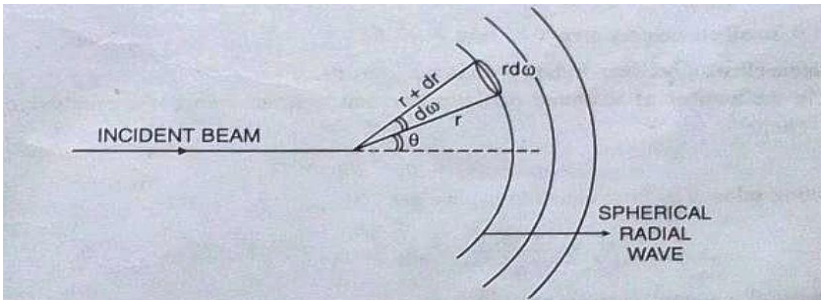

Fig. 1.2

The wave-function ψ_k may be written as a function of (r, θ, ϕ) where r is the radial distance between the two particles; i.e.

$$\psi_k = \psi_k(r,\theta,\phi)$$

The scattering is determined by the asymptotic form of $\psi_k(r,\theta,\phi)$ in the region where V= 0, when the colliding particles are far apart (or $\mathbf{r} \to \infty$). When we represent it, we want it to have two components: one part should represent an incident wave, and the other should represent a scattered radially outgoing wave i.e.

$$\psi_k(r,\theta,\phi) = \lim_{\mathbf{r}\to\infty} e^{i\mathbf{k}.\mathbf{r}} + f(\omega)\frac{e^{ikr}}{r} \qquad \ldots\ldots (2)$$

Let's assume that there is only one such solution for each value of **k**. We will call this the stationary scattering wave-vector **k**. The two terms of the asymptotic form are easily interpreted if we remember the definition of current density vector

$$\boldsymbol{J} = \frac{\hbar}{2im}(\psi^*\nabla\psi - \psi\nabla\psi^*) \qquad \ldots\ldots (3)$$

The plane wave term $e^{i\mathbf{k}.\mathbf{r}}$ represents a wave of unit density and of current density $\frac{\hbar k}{m}$. Keeping only the lowest order in r in mind, the term $f(\omega)\frac{e^{ikr}}{r}$ represents a wave of density $\frac{|f(\omega)|^2}{r^2}$ and of *current density* $\frac{|f(\omega)|^2}{r^2}\frac{\hbar k}{m}$ directed along the direction ω towards increasing r (outgoing-wave). In fact, since the effect of the potential V(r) can be neglected in the asymptotic region, therefore according to classical approximation we can interpret the term $e^{i\mathbf{k}.\mathbf{r}}$ as a beam of mono-energetic particles of momentum $\hbar k$ and of density 1, representing the incident beam and the term $\frac{f(\omega)}{r}e^{ikr}$ is interpreted as a beam of particles emitted radially from the scattering centre and represents a beam of the scattered particles.

In accordance with this interpretation, we can calculate the number of particles emitted per unit time into the solid angle dω located in the direction ω.

Density of scattered particle is

$$\rho_s = \left| f(\omega) \frac{e^{ikr}}{r} \right|^2 = \frac{1}{r^2} |f(\omega)|^2 \qquad \text{….. (4)}$$

If $f(\omega)\frac{e^{ikr}}{r}$ is the scattering wave- function.

From fig. 2 small elementary area $= r.rd\omega = r^2 d\omega$

The volume element between *r* and *r* + *dr* is equal to $r^2 d\omega . dr$

As ρ_s in the number of scattered particles per unit volume, hence the number of particles in this elementary volume,

$$N_s = \rho_s r^2 d\omega \, dr$$

Substituting value of ρ_s from equation (4), we get

$$N_s = \frac{1}{r^2} |f(\omega)|^2 r^2 d\omega \, dr = |f(\omega)|^2 \, dr d\omega \qquad \text{….. (5)}$$

∴ The number of scattered particles per unit time

$$\frac{dN_s}{dt} = |f(\omega)|^2 d\omega \, \frac{dr}{dt} = |f(\omega)|^2 \, dr \, v = |f(\omega)|^2 d\omega . \frac{\hbar k}{m}$$

$$= |f(\omega)|^2 \frac{\hbar k}{m} d\omega \qquad \text{….. (6)}$$

If J is the current density, then $J = \rho v$ …..(7)

Since beam of particles is travelling in the number of particles crossing unit area in the same direction with velocity *v*. The flux of the beam is the number of particles crossing unit area (perpendicular to the beam) per unit time. These are number of particles in a volume of unit cross-section.

But ρ=1 for incident particles.

$$J = v = \frac{\hbar k}{m} \qquad \text{….. (8)}$$

If σ (ω) is the scattering cross-section, then number of particles scattered in solid angle $d\omega$ per unit time is equal to $= J\sigma(\omega)d\omega$

Using equation (8), Number of particles scattered in solid angle $d\omega$ per unit time is

$$= \frac{\hbar k}{m} \sigma(\omega) d\omega \qquad \text{….. (9)}$$

Comparing equation (6) and (9) we get,

$$\frac{\hbar k}{m}\sigma(\omega)d\omega = |f(\omega)|^2\frac{\hbar k}{m}d\omega$$

$$\boldsymbol{\sigma(\omega) = |f(\omega)|^2} \qquad \text{..... (10)}$$

$\boldsymbol{f(\omega)}$ is called the ***Scattering amplitude.***

Total scattering cross section is,

$$\sigma_{\text{total}} = \int |f(\omega)|^2 d\omega. \qquad .....(11)$$

The wave-function ψ_k may be normalised by the relation,

$$\int \psi_k^* \psi_k d\tau = 1$$
$$\int |\psi_k|^2 d\tau = 1 \qquad .....(12)$$

across a large box with periodic boundary conditions.

Therefore, for finding out the normalization constant A, we must take the wave function as

$$\psi_k = \text{Lim}_{r\to\infty} A\left[e^{ik\cdot r} + f(\omega)\frac{e^{ikr}}{r}\right]. \qquad .....(13)$$

The wave-function may be normalised to unit incident flux by choosing,

$$A = \frac{1}{v^{1/2}} = \left(\frac{m}{\hbar k}\right)^{1/2};$$

For simplicity we often choose A equal to 1

The aforementioned argument is incorrect for two reasons:

(i) The incident plane wave current and the scattered wave current do not simply add up to produce the current density vector. The interaction $e^{ik.r}$ and $f(\omega)\frac{e^{ikr}}{r}$ terms
from the previous treatment must be added to these contributions. we intentionally ignored the interferences between incident and scattered waves.

(ii) $\psi_k(r)e^{-iEt/\hbar}$ is the idealised representation of stationary wave in physical situation. Each particle involved in the scattering process must really be represented by a wave-packet made by superimposing stationary waves of idealised form that correspond to wave-vectors with slightly varying magnitudes and directions from **k**. The initial conditions are correctly met by the way that this packet is built. Therefore, wave-packets are required to depict the scattering phenomenon.

1.7 PARTIAL WAVE ANALYSIS

The working out the higher perturbation theory is quite difficult. When the Born approximation fails, it is common to approach the scattering and collision problems using a completely new approach known as the method of partial waves. *The partial wave approach, which mostly applies to spherically symmetric potentials and consists of the expansion of the wave function as a series of spherical harmonics multiplied by a radial wave-function, as it would in the case of a hydrogen atom.* Rayleigh first used this technique to study the scattering of sound waves, and later Faxen and Holtsmark used it to study the scattering of Schrodinger waves. We first demonstrate that a plane wave is equivalent to the sum of a number of spherical waves before talking about scattering.

1.7.1 Plane Wave as the sum of spherical waves

The plane wave travelling along z-axis is given by

$$\psi = e^{ikz}$$

In spherical coordinates (r, θ, ϕ) with $z = r\cos\theta$, it may be expressed as

$$\psi = R(r)\Theta(\theta)\Phi(\phi)$$

$$= e^{ikr\cos\theta} \qquad \text{..... (1)}$$

This is a solution of spherical wave equation;

$$\nabla^2\psi + k^2\psi = 0, k^2 = \frac{2\mu E}{\hbar^2} \qquad \text{.....(2)}$$

μ is *the reduced mass* of the particles.

Substituting ψ=RΘΦ. R, Θ, Φ are the solutions of given separated equations;

$$\frac{d^2R}{dr^2}+\frac{2}{r}\frac{dR}{dr}+\left\{k^2-\frac{l(l+1)}{r^2}\right\}R=0 \qquad .....(3)$$

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\left\{l(l+1)-\frac{m^2}{\sin^2\theta}\right\}\Theta=0 \qquad .....(4)$$

$$\frac{d^2\Phi}{d\phi^2}+m^2\Phi=0 \qquad .....(5)$$

Every surface of constant phase in the plane wave is symmetrical about the direction of propagation (i.e. axis).

Therefore $\Phi(\phi)=$ constant.

This means that equation (5) has the only solution if m=0. It follows that the solution of (4) are Legendre polynomials

$$P_1^{(m=0)}(\cos\theta)=P_l(\cos\theta)$$

So, $\Psi=R(r)\,P_l(cos\theta)$ .....(6)

For $l = 0$, equation (3) can be expressed as

$$\frac{d^2}{dr^2}(rR_0)+k^2(rR_0)=0 \qquad .....(7)$$

$$R_0=A_0\frac{\sin kr}{kr}=A_0j_0(kr) \qquad .....(8)$$

Equation (8) is the solution of equation (7) where $j_0(kr)$is the spherical Bessel's function for $l = 0$.

This case $l = 0$ has strong analogy between equation (3) and Bessel's equation. If A_l are arbitrary constants, then the general solution of (2), having axial symmetry, may be expressed as

$$\psi=e^{ikz}=e^{ikr\cos\theta}=\sum_l R_l(r)P_l(\cos\theta)$$
$$=\sum_l A_l j_l(kr)P_l(\cos\theta) \qquad .....(9)$$

For large values of (kr), the asymptotic form of $j_l(kr)$ is,

$$j_l(kr)\underset{kr>>1}{\longrightarrow}\frac{1}{kr}\sin\left(kr-\frac{l\pi}{2}\right) \qquad .....(10)$$

The value of A_l may be obtained if we multiply both sides of (9) by $P_l(\cos\theta)$ and integrate over all θ Putting cos θ = x in (9) and using orthonormality conditions of $P_l(x)(m=0)$, we get

$$\int_{-1}^{+1} e^{ikrx} P_l(x)dx = \sum_m A_m j_m(kr) \int_{-1}^{+1} P_l(x)P_m(x)dx$$
$$= \sum_m A_m j_m(kr) \cdot \frac{2}{2m+1}\delta_{ml}$$
$$= \frac{2}{2l+1} A_l j_l(kr)$$

$$\text{i.e.} \quad \frac{2}{2l+1} A_l j_l(kr) = \frac{1}{ikr}\left[e^{ikrx} P_l(x)\right]_{-1}^{+1} - \left[\frac{1}{ikr}\int_{-1}^{+1} e^{ikrx} \cdot P_l'(x)dx\right]$$

The second term of R.H.S. in above equation is the order of $1/r^2$ for large values of r and so negligible. Therefore for large values of r, using $P_l(1) = 1$, $P_l(-1) = (-1)^l = e^{i\,l\,\pi}$ we get,

$$\frac{2}{2l+1} A_l \cdot \frac{1}{kr}\sin\left(kr - \frac{l\pi}{2}\right) \approx \frac{1}{ikr}\left[e^{ikr} - e^{il\pi} \cdot e^{-ikr}\right]$$
$$= \frac{1}{ikr} e^{il\pi/2}\left[e^{i}\left(kr - \frac{l\pi}{2}\right) - e^{-i}\left(kr - \frac{l\pi}{2}\right)\right]$$
$$= 2i^l \cdot \frac{1}{kr}\sin\left(kr - \frac{l\pi}{2}\right)$$

This gives,

$$A_i = (2l+1)i^l \qquad \ldots\ldots(11)$$

Therefore equation (9) becomes,

$$\psi = e^{ikz} = \sum_{l=0}^{\infty}(2l+1)i^l jl(kr)P_l(\cos\theta) \qquad \ldots\ldots(12)$$

where equation (10) provides the asymptotic form. According to equation (12), a plane wave is equivalent to the superposition of several spherical waves.

Let's take a look at the scattering problem by considering a plane wave incident along the z-axis in a region having interaction potential function $V(r)$. Then the total wave function may be expressed as

$$\psi(r) = e^{ikz} + f(\theta)\frac{e^{ikr}}{r} \qquad \ldots\ldots(13)$$

First term of the R.H.S. of equation (13) represents incident wave and second term represents scattered wave and equation (13) is a solution of three-dimensional Schrodinger's equation

$$\nabla^2\psi + \frac{2\mu}{\hbar^2}[E - V(r)]\psi = 0 \qquad \ldots\ldots(14)$$

The solution of equation(14) may be given as

$$\psi(r) = \sum_{l=0}^{\infty} R_l(r) Y_{lo}^{(\theta)} \qquad \ldots\ldots(15)$$

This is a superposition of a number of waves. Each term in above equation is called a **partial wave,** corresponding to a particular value of *l.* the function $R_l(r)$ are called radial wave function.

Substituting,

$$\frac{2\mu E}{\hbar^2} = k^2 \text{ and } \frac{2\mu V(r)}{\hbar^2} = U(r) \qquad \ldots\ldots(16)$$

Then equation(14) becomes,

$$\nabla^2\psi + \left[k^2 - U(r)\right]\psi = 0 \qquad \ldots\ldots(17)$$

As there is symmetry about polar axis i.e., z-axis (m = 0) and potential energy function does not involve ϕ, the solution of (17) may be expressed as

$$\psi(r, \theta, \phi) = \psi(r, \theta) = \sum_l R_l(r) P_l(\cos\theta) \qquad \ldots\ldots(18)$$

Setting,

$$\chi_l = rR_l(r) \qquad \ldots\ldots(19)$$

Equation (18) becomes,

$$\psi(r, \theta) = \sum_l r^{-1}\chi_l(r) P_l(\cos\theta) \qquad \ldots\ldots(20)$$

where $\chi_l(r)$ satisfies the equation,

$$\frac{d^2\chi_l}{dr^2} + \left[k^2 - U(r) - \frac{l(l+1)}{r^2}\right]\chi_l = 0 \qquad \ldots\ldots(21)$$

In order to find the general nature of asymptotic behaviour of this equation consider *r* to be so large that U and *l* terms in equation (21) may be ignored, so (21) becomes,

$$\frac{d^2\chi_l}{dr^2} + k^2\chi_l = 0$$

or

$$x_l = e^{\pm ikr} \qquad \ldots\ldots(22)$$

This only produces radial waves.

We define a distance "*a*" such that when $r > a$, *V(r) =0* and when $r < a$, *V(r)* is appreciably finite in order to obtain a better estimate, equation (21) then becomes,

$$\frac{d^2\chi_l}{dr^2} + \left[k^2 - \frac{l(l+1)}{r^2}\right]\chi_l = 0 \qquad \ldots\ldots(23)$$

The solution to this spherical Bessel equation (23) is given by,

$$\chi_l = A\sqrt{(kr)}J_{(l+l/2)} + B\sqrt{(\mathrm{kr})}J_{-l-1/2} \text{ if } l \neq 0 \text{ and } r \neq \infty$$

And

$$J_{l+1/2} = \left(\frac{2kr}{\pi}\right)^{1/2} J_l(kr)$$

$$J_{-l-1/2} = (-1)^{l+1}\left(\frac{2kr}{\pi}\right)^{1/2} \eta_l(kr),$$

$$where \qquad j_l(kr) = \frac{1}{kr}\cos\left\{kr - (l+1)\frac{\pi}{2}\right\}$$

$$= \mathrm{Lim}_{kr\to\infty}\frac{1}{kr}\sin\left(kr - \frac{l\pi}{2}\right)$$

$$\eta(kr) = \mathrm{Lim}_{kr\to\infty}\frac{1}{kr}\sin\left\{kr - \frac{(l+1)\pi}{2}\right\}$$

$$\chi_l = A'rj_l(kr) + B'r\eta_1(kr),$$

$$\frac{\chi_1}{r} = R_l(r) = A'j_l(kr) + B'\eta_l(kr) \qquad \ldots\ldots(24)$$

where A′ and B′ are new amplitudes which deviate from original amplitudes A and B. Let us take δ as phase angle between these amplitudes and put,

$$A' = A_l \cos\delta_l \quad \text{and} \quad B' = -A_l \sin\delta_l$$

$$or \qquad \tan\delta_l = -\frac{B'}{A'}.$$

$$R_l(r) = \frac{A_l}{kr}\left[\cos\delta_l \sin\left(kr - \frac{l\pi}{2}\right) - \sin\delta_l \sin\left\{kr - (l+1)\frac{\pi}{2}\right\}\right]$$
$$= \frac{A_l}{kr}\left[\cos\delta_l \sin\left(kr - \frac{l\pi}{2}\right) + \sin\delta_l \cos\left(kr - \frac{l\pi}{2}\right)\right]$$

Or $$R_l(r) = \frac{A_l}{kr} sin\left(kr - \frac{l\pi}{2} + \delta_l\right) \qquad \text{…..(25)}$$

In this equation δ_l is called the *phase shift* of the partial wave caused by scattering potential *V(r).* In view of this equation (18) becomes,

$$\psi(r,\theta) = \sum_l \frac{A_l}{kr}\sin\left(kr - \frac{l\pi}{2} + \delta_l\right) P_l(\cos\theta)$$
$$= \sum_l \frac{A_l}{kr}\left\{\frac{e^{i\left(kr - \frac{lx}{2} + \delta_l\right)} - e^{-i\left(kr - \frac{l\pi}{2} + \delta_l\right)}}{2i}\right\} \times P_l(\cos\theta) \qquad \ldots\ldots(26)$$

This equation is identical with asymptotic form of equation (13) i.e.

$$\psi = e^{ikz} + f(\theta)\frac{e^{ikr}}{r}$$
$$= \sum_l (2l+1) i^l \cdot \frac{1}{kr}\sin\left(kr - \frac{l\pi}{2}\right) P_l(\cos\theta) + f(\theta)\frac{e^{ikr}}{r}$$
$$= \sum_l (2l+1) i^l \cdot \frac{1}{kr}\left(\frac{e^{i\left(kr - \frac{lx}{2}\right)} - e^{-i\left(kr - \frac{l\pi}{2}\right)}}{2i}\right\} \times P_l(\cos\theta) + r^{-1} f(\theta) e^{ikr} \qquad \ldots\ldots(27)$$

Given that equations (26) and (27) are identical, comparing the coefficients of and from both equations yields,

$$\sum_l A_l \frac{e^i\left(-\frac{l\pi}{2} + \delta_l\right)}{2ikr} P_l(\cos\theta) = \sum_l \frac{(2l+1) i^l e^{-il\pi/2}}{2ikr} \cdot P_l(\cos\theta) + r^{-1} \cdot f(\theta) \qquad \ldots\ldots(28)$$

And

$$\sum_l A_l e^{-i}\left(-\frac{l\pi}{2}+\delta_l\right)\times P_l(\cos\theta)=\sum_l(2l+1)i^l e^{il\pi/2}\cdot P_l(\cos\theta) \qquad .....(29)$$

From equation (29),

$$A_l=(2l+1)i^l e^{i\delta_l}$$

Substituting this value of A_l in (28) we get,

$$\sum_l \frac{(2l+1)l^l e^{i\left(-\frac{l\pi}{2}+\delta_l\right)}}{2ikr}P_l(\cos\theta)=\sum_l\frac{(2l+1)i^l e^{-il\pi/2}}{2ikr}P_l(\cos\theta)+\frac{1}{r}f(\theta)$$

As $i^l = e^{i\,l\pi/2}$, we get

$$f(\theta)=(2ik)^{-1}\sum_{t=0}^{\infty}(2l+1)\left(e^{2i\delta_l}-1\right)P_l(\cos\theta) \qquad .....(31a)$$

$$=\frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\left(\frac{e^{i\delta_l}-e^{-i\delta_l}}{2i}\right)P_l(\cos\theta)$$

$$=\frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\left(\frac{e^{i\delta_l}-e^{-i\delta_l}}{2i}\right)P_l(\cos\theta)$$

$$=\frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\sin\delta_l P_l(\cos\theta) \qquad .....(31b)$$

The differential scattering cross-section is given by,

$$\sigma(\theta)=|f(\theta)|^2=\frac{1}{k^2}\left|\sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)e^{i\delta_l}\sin\delta_l\right|^2 \qquad .....(32)$$

The total elastic cross-section is the integral of equation (32) over the sphere, *i.e.*

$$\sigma_{\text{total}}=2\pi\int_0^{\pi}\sigma(\theta)\sin\theta d\theta$$

$$=\frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l \qquad .....(33)$$

$$\text{since}\int|P_l(\cos\theta)|^2\sin\theta d\theta=\frac{2}{(2l+1)}$$

Here δ_l the phase shift of l^{th} partial wave is unknown parameter and is to be evaluated.

1.8 OPTICAL THEOREM

A general law of scattering theory in physics known as the *optical theorem* relates the *forward scattering amplitude* to the *total cross section* of the scatterer.

It may be noted that the scattering amplitude is complex.

For $\theta = 0$, $P_l(cos\theta) = P_l(cos0^o) = P_l(1) = 1$ for all values of *l*.

Equation (31) gives for $\theta = 0$ gives,

$$f(0) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\, sin\delta_l\, P_l\, cos0)$$

$$= \frac{1}{k}\sum_{l}(2l+1)\, e^{i\delta_l}\, sin\delta_l$$

And so,

$$\boldsymbol{I_m f(0) = \frac{1}{k}\sum_{l}(2l+1)\, sin^2\delta_l}$$

Where, $I_m f(0)$ denotes the imaginary part of $f(0)$.

∴ From equation (33), the total elastic cross-section gives,

$$\boldsymbol{\sigma_{total} = \frac{4\pi}{k} I_m f(0)} \qquad \text{….. (34)}$$

This relation is a special case of a more general relation (including absorption) called the ***Optical theorem.*** It relates the *imaginary part of the forward scattering amplitude* (i.e., at $\theta = 0$) to the *total scattering cross-section*.

1.9 SUMMARY

In this unit, you have studied about the scattering of particles and wave. Also, we have discussed cross-section, differential cross-section and total cross-section. In Stationary scattering wave we got know the relation between scattering cross-section and scattering amplitude i.e., $\sigma(\omega) = |f(\omega)|^2$. Partial wave analysis suggest that plane wave is equivalent to the superposition of a number of spherical waves.

1.10 GLOSSARY

Scattering – The spreading of a stream of particles or a beam of rays

Cross-section – a cross section is the non-empty intersection of a solid body in three-dimensional space with a plane

Differential – an infinitesimal ("infinitely small") change in some varying quantity

Partial – part of the whole

Superposition – the ability of a quantum system to be in multiple states at the same time until it is measured.

Asymptotic – approaching a given value as an expression containing a variable tends to infinity

Phase angle – a measure in degrees of how much one wave leads another wave or lags behind that wave

Phase shift – The displacement of a waveform in time

Scattering amplitude – the probability amplitude of the outgoing spherical wave relative to the incoming plane wave in a stationary-state scattering process.

1.11 REFERENCES

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4. P.A. M. Dirac, The Principles of Quantum Mechanics, Oxford University Press, London

1.12 SUGGESTED READINGS

1. Advanced Quantum Mechanics, Franz Schwabl, Springer

2. Introduction to Quantum Mechanics, David J. Griffiths, Cambridge University Press

3. P.M. Mathews and K. Venkatesan, A Text book of Quantum Mechanics, Tata Mc Graw-Hill, New Delhi.

4. L.I. Schiff, Quantum Mechanics, McGraw-Hill

1.13 TERMINAL QUESTIONS

Short Answer Type Question

1. What do you understand by scattering cross-section? Deduce an expression for the scattering cross-section of particles by a spherically symmetric potential.
2. Define total and differential cross-section. Discuss on the basis of classical theory the scattering process when the angle of deflection is small.
3. Write the short:
   i. Scattering Amplitude
   ii. Optical Theorem

Long Answer Type Question

1. Describe the method of partial waves for the determination of the rigid scattering amplitude for scattering from the spherically symmetric potential.
2. Use method of partial waves to obtain scattering amplitude and cross-section. Show that the imaginary part of forward scattering amplitude is proportional to the total cross-section.
3. Describe and discuss the method of partial waves for an elastic scattering. Give the interpretation and deduce optical theorem.
4. Distinguish between incoming and outgoing waves. Deduce an expression for the total scattering cross-section of particles by a spherically symmetric potential.
5. What is meant by scattering cross-section? Show that the scattering amplitude by the method of partial waves is given by,
   $f(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\ sin\delta_l\ P_l cos\theta)$

UNIT 2 BORN APPROXIMATION

Structure

2.1 Introduction

2.2 Objectives

2.3 Born approximation

2.4 Born approximation and its validity

2.5 Phase shifts

2.5.1 Small Phase Shift

2.5.2 Phase shifts related to potential

2.6 Scattering length and effective range for the low energy scattering

2.6.1 Scattering length and effective range for short ranged potential V(*r)*

2.7 Summary

2.8 Glossary

2.9 References

2.10 Suggested Readings

2.11 Terminal Questions

2.1 INTRODUCTION

The Born approximation often involves substituting the incident field for the total field as the driving field at each point in the scatterer in scattering theory, and specifically in quantum mechanics. The Born approximation was first presented by Max Born in the beginning of the development of quantum theory. It uses the perturbation approach to account for extended body scattering. If the scattered field is small in comparison to the scatterer's incident field, it is accurate.

2.2 OBJECTIVES

After studying this unit, you should be able to-

1. Understand the Born approximation and its validity
2. What is phase shift and how to calculate it
3. Explain Scattering length and its importance in quantum mechanics.
4. Discuss scattering length and effective range for low energy scattering

2.3 BORN APPROXIMATION

The Born approximation can be used to determine the scattering amplitude $f(\theta, \phi)$) and therefore, the differential cross section $\sigma(\theta, \phi) = |f(\theta, \phi)|^2$,if the scattering occurs from localized, weak scattering centers that scattering does not occur far away from the scatterer.

When the potential function is fairly small, the Born approximation is applicable. The idea is simply that of successive approximations. *The Born approximation simply ignores the re-scattering of the scattered waves provided the scattered wave is small compared to the incident wave.*

The total wave-function of the scattering problem with source point at $\mathbf{r}''$ is given by,

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{m}{2\pi\hbar^2}\int G(\mathbf{r},\mathbf{r}'')V(\mathbf{r}'')\psi(\mathbf{r}'')d\tau'' \qquad .....(1)$$

Replacing r by r′ in above equation, we get

$$\psi(\mathbf{r}') = e^{i\mathbf{k}\cdot\mathbf{r}'} - \frac{m}{2\pi\hbar^2}\int G(\mathbf{r}',\mathbf{r}'')V(\mathbf{r}'')\psi(\mathbf{r}'')d\tau''$$

Substituting this value of ψ(**r′**) in the integral of equation representing the total wave-function with source point at **r′** i.e.,

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{m}{2\pi\hbar^2}\int G(\mathbf{r},\mathbf{r}')V(\mathbf{r}')\psi(\mathbf{r}')d\tau' \qquad .....(2)$$

We get,

$$\psi(\mathbf{r}) = e^{i\mathbf{k}.\mathbf{r}} - \frac{m}{2\pi\pi^2}\int G(\mathbf{r},\mathbf{r}')V(\mathbf{r}')e^{i\mathbf{k}.\mathbf{r}'}d\tau'$$
$$+\left(\frac{m}{2\pi\hbar^2}\right)^2\iint G(\mathbf{r},\mathbf{r}')V(\mathbf{r}')G(\mathbf{r}',\mathbf{r}'')V(\mathbf{r}'')d\tau''d\tau' \qquad .....(3)$$

The first iterated form of equation (2) is achieved by the iterative process in equation (3). This procedure is repeatable indefinitely, producing an infinite (Neumann) series that can be assumed to represent a solution provided the series converges. The series meaning is described below.

The first term $e^{i\,\mathbf{k}.\mathbf{r}}$ represents the incident wave-function while the remaining terms correspond to scattered wave-function. The first term in the scattered wave represents single scattering of the incident wave $e^{i\,\mathbf{k}.\mathbf{r}'}$ by the interaction $\boldsymbol{V}(\mathbf{r}')$ in the volume element $d\mathbf{r}'$. This produces a wave which travels from **r′** to the point of observation **r**, and the total wave arising from single scattering is obtained by integration over the region in which the force is effective. In the second term, the incident wave $e^{i\,\mathbf{k}.\mathbf{r}''}$ is scattered at the point r″, $[\boldsymbol{V}(\mathbf{r}'')e^{i\,\mathbf{k}.\mathbf{r}''}]$, travels to the point r′, $[\boldsymbol{G}(\mathbf{r}',\mathbf{r}'')\boldsymbol{V}(\mathbf{r}'')e^{i\,\mathbf{k}.\mathbf{r}''}]$ where it is again scattered and the travels from r′ to r. The total effect of all such scattering is obtained by integration over r″ and r′. Accordingly nth term represents the contribution of waves which have been scattered n-times in the region of interaction before travelling to the point r, where their total contribution is observed.

It may be anticipated that the Neumann series will converge quickly and that the first term in the series will provide an approximation to ψ if the interaction is weak, resulting in a scattering wave that is not too large. This is known as the *First-Born approximation*.

$$\psi = e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{m}{2\pi\hbar^2}\int G(\mathbf{r},\mathbf{r}')V(\mathbf{r}')e^{i\mathbf{k}\cdot\mathbf{r}'}d\tau' \qquad .....(4)$$

The n^{th} Born approximation is the equation where the Neumann series is terminated at the n^{th} term. The Born approximation, by its very nature, eliminates waves that have been multiplicatively scattered more than n-times as a result of the interaction.

Substituting asymptotic form of Green's function, we get

$$\psi = e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}\int e^{-i\mathbf{k}'\cdot\mathbf{r}'}V(\mathbf{r}')e^{ik\cdot\mathbf{r}'}d\tau' \qquad .....(5)$$

$$\psi = e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta,\phi)\frac{e^{ikr}}{r} \qquad .....(6)$$

Hence according to *first Born approximation*, scattering amplitude,

$$f(\theta,\phi) \approx -\frac{m}{2\pi\hbar^2}\int e^{i(k-k')\cdot r'}V(r')d\tau' \qquad .....(7)$$

So, the scattering cross-section is

$$\sigma(\theta,\phi) = \left(\frac{m}{2\pi\hbar^2}\right)^2\left|\int e^{i(k-k')\cdot r'}V(r')d\tau'\right|^2 \qquad .....(8)$$

2.4 CONDITION FOR VALIDITY OF BORN APPROXIMATION

The Born approximation will only be valid when the total wave function does not significantly different from the incident wave function $e^{i\mathbf{k}.\mathbf{r}}$**.** Therefore, it will be valid when the scattered wave $\psi_s(\mathbf{r})$ is small compared $e^{i\mathbf{k}.\mathbf{r}}$ in the region where $V(\mathbf{r})$ is large. In most cases both $V(\mathbf{r})$and $\psi_s(\mathbf{r})$are largest near the origin, so that a rough criterion for the validity of Born approximation is,

$|\psi_s(\mathbf{r})|^2 < 1$ for small values of **r.** ….. (9

The case, in which $\psi_s(\mathbf{r})$ is small when **r** is small but large for intermediate values of **r**, such that $V(\mathbf{r})$ is still considerable, we should apply the criterion carefully. The Born approximation still holds when the criterion is not satisfied. The Born approximation is valid if $\psi_s(\mathbf{r})$ is small everywhere, this is a sufficient condition although this is not a necessary condition.

We can define another criterion for the validity of the Born approximation if we keep in mind that a change in potential behaves similarly to a change in refractive index in optics. As a result, the wave function's phase changes as a result of the potential change. If the phase of the incident wave is not much changed as it passes through the region where it is influenced by the perturbing potential, the overall wave function will not significantly deviate from the starting wave function.

The magnitude of the wave vector at a distance is-

$k = \frac{\sqrt{(2mE)}}{\hbar}$ and near the centre of force it is $\frac{\sqrt{[2m(E-V)]}}{\hbar}$.

The change of phase due to the potential is then given by,

$$\Delta\phi = \int_0^\infty \sqrt{\left(\frac{2m}{n^2}\right)}[\sqrt{[(E-V)]} - \sqrt{E}]dr \qquad \ldots\ldots(10)$$

Implying that the wave function is not significantly different from that in the absence of the potential, if this change in phase is small compared to unity. The first order Born approximation will therefore be valid if,

$$|\Delta\phi| = \left|\sqrt{\left(\frac{2m}{\hbar^2}\right)}\int_0^\infty [\sqrt{(E-V)} - \sqrt{E}]dr\right| << 1 \qquad \ldots\ldots(11)$$

If $V << E$ the criterion may be simplified by expressing equation (11) as a function of the ratio V/E and expanding the square root. Then the criterion becomes,

$$\sqrt{\left(\frac{2mE}{\hbar^2}\right)}\left|\int_0^\infty \left\{\left(1-\frac{V}{E}\right)^{1/2} - 1\right\}dr\right| << 1 \qquad \ldots\ldots(12)$$

$$or \quad \sqrt{\left(\frac{2mE}{\hbar^2}\right)}\left|\int_0^\infty \left\{\left(1-\frac{V}{2E}+\ldots.\right) - 1\right\}dr\right| << 1$$

$$or \quad \sqrt{\left(\frac{2mE}{\hbar^2}\right)}\left|\int_0^\infty \frac{V}{2E}dr\right| << | \text{ since } \frac{V}{E} << 1$$

$$or \quad \sqrt{\left(\frac{m}{2\hbar^2 E}\right)}\left|\int_0^\infty V dr\right| << 1$$

$$or \quad \sqrt{\left(\frac{m}{2\hbar^2 E}\right)}\bar{V}\bar{r} << 1 \qquad \ldots\ldots(13)$$

where $\bar{r}$ is the mean range and $\bar{V}$ is the average potential.

In case, the scattering of high-energy particles by the square potential well with radius a and depth V_0, $V_0 << E$. From equation (13),

$$\sqrt{\left(\frac{m}{2\hbar^2 E}\right)}V_0 a < 1$$

$$E << \frac{m}{2}\left(\frac{V_0 a}{\hbar}\right)^2 \qquad \ldots\ldots(14)$$

Another explanation for the condition of validity of Born Approximation:

The scattered wave should be significantly smaller than the incident wave, which is the criteria for the validity of the Born approximation.

The mathematical representation,

$$|\psi_{sc}(\mathbf{r})| << |\psi_{in}| \text{ i.e. } |\psi_{sc}(\mathbf{r})| << \left|e^{\mathrm{ik.r}}\right| = 1$$
$$|\psi_{sc}(\mathbf{r})|^2 << 1$$

We know,

$$\psi_{sc}(\mathbf{r}) = f(\theta,\phi)\frac{e^{\mathrm{ikr}}}{r}$$

Where,

$$f(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\int e^{i(k-k')\cdot r'}V(r')d\tau'$$

$$\mathbf{k}-\mathbf{k}' = \mathbf{K}$$
$$\psi_{sc}(\mathbf{r}) = -\frac{m}{2\pi\hbar^2}\int e^{i\mathbf{K}\cdot\mathbf{r}'}V(\mathbf{r}')\frac{e^{ikr'}}{r'}d\tau$$

As, $r \to r'$

The intensity of scattered waves will be at its peak close to $r = 0$ or at the scattering centre because they are generally spherical waves and lose strength as they go away from it.

$$|\psi_{sc}(0)| = \left|-\frac{m}{2\pi\hbar^2}\int e^{i\mathbf{K}\cdot\mathbf{r}'}V(\mathbf{r}')d\tau'\frac{e^{ikr'}}{r'}d\tau'\right|$$

Thus, the condition of validity of Born approximation is,

$$|\psi_{sc}(0)|^2 = \left|\frac{m}{2\pi\hbar^2}\int\frac{e^{i(\mathbf{K}\cdot r'+kr')}V(r')d\tau'}{r'}\right|^2 << 1$$

If ***V*(r)** is spherically symmetric, then choosing **K** as polar axis, we can write,

$$d\tau' = dr'r'd\theta'r'\sin\theta'd\phi'$$
$$|\psi_{sc}(0)|^2 = \left(\frac{m}{2\pi\hbar^2}\right)^2\left|\int_0^a\int_0^\pi\int_0^{2\pi}e^{i(\mathbf{K}\cdot r'+kr')}\frac{V(\mathbf{r}')}{r'}r^2\sin\theta'd\theta'd\phi'\right| << 1$$

But,

$$\mathrm{K}.\,\mathbf{r}' = Kr'\cos\theta'$$

$$\int_0^{\pi} e^{iKr'\cos\theta'}\sin\theta' d\theta' = \int_{-1}^{+1} e^{iKr'p}dp = \left\{\frac{e^{iKr'p}}{iKr'}\right\}_{-1}^{+1}$$

$$= \frac{e^{iKr'} - e^{-iKr'}}{iKr'}$$

$$\int_0^{2\pi} d\phi = 2\pi$$

$$|\psi_{sc}(0)|^2 = \left(\frac{m}{2\pi\hbar^2}\right)^2 \left|\int_0^a e^{ikr'}V(r')\frac{e^{iKr'} - e^{-iKr'}}{iK}(2\pi)dr'\right|^2 << 1$$

Near scattering centre, the propagation vectors **K** and k of scattered and incident waves respectively are equal, so that

$$|\psi_{sc}(0)|^2 = \left(\frac{m}{\hbar^2 k}\right)^2 \left|\int_0^a \left(e^{2ikr'} - 1\right)V(r')dr'\right|^2 << 1$$

This is the condition for validity of Born approximation.

2.5 PHASE SHIFTS

Phase shift of the partial wave is caused by scattering potential.

We know that total scattering cross section is given by equation:

$$\sigma_{total} = 2\pi\int_0^{\pi}\sigma(\theta)\,sin\theta\,d\theta$$

$$= \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\,sin^2\delta_l$$

Here δ_l the phase shift of l^{th} partial wave is unknown parameter and is to be evaluated.

The scattering cross section vanishes for $\delta_l = 0$ or 180^0 and the cross section is maximum if the value of $\delta_l = \pm\frac{\pi}{2}, \pm\frac{3\pi}{2}$ etc.

The radial wave function $R(r) = \lim_{r\to\infty}\frac{A_l}{kr}\sin kr - \frac{lr}{2} - \delta_l$

So δ_l is the difference in phase between the asymptotic form of the actual radial function R(r) and the radial function $j_1(kr)$ in the absence of scattering potential (V=0). $j_1(kr)$ will be

maximum when r $\approx \frac{l}{k}$ hence for the value of r (we choose "a") r $\approx a \approx \frac{l}{k}$ we get higher phase difference (since V will vanish beyond 'a' i.e., $r > a$).

2.5.1 Small Phase Shift

The phase shift will be very small if $a << \frac{l}{k}$ .Thus the summation $\sum_{l=0}^{\infty}$ involves the summation of few terms such as $\sum_{l=0}^{l=ak}$.

Calculation of δ_l :

δ_l is calculated by applying boundary condition for the continuity of R_l at $r = a$ in the region $r < a$ and $r > a$

$$\left[\frac{1}{R_l}\frac{dR_l}{dr}\right]_{r<a}\Big|_{at\ r=a} = \left[\frac{1}{R_l}\frac{dR_l}{dr}\right]_{r>a}\Big|_{at\ r=a}$$

But

$$R_l = A_l[\cos\delta_l J_l(kr) - \sin\delta_i \eta_l(kr)]$$

$$so \quad \frac{1}{R_l}\frac{dR_l(r)}{dr} \mid r > a \mid \text{ at } r = a = k\frac{[\cos\delta_l j_l'(ka) - \sin\delta_l \eta_l'(ka)]}{\cos\delta_l j_l(ka) - \sin\delta_l \eta_l(ka)} \mid r > a$$

$$Let \qquad \frac{1}{R_l}\frac{dR_l}{dr} \mid r > a \mid \text{ at } r = a = \gamma_l.$$

$$\gamma_l = k\frac{[j_l'(ka) - \tan\delta_l \eta_l'(ka)]}{j_l(ka) - \tan\delta_l \eta_l(ka)}$$

$$\tan\delta_l = \frac{kj_l'(ka) - \gamma_l j_l(ka)}{k\eta_l'(ka) - \gamma_l \eta_l(ka)} \qquad \ldots\ldots(15)$$

$$j_l'(ka) = j_{l-1}(ka) - \frac{l+1}{ka} j_l(ka),$$

$$and \quad \eta_l'(ka) = \eta_{l-1}(ka) - \tfrac{l+1}{ka}\eta_l(ka)$$

Here γ_l is the ratio of slope to value of the interior wavefunction. Equation (15) can be used once to determine an expression for δ_l when l is large and δ_l anticipated to be small. In the absence of a scattering potential γ_l will differ little from the ratio of slope to value of the solution, in this case. Thus, we put,

$$\gamma_l = k\left[\frac{j_l'(ka)}{j_l(ka)} + \varepsilon_l\right] \qquad \ldots\ldots(16)$$

$$|\varepsilon_l| < \left|\frac{j_l'(ka)}{j_l(ka)}\right| \qquad \ldots\ldots(17)$$

Equation (15) can be written by changing j'_l into j_l so that,

$$\tan\delta_l = \frac{\varepsilon_l (ka)^2 j_l^2(ka)}{\varepsilon_l (ka)^2 j_l(ka)\eta_l(ka) - 1} \qquad \ldots\ldots(18)$$

Which is still exact.

If now we make use of the power series equation for j_l when $l > (ka)^2$ and use the value of j_l in terms of sine and cosine, the inequality (17) becomes,

$$|\varepsilon_l| < \frac{1}{ka}$$

And equation (18) may be approximated as,

$$\delta_l = \frac{\varepsilon_l (ka)^{2l+2}}{[(2l+1)!]^2} = -\frac{\varepsilon_l 2^{2l}(l!)^2 (ka)^{2l+2}}{[(2l+1)!]} \qquad \ldots\ldots(19)$$

By Stirling's formula, we get

$$\log|\delta_1| \approx \log|\varepsilon_l| = 2l[\log(ka) + 1 + \log 2] - 2l\log l$$

The following are explanations regarding δ_l.

(i) $\delta_l > 0$ *for attractive field*

$\delta_l < 0$ *for repulsive field*

(ii) For large *k* and *l*, the phase shift can be calculated by the Born approximation it becomes,

$$\delta_l = -\frac{1}{2k} U(r_0) r_0$$

where r_0 is the classical distance of closest approach. For large *l*, r_0, ρ = impact parameter. The series for total cross-section behaves like

$$\sigma \propto \Sigma(2l+1)\delta_l^2 = \frac{1}{4}\int_0^\infty dp \cdot \rho^3 U^2(\rho)$$

As

$$p\rho = \hbar k\rho.$$

In order that this may converge *U(r)* must decrease with distance at a rate faster than $1/r^2$.

(iii). For a scattering amplitude in forward direction, $f(0)$ will have the form

$$f(0) \propto \Sigma(2l+1)\delta_l \to k\int_0^\infty dp \cdot \rho^3 U(\rho).$$

In order that it may converge $U(\rho)$ must decrease with distance faster than $1/r^3$.

(iv). For low energy scattering by a potential of the asymptotic form c/r^n , the variations of the phase shifts for various l are

$$\begin{aligned} &\delta_l \propto k^{2l+1} && \text{for} \quad 2l < n-3, \\ &\delta_l \propto k^{2l+2} \log k && \text{for} \quad 2l = n-3, \\ &\delta_l \propto k^{n-2} && \text{for} \quad 2l > n-3, \end{aligned}$$

2.5.2 Phase shifts related to potential

The radial equation must be fully solved in order to obtain the phase shift precisely because it solely depends on the asymptotic form of R_l. Certain potentials make this feasible, however in general, some significant information can be inferred regarding δ_l. We compare the function χ_l with the corresponding function $\chi_l^0 \propto r\, j_l(kr)$ to represent the phase shift in terms of the potential; when potential $V = 0$ the relevant equations are

$$\frac{d^2\chi_l}{dr^2} + \left[k^2 - U(r) - \frac{l(l+1)}{r^2}\right]\chi_l = 0 \qquad \ldots\ldots (20)$$

$$\frac{d^2\chi_l(0)}{dr^2} + \left[k^2 - \frac{l(l+1)}{r^2}\right]\chi_l^{(0)} = 0; \text{ with } \chi_l^{(0)} \propto r j_l(kr) \qquad \ldots\ldots (21)$$

multiplying equation (20) by χ_l^0 and (21) by χ_l and then subtracting, we get

$$\chi_l^{(0)}\frac{d^2\chi_l}{dr^2} - \chi_l\frac{d^2\chi_l^{(0)}}{dr^2} - U(r)\chi_l^{(0)}\chi_l = 0$$

$$\frac{d}{dr}\left[\chi_l^{(0)}\frac{d\chi_l}{dr} - \chi_l\frac{d\chi_l^{(0)}}{dr}\right] - U(r)\chi_l^{(0)}\chi_l = 0 \qquad \ldots\ldots (22)$$

Integrating with respect to r, from limits 0 to r, and remembering that χ_l and χ_0^0 vanish at the origin $r = 0$; we get

$$\left\{\chi_l^0\frac{d\chi_l}{dr} - \chi_l\frac{d\chi_l^0}{dr}\right\} - \int_0^r U(r')\chi_l^0(r')\chi_l(r')dr' = 0 \qquad \ldots\ldots (23)$$

It is clear that this relation is independent of χ and χ_l^0. Let us normalize χ and χ_l^0 so that their asymptotic constant is unity, i.e., at $r \to \infty$ we have,

$$\chi_l \to \sin(kr + \Delta l) \text{ and } \chi_l^{(0)} \to \sin\left(kr - \frac{1}{2}\pi\right) \qquad \ldots\ldots (24)$$

This means that,

$$\chi_l^{(0)} = kr j_l(kr);$$

then the bracketed term in (23) (for r→∞) may be expressed as

$$k\sin\left(kr-\tfrac{l\pi}{2}\right)\cos(kr+\Delta l)-\sin(kr+\Delta l)\cos\left(kr-\tfrac{l\pi}{2}\right)$$
$$=-k\sin\left(\frac{l\pi}{2}+\Delta l\right)=-k\sin\delta_l$$

Thus, at r→∞, equation (23) becomes,

$$k\sin\delta_l=\int_0^\infty V(r')\chi_l^0(r')\chi_l(r')dr'$$

$$\sin\delta_l=-\int_0^\infty V(r)rj_l(kr)\chi_l(r)dr \qquad .....25$$

This expression for the phase shift is exact, but is purely formal since χ_l(r) for all values of *r* is not known. However, it is important for an approximate evaluation. Assume, for instance, that χ_l barely differs from

$$\chi_l^{(0)}=krj_l(kr)$$

Then,

$$\sin\delta_l=-k\int_0^\infty U(r)r^2j_l^2(kr)dr \qquad .....(26)$$

This is **Born approximation for phase shifts**. For the approximation to be valid, it is necessary that the potential term *U*(*r*) in equation (20) is very small. This is only possible if either the kinetic energy term k^2 or the centrifugal potential term dominates over U(*r*). In the former case δ_l is expected to be small for all *l* & then we can take,

$$\left(e^{2i\delta_l}-1\right)\rightarrow 2i\delta_l\approx 2i\sin\delta_l$$

Substituting this in, $f(\theta)=(2ik)^{-1}\sum_{l=0}^{\infty}(2l+1)(e^{2i\delta_l}-1)P_l(cos\theta)$

We get,

$$f(\theta)=-\sum_{l=0}^{\infty}(2l+l)\int_0^\infty U(r)r^2j_l^2(kr)drP_l(\cos\theta)$$

This reduces to Born approximation formula.

2.6 SCATTERING LENGTH AND EFFECTIVE RANGE THEORY FOR LOW ENERGY SCATTERING

At low energies, the partial wave approach is of special interest if the incident beam's energy is so low that $ka < 1$ where a is the range of potential, then the only $l = 0$ or s-wave is scattered. In the region with non-zero potential, all other partial waves are so small that they don't change. The scattering amplitude for s-wave is given by,

$$f(\theta) = \frac{1}{k} e^{i\delta_0} \sin\delta_0 \qquad \ldots\ldots(1)$$

We observe that the scattering is isotropic at the centre of the small reference system because the scattering amplitude is independent θ of ϕ and. The total scattering cross-section, naturally,

$$\rho_{\text{total}} = \frac{4\pi}{k^2} \sin^2\delta_0 \qquad \ldots\ldots(2)$$

In the limit $k \to 0$, $\sigma_{total} \to \sigma_0$ called the *low-energy cross-section*. Then we note that,

$$\text{Lim}_{k\to 0}\, k^2 \,\text{cosec}^2\,\delta_0 = \frac{4\pi}{\sigma_0}$$

It is obvious that,

$$\text{Lim}_{k\to 0} \sin\delta_0(k) \to 0$$

i.e., $\delta(k)$ approaches 0 or π in zero energy limit.

It is found that low energy cross-section can be described, instead of δ_0, by two quantities that characterize $V(r)$ completely as far as low energy scattering is concerned. In relation to nucleon-nucleon scattering, Fermi introduced the terms "effective range (r_0)" and "scattering length (a)". The two low energy parameters r_0 and a will be entirely determined by the bound state wave-function if the system has a bound state with a low binding energy. This relationship between the bound state's properties and low energy scattering is interesting but not unexpected since that both were determined by the potential $V(r)$.

2.6.1 Scattering length and effective range for short ranged potential V®

For *s*-wave, the Schroedinger equation is

$$\frac{d^2u}{dr^2} + [k^2 - U(r)]u = 0, U(r) = \frac{2m}{\hbar^2}V(r) \qquad \ldots\ldots(3)$$

Let $u_1(r), u_2(r)$ be the solutions for two energies k_1^2, k_2^2 They satisfy,

$$u_1(0) = 0, u_2(0) = 0 \qquad \ldots\ldots (4)$$

and are normalised such that asymptotically they are

$$\left.\begin{aligned} u_1(r) &\to \tfrac{1}{\sin\delta_1}\sin(k_1 r + \delta_1), \\ u_2(r) &\to \tfrac{1}{\sin\delta_2}\sin(k_2 r + \delta_2), \end{aligned}\right\} \qquad \ldots\ldots(5)$$

From the two equations, we readily obtain

$$\left[u_2\frac{du_1}{dr} - u_1\frac{du_2}{dr}\right]_0^R = (k_2^2 - k_1^2) - \int_0^R u_1 u_2 dr \qquad \ldots\ldots(6)$$

Where R is an arbitrary radial distance.

Let us take two free-particle solutions,

$$\left.\begin{aligned} v_1(r) &\approx \tfrac{1}{\sin\delta_1}\sin(k_1 r + \delta_1) \\ v_2(r) &= \tfrac{1}{\sin\delta_2}\sin(k_2 r + \delta_2) \end{aligned}\right\} \qquad \ldots\ldots(7)$$

From the equations for $v_1(r)\ and\ v_2(r)$ we obtain as in equation (6)

$$\left[v_2\frac{dv_1}{dr} - v_1\frac{dv_2}{dr}\right]_0^R = (k_2^2 - k_1^2) - \int_0^R v_1 v_2 dr \qquad \ldots\ldots(8)$$

On subtraction equation (7) from (8) and using equation (4), (5) and (7) and limiting $R \to \infty$, we get,

$$k_2\cot\delta_2 - k_1\cot\delta_1 - (k_2^2 - k_1^2)\int_0^\infty (u_1 v_2 - v_1 u_2)dr \qquad \ldots\ldots(9)$$

On defining the "scattering length" a by,

$$-\frac{1}{a} = \mathrm{Lim}_{k\to 0}[k\cot\delta(k)] \qquad \ldots\ldots(10)$$

We can write (9), on limiting $k_1 \to 0$ and denoting k_2 by k,

$$k\cot\delta = -\frac{1}{a} + \frac{b}{2}k^2, \qquad \ldots\ldots(11)$$

$$where \quad b = 2\int_0^\infty (v_0 v - u_0 u)dr. \qquad \ldots\ldots(12)$$

The inclusion of factor 2 in equation (12) so that b (or r_0) has the meaning of the range of the potential. According to equation (5) and (7), the integrand above only deviates from zero in the region where $U(r)$ is appreciable. The wavefunction $u(r)$ won't be overly affected by the energy k^2 if $|U(r)| >> k^2$ in this region.

To approximation replacing u, v by u_0, v_0 (for zero energy) in equation (12), i.e., we will use the first two terms of the power series expansion in k^2 or $k\cot\delta$:

Where,

$$k\cot\delta = -\frac{1}{a} + \frac{r_0}{2}\{k_2 + 0\}(k^4) \qquad \ldots\ldots(13)$$

$$where \quad r_0 = 2\int_0^\infty (v_0^2 - u_0^2)dr. \qquad \ldots\ldots(14)$$

r_0 is referred to as the potential's $V(r)$"effective range." The zero energy $u_0(r)$ has the asymptotic form in accord with equation (5) and (10)

$$u_0(r) \to v(r) = \mathrm{Lim}_{k\to 0}(\cos kr + \cot\delta \sin kr) \qquad \ldots\ldots(15)$$
$$= 1 - \frac{r}{a}.$$

By the equations (5) and (7) $v_0^2 - u_0^2$ vanishes outside the "range" of $U(r)$. So, both r_0 and a are determined by $U(r)$ that they are in sensitive to the exact form of $U(r)$ but depend only on some integrand of $U(r)$.
(1) For $k^2 \to 0$, we have from equation (2) and (10)

$$\sigma = \frac{4\pi}{k^2(1+\cot^2\delta)} \to 4\pi a^2 \quad \ldots\ldots(16)$$

(2) From the expression of δ_l, we have δ_0 for $k \to 0$.

$$a = \int_0^\infty rU(r)u_0(r)dr \quad \ldots\ldots(17)$$

where $u_0(r)$ is normalised by the asymptotic behaviour and is different from (15)

$$u_0(r) \to \mathrm{Lim}_{k\to 0}\frac{\sin(kr+\delta)}{k} = (r-a)\cos\delta \quad \ldots\ldots(18)$$

Where cos δ has a value between 1 and -1.

If we use the Born approximation and if it is valid, i.e., u_0 is replaced by the field free solution,

$$r\sqrt{(\pi/2kr)}J_{1/2}(kr) = (1/k)\sin kr \to r \text{ as } k \to 0$$

Then equation (17) becomes

$$a \approx \int_0^\infty U(r)r^2dr \quad \ldots\ldots(19)$$

(3) The sign of '*a*' depends on *U*(*r*). We take the following example for variation of '*a*' with *U*(*r*): Consider a potential well,

$$U(r) = \begin{cases} -\beta^2, r < R \\ 0, r > R \end{cases} \quad \ldots\ldots(20)$$

If $E = -\gamma^2, \gamma > 0$, is a discrete state, then

$$\left(\frac{d^2}{dr^2} - \gamma^2 + \beta^2\right)u_\gamma(r) = 0; r < R$$

$$\left(\frac{d}{dr^2} - \gamma^2\right)u_\gamma(r) = 0; r > R$$

$$u_\gamma(r) = \begin{cases} A\sin\left(\sqrt{\beta^2-\gamma^2}\right)r\} & r < R \\ Be^{-\gamma} & r > R \end{cases}$$

The continuity condition at $r = R$ provides that

$$\tan\left(\sqrt{(\beta^2-\gamma^2)}R\right) = \frac{\sqrt{(\beta^2-\gamma^2)}}{\gamma} \qquad \ldots\ldots(21)$$

The following is seen as the condition βR for the existence of 1, 2, or more discrete states:

For only 1 discrete state,
$\frac{1}{2}\pi < \beta R < \frac{3}{2}\pi.$
For only 2 discrete state,
$\frac{3}{2}\pi < \beta R < \frac{5}{2}$ $\qquad \ldots\ldots(22)$

Now consider the scattering $U(r)$ in equation (20); the wave-function u_k can be written as follows:

$$\left(\frac{d^2}{dr^2} + k^2 + \beta^2\right)u_k = 0, r > R.$$
$$\left(\frac{d^2}{d^2} + k^2\right)u_k = 0, r > R \qquad \ldots\ldots(23)$$
$$u_\gamma(r) = C\sin\left(\sqrt{(\beta^2+k^2)}r\right), r < R$$
$$= D\sin(kr+\delta), r > R \qquad \ldots\ldots(23a)$$

Apply continuity condition at $r = R$

$$k\cot(kR+\delta) = \sqrt{(\beta^2+k^2)}\cot\left(\sqrt{(\beta^2+k^2)}R\right) \qquad \ldots\ldots(24)$$

$$k\cot\delta = \frac{k\tan\left(\sqrt{(\beta^2+k^2)}R\right)\tan kR + \sqrt{(\beta^2+k^2)}}{\tan\left(\sqrt{(\beta^2-k^2)}R\right) - \frac{1}{k}\sqrt{(\beta^2+k^2)}\tan kR} \qquad \ldots\ldots(24a)$$

By the equation (10), a comes out to be,

$$a = R - \frac{1}{\beta}\tan\beta. \qquad \ldots\ldots(25)$$

As a result, the scattering length a vanishes as $\beta \to \infty$. As βR increases from 0, a decrease. As $\beta R \to \pi/2$, a becomes negatively infinite. When the energy is 0, the cross-section σ possesses "*resonance*," and it becomes infinite.

The following formula can be used to determine the range r_0 for rectangular potential:

We obtain from (23a) and the $u_k(r)$ for $k \to 0, r \to \infty$ in (15), we get

$$u_0 = \left(1 - \frac{R}{a}\right)\frac{\sin \beta r}{\sin \beta R}, 0 < r < R$$

And with equation (15), for v_0, we have from equation (12)

$$r_0 = 2R - 2\frac{R^2}{2} + \frac{3R^{2R^3}}{3a^2} + \left(1 - \frac{R}{a}\right)^2\left(\frac{1}{\beta \tan \beta R} - \frac{R}{\sin^2 \beta R}\right) \quad \ldots\ldots(26)$$

If $\beta R = (n + 1/2)\,\pi, n = 0,1,2,\ldots\ldots;$ a stands to $\pm\infty$ and equation (26) simplifies and the total cross section σ in terms of a and r_0 is

$$\sigma = \frac{4\pi a^2}{1 + a(a - r_0)k^2 + \left(\frac{1}{2}ar_0\right)k^4}$$

2.7 SUMMARY

For weak scattering potentials and high incident energy, the Born approximation remains true. In other words, the scattered wave can be considered as a plane wave when the average interaction energy between the incident particle and the scattering potential is significantly lower than the incident kinetic energy of the particle. Low-energy scattering is described by scattering length in the quantum mechanics. In the context of quantum mechanics, partial-wave analysis is a method for resolving scattering problems by decomposing each wave into its constituent angular-momentum components and solving using boundary conditions.

2.8 GLOSSARY

Approximation- nearly exact

Successive- following in order

Differential- an infinitesimal ("infinitely small") change in some varying quantity

Range- the distance or extent between possible extremes

Scattering- a change in the direction of motion of a particle because of a collision with another particle

Asymptotic- approaching a given value as an expression containing a variable tends to infinity

Cross-section- a section made by a plane cutting anything transversely

2.9 REFERENCES

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2.11 TERMINAL QUESTIONS

1. Calculate the scattering amplitude for a central potential in the first-Born approximation and discuss its condition of validity.

2. Explain the method of partial waves to calculate the phase shifts and scattering amplitude.

3. Discuss the scattering length and effective range theory for low energy scattering.

4. What is Born approximation? Explain the condition for validity of Born approximation.

5. What is phase shift? Calculate phase shift δ_l.

UNIT 3 PERTURBATION THEORY I

Structure

3.1 Introduction

3.2 Objectives

3.3 Time dependent perturbation theory

3.4 Constant perturbation

3.5 Transition probability: Fermi's-Golden rule

3.6 Harmonic perturbation

3.7 Selection rules for dipole radiation

3.8 Summary

3.9 Glossary

3.10 References

3.11 Suggested Readings

3.12 Terminal Questions

3.1 INTRODUCTION

In quantum mechanics exact solution of the problems cannot be obtained, so we should opt for the approximate solutions. Physics is said to be a science of approximations. In quantum mechanics different methods of approximation have been formulated to get nearly accurate evaluation of energy values and wave function.

For any perturbed quantum mechanical system, we use approximation methods instead of simple Schrodinger equation to find out wave function and energy Eigen values of the system.

Hence, perturbation theory is a tool or a systematic procedure for obtaining approximate solutions to the perturbed problems by using solutions for unperturbed case.

Perturbation theory was developed by Schrödinger in 1926 and are of two types:

- Time independent or Stationary perturbation theory
- Time dependent perturbation theory

What is Perturbation?

Perturbation is a small change/ disturbance

Perturbation in quantum mechanics is a small change in Hamiltonian of the system

Hamiltonian means the total energy (K.E. + V)

Perturbation is the change in potential of the system

For any perturbed quantum mechanical system, we cannot use simple Schrodinger Equation to find out wave function or Eigen function and energy Eigen values of the system.

When the Hamiltonian of a system depends on the time, there are no stationary state solutions of Schrodinger's equation. Thus, the identification of a bound state with discrete energy levels and stationery eigenfunctions must be modified.

3.2 OBJECTIVES

After studying thus unit, you should be able to-

- Understand time dependent perturbation theory
- Explain Constant perturbation
- Explain Harmonic perturbations
- Understand Transition probability: Fermi's-Golden rule
- Discuss Selection rules for dipole radiation

3.3 TIME DEPENDENT PERTURBATION THEORY OR METHOD OF VARIATION OF CONSTANTS

In this method Hamiltonian is divided into two parts as usual, i.e. The Perturbed Hamiltonian,

$H = H^0 + H'$

Where H^0 is simple unperturbed Hamiltonian and H' is small time dependent perturbations term and has the effect of causing transitions between Eigen-states of H^0 that would be stationary in the absence of H'.

It is generally impossible to obtain exact solution of the Schrodinger equation when the Hamiltonian depends upon time. Therefore, such an equation is solved by time- dependent perturbation theory also called the method of variation of constants.

Total Hamiltonian:

$$H = H^0 + H' \qquad \text{.... (1)}$$

Where the unperturbed Hamiltonian H^0 can be solved for its normalized eigenfunction ϕ_n and its eigen value E_n i.e., we have

$$H^0\phi_n = E_n\phi_n \qquad \text{..... (2)}$$

Perturbation term is H' very small. Since H' depends upon time, the stationary solution of the actual Schrodinger equation does not exist.

Hence time-dependent Schrodinger equation is:

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi \qquad \text{..... (3)}$$

The energy Eigen-states of such a system are stationary: the time enters only in the phase according to

$$\Psi(t) = \sum_n a_n(t)\phi_n(\boldsymbol{r})e^{-i\omega_n t} \qquad \text{..... (4)}$$

$$\omega_n = \frac{E_n}{\hbar}$$

Where $a_n's$ are time-dependent constants and $\phi_n(\boldsymbol{r})$ is time-independent.

This equation represents solution of equation (3), therefore substituting value of ψ and H from (1) and (4) in (3), we get:

$$i\hbar\frac{\partial}{\partial t}[\sum_n a_n(t)\phi_n(\boldsymbol{r})e^{-i\frac{E_n}{\hbar}t}] = (H^0 + H')[\sum_n a_n(t)\phi_n(\boldsymbol{r})e^{-i\frac{E_n}{\hbar}t}]$$

or

$$[i\hbar\sum_n \dot{a}_n(t)\phi_n(\boldsymbol{r})e^{-i\frac{E_n}{\hbar}t} + \sum_n a_n E_n\,\phi_n(\boldsymbol{r})e^{-i\frac{E_n}{\hbar}t}]$$

$$= \sum_n H^0\, a_n\phi_n(\boldsymbol{r})\, e^{-i\frac{E_n}{\hbar}t} + \sum_n H'\, a_n\phi_n(\boldsymbol{r})e^{-i\frac{E_n}{\hbar}t}$$

Where, $\frac{d}{dt}a_n(t) = \dot{a}_n$

Using equation (2) i.e. $H^0\phi_n = E_n\phi_n$, we get

$$[i\hbar \sum_n \dot{a}_n\, \phi_n(\boldsymbol{r}) e^{-i\frac{E_n}{\hbar}t} + \sum_n a_n E_n \phi_n(\boldsymbol{r})\, e^{-i\frac{E_n}{\hbar}t}$$

$$= \sum_n a_n\, E_n \phi_n(\boldsymbol{r}) e^{-i\frac{E_n}{\hbar}t} + \sum_n a_n\, H'\phi_n(\boldsymbol{r}) e^{-i\frac{E_n}{\hbar}t}]$$

Or $$[i\hbar \sum_n \dot{a}_n\, \phi_n(\boldsymbol{r}) e^{-i\frac{E_n}{\hbar}t} = \sum_n a_n\, H'\phi_n(\boldsymbol{r}) e^{-i\frac{E_n}{\hbar}t}] \quad \text{.....(5)}$$

Multiplying both sides by ϕ_k^* and integrating over configuration space, we get

$$\phi_n(\boldsymbol{r}) \to \phi_n$$

$$[i\hbar \sum_n \dot{a}_n\, e^{-i\frac{E_n}{\hbar}t} \int \phi_k^*\, \phi_n\, d\tau = \sum_n a_n\, e^{-i\frac{E_n}{\hbar}t} \int \phi_k^* H'\phi_n d\tau]$$

Now using orthonormality condition of $\phi's$, i.e.

$$\int \phi_k^*\, \phi_n\, d\tau = \delta_{kn}$$

δ_{kn} = 0 for n ≠ k

= 1 for n = k

We get, $$i\hbar\, \dot{a}_n\, e^{-i\frac{E_n}{\hbar}t}\, \delta_{kn} = \sum_n a_n\, e^{-i\frac{E_n}{\hbar}t} \int \phi_k^* H'\phi_n d\tau$$

Because in L.H.S. all terms will be zero except *k*th term due to the properties of Kronecker delta δ_{kn}, we have,

$$i\hbar\, \dot{a}_k\, e^{-i\frac{E_n}{\hbar}t} = \sum_n a_n\, e^{-i\frac{E_n}{\hbar}t} \int \phi_k^* H'\phi_n d\tau \quad \text{.....(6)}$$

The integral $\int \phi_k^* H'\phi_n d\tau$ at right hand side is a matrix

$$< k|\, H'|\, n > = H'_{kn}$$

So $i\hbar\, \dot{a}_k = \sum_n a_n\, e^{\frac{i(E_k - E_n)t}{\hbar}} H'_{kn}$ .....(7)

$$\frac{E_k - E_n}{\hbar} = \omega_{kn} \qquad \text{…..(8)}$$

ω_{kn} is the Bohr's frequency.

Time dependent constants a_n's is given by

$$\dot{a}_k = (i\hbar)^{-1} \sum_n a_n H'_{kn} e^{i\omega_{kn}t}$$

$$= (i\hbar)^{-1} \sum_n a_n < \mathrm{k}| H'| \mathrm{n} > e^{i\omega_{kn}t} \qquad \text{…..(9)}$$

If we replace H' by $\lambda H'$, where λ is the parameter, then coefficient *a*'s can be expressed in parameter λ as follows,

$$a_n = a_n^{(0)} + \lambda\, a_n^{(1)} + \lambda^2 a_n^{(2)} + \ldots\ldots \qquad \text{\ …..(10)}$$

Substituting the value of a_n in equation (9) we get,

$$\dot{a}_k^{(0)} + \lambda\, \dot{a}_k^{(1)} + \lambda^2 \dot{a}_k^{(2)} + \ldots\ldots = (i\hbar)^{-1} \sum_n a_n^{(0)} + \lambda\, a_n^{(1)} + \lambda^2 a_n^{(2)} + \ldots\ldots) H'_{kn}\, e^{i\omega_{kn}t}$$

Comparing coefficients of different powers of λ on both sides.

Equating coefficient of λ^0, $i\hbar\, \dot{a}_k^{(0)} = 0$ ……(a)

Equating coefficient of λ, $i\hbar\, \dot{a}_k^{(1)} = \sum_n a_n^{(0)}\ H'_{kn}\, e^{i\omega_{kn}t}$ ……(b)

….. …..

….. …..

In general,

$$i\hbar\, \dot{a}_k^{(s+1)} = \sum_n a_n^{(s)}\ H'_{kn}\, e^{i\omega_{kn}t} \qquad \text{……(c)}$$

Where s = 0,1, 2, … …..(11)

So, we can get desired perturbation.

Zeroth order calculation: From (11), we have

$$i\hbar\,\dot{a}_k^{(0)} = 0 \quad \text{or } \dot{a}_k^{(0)} = 0 \quad \text{i.e. } \frac{d}{dt}a_k^{(0)} = 0$$

Integrating, we obtain,

$$a_k^{(0)} = constant\ in\ time.$$

For convenience without loss of generality, we may put,

$$a_k^{(0)} = <k|\,m> = \delta_{km}$$

As the initial state m is one of a discrete or continuous set.

Accordingly, $a_k^{(0)} = 1\ for\ k = m\ i.e.\ a_m^{(0)}$=1

And $a_k^{(0)} = 0\ if\ k \neq m$

Thus, in the sum, we have only one term and equation (9) may be expressed as

$$\dot{a}_k = (i\hbar)^{-1} <\mathrm{k}|\,H'|\,\mathrm{n}>\, e^{i\omega_{kn}t} \quad \text{.....(12)}$$

First order Perturbation:

Integration of (12), gives

$$a_k^{(1)}(t) = (i\hbar)^{-1} \int_{-\infty}^{t} <k|\,H'|\,n>\, e^{i\omega_{kn}t}\,dt \quad \text{.....(13)}$$

The constant of integration is taken to be zero in order that $a_k^{(1)}$ be zero at $t = -\infty$ (before the perturbation is applied).

3.4 CONSTANT PERTURBATION

Let us consider a perturbation that is constant in time and that it operates only during the time 0 to *t*, i.e.

$$H'_{km}=< k|\, H'|\, m >= \begin{cases} 0 \\ 0 \end{cases} < k|\, H'|\, m > \begin{cases} for\ -\infty < t' < 0 \\ for\ 0 \le t' \le t \\ for\ t' > t \end{cases} \qquad \text{.....(14)}$$

From equation (13) and (14), we get

$$a_k^{(1)}(t) = (i\hbar)^{-1} \int_0^t < k|\, H'|\, m > e^{i\omega_{km}t'}\, dt'$$

$$= (i\hbar)^{-1} < k|\, H'|\, m > \int_0^t e^{i\omega_{km}t'}\, dt'$$

$$= (i\hbar)^{-1} < k|\, H'|\, m > \left[\frac{e^{i\omega_{km}t'}}{i\omega_{km}}\right]_0^t$$

$$= (i\hbar)^{-1} < k|\, H'|\, m > \left[\frac{e^{i\omega_{km}t}-1}{i\omega_{km}}\right]$$

$$= \frac{<k|H'|m>}{\omega_{km}\hbar}(e^{i\omega_{km}t}-1) \qquad \text{.....(15)}$$

Thus, to the first order, the probability of the system from m^{th} state to kth state is given by

$$|a_k^{(1)}(t)|^2 = \frac{|< k|\, H'|\, m >|^2}{\omega_{km}{}^2\hbar^2}\, |e^{i\omega_{km}t}-1|^2 \qquad \text{.....(16)}$$

Using the relation,

$$\lim_{x\to 0}(e^{ix}-1) = 2ie^{ix/2}\sin\frac{x}{2} = 2i\sin\frac{x}{2}$$

$$\text{Or } |e^{ix}-1|^2 = 4\sin^2\frac{x}{2}$$

$$\text{i.e., } |e^{i\omega_{km}t}-1|^2 = 4\sin^2\left(\frac{\omega_{km}t}{2}\right)$$

$$|a_k^{(1)}(t)|^2 = \frac{4|< k|\, H'|\, m >|^2}{\omega_{km}{}^2\hbar^2}\sin^2\left(\frac{\omega_{km}t}{2}\right) \qquad \text{.....(17)}$$

Physical interpretation: We plot $\frac{\sin^2\left(\frac{\omega_{km}t}{2}\right)}{\omega_{km}{}^2}$ as a function of ω_{km}. The plot is shown in fig. 1

The major maxima of probability curve occur at ω_{km}= 0 i.e., for $E_k - E_m$.

$$\text{If we put } \omega_{km} = x \text{ in } \frac{\sin^2\left(\frac{\omega_{km}t}{2}\right)}{\omega_{km}{}^2} \text{ we get,}$$

$$\frac{sin^2(\frac{\omega_{km}t}{2})}{{\omega_{km}}^2} = \frac{sin^2(\frac{xt}{2})}{x^2} = \frac{1}{x^2}\left[\frac{xt}{2} - \frac{(xt/2)^3}{3} + \frac{(xt/2)^5}{5} - \ldots.\right]^2$$

$= \frac{1}{x^2}\ (\frac{xt}{2})^2$, if higher powers are neglected because their values are very small

$= \frac{t^2}{4}$

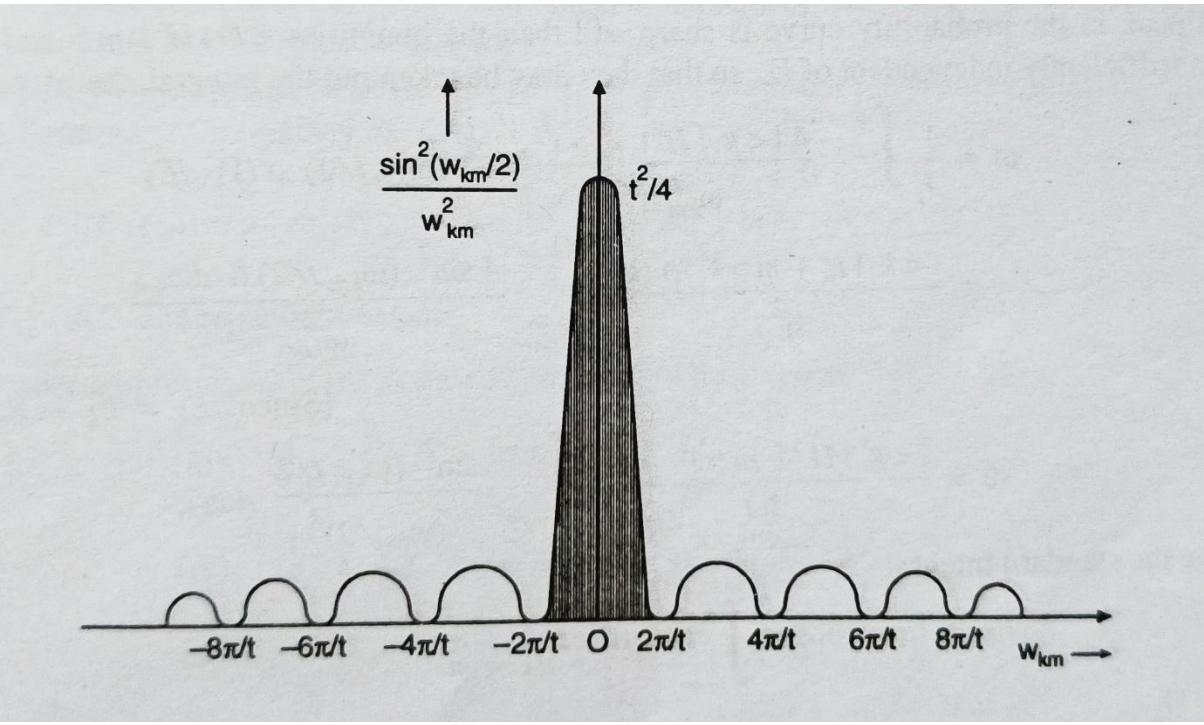

Fig:3.1

The hight of main peak is $\frac{t^2}{4}$ and the intensity of probability curve touches the ω_{km} axis at points where $\frac{sin^2(\frac{xt}{2})}{x^2} = 0$.

This occurs at points where,

$$\frac{xt}{2} = \pm r\pi \ or\ x = \pm\frac{2\pi r}{t}$$

Where *r* is an integer (i.e., *r* =0,1,2, 3, …)

Thus, $x = \omega_{km} = \pm\frac{2\pi r}{t} = 0, \pm\frac{2\pi}{t}, \pm\frac{4\pi}{t}, \pm\frac{6\pi}{t}, \ldots.$ i.e., width of the peak is proportional to 1/*t*; the area under the curve is proportional to *t* i.e., time of application of the perturbation.

Constant perturbation for a definite time is analogous to single slit diffraction experiment are applicable to problems of excitation and emission of radiation in elementary systems.

Now we look for the figure's physical interpretation: When *r* is large enough, most transitions to new states occur under the primary peak because its area is much larger than those of its neighbouring peaks.

There are transitions in the system and it is noticed that there is a clear transition rate from a set initial state to a final state if we have a system with the Hamiltonian Ho and if this system interacts with an external agency with an interaction Hamiltonian H.

3.5 THE TRANSITION PROBABILITY: FERMI-GOLDEN RULE

Let's assume that the unperturbed Hamiltonian H_o has a continuous spectrum and that transitions are occurring from one state to another along the continuum. This is how most physical problems work, such as the scattering problem, where the scattered states have continuum eigenvalues of the Hamiltonian.

If the transition takes place to state k of energy between E_k and E_k+dE_k and the energy density of states is given by $\rho(k)$ at this stage, then the transition probability per unit time is defined as

$$\omega = \frac{1}{t}\int |a_k^{(1)}(t)|^2 \rho(k)\, dE_k \qquad \text{.....(18)}$$

where $\rho(k)$ gives the number of final states in the energy interval from E_k to E_k+dE_k. If t is large enough, the central peak in the probability curve is sharp and then the quantities

$< k\ |H'|\ m >$ and $\rho(k)$ may be regarded as sufficiently independent of E_k, so that they may be taken out the integral, therefore,

$$\omega = \frac{1}{t}\int_{-\infty}^{+\infty} \frac{4|<k|H'|m>|^2}{\omega_{km}^2\hbar^2}\sin^2(\omega_{km}t/2)\rho(k)dE_k$$
$$= \frac{|<k|H'|m>|^2\rho(k)}{\hbar^2 t}\int_{-\infty}^{+\infty}\frac{4\sin^2(\omega_{km}t/2)\hbar d\omega_{km}}{\omega_{km}^2}$$
$$\omega = \frac{|<k|H'|m>|^2\rho(k)}{\hbar t}\int_{-\infty}^{+\infty}\frac{\sin^2(\omega_{km}t/2}{(\omega_{km}/2)^2}d\omega_{km} \qquad .....(19)$$

we have the standard integral

$$\int_{-\infty}^{+\infty}\frac{\sin^2 x}{x^2}dx = \pi$$

Substituting

$$\frac{\omega_{km}t}{2} = x, \text{ i.e. } \omega_{km} = \frac{2x}{t}, \text{ so } d\omega_{km} = \frac{2}{t}dx$$
$$\int_{-\infty}^{+\infty}\frac{\sin^2(\omega_{km}t/2}{(\omega_{km}/2)^2}d\omega_{km} = \int_{-\infty}^{+\infty}\frac{\sin^2 x}{\left(\frac{x}{t}\right)^2}\cdot\left(\frac{2}{t}dx\right)$$
$$= 2t\int_{-\infty}^{+\infty}\frac{\sin^2 x}{x^2}dx = 2\pi t \qquad .....(20)$$

Substituting this in (19), we get

$$\omega = \frac{|<k|H'|m>|^2\rho(k)}{\hbar t}\cdot 2\pi t = \frac{2\pi}{\hbar}\rho(k)|<k|H'|m>|^2 \qquad .....(21)$$

Equation (21) is the important result of time-dependent perturbation theory and called as **Fermi-Golden Rule**. The **Fermi-Golden Rule** is a key result of time-dependent perturbation theory. This relation has been successfully used to determine transition probabilities between two states and to determine their corresponding life spans. It has provided the results that were actually found experimentally, particularly in β-decay.

3.6 HARMONIC PERTURBATION

Perturbation theory studies how quantum systems respond to outside disturbances. Harmonic perturbation is a rare specific case of time-dependent perturbation for which an exact analysis is available. If the perturbation is harmonic of frequency ω, i.e.

$$< k|\, H'(t')|\, m > | \text{ or } H'_{km}(t') = \begin{cases} 0 \; for \; -\infty < t' < 0 \\ 2 < k|\, \mathrm{H_0}'|\, m > \; sin\, \omega t' \; for \; 0 \le t' \le t \\ 0 \; for \; t' < t \end{cases} \qquad \text{.....(23)}$$

$< k|\, \mathrm{H_0}'|\, m >$ is independent of time.

The first order amplitude $a_k^{(1)}(t')$ at time t', would then be given as

$$a_k^{(1)}(t' \ge t) = (i\hbar)^{-1} \int_0^1 < k|H'|m > e^{i\omega_{km}t'} dt'$$

$$= (i\hbar)^{-1} \int_0^t 2 < k|H_0'|m > \sin\omega t' e^{i(\omega_{km}t'} dt'$$

$$= \frac{2 < k|H_0'|m >}{i\hbar} \int_0^{'} \frac{e^{i\omega t'} - e^{-i\omega t'}}{2i} e^{i\omega_{km}t'} dt'$$

$$= -\frac{\langle k|H_0'|m >}{\hbar} \int_0^t \left\{ e^{i(\omega_{km}+\omega)t'} - e^{i(\omega_{km}-\omega)t'} \right| dt'$$

$$= -\frac{< k|H_0'|m >}{\hbar} \left[\frac{e^{i(\omega_{km}+\omega)t'}}{i(\omega_{km}+\omega)} - \frac{e^{i(\omega_{km}-\omega)r'}}{i(\omega_{km}-\omega)} \right]_0^{'}$$

i.e. $$a_k^{(1)}(t') = -\frac{< k|\, \mathrm{H_0}'|\, m>}{i\hbar} \left[\frac{e^{i(\omega_{km}+\omega)t} - 1}{\omega_{km}+\omega} - \frac{e^{i(\omega_{km}-\omega)t} - 1}{\omega_{km}-\omega} \right] \qquad \text{.....(24)}$$

The form of this equation suggests that,

(i) The first order amplitude depends on perturbation duration t and not on instantaneous time t'.

(ii) The amplitude is appreciable only when the denominator of the one or the other terms is practically zero.

The first term is important when $\omega_{km} = -\omega$ or $E_k \approx E_m - \hbar\omega$ and the second term is important when $\omega_{km} = \omega$ or $E_k \approx E_m + \hbar\omega$ .Thus the first order effect of a harmonic perturbation (i.e., perturbation that varies sinusoidally with time) with angular frequency ω is to transfer or to receive from the system on which it acts the Planck's energy quantum $\hbar\omega$.

In the special case in which the initial state m is a discrete bound state and the final state k is one of the continuous sets of dissociated states. Then $E_k > E_m$ and only second term in equation (24) need to be considered. In this case the first order probability of finding the system in k^{th} state after the perturbation is removed is given by

$$|a_k^{(1)}(t' \geq t)|^2 = \frac{4\,|<k|\,H_0'\,|\,m>|^2 \sin^2\frac{(\omega_{km}-\omega)t}{2}}{\hbar^2(\omega_{km}-\omega)^2} \qquad \text{.....(25)}$$

3.7 SELECTION RULES FOR DIPOLE RADIATION

An electric dipole separates the positive and negative electric charges in any electromagnetic system. A simple illustration of this system is a pair of charges with the same magnitude but the opposite sign, separated by a small distance.

Electric dipole radiation (EDR) is the Electromagnetic radiation (EMR) generated by an oscillating electric dipole (pair of opposite charges) or by an electric dipole that cycles through changes in the location of the charges at some frequency.

The dipole transitions between states *f, i,* are possible only if,

$$<\mathbf{er}>_{fi} \neq \mathbf{0} \;\; or \;\; \boldsymbol{e}<\mathbf{r}>_{fi} \neq \mathbf{0}$$

In this case, the states that are being considered have definite angular momenta, The selection rule governing the change in angular momentum is then provided by this condition.

From the properties of spherical harmonics, it follows that

$$\int (Y_{l_f m_f})^* Y_{l_i m_i} d\tau \neq 0 \;\text{ only if }\; l_f\text{-}l_i = \pm 1$$

This result can be obtained more generally if it is assumed that **r** is a vector operator or a spherical tensor of rank one. Hence its matrix element between the angular momentum eigen states is proportional to Clebsch - Gordan coefficient $< l_i\, m_i ;\, l_f\, m_f >$ by Wigner Eckart theorem. Consequently, if $|\Delta l| = |l_i - l_f|$ exceeds one. The matrix elements for Δl vanishes because **r** is of odd parity.

The selection rule for l remains $\Delta l = \pm 1$. From the properties of Clebsch - Gordan coefficient it is also clear that $\Delta m = m_f - m_i$ is restricted to $\Delta m = \pm 1,0$. The polarisation vector **A** determines which of these cases can occur. For example, of **A** is along z-ais, then $\mathbf{r}_{(\mathbf{A})_{\mathbf{fi}}} = z_{fi}$, as z = r cos$\theta$. Which is independent of ϕ this corresponds to m = 0 in Clebsch - Gordan coefficients and hence the selection rule from *m* is $\Delta m = 0$

Thus, the selection rules are $\Delta m = 0$ and $\Delta l = \pm 1$.

The transitions which occur under dipole selection rules are called allowed transitions.

3.8 SUMMARY

In this unit, you have studied the time dependent perturbation theory also called as method of variation of constants. The time dependent perturbation term is small and since this term depends upon time, the stationery solution of the actual Schrodinger equation does not exist. Also, you have studied about constant perturbation, transition probability harmonic perturbation and selection rule for dipole transition.

3.9 GLOSSARY

Perturbation – a deviation of a system caused by an outside influence

Constant – something that does not or cannot change or vary

Hamiltonian – the Hamiltonian of a system is an operator corresponding to the total energy of that system

Dipole – a pair of equal and opposite electric charges or magnetic poles of opposite sign separated especially by a small distance

Parity - the flip in the sign of one spatial coordinate

3.10 REFERENCES

1. Advanced Quantum Mechanics, B.S. Rajput, Pragati Prakashan, Meerut

2. Advanced Quantum Mechanics, Satya Prakash, Kedar Nath Ram Nath, Meerut

3. Advanced Quantum Mechanics, J.J.Sakurai, Pearson

4. P.A. M. Dirac, The Principles of Quantum Mechanics, Oxford University Press, London

3.11 SUGGESTED READINGS

1. Advanced Quantum Mechanics, Franz Schwabl, Springer

2. Introduction to Quantum Mechanics, David J. Griffiths, Cambridge University Press

3. P.M. Mathews and K. Venkatesan, A Text book of Quantum Mechanics, Tata Mc Graw-Hill, New Delhi.

4. L.I. Schiff, Quantum Mechanics, McGraw-Hill

3.12 TERMINAL QUESTIONS

Short Answer type questions

1. Write short notes on
   i. Constant Perturbation
   ii. Harmonic Perturbation

2. Give the outline for outline of the derivation of the "dipole selection rule" $\Delta m = 0, \pm 1$ and $\Delta l = \pm 1$.
3. What is Perturbation theory? Explain time dependent Perturbation theory.
4. Show that the first order effect of a time dependent perturbation, varying sinusoidally in time, leads to emission or absorption of energy.

Long Answer type questions

1. Discuss the first order time dependent perturbation theory and derive the Fermi Golden rule for the transition rate from a given initial state to a final state of continuum.
2. Prove that the transition probability per unit time is

   $\frac{2\pi}{\hbar}\rho(k)\ |H'_{km}|^2$

   Where $\rho(k)$ denotes the density of final states and H'_{km} is the matrix element of the perturbation term.

3. Give the time dependent perturbation theory for the case of a perturbation which is constant in time except; that it is switched on at $t = 0$ and switched off at time t.

   Describe the method of variation of constants as applied to time dependent perturbation. Illustrate by simple examples.
4. Discuss briefly the time dependent perturbation theory and derive an expression for the transition probability to a group of states per unit time.

UNIT 4 PERTURBATION THEORY II

Structure

4.1 Introduction

4.2 Objectives

4.3 Adiabatic approximation

4.4 Sudden approximation

4.5 Semi classical treatment of an atom with electromagnetic radiation

4.5.1 For absorption

4.5.2 For emission

4.5.3 Interpretation of terms of absorption and emission

4.6 Summary

4.7 Glossary

4.8 References

4.9 Suggested Readings

4.10 Terminal Questions

4.1 INTRODUCTION

So far, time-independent perturbations and only periodic time dependent perturbations have been considered. One of the general time-dependent difficulties in quantum mechanics is the on/off switching of a perturbing factor, such as an external field. In general, solving the details of turning on or off time-dependent disturbances is too difficult. The abrupt and adiabatic approximations, however, are two significant limiting situations that may be examined in depth and with some degree of accuracy.

4.2 OBJECTIVES

After studying this unit, you should be able to-

- Explain adiabatic approximation
- Explain adiabatic approximation
- Understand Semi classical treatment of an atom with electromagnetic radiation

4.3 ADIABATIC APPROXIMATION

In standard time dependent perturbation theory, weak time dependent perturbation is assumed. When we assume the time dependent perturbation is slow, then it is called adiabatic approximation or we can say in adiabatic approximation the perturbation is varying slowly with time. According to this approximation, we expect on physical ground that solution of the Schrodinger equation can be approximated by means of stationary eigen functions of the instantaneous Hamiltonian, so that a particular eigen function at one time goes over continuously into corresponding eigen function at a later time.

The detailed response of a system to a time-dependent disturbance depends on the perturbation's time scale. Consider a simple pendulum that oscillates back and forth in a vertical plane with no friction or air resistance. If we move the support "fast," the bob will move in a highly chaotic manner. The bob will continue to oscillate smoothly, in the same plane (or one parallel to it), and with the same amplitude if we move the support "gradually," on the other hand.

"The adiabatic process is characterised by this slow change in the external conditions."

Now we solve Schrodinger's equations:

$$i\hbar \frac{\partial \psi}{\partial t} = H(t)\psi \qquad \text{.....(1)}$$

Where $H(t)$ changes slowly over time. In this condition it is expected that equation (1) should give a good approximation by solving at each instant of time assuming that H is constant and is equal to the instantaneous value $H'(t')$, where t' is the time at which is H required. For $t' = t = constant$ the stationary state wave function is obtained and would satisfy the equation,

$$H'(t')\,\psi_n(\boldsymbol{r}, t') = E_n(t')\,\psi_n(\boldsymbol{r}, t') \qquad \text{.... (2)}$$

The approximate solution is,

$$\psi_n = \phi_n(t) \exp\left\{-\frac{i}{\hbar}\int_0^t E_n(t')dt\right\} \qquad \text{.....(3)}$$

$$\Psi = \sum_n a_n(t)\phi(t) \exp\left\{-\frac{i}{\hbar}\int_0^t E_n(t')dt'\right\} \qquad \text{.....(4)}$$

Substituting equation (4) in equation (1), you get

$$i\hbar\left[\sum_n\left(\dot{a}_n(t)\phi_n(t)+a_n\frac{\partial\phi_n}{\partial t}\right)\exp\left\{-\frac{i}{\hbar}\int_0^t E_n(t')dt^t\right\}+\sum_n a_n\phi_n E_n\exp\left\{-\frac{i}{\hbar}\int_0^t E_n(t')dt'\right\}\right]$$

$$= H\sum_n a_n\phi_n\exp\left\{-\frac{i}{\hbar}\int_0^t E_n(t')dt'\right\}$$

$$= \sum_n a_n\phi_n E_n\exp\left\{-\frac{-i}{\hbar}\int_0^t E_n(t')dt'\right\}$$

or

$$i\hbar\sum_n\left(\dot{a}_n\phi_n+a_n\frac{\partial\phi_n}{\partial t}\right)\exp\left\{-\frac{i}{\hbar}\int_0^t E_n(t')dt\right\}=0$$

or

$$\sum_n^{\Sigma}\left(\dot{a}_n\phi_n+a_n\frac{\partial\phi_n}{\partial t}\right)\exp\left\{-\frac{i}{\hbar}\int_0^t E_n(t)dt'\right\}=0 \qquad .....(5)$$

Multiplying by $\psi_m^*\ exp\left\{\frac{i}{\hbar}\int_0^t E_m'(t')\,dt'\right\}$ and integrating over all space, we get

$$\int\sum_n\dot{a}_n\phi_n\phi_m^*\exp\left\{-\frac{i}{\hbar}\int_0^t(E_n-E_m)dt'\right\}d\tau+\frac{\Sigma}{n}a_n\int_{m_m}\frac{\partial\theta_n}{\partial t}$$
$$\exp\left\{-\frac{i}{\hbar}\int_0^1(E_n-E_m)dt'\right\}d\tau=0$$

Using condition of orthonormality, we get

$$\dot{a}_m=-\sum_n a_n\int\phi_m^*\frac{\partial\phi_n}{\partial t}\exp\left\{-\frac{i}{\hbar}\int_0^1(E_n-E_m)dt'\right\}d\tau$$
$$=-\sum_n a_n\int\phi_m^*\frac{\partial\phi_n}{\partial t}d\tau,\exp\left\{-\frac{i}{n}\int_0^1(E_n-E_m)dt'\right\} \qquad .....(6)$$

Evaluation of,

$$\int \phi_m^* \frac{\partial \phi_n}{\partial t} d\tau = \left\langle \phi_m \mid \dot{\phi}_n \right\rangle$$

We have $H(t)\ \phi_n(t) = E_n(t)\ \phi_n(t)$ …. (7)

Differentiating equation (7) with respect to t, we get,

$$\frac{\partial H}{\partial t}\phi_n + H\frac{\partial \phi_n}{\partial t} = \frac{\partial E_n}{\partial t}\phi_n + E_n\frac{\partial \phi_n}{\partial t}$$

Multiplying by ϕ_m^* and integrating over all space, we get,

$$\int \phi_m^* \frac{\partial H}{\partial t}\phi_n d\tau + \int \phi_m^* H\frac{\partial \phi_n}{\partial t} d\tau = \frac{\partial E_n}{\partial t}\int \phi_m^* \phi_n d\tau + E_n \int \phi_m^* \frac{\partial \phi_n}{\partial t} d\tau$$

As $\int \phi_m{}^* \phi_n d\tau = 0$ and H is Hermitian, we get

$$\int \phi_m{}^* \frac{\partial H}{\partial t}\phi_n d\tau + \int (H\phi_m)^* \frac{\partial \phi_n}{\partial t} d\tau = E_n \int \phi_m^* \frac{\partial \phi_n}{\partial t} d\tau$$

As $H\phi_m = E_m\phi_m$

$$\therefore \quad \int \phi_m{}^* \frac{\partial H}{\partial t}\phi_n d\tau + E_m \int \phi_m{}^* \frac{\partial \phi_n}{\partial t} d\tau = E_n \int \phi_m{}^* \frac{\partial \phi_n}{\partial t} d\tau$$

$$\text{i.e.} \quad (E_m - E_n)\int \phi_m^* \frac{\partial \phi_n}{\partial t} d\tau = -\int \phi_m^* \frac{\partial H}{\partial t}\phi_n d\tau$$

$$\int \phi_m{}^* \frac{\partial \phi_n}{\partial t} d\tau = -\frac{\int \phi_m{}^* \frac{\partial H}{\partial t}\phi_n d\tau}{E_m - E_n} \qquad \ldots\ldots (8)$$

$$= \frac{\int \phi_m{}^* \frac{\partial H}{\partial t}\phi_n d\tau}{E_n - E_m} (\text{ for } n \neq m)$$

This gives

Substituting this value in (6), we get

$$\dot{a}_m = -\sum_{n\neq m} \frac{a_n\left(\int \phi_m{}^* \frac{\partial H}{\partial t}\phi_n d\tau\right)\exp\left\{-\frac{i}{\hbar}\int_0^t (E_n - E_m)dt'\right\}}{E_n - E_m}$$

$$\dot{a}_m = -\sum_{n\neq m} a_n \frac{\left(\int \phi_m{}^* \frac{\partial H}{\partial t}\phi_n d\tau\right)\exp\left\{-\frac{i}{\hbar}(E_n - E_m)t\right\}}{E_n - E_m} \qquad \ldots\ldots (9)$$

Applying the method of variation of constants.

Let the system with a_k= 1 and a_n= 0 for $n \neq k$. Solving this by successive approximations

$$\dot{a}_m = -\frac{<m|\frac{\partial H}{\partial t}|k>}{E_k - E_m} exp\left\{-\frac{i}{\hbar}(E_k - E_m)t\right\} \qquad \ldots.. (10)$$

$$\text{Where} < m\left|\frac{\partial H}{\partial t}\right| k > = \int \phi_m^* \frac{\partial H}{\partial t}\phi_k \, d\tau$$

To evaluate the matrix element, we can neglect the slow change of $\left(\frac{\partial H}{\partial t}\right)_{mk}$ and integrate equation (10), so that

$$a_m = -\frac{< m|\frac{\partial H}{\partial t}|k >}{E_k - E_m}\int_{-\infty}^{t} e^{-\frac{i}{\hbar}(E_k - E_m)t}dt$$

$$= -\frac{i\hbar}{(E_k - E_m)^2} < m\left|\frac{\partial H}{\partial t}\right| k > \left\{\exp\left(-\frac{i}{\hbar}(E_k - E_m)t\right) - 1\right\}$$

We know, $E_k - E_m = \hbar\omega_{mk}$ ….. (11)

$$a_m = \frac{1}{i\hbar\omega_{mk}^2} < m\left|\frac{\partial H}{\partial t}\right| k > \{exp(-i\omega_{mk}t) - 1\} \quad \ldots.. (12)$$

∴ The total probability in the interval 0 to *t* is given by $|a_m|^2 = \frac{\left|<m|\frac{\partial H}{\partial t}|k>\right|^2}{\hbar^2\omega_{mk}^4}$

From Condition $|a_k|^2 << 1$,

$$\hbar\omega_{mk}^2 \left| < m\left|\frac{\partial H}{\partial t}\right| k > \right| << 1$$

Thus, for adiabatic approximation $< m \left|\frac{\partial H}{\partial t}\right| k >$ should be significant.

The example of adiabatic approximation occurs in the collision of gas molecules. When the gas molecules collide with each other than the process may be regarded as adiabatic in which the electrons remain in their original state and energy of the gas molecules system remains unchanged.

4.4 SUDDEN APPROXIMATION

The sudden approximation occurs when,

i. The perturbing term $H'(t)$ is very small.

ii. And the perturbing term changes suddenly (rapidly) during a finite interval of time t_0.

The change in the Hamiltonian is discontinuous on different times in the sudden approximation.

Let t_0 be the duration for which the perturbation is applied, then to consider sudden approximation we have,

$$\dot{a}_m = \frac{<m|\frac{\partial H}{\partial t}|k>}{E_k - E_m} exp\left\{-\frac{i}{\hbar}(E_k - E_m)t\right\} \quad \text{..... (1)}$$

In sudden approximation the variation of $\frac{\partial H}{\partial t}$ cannot be neglected; so

$$a_m = \int_0^{t_0} \frac{<m|\frac{\partial H}{\partial t}|k>}{E_k - E_m} exp\left\{-\frac{i}{\hbar}(E_k - E_m)t\right\} dt$$

$$= \left\{\frac{< m|H(t)|k >}{E_k - E_m} \exp\left\{-\frac{i}{\hbar}(E_k - E_m)t\right\}\right\}_0^{t_0}$$

$$- \int_0^{t_0} \frac{<m|H(t)|k>}{E_k - E_m} \exp\left\{-\frac{i}{\hbar}(E_k - E_m)t\right\} . \left\{-\frac{i}{\hbar}(E_k - E_m)\right\} dt \quad \text{..... (2)}$$

By the help of uncertainty relation $\Delta E\, \Delta t \approx \hbar$, is expressed (since $\Delta t = t_0$ *is very small*) as,

$$\frac{\hbar}{\Delta E} >> t_0 \qquad \text{..... (3)}$$

The physical interpretation of this condition is that of the energy of the system changes by an amount ΔE. In a time t_0 which is much less than the characteristics time associated with this energy change, then the state of the system remains unchanged (i.e., there is no transition) and so $< m|H(t)|k >$ = 0 so equation (2) becomes,

$$a_m = \frac{i}{\hbar} \int_0^{t_0} < m|H(t)|k > \exp\left\{-\frac{i}{\hbar}(E_k - E_m)t\right\} dt \qquad \text{..... (4)}$$

If ω_{mk} is the angular frequency of the transition from initial state *k* to a final state *m*, then

$$\omega_{mk} = \frac{E_m - E_k}{\hbar}$$

$$a_m = \frac{i}{\hbar} \int_0^{t_0} < m|H(t)|k > e^{i\omega_{mk}t}\, dt \qquad \text{..... (5)}$$

When perturbation is switched on suddenly, $H(t)$ changes instantaneously in time Δt which is small compared to period $\frac{1}{\omega_{mk}}$ so that the factor $e^{i\omega_{mk}t}$ in the above integral changes a little and hence can be taken outside the integral, then we get,

$$a_m = \frac{i}{\hbar}\, e^{i\omega_{mk}t} \int_0^{t_0} < m|H(t)|k > \, dt$$

$$= \frac{i}{\hbar}\, e^{i\omega_{mk}t} < m|H(t_0) - H(0)\,|k > t_0$$

$$= \frac{it_0}{\hbar}\, e^{i\omega_{mk}t} < m|H'|k > \qquad \text{..... (6)}$$

Where, $H' = H(t_0) - H(0)$ and its value is maximum during the sudden switch on.

Hence the sudden probability of the transition from state *k* to a state *m* will be given by,

$$|a_m|^2 = \frac{t_0^2}{\hbar^2}|< m|H'|k >|^2 \approx \frac{|<m|H'|k>|^2}{\hbar^2\omega_{mk}^4} \quad \ldots\ldots (7)$$

This is the equation which is used to evaluate the probability for transition under the influence of sudden perturbation. Sudden perturbation should be sufficiently small, so that the perturbation theory may be applied.

4.5 SEMI CLASSICAL TREATMENT OF AN ATOM WITH ELECTROMAGNETIC RADIATION OR APPLICATION OF TIME INDEPENDENT THEORY TO SEMI -CLASSICAL THEORY OF RADIATION

We are quite interested in studying processes that emit or absorb a single photon. But for this, the electromagnetic field must be quantised, which is covered in a more advanced course. As a result, we must rely on the so-called semi-classical radiation theory in this course, which treats the radiation field as a classical field. The interactions between the radiation field and the particles are then represented by specific Hamiltonian interaction terms, which are dealt with time-dependent perturbation theory. The particles and their Coulomb interactions are handled in a quantum mechanical manner.

This is the reason the theory is known as a semi-classical radiation theory.

This semi classical treatment describes approximately but correctly the influence of an external radiation on particles giving absorption and induced emission, but not the influence of particles on the fields (spontaneous emission).

The theory will be semi-classical due to the fact that we shall treat the motion of the atoms to be quantised and the electromagnetic field to be classical represented by continuous potentials $\boldsymbol{A}$ and $\boldsymbol{\psi}$.

From the knowledge of classical electrodynamics, it is known that for transverse electromagnetic waves the vector potential $\boldsymbol{A}$ satisfies the equations:

$$\left.\begin{aligned} \nabla^2\mathbf{A} - \tfrac{1}{c^2}\tfrac{\partial \mathbf{A}}{\partial t} = 0 \\ and \qquad \operatorname{div}\mathbf{A} = \nabla\cdot\mathbf{A} = 0 \end{aligned}\right\} \qquad \ldots\ldots(1)$$

A typical plane wave-monochromatic solutions applicable to physical situations of equations (1), representing a real potential with the real polarization vector $Re\mathbf{A_0} = |\mathbf{A_0}|$ and propagation vector ***k*** can be written as

$$\mathbf{A}(\mathbf{r},t) = \mathbf{A}_0 e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} + A_0^* e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \qquad \ldots\ldots(2a)$$

$$= 2|\mathbf{A}_0|\cos(\mathbf{k}\cdot\mathbf{r}-\omega t+\alpha);$$

$$\mathbf{A}_0 = |\mathbf{A}_0|e^{i\alpha} \qquad \ldots\ldots(2b)$$

Equation **(2a)** is satisfied if ω = *kc*, *k* being magnitude of propagation vector **k** and **(2b)** is satisfied if constant complex vector $\mathbf{A_0}$ is perpendicular to **k**.

The electric field associated with vector potential **A** (equation (1), ϕ=0) is

$$\mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} = -\frac{2\omega}{c}|A_0|\sin(\mathbf{k}\cdot\mathbf{r}-\omega t+\alpha) \qquad \ldots\ldots(3)$$

The intensity of radiation i.e., Flow of energy per unit area per second is given by well-known **Poynting's vector**

$$\mathbf{I} = \frac{c}{4\pi}(\mathbf{E}\times\mathbf{B}). \quad \text{(C.G.S. System)} \qquad \ldots\ldots(4)$$

In free space $|\mathbf{E}| = |\mathbf{B}|$ and **E** is normal to **B**. Thus, in free space **(E×B)** is a vector of magnitude $|E|^2$and direction **k** *i.e.*

$$I = \frac{c}{4\pi}\cdot\frac{4\omega^2}{c^2}|A_0|^2\sin^2(\mathbf{k}\cdot\mathbf{r}-\omega t+\alpha)$$

Mean Poynting vector:

$$\bar{\mathbf{I}} = \frac{\omega^2}{2\pi c}|A_0|^2$$

[Since time averaged magnitude of $\sin^2(\mathbf{k}\cdot\mathbf{r} - \omega t + \alpha)$ is $\frac{1}{2}$]

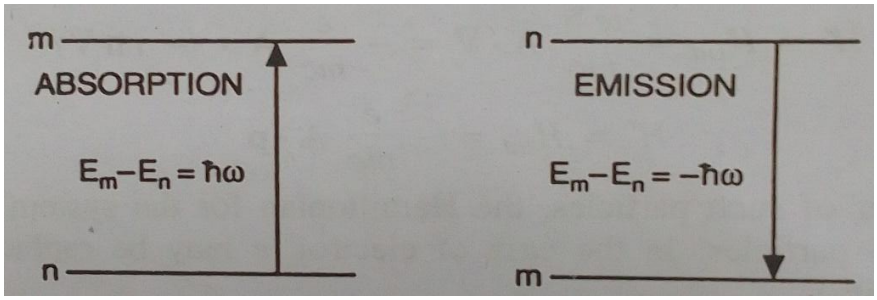

Fig.4.1

The first order correction to Hamiltonian for a charged particle interaction with electromagnetic field is given by:

$$H'_{int} = -\frac{e}{mc}(\mathbf{A}\cdot\mathbf{p}) = \frac{ie\hbar}{mc}\mathbf{A}\cdot\nabla$$
$$= \frac{ie\hbar}{mc}\left[\mathbf{A}_0 e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} + \mathbf{A}_0{}^* e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\right]\cdot\nabla \qquad \ldots\ldots(6)$$

Assuming nth state as initial state, then Zero order perturbation equation for a final state m becomes,

$$i\hbar\dot{a}_m^{(1)}(t) = (H'_{int})_{mn}e^{i\omega_{mn}t} \qquad \text{where } \boldsymbol{\omega_{mn}} = \frac{E_m - E_n}{\hbar}$$

$$= H'_{mn}e^{i(\omega_{mn}-\omega)t} + H''_{mn}e^{i(\omega_{mn}+\omega)t} \qquad \ldots\ldots (7)$$

where,

$$H'_{mn} = \frac{ie\hbar}{mc}\int \psi_m^{0*}\, e^{i(\mathbf{k}.\mathbf{r})}(\mathbf{A_0}.\boldsymbol{\nabla})\psi_n^0\, d\tau$$

$$H'_{mn} = \frac{ie\hbar}{mc}\int \psi_m^{0*} e^{i(\mathbf{k}.\mathbf{r})}(\boldsymbol{A_0}.\boldsymbol{\nabla})\psi_n^0\, d\tau \qquad \ldots\ldots (8)$$

If harmonic perturbation of frequency ω is switched on at t=0, then equation (7) on integration with respect to *t* gives,

$$a_m^{(1)}(t) = \frac{1}{i\hbar}\left[\int_0^t H'_{mn} e^{i(\omega_{mn}-\omega)t}dt + \int_0^t H''_{mn} e^{i(\omega_{mn}+\omega)t}dt\right]$$
$$= H'_{mn}\frac{1-e^{i(\omega_{mn}-\omega)t}}{\hbar(\omega_{mn}-\omega)} + H''m_{mn}\frac{1-e^{i(\omega_{mn}+\omega)t}}{\hbar(\omega_{mn}+\omega)} \quad \ldots\ldots(9a)$$

using $\omega_{mn} = \frac{E_m - E_n}{\hbar}$, we get,

$$a_m^{(1)}(t) = H'_{mn}\left\{\frac{1-e^{i(E_m-E_n-\hbar\omega)t/\hbar}}{E_m-E_n-\hbar\omega}\right\} + H''_{mn}\left\{\frac{1-e^{i(E_m-E_n+\hbar\omega)t/\hbar}}{E_m-E_n+\hbar\omega}\right\} \quad \ldots\ldots (9b)$$

Out of the two terms in equation (9) only one term at a time is to be considered.

If $E_m - E_n - \hbar\omega$ or $E_m - E_n = \hbar\omega$, the first term will be very large compared with the second; but if

$$E_m - E_n + \hbar\omega \text{ or } E_m - E_n = -\hbar\omega$$

the second term will be large compared to first, while if neither of these conditions is satisfied, the probability of transition is vanishingly small. This means that the transitions are probable only if,

$$E_m - E_n = \pm\hbar\omega \quad \ldots\ldots (10)$$

which is Bohr's frequency condition, which thus emerges as a deduction rather than a postulate.

One of these two probability relates to radiation from the field being **absorbed**, and the other to radiation being **emitted** by the field. It is rather amazing that we have energy quantization even if we did not initially assume an electromagnetic field quantization. Equation (10) makes the assumption that there is energy conservation between the particle and the field.

4.5.1 For Absorption

$E_m > E_n$ the probability is maximum for $\omega_{mn} = \omega$ or

$E_m - E_n = \hbar\omega$ and first term of (9b) predominates while the second term is negligible. Thus, for absorption

$$a_m^{(1)}(t) = H'_{mn}\left\{\frac{1-e^{i(\omega_{mn}-\omega)t}}{\hbar(\omega_{mn}-\omega)}\right\} \quad \ldots\ldots (11)$$

The probability of finding the system in *m*-state at the end of the interval *t* is

$$|a_m^{(1)}(t)|^2 = |H'_{mn}|^2\left\{\frac{4\,sin^2\frac{1}{2}(\omega_{mn}-\hbar\omega)t}{\hbar^2(\omega_{mn}-\omega)^2}\right\}. \quad \ldots\ldots (12)$$

Thus, for absorption the probability is proportional to $|H'_{mn}|^2$.

We have just taken one frequency ω into consideration thus far. Since the probability $|a_m^{(1)}(t)|^2$ is very small except when $\omega_{mn} = \omega$; the random motion of emitting and absorbing atoms produces a Doppler broadening of spectral lines and the radiation present in the initial state has a continuum of frequencies. If the intensity in the smaller angular frequency range $\Delta\omega$ is $I(\omega)\Delta\omega$ the magnitude of the Poynting vector is,

$$\dot{I}(\omega)\Delta\omega = \frac{\omega^2}{2\pi c}|\mathbf{A}_0|^2 \text{ or } |\mathbf{A}_0|^2 = \frac{2\pi c}{\omega^2}I(\omega)\Delta\omega \quad \ldots\ldots (13)$$

Here $\mathbf{A_0}$ is the vector potential amplitude and characterises the frequency range.

The transition probability for absorption is,

$$|a_m^{(1)}(t)|^2 = \sum_n \frac{8\pi e^2}{m^2 c\omega^2}\, I(\omega)\Delta\omega\left|\int\int \psi_m^{0*}\, e^{i(\mathbf{k}.\mathbf{r})}\, gradA\, \psi_n^0\, d\tau\right|^2 . \frac{\sin^2\{(\omega_{mn}-\omega)t/2\}}{(\omega_{mn}-\omega)^2} \quad \ldots\ldots (14)$$

where *gradA* is the component of the gradient operator along the polarization vector $\mathbf{A_0}$. On account of being no phase relations between the radiation components of different frequencies, the contributions to the probability from various frequency ranges are additive. Each frequency range Δω in equation (14) can be made infinitesimal and then the summation can be replaced by an integration. As the time factor has a sharp maximum at ω = ω_{mn} the other factors involving can be taken outside the integral and the limits on ω can be extended to $\pm\infty$ .By doing so the transition probability per unit time for an upward and (absorption) becomes.

$$\frac{1}{t}\left|a_m^{(1)}(t)\right|^2 = \frac{8\pi e^2}{m^2 c\omega_{mn}^2} I(\omega_{mn}) \left| \int \psi_m^{0*} e^{i\mathbf{k}\cdot\mathbf{r}} \operatorname{grad}_A \psi_n^0 d\tau \right|^2 \times \int_{-\infty}^{+\infty} \frac{\sin^2\left\{(\omega_{mn}-\omega)\frac{1}{2}t\right\}}{t(\omega_{mn}-\omega)^2} d\omega$$

$$= \frac{4\pi^2 e^2}{m^2 c\omega_{mn}^2} I(\omega_{mn}) \left| \int \psi_m^{0*} e^{i\mathbf{k}\cdot\mathbf{r}} \operatorname{grad}_A \psi_n^0 d\tau \right|^2 \qquad \ldots\ldots(15)$$

$$\text{since} \int_{-\infty}^{+\infty} \frac{\sin^2\left\{(\omega_{mn}-\omega)\frac{1}{2}t\right\}}{\{(\omega_{mn}-\omega)/2\}^2} \cdot d\omega = 2\pi t \Bigg]$$

Where $\mathbf{k} = \frac{\omega_{mn}}{c}$

4.5.2 For Emission

For emission or for the downward transition there is a similar result, the only difference being that $e^{i(\mathbf{k}.\mathbf{r})}$ is replaced by $e^{-i(\mathbf{k}.\mathbf{r})}$ i.e., the *transition probability per unit time of a downward transition* $E_m{}' \approx E_n - \hbar\omega$*) is given by,*

$$\frac{1}{t}\left|a_m^{(1)}(t)\right|^2 = \frac{4\pi^2 e^2}{m'^2 c\omega_{nm'}^2} I(\omega_{nm'}) \left| \int \psi_{m'}^{*} e^{-i\mathbf{k}\cdot\mathbf{r}} \operatorname{grad}_A \psi_n^0 d\tau \right|^2 \qquad \ldots\ldots(16)$$

Where $\mathbf{k} = \frac{\omega_{mn}{}'}{c}$

4.5.3 Interpretation of terms of absorption and emission

Equation (15) and (16) represent the transition probabilities of the particle per unit time between stationary states under the influence of a classical radiation field.

Let us now interpret these expressions in terms of absorption and emission of quanta of electromagnetic radiation by assuming that such quanta exist and provide the energy units of the radiation field and that energy is conserved between the field and that particle.

In an upward transition the particle gains the amount of energy $E_m - E_n$ under the influence of angular frequency ω_{mn}. The quantum energy of this radiation is $E_m - E_n \approx \hbar\omega_{mn}$, so that we may consider hat the upward transition of the particle is associated with the absorption of the one quantum from the radiation field.

Similarly, the downward transition may be considered to be associated with emission of the quantum whose energy corresponds to the frequency of the radiation field. According to

equation (16) the transition probability of emission per unit time is proportional to the intensity of the radiation present. The process of emission is therefore called the *induced emission.*

If we rewrite equation (16) in terms of the reverse transition to that which appears in (15). Equation (15) describes the transition from an initial lower state *n* to a final upper state m, equation (16) can be made to describe the transition from an initial upper state m to a final lower state *n* if *n* is replaced by *m* and m' by *n.* Then equation (16) takes the form

$$\frac{4\pi^2 e^2}{m^2 c\omega_{mn}^2} I(\omega_{mn}) \left| \int \left(\psi_n^{0*} e^{-ik\cdot r}\right) \nabla_A \psi_{ni}^0 d\hbar \right|^2 \quad \ldots\ldots (17)$$

It can be seen that the integral is just negative of the complex conjugate of integral in (15). The squares of magnitudes of both integrals in (15) and (17) are equal. This implies that the transition probabilities of absorption and induced emission between any pair of states are the same.

4.6 SUMMARY

In this unit, you have studied about adiabatic approximation, in which the perturbation is turned on very slowly. Adiabatic approximation occurs in the collision of gas molecules. In sudden approximation the Hamiltonian changes rapidly for a very short but finite time interval. Also, you have understood that the transition probabilities of absorption and induced emission between any pair of states are the same.

4.7 GLOSSARY

Perturbation – a deviation of a system caused by an outside influence

Adiabatic – The gradual change in the external conditions

Sudden – The quick change

Approximation – nearly same but not exact

Absorption – a process by which radiation is absorbed and converted into energy

Emission – the process by which a higher energy quantum mechanical state of a particle becomes converted to a lower one through the emission of a photon, resulting in the production of light

Induced – to cause or produce

Transition – alteration of a physical system from one state or condition to another

Probability – something that is likely to happen

4.8 REFERENCES

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2. Advanced Quantum Mechanics, Satya Prakash, Kedar Nath Ram Nath, Meerut

3. Advanced Quantum Mechanics, J.J.Sakurai, Pearson

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4.9 SUGGESTED READINGS

1. Advanced Quantum Mechanics, Franz Schwabl, Springer

2. Introduction to Quantum Mechanics, David J. Griffiths, Cambridge University Press

3. P.M. Mathews and K. Venkatesan, A Text book of Quantum Mechanics, Tata Mc Graw-Hill, New Delhi.

4. L.I. Schiff, Quantum Mechanics, McGraw-Hill

4.10 TERMINAL QUESTIONS

Short Answer type question

1. Write Short notes on:

i. Adiabatic approximation
ii. Sudden approximation

2. On the basis of time dependent perturbation theory, briefly outline the theory of emission and absorption in atomic systems.
3. Explain semi classical theory of radiation.

Long Answer type question

1. Give the theory of induced emission and absorption of radiation on the basis of time dependent perturbation theory.
2. Develop the semi classical radiation theory and use it to determine the conditions for allowed transitions.
3. Explain Adiabatic approximation in detail.
4. Explain Sudden approximation in detail.
5. Give an account of adiabatic and sudden approximations. Show that approximation can be applied to the extra nuclear electron initially present in the hydrogen atom and is superior to the other approximation methods that might be used.

UNIT 5 RELATIVISTIC QUANTUM MECHANICS

Structure

5.1 Introduction

5.2 Objectives

5.3 Klein-Gordon equation

5.4 Dirac's Equation

5.5 Plane Wave Solutions

5.6 Interpretation of negative energy states

5.7 Summary

5.8 Glossary

5.9 References

5.10 Suggested Readings

5.11 Terminal Questions

5.1 INTRODUCTION

Till now we have dealt with non-relativistic quantum mechanics. A free particle satisfying Schrodinger equation has the non-relativistic energy $E = p^2/2m$. Non-relativistic Quantum Mechanics is applicable for particles with velocity much smaller than the velocity of light (v << c). But for relativistic particles, i.e., particles with velocity comparable to the velocity of light (e.g., electrons in atomic orbits), we need to use relativistic Quantum Mechanics. For relativistic Quantum Mechanics, we need to formulate a wave equation which is consistent with relativistic transformations (Lorentz transformations) of special theory of relativity. A characteristic feature of relativistic wave equations is that the spin of the particle is built into the theory from the beginning and cannot be added afterwards. (Schrodinger equation does not have any spin information; we need to separately add spin wave function.) it makes a particular relativistic equation applicable to a particular kind of particle (with a specific spin) i.e, a relativistic equation which describes scalar particle(spin=0) cannot be applied for a fermion(spin=1/2) or vector particle(spin=1). Before discussion relativistic QM, let us briefly summarise some features of special theory of relativity here. Specification of an instant of time t and a point $\vec{r}$ = (x, y, z) of ordinary space defines a point in the space-time. We'll use the notation

$$x^\mu = (x^0, x^1, x^2 x^3) \quad \text{or} \quad x^\mu = (x^0, x^i) \text{ where, } x^0 = ct \text{ , } \mu = 0,1,2,3$$

This notation is given for four vectors. Now if we consider two events in space time $(x^0, x^1, x^2 x^3)$ and $(x^0 + dx^0, x^1 + dx^1, x^2 + dx^2, x^3 + dx^3)$ In three dimensional space we define the distance between two points. We generalize the notion of the distance between two points in space to the interval between two points in the space-time, say, ds. For ds to be same for all observer (i.e., in all inertial frames), it must be invariant under Lorentz transformations and rotations. The interval is defined as:

$$ds^2 = g_{\mu\nu} dx^\mu dx^\nu$$

Where, $g_{\mu\nu}$ is the metric of the space-time. In Minkowski space

$$g\mu\nu = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

So,

$$ds^2 = (cdt)^2 - ((dx^1)^2 + ((dx^2)^2 + ((dx^3)^2) = (cdt)^2 - (d\vec{r})^2$$

Under Lorentz transformation x^μ transforms as $x'^\mu = \Lambda^\mu{}_\nu x^\nu$ where, $\Lambda^\mu{}_\nu$ is a 4×4 matrix representing the Lorentz transformation operator. For example, the operator for x^1 axis can be given as:

$$\Lambda^\mu_\nu = \begin{bmatrix} \gamma & -\gamma\beta & 0 & 0 \\ -\gamma\beta & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Where, β= v/c and $1/\sqrt{1-(v/c)^2}$. Hence, the transformed coordinates under x^1 axis represent:

$$ct' = \gamma\left(ct - \frac{v}{c}x^1\right), x'^1 = \gamma\left(x^1 - \frac{v}{c}ct\right), x'^2 = x^2, x'^3 = x^3$$

Problem: Prove that ds^2 is invariant.

Solution: $ds'^2 = (cdt')^2 - ((dx'^1)^2 + ((dx'^2)^2 + ((dx'^3)^2)$

$$= \gamma^2(cdt - \beta dx'^1)^2 - \gamma^2(cdt - \beta cdt)^2 - (dx^2)^2 - (dx^3)^2$$

$Hence, \quad ds'^2 = ds^2$

ds^2 is Lorentz invariant. It can be both positive and negative unlike spatial distance which is always positive. If:

$ds^2 > 0$ i.e., $(cdt^2) > (\overrightarrow{dr})^2$, the interval is called "time-like"

$ds^2 < 0$ i.e., $(cdt^2) < (\overrightarrow{dr})^2$, the interval is called "space-like"

$ds^2 = 0$ i.e., $(cdt^2) = (\overrightarrow{dr})^2$, the interval is called "light-like"

Covariant & Contravariant vectors: Any quantity which transforms like x^μ under Lorentz transformation is called a contravariant vector while anything which transforms like $\frac{\partial}{\partial x^\mu}$ is called covariant vector. General convention for contravariant vector is a^μ (i.e., is in the superscript) and for covariant vector a_μ (i.e., μ is in the subscript) i.e., $\frac{\partial}{\partial x^\mu} = \partial\mu$. The inner product of a covariant vector and a contravariant vector is a Lorentz invariant (i.e., scalar). The relation between contra and covariant vectors is given as follows:

$$x_\mu = \sum_\nu g_{\mu\nu} x^\nu$$

After implementing the convention of summation over repeated indices we can write the above equation as $x_\mu = g_{\mu\nu} x^\nu$ where ν can be repeated again and hence can be summed over. Similarly $x^\mu = g^{\mu\nu} x_\nu$. In Minkowski space $g_{\mu\nu} = g^{\mu\nu}$. So, we have

$$x_0 = g_{0\nu} x^\nu = g_{00} x^0 + g_{01} x^1 + g_{02} x^2 + g_{03} x^3 = g_{00} x^0 = x^0$$

$$x_1 = g_{1\nu} x^\nu = g_{10} x^0 + g_{11} x^1 + g_{12} x^2 + g_{13} x^3 = g_{11} x^1 = -x^1$$

Similarly,

$$x_2 = -x^2 \; and \; x_3 = -x^3$$

Differential Operators:

$$\partial_\mu = \frac{\partial}{\partial x^\mu} = \left(\frac{1}{c}\frac{\partial}{\partial t}, \frac{\partial}{\partial x^1}, \frac{\partial}{\partial x^2}, \frac{\partial}{\partial x^3}\right)$$

$$\partial_\mu = (\partial_0, \partial_1, \partial_2, \partial_3) = \left(\frac{1}{c}\frac{\partial}{\partial t}, \vec{\nabla}\right)$$

Similarly,

$$\partial^\mu = g^{\mu\nu}\partial_\nu = \left(\frac{1}{c}\frac{\partial}{\partial t}, -\vec{\nabla}\right)$$

The Lorentz invariant second order differential operator or the d'Alembertian operator is given by following relation:

$$\square = \partial_\mu \partial^\mu = \left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2}, -\overrightarrow{\nabla^2}\right)$$

As we know the relativistic mass $mr = \gamma m$ and energy $E = m_r c^2 = \gamma mc^2$. The energy-momentum 4-vector is $p^\mu = (E/c, \vec{p})$ where $\vec{p} = \gamma m \vec{v}$. So,

$$p^2 = g_{\mu\nu}p^\mu p_\nu = p^\mu p_\nu = (E/c)^2 - (\vec{p})^2 = \frac{(\gamma mc^2)^2}{c^2} - (\gamma m\vec{v})^2) = m^2c^2$$

So, the relativistic energy momentum relation is given by:

$$E^2 = c^2p^2 + m^2c^4$$

5.2 OBJECTIVES

Till now we have considered non-relativistic quantum mechanics and it is not applicable to the phenomenon involving particles moving with relativistic velocities. Hence, it is desirable to include the requirements imposed on our theory by the relativistic theory, at least required by special theory of relativity which deals with inertial systems. Since the use of general theory is not essential due to negligible gravitational field in atomic systems. This concept can be imposed in two following ways:

1) Implementing the concepts of special theory of relativity,
2) Formulating quantum theory in Lorentz invariant form.

5.3 KLEIN-GORDON EQUATION

Schrodinger proposed a relativistic form of his non-relativistic equation (at the same time when he developed his non-relativistic equation. Klein and Gordon developed this equation at a later time and is known as Klein-Gordon equation. Schrodinger used the energymomentum dispersion relation. Using the correspondence principle:

$$\hat{H}\psi = i\hbar\frac{\partial\psi}{\partial t} \qquad (1)$$

The non-relativistic Schroedinger equation is

$$-\frac{\hbar^2}{2m}\nabla^2\psi(r,t) = i\hbar\frac{\partial\psi(r,t)}{\partial t} \qquad (2)$$

Since transformations (under which the requirement of Special theory of relativity is invariant) to be considered are linear transformations.

$$\bar{x}^\mu = a^\mu_\nu . x^\nu \qquad (3)$$

This leaves invariant metric tensor $g_{\mu\nu}$

$$g_{\mu\nu} = \begin{cases} 1 \; for \; \mu = \nu \\ 0 \; for \; \mu \neq \nu \end{cases} \text{ where } g_{11}=g_{22} = g_{33} = g_{44} = 1 \; and \; g_{\mu\nu} = 0 \; for \; \mu \neq \nu$$

Equation (2) in tensor notations in Minkowski space (where Special theory of relativity treats spatial and temporal variables) can be given as:

$$-\frac{\hbar^2}{2m} g^{\mu\nu} \frac{\partial}{\partial x^{\mu}} \frac{\partial}{\partial x^{\nu}} \psi(x^{\alpha}) = -\hbar c \frac{\partial}{\partial x^{4}} \psi(x^{\alpha}) \qquad (4)$$

Where, $x^4 = ict$

This equation is invariant under linear transformation of space co-ordinates alone, but not invariant under Lorentz transformation in special relativity. Under these transformations this equation can become of second order in new time coordinates and mixed space time second order partial derivatives will appear. Such a result is not surprising since the Hamiltonian used here was non-relativistic. This is due to the use of non-relativistic Hamiltonian.

$$\widehat{H} = E = \pm\sqrt{c^2p^2 + m^2c^4} \qquad (5)$$

Schroedinger equation will become:

$$\pm[\sqrt{c^2p^2 + m^2c^4}]\psi = i\hbar\frac{\partial\psi}{\partial t} \qquad (6)$$

There are two difficulties in the interpretation of above equation:

First related to interpret sign ±. There is no problem in classical mechanics since energy can continuously vary with a gap of $2mc^2$ between lowest positive and highest negative value. If any particle has any type of energy other can be ignored. But in quantum mechanics energy can change discontinuously.

Second difficulty arises when $\pm[\sqrt{c^2p^2 + m^2c^4}]\psi = i\hbar\frac{\partial\psi}{\partial t}$.

We cannot interpret the square root of any operator & if we expand it binomially there will be space and time derivative in unsymmetrical form, so it will not be Lorentz invariant & will be difficult to solve. So Klein-Gordon modified this Schrödinger equation as:

$$\widehat{H}\psi = i\hbar\frac{\partial\psi}{\partial t}$$

$$H^2\psi = i\hbar\hat{H}\frac{\partial\psi}{\partial t} = i\hbar\frac{\partial\hat{H}\psi}{\partial t}$$

$$H^2\psi = -\hbar^2\frac{\partial^2\psi}{\partial t^2} \qquad (7)$$

Equation (7) is relativistic Schroedinger equation & also known as Klein-Gordon equation. For relativistic free particle K.G. equation is:

$$(-\hbar^2c^2\nabla^2 + m^2c^4)\psi = -\hbar^2\frac{\partial^2\psi}{\partial t^2} \qquad (8)$$

This equation may be written as:

$$(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{m^2c^2}{\hbar^2})\psi = 0 \qquad (9)$$

$$\left[\square - \frac{m^2c^2}{\hbar^2}\right]\psi = 0 \qquad (10)$$

where, $\square = \nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} = \frac{\partial}{\partial x^\mu}\frac{\partial}{\partial x^\nu}$ is called the D' Alembertian operator.

In coordinate representation

$$\left(g^{\mu\nu}\frac{\partial}{\partial x^\mu}\frac{\partial}{\partial x^\nu} - k^2\right)\psi(x^\alpha) = 0, \text{ where } k=\frac{mc}{\hbar} \qquad (11)$$

Problem: Derive continuity equation for the KG equation.

Solution: The KG equation describes the relativistic dynamics of a scalar particle. The plane wave solution of the KG equation is

$$\phi(x) = Ne^{-i(Et-\vec{p}.\vec{x})} \qquad 11(a)$$

Where, N is normalization constant and energy E can be both positive and negative.

Multiply above equation by $\phi^*(x)$ we get

$$\phi^*(x)\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2\right)\phi(x) = -\frac{m^2c^2}{\hbar^2}\phi^*(x)\phi(x) \qquad 11(b)$$

Taking the complex conjugate of equation (9) and post-multiply with $\phi(x)$, which gives

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\phi^*(x)\right)\phi(x) - \left(\nabla^2\phi^*(x)\right)\phi(x) = -\frac{m^2c^2}{\hbar^2}\phi^*(x)\phi(x) \qquad 11(c)$$

Subtracting 11(c) from 11(b)

$$\phi^*(x)\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\phi(x) - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\phi^*(x)\phi(x) - (\phi^*(x)\nabla^2\,\phi(x) - \phi(x)\nabla^2\,\phi^*) = 0$$

$$\text{Or } \frac{1}{c}\frac{\partial}{\partial t}\left[\frac{i\hbar}{2mc}\left(\phi^*\frac{\partial\phi}{\partial t} - \frac{\partial\phi^*}{\partial t}\phi\right)\right] + \vec{\nabla}.\left[\frac{\hbar}{2im}(\phi^*\nabla\phi - (\nabla\phi^*)\phi\right] = 0$$

Thus, $\frac{1}{c}\frac{\partial}{\partial t}\rho + \vec{\nabla}.\vec{j} = 0$

$$\text{Or } \partial_\mu j^\mu = 0$$

This is the continuity equation for the KG equation where

$$j^0 = \rho = \frac{i\hbar}{2mc}\left(\phi^*\frac{\partial\phi}{\partial t} - \frac{\partial\phi^*}{\partial t}\phi\right)$$

$$\text{And } \vec{j} = \left[\frac{\hbar}{2im}(\phi^*\nabla\phi - (\nabla\phi^*)\phi\right]$$

Recall the continuity equation for Schrodinger equation ρ is the probability density and $\vec{j}$ is the probability current. Continuity equation has the interpretation of conservation of probability. It tells that if the probability of finding a particle in some region decreases, the probability of finding it outside that region increases, i.e., there is a flow of probability current so that the total probability remains conserved. Since the KG eqn also satisfies the same continuity equation, it is natural to interpret ρ as the probability density and $\vec{j}$ as the probability current.

MAJOR PROBLEMS WITH K-G EQUATION

There are two major problems with the KG equations which have been listed below:

(1) The equation has both positive and negative energy solutions. The negative energy solution poses a problem. For large $\vec{p}$ we can have large negative energy, i.e., the system become unbounded from below. So, we can extract any arbitrary large amount of energy from the system by pushing it into more and more negative energy states. One may say, we truncate the physical space to be the positive energy states only i.e, only *E* are physical. But then the eigenstates don't form a complete basis states, (both +ve and –ve energy states are Fourier modes of ϕ); if we don't have completeness

relation, we cannot have superposition principle too i.e., we cannot expand a state in the basis of ϕ and a perturbation may cause the system to jump to a negative energy states. Since -ve energy states are valid solutions of the KG equation, we cannot stop that. So, just interpreting negative energy states as nonphysical does not work.

(2) The second problem is associated with the probability density. Since $\rho=2N^2E$, i.e. ρ is negative if E is negative. But for interpretation of probability density it must be a positive quantity. Though in QM, KG equation looks awkward at this moment, but in QFT this is a valid equation for scalar (spin=0) particles. Feynman and Stückelberg interpreted the positive energy states as particles propagating forward in time and negative energy states are propagating backward in time and thus represent antiparticles propagating forward in time. But we'll not discuss those developments here.

5.4 DIRAC'S RELATIVISTIC EQUATION

The Dirac equation is a relativistic quantum mechanical wave equation for spin-1/2 particles (e.g., electrons), which was derived by Dirac in 1928. The difficulties in finding a consistent single-particle theory from the Klein–Gordon equation led Dirac to search for an equation that

- had a positive-definite conserved probability density and
- was first order both in time and space

Dirac approached the problem of finding a relativistic wave equation:

$$\hat{H}\psi(r,t) = i\hbar\frac{\partial\psi(r,t)}{\partial t} \qquad (1)$$

Dirac formulated an equation to avoid the difficulties arising in K.G. equations on basis of requirements of Lorentz invariance which demand that an equation which is linear in **H** and hence in **E** must be linear in **p**. Dirac assumed that the Hamiltonian H is linear in energy and momentum. The simplest linearized Hamiltonian for a free particle is

$$H = c\vec{\alpha}.\boldsymbol{p} + \beta mc^2 \qquad (2)$$

Where α & β are independent of E & p (thus commutes with r).

Substituting H from (2) into (1)

$$(c\vec{\alpha}.\boldsymbol{p} + \beta mc^2)\,\psi(r,t) = i\hbar\frac{\partial\psi(r,t)}{\partial t} \qquad (3)$$

$$[c\vec{\alpha}.(-i\hbar\boldsymbol{\nabla}) + \beta mc^2]\psi(r,t) = i\hbar\frac{\partial\psi(r,t)}{\partial t}$$

$$\text{Or } \left(i\hbar\frac{\partial}{\partial t} + i\hbar c\vec{\alpha}.\boldsymbol{\nabla} - \beta mc^2\right)\psi(r,t) = 0 \quad \textbf{(4)}$$

For simplicity we can write E for $i\hbar\frac{\partial}{\partial t}$ and p for $-i\hbar\nabla$ thus, we get

$$(E - c\vec{\alpha}.\boldsymbol{p} + \beta mc^2)\psi(r,t) = 0 \qquad \textbf{(5)}$$

Also we can put $\vec{\boldsymbol{\alpha}} = \boldsymbol{i\alpha_x + j\alpha_y + k\alpha_z}$ $\boldsymbol{and}$ $\boldsymbol{p = ip_x + jp_y + kp_z}$ in equation (5)

$$(c\alpha_x p_x + c\alpha_y p_y + c\alpha_z p_z + \beta mc^2)\psi = E\psi \qquad (6)$$

Where $\alpha_x, \alpha_y, \alpha_z$ & β have following properties

(i) $\alpha_x^2 = \alpha_y^2 = \alpha_z^2 = \beta^2 = 1$

(ii) $\alpha_x\alpha_y + \alpha_y\alpha_x = 0, \alpha_y\alpha_z + \alpha_z\alpha_y = 0, \alpha_z\alpha_x + \alpha_x\alpha_z = 0$

(iii) $\alpha_x\beta + \beta\alpha_x = \alpha_y\beta + \beta\alpha_y = \alpha_z\beta + \beta\alpha_z = 0$

i.e., their squares are unity and; they anti-commute with one another in pairs.

Matrices for $\vec{\alpha}$ and β

The squares of all four matrices are unity; such that their eigenvalues are +1 and -1. Arbitrarily taking β as the matrix that is to be diagonalised, so that all +1 and -1 eigenvalues are grouped together. So, the matrix β can be expressed as:

$$\beta = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Which is an abbreviation of

$$\beta = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

All the four matrices $\alpha_x, \alpha_y, \alpha_z$ & β are such that their squares are unity and they anti-commute with each other in pairs. Since we know that Pauli's spin matrices also satisfy the above properties, given by:

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_x = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Since a 2×2 matrix has four elements, so, there are only four independent 2×2 matrices. Three of these are $\sigma_x, \sigma_y, \sigma_z$. The only other matrix linearly independent of these three is

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Which is a unit matrix and therefore commutes rather than anti-commutes with every σ. Now, we show that the Dirac Matrices must be even-dimensional.

Let's take β as N×N diagonal matrix:

$$\beta = \begin{bmatrix} b_1 & & 0 \\ & b_i & \\ 0 & & b_N \end{bmatrix}$$

As β^2=1, $b_i^2 = 1, b_i = \pm 1(1,2,\ldots . N)$

Also, since $\alpha_k^2 = \beta^2$=1(k = x, y, z); det$\alpha_k or\ det\beta \neq 0$

This implies that matrices $\alpha_k (k = x, y, z)\ and\ \beta$ has an inverse

Since β anti-commutes with each component of α_k, we have;

$$\alpha_k \beta + \beta\, \alpha_k = 0$$

Or $\beta\, \alpha_k = -\alpha_k \beta$

Multiply with inverse of α_k we get

$$\alpha_k^{-1} \beta\, \alpha_k = -\beta$$

Taking trace on both sides

$Trace(\alpha_k^{-1}\beta\,\alpha_k) = -Trace\,\beta$ since, Trace (ABC)=Trace (CAB)

Thus, Trace (β) = -Trace (β) or, Trace (β)=0

Similarly, Trace (α_k)=0

Thus, this shows that the trace of each of the matrices must be zero. Also we know that Dirac matrices must be even dimensional. Therefore, we cannot use 3×3 matrices. The next simplest choice is 4×4 matrices.

As the eigenvalues of all four matrices are +1 and -1. We can arbitrarily take β as grouped matrices of ±1 eigenvalues:

$$\beta = \begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix}$$

$$\beta = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

As β anti-commutes with $\vec{\alpha}$ we have

$$\alpha_k\beta + \beta\,\alpha_k = 0$$

The, jl element of which is$(\alpha_k)_{jl}(\beta_j + \beta_l) = 0$; here, if $\beta_j = \beta_l$ then $(\alpha_k)_{jl} = 0$ whereas, if β_j and β_l have opposite signs then, $(\alpha_k)_{jl}$ need not to be zero. Therefore,

$$\alpha_k = \begin{bmatrix} 0 & \alpha_{x1} \\ \alpha_{x2} & 0 \end{bmatrix}$$

Where, α_{x1} has m rows and n columns while α_{x2} has n rows and m columns. Also square of α_k is unit matrix.

Or $\alpha_{x1}\alpha_{x2} = 1$ and $\alpha_{x2}\alpha_{x1} = 1$, but no two matrices exit that satisfy this condition simultaneously if m ≠ n. Therefore, we must have m=n=2 for 4×4 matrix. It is apparent that $\alpha_y and\ \alpha_z$ can be taken in similar form.

Using Pauli's spin matrices:

$$\alpha_x = \begin{bmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

Similarly,

$$\alpha_y = \begin{bmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix}$$

And,

$$\alpha_z = \begin{bmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}$$

The four components of $\psi's$: If the Dirac operators are to involve 4×4 matrices. Then the Dirac operands must have the four components, that is Dirac ψ function, must have the form

$$\psi = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix}$$

where each of four components is an ordinary function of x, y, z and t. The time dependence of a Dirac pertaining to a system whose Hamiltonian is H is determined through the equation

$$H\psi = i\hbar \frac{\partial \psi}{\partial t}$$

Where

$$\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial t} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} = \begin{bmatrix} \partial\psi_1/\partial t \\ \partial\psi_2/\partial t \\ \partial\psi_3/\partial t \\ \partial\psi_4/\partial t \end{bmatrix}$$

The Dirac Equation:

The equation $H\psi = E\psi$ can now be written as

$$(c\vec{\alpha}.p + \beta mc^2)\psi = E\psi$$

$$(c\alpha_x p_x + c\alpha_y p_y + c\alpha_z p_z + \beta mc^2)\psi = E\psi$$

To write it in more explicit form we replace α and β by specific matrices using ψ with four component column symbol.

$$\begin{bmatrix} mc^2 & 0 & cp_z & c(p_x - ip_y) \\ 0 & mc^2 & c(p_x + ip_y) & -cp_z \\ cp_z & c(p_x - ip_y) & -mc^2 & 0 \\ c(p_x + ip_y) & -cp_z & 0 & -mc^2 \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} = E \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix}$$

So that this equation reduces to the four simultaneous equations

$$(mc^2)\psi_1 + cp_z\psi_3 + c(p_x - ip_y)\psi_4 = E\psi_1$$

$$(mc^2)\psi_2 + cp_z\psi_4 + c(p_x - ip_y)\psi_3 = E\psi_2$$

$$(-mc^2)\psi_3 + cp_z\psi_1 + c(p_x + ip_y)\psi_2 = E\psi_3$$

$$(-mc^2)\psi_4 + cp_z\psi_2 + c(p_x + ip_y)\psi_1 = E\psi_4$$

These equations may also be expressed as follows:

$$\{(E - mc^2)\psi_1 - cp_z\psi_3 - c(p_x - ip_y)\psi_4 = 0\}$$

$$\{(E - mc^2)\psi_2 - c(p_x + ip_y)\psi_3 + cp_z\psi_4 = 0\}$$

$$\{(E + mc^2)\psi_3 - cp_z\psi_1 - c(p_x - ip_y)\psi_2 = 0\}$$

$$\{(E + mc^2)\psi_4 + c(p_x - ip_y)\psi_1 - cp_z\psi_2 = 0\}$$

Finally we can replace p_x $by - i\hbar\frac{\partial}{\partial x}$ and get:

$$(E - mc^2)\psi_1 + i\hbar c\frac{\partial\psi_3}{\partial z} + i\hbar c(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y})\psi_4 = 0$$

$$(E - mc^2)\psi_2 + i\hbar c\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)\psi_3 - i\hbar c\frac{\partial\psi_4}{\partial z} = 0$$

$$(E + mc^2)\psi_3 + i\hbar c\frac{\partial\psi_1}{\partial z} + i\hbar c(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y})\psi_2 = 0$$

$$(E+mc^2)\psi_4 + i\hbar c\left(\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right)\psi_1 - i\hbar c\frac{\partial \psi_2}{\partial z} = 0$$

Problem: If $\vec{\alpha}$ represents three Dirac matrices $\alpha_x, \alpha_y, \alpha_z$ and B and C are usual three dimensional vectors, then show that

$$(\vec{\alpha}.B)(\vec{\alpha}.C) = B.C + i\vec{\sigma}'.B \times C$$

Where, $\vec{\sigma}' = \begin{bmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{bmatrix}$ is a 4×4 matrix. $\vec{\sigma}$ being a 2×2 matrices.

Solution: $(\vec{\alpha}.B)(\vec{\alpha}.C) = (\alpha_x B_x + \alpha_y B_y + \alpha_z B_z)(\alpha_x C_x + \alpha_y C_y + \alpha_z C_z)$

$$= \alpha_x^2 B_x C_x + \alpha_y^2 B_y C_y + \alpha_z^2 B_z C_z + \alpha_x \alpha_y (B_x C_y - B_y C_x) + \alpha_y \alpha_z (B_y C_z - B_z C_y) + \alpha_z \alpha_x (B_z C_x - B_x C_z)$$

Since, $\alpha_x \alpha_y = -\alpha_y \alpha_x etc.$

Also, $\alpha_x^2 = \alpha_y^2 = \alpha_z^2 = 1$

But, $$\alpha_x \alpha_y = \begin{bmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{bmatrix}\begin{bmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{bmatrix} = \begin{bmatrix} \sigma_x \sigma_y & 0 \\ 0 & \sigma_x \sigma_y \end{bmatrix}$$

$$= \begin{bmatrix} i\sigma_z & 0 \\ 0 & i\sigma_z \end{bmatrix} = i\begin{bmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{bmatrix} = i\sigma_z'$$

Similarly, $\alpha_y \alpha_z = i\sigma_x'$ and $\alpha_z \alpha_x = i\sigma_y'$

Thus, $$(\vec{\alpha}.B)(\vec{\alpha}.C) = B.C + i\begin{bmatrix} \sigma_x' & \sigma_y' & \sigma_z' \\ B_x & B_y & B_z \\ C_x & C_y & C_z \end{bmatrix}$$

$$= B.C + i\vec{\sigma}'.B \times C$$

Problem: If $\vec{\alpha}$ and β are Dirac matrices, prove that

(i) $\alpha_x = \frac{1}{2}[\alpha_x \alpha_y,\ \alpha_y]$

(ii) $\alpha_x \alpha_y \alpha_z = \frac{1}{2}[\alpha_x \alpha_y \alpha_z \beta,\ \beta]$

(iii) $Trace(\vec{\alpha}.B)(\vec{\alpha}.C) = 4\ B.C$

Solution: If $\vec{\alpha} = (\alpha_x, \alpha_y, \alpha_z)$ and β are Dirac matrices, then they must obey following properties:

1. The squares of all matrices is unity
   $\alpha_x^2 = \alpha_y^2 = \alpha_z^2 = \beta^2 = 1$
2. All four matrices anticommute in pairs
   $\alpha_x\alpha_y = -\alpha_y\alpha_x etc.$

(i) We have $[\alpha_x\alpha_y, \alpha_y] = \alpha_x\alpha_y\alpha_y - \alpha_y\alpha_x\alpha_y$

$= \alpha_x\alpha_y^2 + \alpha_x\alpha_y\alpha_y$

$= \alpha_x\alpha_y^2 + \alpha_x\alpha_y^2 = \alpha_x + \alpha_x$

Therefore, $\alpha_x = \frac{1}{2}[\alpha_x\alpha_y, \alpha_y]$

(ii) $[\alpha_x\alpha_y\alpha_z\beta, \beta] = \alpha_x\alpha_y\alpha_z\beta\,\beta - \beta\alpha_x\alpha_y\alpha_z\beta$

$= \alpha_x\alpha_y\alpha_z\beta^2 + \beta\alpha_x\alpha_y\alpha_z\beta$

$= 2\alpha_x\alpha_y\alpha_z$

$Therefore,\ \alpha_x\alpha_y\alpha_z = \frac{1}{2}[\alpha_x\alpha_y\alpha_z\beta, \beta]$

(iii) If $\alpha_x, \alpha_y, \alpha_z$ are Cartesian components of $\vec{\alpha}$ and similarly B and C have Cartesian components, then we have

$$(\vec{\alpha}.B)(\vec{\alpha}.C) = (\alpha_xB_x + \alpha_yB_y + \alpha_zB_z)(\alpha_xC_x + \alpha_yC_y + \alpha_zC_z)$$

$$= \alpha_x^2B_xC_x + \alpha_y^2B_yC_y + \alpha_z^2B_zC_z + \alpha_x\alpha_y(B_xC_y - B_yC_x) + \alpha_y\alpha_z(B_yC_z - B_zC_y) + \alpha_z\alpha_x(B_zC_x - B_xC_z)$$

$$Since,\quad \alpha_x^2 = \alpha_y^2 = \alpha_z^2 = \begin{bmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{bmatrix}$$

$$\alpha_x\alpha_y = \begin{bmatrix}0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\\ 0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\end{bmatrix}\begin{bmatrix}0 & 0 & 0 & -i\\ 0 & 0 & i & 0\\ 0 & -i & 0 & 0\\ i & 0 & 0 & 0\end{bmatrix} = \begin{bmatrix}i & 0 & 0 & 0\\ 0 & -i & 0 & 0\\ 0 & 0 & i & 0\\ 0 & 0 & 0 & -i\end{bmatrix}$$

$$\alpha_z\alpha_x = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}\begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix}$$

$$\alpha_y\alpha_z = \begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & i & 0 \end{bmatrix}$$

Substituting these values we get

$$(\vec{\alpha}.B)(\vec{\alpha}.C) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}(B_xC_x + B_yC_y + B_zC_z) + \begin{bmatrix} i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & -i \end{bmatrix}(B_xC_y - B_yC_x) + \begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix}(B_zC_x - B_xC_z) + \begin{bmatrix} 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & i & 0 \end{bmatrix}(B_yC_z - B_zC_y)$$

As the Trace of a matrix is the sum of its diagonal terms, we now have

$$\text{Trace } (\vec{\alpha}.\boldsymbol{B})(\vec{\alpha}.\boldsymbol{C}) = 4((B_xC_x + B_yC_y + B_zC_z) + 0 + 0 + 0$$

$$= 4\,\boldsymbol{B}.\boldsymbol{C}$$

5.5 DIRAC'S FREE PARTICLE SOLUTION OR PLANE WAVE SOLUTIONS

The wave function ψ has four components and the Dirac equation is exactly a set of 4 first order linear partial differential equations. The plane wave solutions have the form:

$$\psi_j(r,t) = u_j e^{i(k.r-\omega t)} \qquad \text{….. (1)}$$

where, j=1,2,3,4

u_j are numbers

Making substitutions in Dirac's equation, we get

$$\{(E - mc^2)u_1 - cp_z u_3 - c(p_x - ip_y)u_4 = 0\}$$

$$\{(E - mc^2)u_2 - c(p_x + ip_y)u_3 + cp_z u_4 = 0\}$$

$$\{(E + mc^2)u_3 - cp_z u_1 - c(p_x - ip_y)u_2 = 0\}$$

$$\{(E + mc^2)u_4 + c(p_x - ip_y)u_1 - cp_z u_2 = 0\} \quad \text{.....(2)}$$

$$\begin{bmatrix} (E - mc^2) & 0 & -cp_z & -c(p_x - ip_y) \\ 0 & (E - mc^2) & -c(p_x + ip_y) & cp_z \\ -cp_z & -c(p_x - ip_y) & (E + mc^2) & 0 \\ -c(p_x + ip_y) & cp_z & 0 & (E + mc^2) \end{bmatrix} = 0$$

Or $(E^2 - m^2c^4 - c^2\boldsymbol{p}^2)^2 = 0$ .....(3)

This is in agreement with momentum energy relation for a free particle.

Or $$E = \pm(\boldsymbol{p}^2c^2 + m^2c^4)^{1/2}$$

i.e., the relation between E & p is in agreement with Schrodinger picture.

Hence, we can assign numerical values of two of u's. At first we take:

$$E_+ = +(\boldsymbol{p}^2c^2 + m^2c^4)^{1/2}$$

There are two linearly independent solutions that can be given as:

$$u_1 = 1, u_2 = 0, u_3 = \frac{cp_z}{E_+ + mc^2}, u_4 = \frac{c(p_x + ip_y)}{E_+ + mc^2}$$

$$u_1 = 0, u_2 = 1, u_3 = \frac{c(p_x - ip_y)}{E_+ + mc^2}, u_4 = \frac{-cp_z}{E_+ + mc^2} \quad \text{.....(4)}$$

Similarly if we choose the negative square root

$$E_- = -(\boldsymbol{p}^2c^2 + m^2c^4)^{1/2},$$

We obtain two new solutions from first two equation of (2)

$$u_1 = \frac{cp_z}{E_- - mc^2}, u_2 = \frac{c(p_x - ip_y)}{E_- - mc^2}, u_3 = 1, u_4 = 0$$

$$u_1 = \frac{c(p_x - ip_y)}{E_- - mc^2}, u_2 = \frac{-cp_z}{E_- - mc^2}, u_3 = 0, u_4 = 1$$

.....(5)

Each of these solutions can be normalized

$$\psi^*\psi = 1,$$

$$u_1^* u_1 + u_2^* u_2 + u_3^* u_3 + u_4^* u_4 = 1$$

$$N^2\left[1 + 0 + \frac{c^2 {p_z}^2}{(E_+ + mc^2)^2} + \frac{c^2({p_x}^2 + {p_y}^2)}{(E_+ + mc^2)^2}\right] = 1$$

Thus,

$$N = \left[1 + \frac{\boldsymbol{p^2c^2}}{(E_+ + mc^2)^2}\right]^{-1/2}$$

PROBABILITY DENSITY AND CURRENT DENSITY

Let us check whether the Dirac equation leads to the correct probability density. The Dirac equation for free particle is given as

$$(\boldsymbol{E - c\vec{\alpha}.p - \beta mc^2})\boldsymbol{\psi} = \mathbf{0},$$

Where E and p are operators given by

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

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

So,

$$\left(i\hbar\frac{\partial\psi}{\partial t} + i\hbar c\vec{\alpha}.\nabla\psi - \beta mc^2\psi\right) = 0, \quad \text{....(1)}$$

A Hermitian conjugate equation gives $\left(-i\hbar\frac{\partial\psi^\dagger}{\partial t} - i\hbar c\nabla\psi^\dagger.\vec{\alpha} - \psi^\dagger\beta mc^2\right) = 0$ (2)

Recall $\vec{\alpha}$ *and* β are Hermitian. Multiplying (1) on left by $\psi^\dagger$ and (2) on right by ψ.

$$\left(i\hbar\psi^{\dagger}\frac{\partial\psi}{\partial t}+i\hbar c\psi^{\dagger}\vec{\alpha}.\nabla\psi-mc^{2}\psi^{\dagger}\beta\psi\right)=0$$

$$\left(-i\hbar\frac{\partial\psi^{\dagger}}{\partial t}\psi-i\hbar c\nabla\psi^{\dagger}.\vec{\alpha}\psi-mc^{2}\psi^{\dagger}\beta\psi\right)=0$$

On subtracting,

$$\left(i\hbar\frac{\partial}{\partial t}(\psi^{\dagger}\psi)+i\hbar c\nabla.(\psi^{\dagger}\vec{\alpha}\psi)\right)=0$$

This equation may be expressed as

$$\left(\frac{\partial}{\partial t}(\psi^{\dagger}\psi)+\nabla.(\psi^{\dagger}c\vec{\alpha}\psi)\right)=0$$

Comparing this equation with equation of continuity $\frac{\partial P}{\partial t}+\nabla.S=0$, we get

Probability density $P(\boldsymbol{r},t)=(\psi^{\dagger}\psi)$

And Current density $S(\boldsymbol{r},t)=(\psi^{\dagger}c\vec{\alpha}\psi)$

This expression for probability density is familiar. The current density expression looks more plausible if we note $c\vec{\alpha}$ is the velocity of the particle in usual sense

$$i\hbar\frac{\partial x}{\partial t}=[x,H]=[x,c\vec{\alpha}.p+\beta mc^{2}]=i\hbar c\vec{\alpha}$$

Since $[x,\vec{p}]=2\hbar$

Therefore,

$$\frac{dx}{dt}=c\vec{\alpha}$$

This implies however, that the Eigen values of velocity operator are $c\vec{\alpha}$. This result is often attributed to Zitterhewegung and interpreted by uncertainty principle. A very precise measurement of instantaneous velocity (distinct from momentum in the relativity theory) requires the accurate measurement of the position of the particle at two slightly different times. Such accurate position measurements imply that the momentum of the particle is

completely unknown, so that very large momenta of the particle become possible and large velocities result.

5.6 NEGATIVE ENERGY STATE OF ELECTRON: THEORY OF POSITRON

Dirac equation in electromagnetic field is given as:

$$[E - e\phi - \vec{\alpha}.(cp - eA) - \beta mc^2]\psi = 0 \qquad \ldots..(1)$$

This equation may be written as four equivalent equations, two corresponding to positive energy states and two corresponding to negative energy states of the particle. On physical grounds negative energy states can be ignored according to classical mechanics but according to quantum mechanics, since energy changes takes place discontinuously and the transition from positive to negative energy states and vice versa are possible. Assuming α to be real and β to be purely imaginary or zero, complex conjugate of equation (1) can be given as:

$$[(-E - e\phi) - \vec{\alpha}.(-\boldsymbol{cp} - \boldsymbol{eA}) + \boldsymbol{\beta mc^2}]\,\psi^* = 0$$

$$[(E + e\phi) - \vec{\alpha}.(-\boldsymbol{cp} + \boldsymbol{eA}) - \boldsymbol{\beta mc^2}]\,\psi^* = 0 \qquad (2)$$

Where, $E = i\hbar\frac{\partial}{\partial t}$ and $p = i\hbar\nabla$

Solution of ψ from (1) belongs to negative value of $(E - e\phi)$, &

Solution of ψ^* from (2) belongs to positive value of $(E + e\phi)$

Which means that operator in (2) is obtained if one substitutes -e instead of e in equation (1). Thus, the negative solution of (1) refers to motion of new kind of particle having mass of an electron but opposite charge. Such particles have been produced during experiments and are termed as positrons. We cannot however assert that the negative energy solutions represent positrons, as this would make the dynamical relations all wrong. For instance is it certainly not true that a positron has a negative kinetic energy. We must therefore establish the theory of positron on a somewhat different aspect.

Dirac proposed that nearly all the negative energy states are occupied with one electron in each state in accordance with Pauli Exclusion Principle and there are no positive energy electrons; so that electrons can no longer reduce in their energy as all the negative energy states are full. This explains the ground state definition of a field to be vacuum state in the new assumption. Thus the normal state of vacuum consists of an infinite density of negative energy electrons. It is assumed that there are no electromagnetic or gravitational effects of these electrons but the deviations from the normal state produced by emptying one or more the negative energy states can be observed.

Evidently Dirac Relativistic equation gives two regions of the continuous energy spectrum of a free electron

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

For minimum energy of electron p=0; therefore when these direct electrons are addressed the energy difference between positive and negative energy states is separated by a gap equals to $2mc^2$. Both in the positive and negative energy states, the electrons can take continuous values of energy states, upto infinity. The positive branch of energy is similar to the classical relativistic energy; but the negative energy is energy states of electron has no classical analog.

Now the transition from negative energy states to positive energy states will create an unoccupied negative energy states. Physically this unoccupied negative energy state will now appear as something with a positive energy, since to make it disappear or to fill it up we should have to add to it an electron with negative energy. **These unoccupied negative energy states are called holes or positrons.**

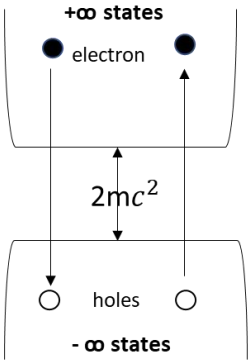

Fig.5.1 Dirac's picture of positive and negative energy states of electron

Thus the absence of a negative energy electron with spin up is equivalent to the presence of a positive energy and positively charged "hole" with spin down. So, "hole" represents the antiparticle of the electron (i.e, positron). So, the unfilled negative energy states according to Dirac, represent positive energy antiparticles. Thus in order to give stability to the +ve energy states, Dirac predicted the existence of positron(Actually, when Dirac wrote this equation, positron was not known and he thought proton which is a positively charged particle might be the antiparticle of electron!). Anderson discovered positron in 1932 to win the Nobel Prize.

The assumptions require there to be a distribution of electrons of infinite density everywhere in the well. A perfect vacuum is a region where all the states of positive energy are unoccupied. In a perfect vacuum, Maxwell's equation

$$\nabla . \boldsymbol{E} = 0$$

Must, of course, be valid. This means that the infinite distribution of negative energy electrons does not contribute to the electron field. Only departure from the distribution in vacuum will contribute to the electronic density ρ_0 in Maxwell equation.

$$\nabla . E = 4\pi\rho_0$$

Thus, there will be a contribution –e for each occupied state of positive energy and a contribution of e for each unoccupied state of negative energy.

Dirac required considering infinite number of electrons filling up the negative energy states to describe a stable "single" electron with positive energy. So, in that sense, it is no-longer a "single-particle" theory! Exciting a negative energy electron to a positive energy state, ie. Creating a physical electron from the vacuum also creates a "hole" in the Dirac sea or a positive energy positron, which corresponds to the process of creating an $e-e+$ pair! Appropriate theory to describe the particle creations or destruction is the Quantum Field Theory Dirac's theory thus suggests moving to quantum field theory.

This at once leads to the conclusion that in the collision of an electron with a positron, the calculation of this process on the **Dirac theory** of the positron, where the positron is considered as an unoccupied state of negative energy, would lead to a result different from that which we should get if we did the calculation considering the positron as an independent positively charged particle in a state of positive energy whose behaviour is described by the Dirac equation.

It is possible for a negative energy electron to absorb radiation and be excited into a positive energy state. In this process we observe an electron of charge –e and energy +E and in

addition a hole in the negative energy sea. The hole shows absence of an electron of charge –e and energy +E i.e. positron. It is called pair production on the basis of the hole theory. Correspondingly electron jumps in the negative energy sea with emission of radiation and leads to electron-positron annihilation.

Dirac equation predicts the correct hydrogen-atom energy spectrum and g value of the electron to high accuracy. Moreover positron predicted by the theory has been experimentally observed. This theory gives the existence of antiparticles as well as particles. The particles are described by positive energy solution for Dirac equation and in present case are electrons of mass m and charge –e, the antiparticles are described by negative energy solution; and in the present instance are positrons of mass m and charge +e.

Thus, the hole theory results to a new fundamental symmetry in nature "*To each particle there is an antiparticle and in particular the existence of electrons implies the existence of positrons*."

5.7 SUMMARY

Schrodinger proposed a relativistic form of his non-relativistic equation (at the same time when he developed his non-relativistic equation. This equation was further developed by Klein and Gordon known as Klein-Gordon equation. Here we have discussed only free relativistic equations. If we consider Dirac equation in for hydrogen atom (i.e., Dirac equation in central potential), the fine structures are observed in the energy eigenvalues. One can also include interaction with radiations by introducing the gauge fields. Along with this theory of positron or negative energy state of electron has also been discussed. The reverse process would consist in creation of an electron and a positron from electromagnetic radiation as elaborated above.

5.8 GLOSSARY

Interpret- clarify

Confined- restricted

Undergo- suffer

Maintain- sustain

Interactions- exchanges

Equivalent- equal to something

5.9 REFERENCES

1. Quantum Mechanics, Satya Prakash, Swati Saluja, Kedar Nath Ram Nath, Meerut
2. Advanced Quantum Mechanics, J.J.Sakurai, Pearson

5.10 SUGGESTED READINGS

1. Introduction to Quantum Mechanics, David J. Griffiths, Cambridge University Press
2. Advanced Quantum Mechanics, B.S. Rajput, Pragati Prakashan

5.11 TERMINAL QUESTIONS

1.Derive the Klien Gordon equation and apply it to a particle in the Coulombian field.

2. Derive the Klien Gordon relativistic wave equation of a free particle. Determine the current density and probability density. Also give the shortcomings of Klien Gordon equations.

3. Discuss Dirac's relativistic equation for free particle. If $\vec{a}$ are Dirac's matrices, prove that

trace $(\vec{a}.\vec{B})(\vec{a}.\vec{C}) = 4\vec{B}.\vec{C}$

Where, $\vec{B}$ and $\vec{C}$ are three dimensional vectors.

3. Using Dirac's equations obtain the energies of the bound states of the hydrogen atom and discuss the hyperfine splitting of first two levels.

4. (a) Show that L=r × p does not commute with the free particle's Dirac Hamiltonian. While J= L+S does where,

$$\vec{s} = \frac{1}{2}\hbar\vec{\Sigma} = \begin{bmatrix} \vec{\sigma} & \vec{\sigma} \\ \vec{\sigma} & \vec{\sigma} \end{bmatrix}$$

(b) Evaluate $(\vec{\alpha}.\vec{B})(\vec{\alpha}.\vec{C})$

5. (a) Show that the probability is indefinite in relativistic Klein-Gordan theory.

(b) How did Dirac overcome this?

(c) Can you neglect the negative energy state solutions of the Dirac equations.

6.Explain the following:

(a) Dirac particle has spin $\frac{1}{2}$

(b) Spin-orbit energy is a consequence of Dirac equation.

7. Find the solution of Klein-Gordon equation and interpret the charge and current densities associated with it.

8. Derive Dirac's relativistic wave equation. Obtain from it the equation of continuity. Hence define the probability and current densities.

9. Explain how Dirac arrived at a linear equation starting from the relation

$$E^2 = c^2p^2 + m^2c^4$$

10. Show that a particle obeying the Dirac equation is endowed with a spin momentum.

11. Write short notes on:

(a) Klein-Gordon equation

(b) Dirac matrices

(c) Dirac equation and electron spin

(d) Negative energy states of an electron.

12. Show how Dirac's relativistic wave equation for an electron leads to the theory of positrons.

13. Dirac wrote Hamiltonian for free particle as

$$H = c\vec{\alpha}.\vec{p} + \beta mc^2$$

What are the reasons to choose $\vec{\alpha}$ and β as 4×4 matrices with elements independent of position and momentum of the particle?

UNIT 6 SPIN THEORY

Structure

6.1 Introduction

6.2 Objectives

6.3 What are Anti particles?

6.3.1 Negative Energy State of Electron

6.4 Spin of Electron

6.4.1 Stern-Gerlach Experiment

6.4.2 Mathematical Formulation of Spin

6.4.3 The Pauli Matrices

6.5 Magnetic Moment of an Electron due to Spin

6.6 Energy values in a coulomb potential

6.7 Summary

6.8 Glossary

6.9 References

6.10 Suggested Readings

6.11 Terminal Questions

6.1 INTRODUCTION

Spin theory plays a very fundamental role in particle physics and it is an important ”tool” to gain insight especially into the theory of strong interactions or the colour force between gluons and quarks, the building blocks of hadrons. The spin property is peculiar to quantum theories. It is not predicted by the non-relativistic theory, but inserted” by hand” to explain experimental facts. In a relativistic approach it is however an automatic and inherent property

6.2 OBJECTIVES

After studying thus unit, you should be able to-

- Understand anti-particles and negative energy state of electron
- Explain the spin of the electron
- Explain Pauli matrices and magnetic moment of an electron due to spin
- Understand the energy values in a coulomb potential

6.3 WHAT ARE ANTI PARTICLES?

In the standard model for describing fundamental particles and interactions, every particle has an antiparticle. For example, the positron is the antiparticle of the electron. It has identical mass, but has a positive charge. If an electron encounters a positron, they annihilate with the transformation of their mass energies into two gamma rays. However, to better understand the concept, let’s discuss it firstly from the perspective of time.

Consider a structureless point particle. Classically, its kinematical state at any time t consists simply of the three components of its three-position $z(t)$. We assume that $z(t)$ is a continuous function of t that is sufficiently differentiable for our purposes. In special relativity, we form the four-position z^{μ} of the particle:

$$Z^{\mu} = (t, z),$$

where we shall always use units in which $c = 1$. The continuous function $z(t)$ specifies the path of the particle in Minkowski spacetime-its worldline. To parameterize its "length", in a Lorentz-invariant way, we consider an infinitesimal differential element of the path,

$$dz\mu\,(t) = (dt, dz(t)),$$

where $dz(t)$ is the infinitesimal change in position $z(t)$ in the infinitesimal time interval from t to $t + dt$. We now consider the Lorentz-invariant quantity

$$d\tau^2(t) \equiv dz^\mu(t) dz_\mu(t) \equiv dt^2 - dz^2(t) \quad \ldots(1)$$

where we employ a (+, −, −, −) metric. What we would like to do is define a quantity $d\tau(t)$ that would provide a measure of "length" along the worldline. But the Lorentz-invariant expression (1) involves not dτ, but rather the square of dτ. Thus, dτ can only be defined up to a sign:

$$d\tau \equiv \pm\sqrt{dz^\mu dz_\mu} \quad \ldots(2)$$

To investigate the meaning of this ambiguity in the sense of $d\boldsymbol{\tau}$, let us consider the special case in which the particle is instantaneously at rest, with respect to our own inertial coordinate system:

$$dz = 0$$

In this case, we find

$$d\boldsymbol{\tau} = \pm dt$$

The solution $d\boldsymbol{\tau} = dt$ for a particle at rest is the one usually presented in introductory texts on special relativity: such a $d\boldsymbol{\tau}$ is obviously equal to the passage of time as measured in the instantaneous rest frame of the particle. For a particle undergoing arbitrary relativistic motion,

we assume that the particle itself possesses its own "cumulative time" or "age", which we term the proper time, that can be calculated by summing up all of the dτ along its worldline:

$$\tau(\mathcal{E}) \equiv \int_{\mathcal{E}_0}^{\mathcal{E}} d\tau$$

where $\boldsymbol{\tau}$(E) is the proper time at event E on the worldline, and where the event E_0 on the worldline defines the (arbitrary) origin of $\boldsymbol{\tau}$. Since the worldline of any classical particle passes through each constant- t hyperplane once and only once, we can replace the events E and E_0 by their corresponding coordinate times t and t_0, and hence determine $\boldsymbol{\tau}$ as a function of t:

$$\tau(t) = \int_{t_0}^{t} dt' \frac{d\tau}{dt'} = \int_{t_0}^{t} dt' \frac{1}{\gamma(t')} \quad \ldots(3)$$

where we have made use of Eq. (1):

$$\frac{d\tau(t)}{dt} = \sqrt{1 - \left(\frac{dz(t)}{dt}\right)^2} \equiv \sqrt{1 - v^2(t)} \equiv \frac{1}{\gamma(t)}.$$

when the speed $\boldsymbol{v}$ of the particle is much smaller than the speed of light, the factor $\boldsymbol{\gamma(t)}$ is close to unity, and the passage of proper time is indistinguishable from that of coordinate time; but if the particle's motion is such that its speed rises to an appreciable fraction of the speed of light, the factor $\boldsymbol{\gamma(t)}$ rises above unity, and the particle "ages" more slowly. In all cases, however, the particle gets older: special relativity only seems to modify the rate; it warps our view of the world, but it does not throw it into reverse.

Let us now consider the other solution in Eq. (2) for a particle at rest, namely,

$$d\boldsymbol{\tau} = -dt.$$

Even to a student possessing a good knowledge of special relativity, Eq. (4) does not look familiar at all. It seems to imply that a particle at rest with respect to our Lorentz coordinate system might somehow believe that time evolves in the opposite direction to what we do! For example, if we determine that some spacetime event E′ is definitely earlier than another event E″ (i.e., E′ lies within the backward light cone of E″), then a particle whose own "proper time" obeys (4) would insist, to the contrary, that E′ is definitely later than E″ (i.e., from the particle's point of view, E′ lies within the forward light cone of E″).

The problem is that, by the principles of relativity, such a particle is just as valid an observer of the universe as we are: it agrees with us that the speed of light is unity in all inertial frames. We have no physically acceptable justification for dismissing its counterintuitive view of the world. We must conclude that both of the solutions (2) are equally valid definitions of the passage of proper time.

Stueckelberg and Feynman made the following realisation: a particle for which dτ evolves in the opposite sense to the *dt* in our particular Lorentz frame of reference is simply in antiparticle motion with respect to us. Of course, there are no classical forces that can change "particle motion" into "antiparticle motion" - the two regimes are as disjoint as the interiors of the forward and backward lightcones; but, even classically, this does not bar the possibility that a particle might have always been in antiparticle motion.

Following this argument to its logical conclusion, it could be noted that there is a similar ambiguity of sign when parameterizing path lengths in Euclidean space, since there the invariant interval is also squared:

$$dl^2 \equiv dz^2$$

and hence we could equally well measure length one way along the path, or in the opposite way. But we are already used to the idea that, at a fundamental level, travelling to the left is no more difficult than travelling to the right. The crucial difference in Minkowski space is precisely the fact that classical forces do not reverse the sense in which "time is traversed"; our intuition with Galilean mechanics is rooted firmly in the belief that everyone agrees on the direction that time is travelling. Relativistically boosting to another frame of reference "warps" the rate at which clocks tick, but it does not reverse it; in contrast, time-reversal is a discrete symmetry, and cannot be brought into contact with "intuitive" physics by a continuous transformation.

6.3.1 NEGATIVE ENERGY STATE OF ELECTRON

We have Dirac equation in electromagnetic field as:

$$\left[\mathbf{E} - e\phi - \vec{\alpha} \cdot (c\mathbf{p} - e\mathbf{A}) - \beta mc^2\right]\psi = 0 \quad \ldots(1)$$

This equation may be written as four equivalent equations, two corresponding to positive energy and the remaining two corresponding to negative energy states of the particle. According to classical mechanics negative energy states can be excluded on physical grounds; but according to quantum mechanics, it is not so because energy changes take place discontinuously and the transition from positive to negative energy states and vice-versa are possible.

If equation (1) is expressed as a matrix equation assuming all the elements of matrices representing α_x, α_y, α_z to be real and all those of matrix representing β to be purely imaginary or zero, then if we take complex conjugate of (1) remembering

$$E = i\hbar\frac{\partial}{\partial t} \text{ and } p = -i\hbar\nabla$$

we get,

$$\left[(-E - e\phi) - \vec{\alpha} \cdot (-c\mathbf{p} - e\mathbf{A}) + \beta mc^2\right]\psi^* = 0$$
$$\left[E + e\phi] - \vec{\alpha} \cdot (c\vec{\mathbf{p}} + e\vec{\mathbf{A}}) - \beta mc^2\right]\psi^* = 0 \qquad \ldots(2)$$

Thus, each solution of the wave-equation (1) has for its complex conjugate a solution of (2). Further if the solution ψ of (1) belongs to a negative value for $(E - e\phi)$ the corresponding solution ψ^* of equation (2) will belong to a positive energy for $(E + e\phi)$. But the operator in equation (2) is just what one would get if one substitutes $-e$ for e in the operator of (1). It follows that each negative energy solution of the wave-equation is obtained from (1) by substitution of $-e$ for e. Thus, the latter solution represents an electron of charge +e (instead of − ve as we had up to the present) moving through the given electromagnetic field.

Thus, the unwanted solution of (1) is connected with the motion of an electron of charge +e. [It is not possible, of course with an arbitrary electromagnetic field, to separate the solution of (1) definitely into those referring to positive and those referring to negative values for $(E - e\phi)$, as such a separation would imply the transitions from one kind to the other do not occur. The preceding discussion is therefore only a rough one, applying to the case when such a separation is approximately possible].

In this way we are led to infer that the negative energy solutions of (1) refer to the motion of a new kind of particle having the mass of an electron and opposite charge. Such particles have been observed experimentally and are called positrons. We cannot however assert that the negative energy solutions represent positrons, as this would make the dynamical relations all wrong. For instance, is it certainly not true that a positron has a negative kinetic energy. We must therefore establish the theory of positron on a somewhat different footing.

Dirac proposed that nearly all the negative energy states are occupied with one electron in each state in accordance with Pauli exclusion principle and there are no positive energy electrons; so that electrons can no longer reduce their energy as all the negative energy states are full. This explains the ground state definition of a field to be vacuum state in the new definition. Thus, the normal state of vacuum consists of an infinite density of negative energy electrons. It is assumed that there are no electromagnetic or gravitational effects of these electrons but the deviations from the normal state Fig. 6.1 Dirac picture of positive and negative energy produced by emptying one or more of the negative energy states can be observed.

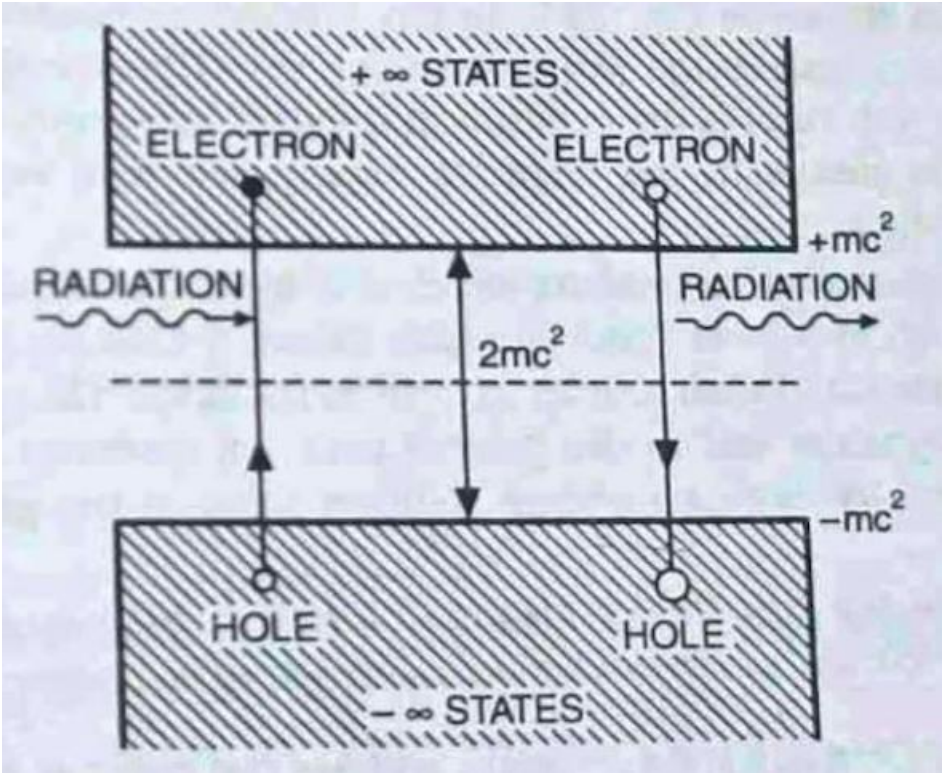

Fig. 6.1

Evidently Dirac relativistic equation gives two regions of the continuous energy spectrum of a free electron

$$E = \pm\sqrt{\left(p^2c^2 + m^2c^4\right)}$$

For minimum energy of electron p=0; therefore, when these Dirac electrons are at rest, the energy difference between positive and negative energy states is separated by a gap negative energy state, the electrons can take continuous values of energy states, up to infinity. The positive branch of energy is similar to the classical relativistic energy; but the negative energy states of a free electron have no classical analogue.

Now the transition from negative energy state to positive energy state will create an unoccupied negative energy state. Physically this unoccupied negative energy state will now appear as something with a negative energy. These unoccupied negative energy states are called holes or positrons.

The assumptions require there to be a distribution of electrons of infinite density everywhere in the well. A perfect vacuum is a region where all the states of positive energy are unoccupied and all those of negative energy are occupied. In a perfect vacuum, Maxwell's equation

$$\nabla \cdot E = 0$$

must, of course, be valid. This means that the infinite distribution of negative energy electrons does not contribute to the electron field. Only departure from the distribution in a vacuum will contribute to the electric density ρ_0 in Maxwell equation.

$$\nabla \cdot E = 4\pi\rho_0$$

Thus, there will be a contribution -e for each occupied state of positive energy and a contribution of e for each unoccupied state of negative energy.

The exclusion principle will operate to prevent a positive energy electron ordinarily from making transitions to states of negative energy. It will be still possible for such an electron to drop into an occupied state of negative energy. In this case we should have an electron and positron disappearing simultaneously, their energy being emitted in the form of radiation. The reverse process would consist in the creation of an electron and a positron from electromagnetic radiation.

It is possible for a negative energy electron to absorb radiation and be excited into a positive-energy state as shown in Fig.6.1. In this process we observe an electron of charge $-|e|$ and energy + E and in addition a hole in the negative energy sea. The hole shows the absence of an electron of charge $-|e|$ and energy +E; that is the positron. It is called pair production on the basis of the hole theory. Correspondingly electron jumps in the negative energy sea with emission of radiation and lead to electron-positron annihilation.

Dirac equation predicts the correct hydrogen-atom energy spectrum and g value of the electron to high accuracy. Moreover, the positron predicted by the theory has been experimentally observed. This theory gives the existence of antiparticles as well as particles. The particles are described by positive energy solution for Dirac equation and in the present case are electrons of mass m and charge −|e|, the antiparticles are described by negative energy solution; and in the present instance are positrons of mass m and charge +|e|.

Thus, the hole theory results to a new fundamental symmetry in nature "To each particle there is an antiparticle and in particular the existence of electrons implies the existence of electron implies the existence of positrons.

6.4 SPIN OF ELECTRON

In 1922, at a time, the hydrogen atom was thought to be understood completely in terms of Bohr's atom model, two assistants at the University of Frankfurt, Otto Stern and Walther Gerlach, performed an experiment which showed that the electrons carry some intrinsic angular momentum, the spin, which is quantized in two distinct levels. This was one of the most important experiments done in the twentieth century, as its consequences allowed for many interesting experimental and theoretical applications.

6.4.1 Stern-Gerlach Experiment

In the Stern-Gerlach experiment silver atoms, carrying no orbital angular momentum but with a single electron opening up a new s-orbital 2(l=0), were sent through a special magnet which generates an inhomogeneous magnetic field, see Fig. 6.2. The properties of the silver atom in this state are such that the atom takes over the intrinsic angular momentum, i.e., spin, of this outermost single electron.

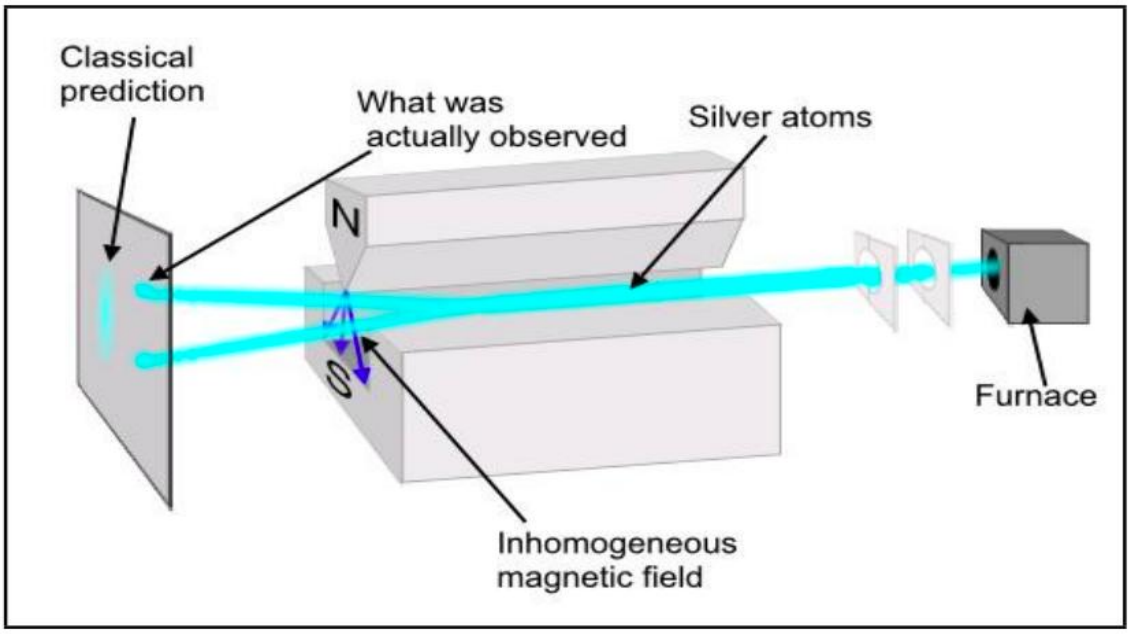

Fig. 6.2: Stern-Gerlach Experiment: The inhomogeneous magnetic field exerts a force on the silver atoms, depending on the spin z-component. Classically a continuous distribution is expected, but the experiment reveals only two values of the spin z-component

The inhomogeneity of the magnetic field causes a force acting on the magnetic dipole in addition to the torque

$$\vec{F} = -\vec{\nabla}V = \vec{\nabla}(\vec{\mu}\vec{B}),$$

where $V = H$ if the particle is at rest. Since the force depends on the value of the spin, it can be used to separate different spins. Classically, the prediction would be a continuous distribution, bounded by two values, representing spins parallel and antiparallel to the direction of the magnetic field. All the spins which are not perfectly (anti-)aligned with the magnetic field would be expected to have components in that direction that lie in between these maximal and minimal values. We can write the magnetic field as a homogeneous and an inhomogeneous part, such that it is oriented parallel to the z-axis, i.e., $B_x = B_{y=0}$,

$$\vec{B} = B_z \vec{e}_z = (B_{\text{hom}} + \alpha z)\vec{e}_z.$$

The force can then be expressed via the z-component of the spin $\vec{S}$, which in the quantum mechanical formalism will be an operator

$$F_z = \alpha\gamma S_z.$$

The separation of the particles with different spin then reveals experimentally the eigenvalues of this operator.

The result of the experiment shows that the particles are equally distributed among two possible values of the spin *z*-component, half of the particles end up at the upper spot ("spin up"), the other half at the lower spot ("spin down"). Spin is a angular momentum observable, where the degeneracy of a given eigenvalue *l* is *(2l+1)*. Since we observe two possible eigenvalues for the spin *z*-component (or any other direction chosen), see Fig. 6.3, we conclude the following value for *s*

$$2s + 1 = 2 \Rightarrow s = \frac{1}{2}$$

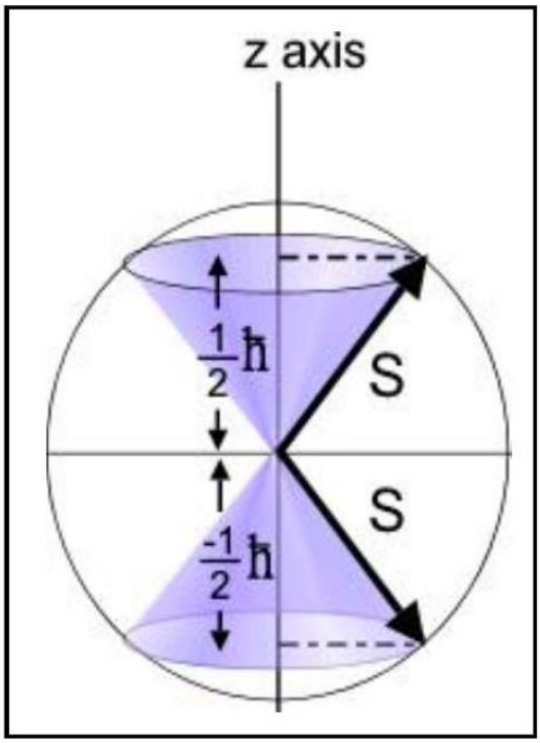

Figure 6.3: Spin $\frac{1}{2}$: The spin component in a given direction, usually the zdirection, of a spin $\frac{1}{2}$ particle is always found in either the eigenstate "$\uparrow$" with eigenvalue $+\frac{1}{2}$ or "$\downarrow$" with eigenvalue $-\frac{1}{2}$.

Result: Two additional quantum numbers are needed to characterise the nature of the electron, the spin quantum number s and the magnetic spin quantum number m_s = -s, ⋯, + s. So we can conclude that spin is quantized and the eigenvalues of the corresponding observables are given by

$$S_z \to \hbar m_s = \pm\frac{\hbar}{2} \quad , \quad \vec{S}^2 \to \hbar^2 s(s+1) = \frac{3}{4}\hbar^2.$$

The spin measurement is an example often used to describe a typical quantum mechanical measurement. Let us therefore elaborate this example in more detail. Consider a source emitting spin $\frac{1}{2}$ particles in an unknown spin state. The particles propagate along the y-axis and pass through a spin measurement apparatus, realised by a Stern-Gerlach magnet as described in Fig. 6.2, which is oriented along the z-axis, see Fig. 6.4.

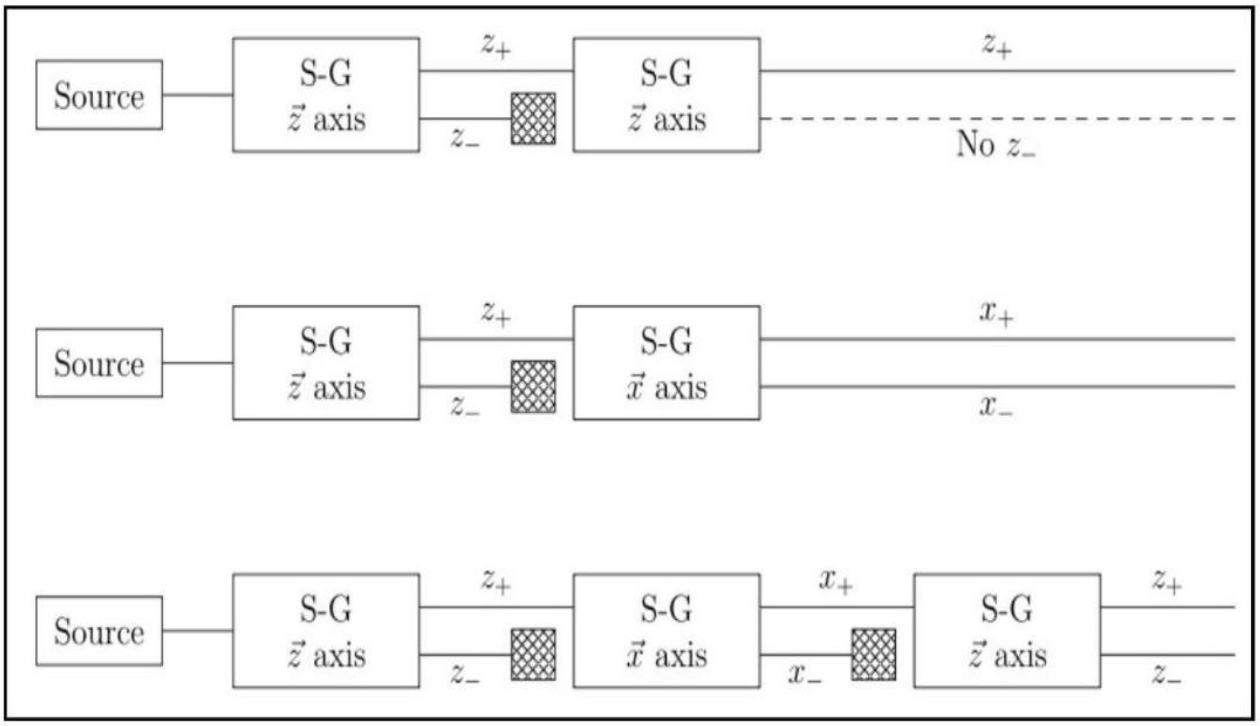

Figure 6.4: Spin $\frac{1}{2}$ measurement: Spin measurements change the state of the particles, if they are not in an eigenstate of the corresponding operator. Therefore subsequent measurements along perpendicular directions produce random results.

All particles leaving the Stern-Gerlach apparatus are then in an Eigen-state of the S_z operator, i.e., their spin is either "up" or "down" with respect to the z-direction. Let's now concentrate on the “spin up” particles (in z-direction), that means we block up the “spin down” in some way, and perform another spin measurement on this part of the beam. If the second measurement is also aligned along the z-direction then all particles will provide the result “spin up”, since they are all already in an Eigen-state of S_z (see the upper part of Fig. 6.4). The measurement of a particle being in an Eigen-state of the corresponding operator leaves the state unchanged, therefore no particle will "flip" its spin.

If, however, we perform the spin measurement along a direction perpendicular to the z-axis, let's choose the x-axis, then the results will be equally distributed among "spin up" or "spin down" in x-direction (see the middle part of Fig. 6.4). Thus, even though we knew the state of the particles beforehand, in this case the measurement resulted in a random spin flip in either of the measurement directions. Mathematically, this property is expressed by the nonvanishing of the commutator of the spin operators

$$[S_z, S_x] \neq 0.$$

If we finally repeat the measurement along the *z*-direction the result will be random again (see the lower part of Fig. 6.4). We do not obtain precise information about the spin in different directions at the same time, due to the non-vanishing of the commutator there holds an uncertainty relation for the spin observables.

Of course, we could also choose an orientation of the Stern-Gerlach magnet along some arbitrary direction. Let us assume we rotate the measurement apparatus by an angle θ (in the *z*-*x* plane), then the probability P_+ to find the particle with "spin up" and P_- to find the particle with "spin down" (along this new direction) is given by

$$P_+ = \cos^2 \frac{\theta}{2} \text{ and } P_- = \sin^2 \frac{\theta}{2}, \text{ such that } P_+ + P_- = 1.$$

6.4.2 Mathematical Formulation of Spin

It is important to mathematically express the theoretical formulation of spin. So, we will describe spin by an operator, more specifically by a 2×2 matrix, since it has two degrees of freedom and we choose convenient matrices which are named after Wolfgang Pauli.

6.4.3 The Pauli Matrices

The spin observable $\vec{S}$ is mathematically expressed by a vector whose components are matrices

$$\vec{S} = \frac{\hbar}{2}\vec{\sigma},$$

where the vector $\vec{\sigma}$ contains the so-called Pauli matrices $\sigma_x, \sigma_y, \sigma_z$:

$$\vec{\sigma} = \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Then the spin vector $\vec{S}$ (or the Pauli vector $\vec{\sigma}$) can be interpreted as the generator of rotations in the sense that there is a unitary operator U(θ)

$$U(\theta) = e^{\frac{i}{\hbar}\vec{\theta}\vec{S}} = \mathbf{1}\cos\frac{\theta}{2} + i\hat{n}\vec{\sigma}\sin\frac{\theta}{2},$$

generating rotations around the $\vec{\theta}$-axis by an angle $|\vec{\theta}|$ of the state vectors in Hilbert space. The scalar product $\vec{\theta}\vec{\sigma}$ is to be understood as a matrix

$$\vec{\theta}\vec{\sigma} = \theta_x\sigma_x + \theta_y\sigma_y + \theta_z\sigma_z.$$

What's very interesting to note here is the fact that a spin $\frac{1}{2}$ particle has to be rotated by 2 × 2π = 4π (!) in order to become the same state, very much in contrast to our classical expectation. It is due to the factor $\frac{1}{2}$ in the exponent.

6.5 MAGNETIC MOMENT OF AN ELECTRON DUE TO SPIN

To fully understand the concept of spin, we have to review the properties of a classical charged particle rotating about its own symmetry axis. The angular momentum due to this rotation, $\vec{S}$, will create a magnetic dipole moment $\vec{\mu}$, proportional to the angular momentum

$$\vec{\mu} = \gamma\vec{S} = g\frac{q}{2mc}\vec{S},$$

where γ is the gyromagnetic ratio and g is just called the g-factor. For the electron we have:

$$\vec{\mu} = \gamma_e \vec{S} = -g_e \frac{e}{2m_e c} \vec{S} = -g_e \frac{\mu_B}{\hbar} \vec{S}.$$

The g-factor of the electron equals two, $g_e = 2$, although for a classical angular momentum, it should be equal to 1. The fact that the spin of the electron contributes twice as strong to the magnetic moment as its orbital angular momentum, is called the anomalous magnetic moment of the electron. The constant μ_B is known as Bohr's magneton B.

If such a magnetic dipole is subject to an external (homogeneous) magnetic field $\vec{B}$ it starts to precess, due to the torque $\vec{\Gamma}$, known as the Larmor torque, exerted by the magnetic field

$$\vec{\Gamma} = \vec{\mu} \times \vec{B} = \gamma \vec{S} \times \vec{B},$$

The potential energy corresponding to this torque is given by:

$$H = -\vec{\mu}\vec{B}.$$

Thus, the Hamiltonian for a particle with spin in an exterior magnetic field of strength $\vec{B}$ is of the form:

$$H = -\gamma \vec{S}\vec{B}.$$

6.6 ENERGY VALUES IN A COULOMB POTENTIAL

The solution of the quantum mechanical problem of determining the energy levels of a (bound) particle in the presence of an attractive Coulomb potential, i.e., the hydrogen atom with centre-of-mass coordinate removed, was a spectacular achievement by Schrodinger, published in the same paper in which his famous equation was first introduced,1 early in 1926.

Here's how the problem goes. The Hamiltonian for the Coulomb potential is given by:

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r},$$

with the first and second terms representing the kinetic and potential energies, respectively of a particle with mass m (this is the reduced mass of the electron if this Hamiltonian arises from the hydrogen problem). Since the Coulomb potential is central, the solution for the angular part of the wave function is standard, and one is left with the radial equation. The radial equation for u (ρ) ≡ r R(r), where R(r) is the radial part of the wave function and ρ ≡ kr, with k ≡ $\sqrt{(-2mE)}/\hbar$, is usually rendered in dimensionless form; it is given by

$$\frac{d^2u}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{\ell(\ell+1)}{\rho^2}\right] u.$$

Here, ℓ is the azimuthal quantum number, $\rho_0 \equiv 2/(ka0)$ with $a_0 \equiv 4\pi_0\hbar^2/(me^2)$ the Bohr radius, and E < 0 indicates that we are considering bound states. Asymptotic solutions are then 'peeled off' by examining the behaviour as ρ → ∞ and ρ → 0. A more general consideration rules out solutions that diverge at the origin; when this is addressed at all, it is based on normalization and/or conditions of hermiticity. However, the elimination of such solutions on general grounds is premature in some cases.

6.7 SUMMARY

In this unit, you have studied about anti-particles and negative energy state of the electron. Also spin of the electron and Pauli matrices are discussed. Magnetic moment of the electron due to spin is explained.

6.8 GLOSSARY

Infinitesimal- extremely small

Anti-particle- every type of particle is associated with an antiparticle with the same mass but with opposite physical charges

Spin- to rotate or cause to rotate rapidly, as on an axis

Moment- the property of a magnet that interacts with an applied field to give a mechanical moment.

Invariant- unchanging;

Inhomogeneous- not uniform

Normalization- the scaling of wave functions so that all the probabilities add to 1

6.9 REFERENCES

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6.10 SUGGESTED READINGS

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2. Introduction to Quantum Mechanics, David J. Griffiths, Cambridge University Press

3. P.M. Mathews and K. Venkatesan, A Text book of Quantum Mechanics, Tata Mc Graw-Hill, New Delhi.

4. L.I. Schiff, Quantum Mechanics, McGraw-Hill

6.11 TERMINAL QUESTIONS

1. Write a short note on Pauli's exclusion principle and his theory of spin.

2. What are antiparticles? Explain the negative energy state of the electron.

3. Explain spin of the electron and Stern-Gerlach experiment.

4. Describe magnetic moment of an electron due to spin in detail.

UNIT 7 IDENTICAL PARTICLES

Structure

7.1 Introduction

7.2 Objectives

7.3 Identical Particles

7.4 Symmetric and anti-symmetric functions for many-particle system

7.5 Exchange Degeneracy

7.6 Classical Fields

7.7 Schwinger's Action Principle

7.8 Lagrangian and Hamiltonian Densities and Field Equation

7.9 Quantum Structure of Free Fields

7.10 Summary

7.11 Glossary

7.12 References

7.13 Suggested Readings

7.14 Terminal Questions

7.1 INTRODUCTION

Identical particles are those particles in a system for which the system remains unaltered by interchanging the particles. As each particle is described quantum mechanically by a wave packet, these particles can be distinguished from one another, only if their wave packers do not overlap. So, we can simply say that the particles that can't be distinguished by means of any inherent property can be said to be "identical particles", like electrons. Otherwise, they would not be identical in all respects. In classical mechanics identical particles do not lose their identity despite the identity of their physical properties due to the existence of sharply definable trajectories for individual particles since each particle can be followed during the course of an experiment.

7.2 OBJECTIVES

After studying this unit, you should be able to-

- Understand identical particle
- Define symmetric and anti-symmetric wave functions
- Explain exchange degeneracy
- Describe classical fields and Schwinger's action principle
- Explain Lagrangian and Hamiltonian densities and field equations
- Describe quantum structure for free fields

7.3 IDENTICAL PARTICLES

The word identical in quantum mechanics is to describe the particles that can be substituted for each other under the most general possible circumstances with no change in physical situation of the system. In quantum mechanics a particle can be described by a wave packet of finite size, spread and the exact specification of the position and momentum of the particle simultaneously is restricted by Heisenberg's uncertainty principle $\Delta q\ \Delta p \approx h$, therefore there is no way of keeping track of individual particles separately, specially if they interact with each other to an appreciable extent. Hence in quantum mechanics the wave functions of the

particles overlap considerably. As a result the quantum mechanical particles can not be distinguished. To give an example of the quantum particles consider the conduction electrons in metals.

Density of electrons $\approx 10^{28}/m^3$

$\therefore$ Volume available for each electron = $10^{-28}/m^3$

For a 1 eV electron momentum, p $= (2mE)^{1/2}$

$= [2x (9.1 \times 10^{-31} kg) (1 \times 1.6 \times 10^{-19} joule)]^{1/2}$

$= 0.5 \times 10^{-24}$ kg-m/sec

$\therefore$ Uncertainty of this electron in the position,

$$\Delta q \approx \frac{h}{\Delta p} = \frac{6.6 \times 10^{-34}\ joule - sec}{0.5 \times 10^{-24} joule\ sec/metre}$$
$$\approx 1.3 \times 10^{-9}\ metre$$

$\therefore$ Volume of conduction electron $= \frac{4}{3}\pi r^3 = \frac{4}{3} \times 3.14 \times (1.3 \times 10^{-9}\ metre)^3$

$$\approx 10^{-27} metre^3$$

Comparing the volume of conduction electron to the volume available to it, it can be concluded that the electron wave function, overlap considerable, i.e., conduction electron cannot be identified separately and hence they are indistinguishable.

Thus, there are two general categories of particles:

(i) Classical particles which are identical but distinguishable,

(ii) Quantum particles which are identical and indistinguishable.

It is to be noted that when quantum particle density is sufficiently low so that their uncertainty is small in comparison to the volume available to them, they also obey classical statistics, otherwise we must use quantum statistics.

7.4 SYMMETRIC AND ANTI-SYMMETRIC FUNCTIONS FOR MANY PARTICLES SYSTEM

The Schroedinger equation for *n* identical particles is written as:

$$H(1,2,\ldots n)\psi(1,2,\ldots n,t) = i\hbar\frac{\partial}{\partial t}\psi(1,2,\ldots n,t),$$

where each of the numbers represents all the coordinates (positional and spin) of one of the particles. The Hamiltonian *H* is symmetrical in its arguments due to the identity of particles. The identity of particles means that they can be substituted for each other without changing *H* or indeed any other observable.

There are two kinds of solutions of wave function ψ of eqn. (1) that have symmetric properties of particular interest.

(i) Symmetric wave function Ψ_s: A wave function is symmetric if the interchange of any pair of particles among its arguments leave the wave function unchanged.

(ii) Antisymmetric wave function ψ_A: A wave function is antisymmetric if the interchange of any pair of particles among its arguments changes the sign of the wave function.

It may now be pointed out that the symmetry character of a wave function does not change with time. If ψ_s is symmetric at a particular time t then $H\psi_s$ is also symmetric and according to equation (1), $\frac{\partial\psi_s}{\partial t}$ is symmetric at time t. Since ψ_s and $\frac{\partial\psi_s}{\partial t}$ are symmetric at time t, ψ_s at infinitesimally latter time t + dt given by $\psi_s + \frac{\partial\psi_s}{\partial t}dt$ is also symmetric. Such a step-by-step integration of the wave function can in principle be continued for arbitrary large time intervals and ψ_s is seen to remain symmetric always.

Similarly, if ψ_A is anti-symmetric wave function at any time t, then $H\psi_A$ and hence $\frac{\partial_A}{\partial t}$ are anti-symmetric and the integration of the wave function ψ_A shows that ψ_A is always anti-symmetric.

If P is an exchange operator, then we must have

$P\Psi_s(1, 2) = \Psi_s(2, 1)$

$P\Psi_A(1, 2) = -\Psi_A(2, 1)$

This symmetry property of the wave function has a relationship with the spin of the particle. This relationship is listed here in the following postulates.

1. The identical particles having an integral spin quantum number are described by symmetric wave function, i.e.,

$$P\Psi_s(1, 2, 3 \ldots r, \ldots s, \ldots n) = +\psi_s(1, 2, 3, \ldots s, \ldots r, \ldots n)$$

This class of particles, i.e., the particles described by symmetric wave functions are known as Bose particles or Bosons and obey Bose-Einstein Statistics. The examples of Bosons are photons (spin 1), neutral helium atoms in normal state ($s = 0$) etc.

2. The identical particles having half odd integral spin quantum number are described by anti-symmetric wave functions, i.e.

$$P\Psi_A(1, 2, \ldots r, \ldots s, \ldots n) = -\Psi_A(1, 2, \ldots s, \ldots r, \ldots n)$$

This class of particles i.e., the particles described by anti-symmetric wave function obey Fermi-Dirac statistics and the particles are known as Fermi-particles or Fermions. The examples of Fermions are electrons, protons, neutrons, muons (all spin $\frac{1}{2}$).

7.5 EXCHANGE DEGENERACY

In quantum mechanics, an energy-level can say to be degenerate if it corresponds to two or more measurable states of a quantum system. Also, two or more different states of a quantum mechanical system are said to be degenerate if they give the same value of energy upon measurement. The number of different states corresponding to a particular energy level is known as the degree of degeneracy of the level.

We shall now show that ψ_S or ψ_A can be constructed from a general unsymmetrized solution ψ of eqn. (1). If the arguments of the wave function ψ are permuted in any way, then the resulting wave function is also a solution of eqn. (1). This is because same permutation applied throughout eqn. (1) does not impair its validity as it corresponds simply to a relabelling of the particles. Since *H* is symmetric, permuted *H* will be same as original *H* and the resulting equation in same as eqn. (1) for the permuted ψ. In this way n! solutions can be obtained from any one solution, each of which corresponds to one of the n! permutations of the n arguments of ψ. Evidently any linear combination of these functions is also a solution of the wave equation (1). The sum of all these functions is symmetric (unnormalized) wave function ψ_S, since the interchange of any pair of particles changes any one of the component functions into another of them and the latter into the former, leaving the entire wave function unchanged.

An anti-symmetric unnormalized wave function can be constructed by adding together all the permuted wave functions that arise from the original solution by means of an even number of interchanges of pairs of particles and subtracting the sum of all the permuted wave functions that arise by means of an odd number of interchanges of pairs of particles in the original solution.

In the case where the Hamiltonian does not depend upon time, stationary state solutions

$$\psi\ (1,\ 2 \ldots n) = \phi\ (1,\ 2 \ldots n) e^{-iEnt/\hbar}$$

can be found and the time independent Schroedinger's equation. can be written as

There is n! solutions of this equation (Eigen-functions) derived from $\phi\ (1,\ 2 \ldots\ n)$ by means of permutations degenerate* and this type of degeneracy is called exchange degeneracy.

Let us now consider a two-particle wave function

$\psi(1s_1,2s_2)$. For a two-particle wave function, the Schroedinger's time independent equation is written as

$$H(1,2)\,\psi(1,2) = E\psi(1,2)$$

The 2! = 2 solutions of this equation are $\psi(1,2)$ and $\psi(2,1)$. The solutions correspond to a single energy state E.

The symmetric wave function can be written as

$$\Psi_s = \psi(1,2) + \psi(2,1)$$

and the anti-symmetric wave function is written as

$$\psi_A = \psi(1,2) - \psi(2,1)$$

Similarly for a system of 3 particles, the Schroedinger's equation is

$$H(1,2,3)\,\Psi(1,2,3) = E\,\Psi(1,2,3)$$

This eqn. has 3! = 6 solutions corresponding to the same eigen values E. The six possible functions obtained by exchanging the indices of the particles are

$$\Psi(1,2,3),\ \Psi(2,3,1),\ \Psi(3,2,1),\ \Psi(1,3,2),\ \Psi(2,1,3),\ \Psi(3,1,2)$$

Out of these six functions, those arising by an even number of interchanges of the pairs of particles in original wave function Ψ (1, 2, 3), are

$$\Psi(1,2,3),\ \Psi(2,3,1),\ \psi(3,1,2)$$

and the functions arising by an odd number of interchanges of pairs of particles in original function ψ (1, 2, 3) are

$$\Psi(1,3,2),\ \Psi(2,1,3),\ \Psi(3,2,1)$$

So, the symmetric wave function can be written as

$$\Psi_s = \psi(1,2,3) + \psi(2,3,1) + \psi(3,1,2) + \psi(1,3,2) + \psi(2,1,3) + \psi(3,2,1)$$

and the anti-symmetric wave function is

$$\psi_A = \psi(1,2,3) + \psi(2,3,1) + \psi(3,1,2) - \{\psi(1,3,2) + \psi(2,1,3) + \psi(3,2,1)\}$$

Here Ψ_s and Ψ_A are unnormalized wave functions.

Average Value and Quantum Statistics

The average value of any dynamical quantity p in state ψ is given by

$$\langle p \rangle = \frac{\int \psi^* P \psi d\tau}{\int \psi^* \psi d\tau}$$

where P is the operator corresponding to the dynamical quantity p. For example, the operator P associated with energy E is $i\hbar\ \partial/\partial t$ and the operator P associated with momentum p is $-i\hbar\ \nabla$.

If ψ is the normalised function, then $\int \psi^* \psi \, d\tau = 1$, therefore

$$\left\langle p >= \int \psi^* P \psi d\tau \right.$$

The symmetric and anti-symmetric normalised Eigen-functions lead to the following results and

$$\langle p_s \rangle = \int \Psi_s P^* \psi_s d\tau$$
$$\langle p_A \rangle = \int \Psi_A \cdot P \psi_A d\tau.$$

A little consideration shows that for symmetric solution an exchange of coordinates of particles leaves both ψ_s and ψ_s^* unaltered. Consequently $\langle p_s \rangle$ remain unchanged. In the case of anti-symmetric solution an exchange of coordinates changes the signs of both ψ_A and ψ_A^*. Consequently $\langle p_A \rangle$ again remains unchanged. Therefore, we conclude that any interchange of two particles leaves the average or the observed property of the system unaffected. Therefore, from the quantum mechanical point of view the similar particles can not be distinguished.

7.6 CLASSICAL FIELDS

Classically the behaviour of the quantum of radiation is described by Maxwell's field equations, which are four fundamental equations given by:

$$\begin{aligned}
\operatorname{div} \mathbf{D} &= \rho \text{ or } \nabla \cdot \mathbf{D} = \rho \\
\operatorname{div} \mathbf{B} &= 0 \text{ or } \nabla \cdot \mathbf{B} = 0 \\
\operatorname{curl} \mathbf{E} &= -\tfrac{\partial \mathbf{B}}{\partial t} \text{ or } \nabla \times \mathbf{E} = -\tfrac{\partial \mathbf{B}}{\partial t} \\
\operatorname{curl} \mathbf{H} &= \mathbf{J} + \tfrac{\partial \mathbf{D}}{\partial t} \text{ or } \nabla \times \mathbf{H} = \mathbf{J} + \tfrac{\partial \mathbf{D}}{\partial t}
\end{aligned}$$

In above equations the notations have the following meanings:

D = electric displacement vector in coulomb/m^2

ρ = charge density in coulomb/m^3

B = magnetic induction in weber/m^2 or Tesla

E = electric field intensity in volt/m or N/coulomb

H = magnetic field strength in amp/m-turn

Each of Maxwell's equations represents a generalization of certain experimental observation: Equation (1) represents the differential form of Gauss's law in electrostatics which in turn is derived from Coulomb's law. Equation (2) represents Gauss's law in magnetostatics which is usually said to represent the fact that the isolated magnetic poles do not exist in our physical world. Equation (3) represents the differential form of Faraday's law of electromagnetic induction and finally equation (4) represents Maxwell's modification of Ampere's law to include time varying fields. It is clear that Maxwell's equations represent mathematical expressions of certain experimental results.

According to equation (2) div **B** = 0, i.e., field vector **B** is solenoidal and it is well known that the div of curl of any vector is always zero, hence **B** can be expressed as a curl of a vector **A** (say) i.e.

$$\mathbf{B} = \text{curl } A = \nabla \times \mathbf{A}.$$

where **A** is called electromagnetic vector potential.

Substituting value of **B** from (5) in (3), we get

$$\operatorname{curl}\mathbf{E} = -\frac{\partial}{\partial t}(\operatorname{curl}\mathbf{A})$$
$$\operatorname{curl}\left(\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t}\right) = 0$$

This implies that the vector $\left(\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t}\right)$ has zero curl, i.e. $\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t}$ is irrotational and we know that the curl of gradient of any scalar function is always zero and hence the vector $\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t}$ can be expressed as the gradient of potential, i.e.

$$\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t} = -\operatorname{grad}\phi$$
$$\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} - \operatorname{grad}\phi = -\frac{\partial \mathbf{A}}{\partial t} - \nabla\phi$$

Equations (5) and (6) derived from homogeneous equations (2) and (3), express the electromagnetic field vectors **E** and **B** in terms of electromagnetic vector and scalar potentials A and ϕ. These electromagnetic potentials play a very important role in relativistic electrodynamics. The inhomogeneous Maxwell's equations (1) and (4) may be expressed as follows: As $D = \varepsilon E$, *we* have from

(1)

$$\operatorname{div}\mathbf{E} = \frac{\rho}{\varepsilon}$$

using (6) we get:

$$\operatorname{div}\left(-\frac{\partial \mathbf{A}}{\partial t} - \operatorname{grad}\phi\right) = \frac{\rho}{\varepsilon}$$
$$\operatorname{div}\operatorname{grad}\phi + \frac{\partial}{\partial t}(\operatorname{div}\mathbf{A}) = -\frac{\rho}{\varepsilon}$$
$$\nabla^2\phi + \frac{\partial}{\partial t}(\nabla \cdot \mathbf{A}) = -\frac{\rho}{\varepsilon}$$

Adding and subtracting $\mu \in \frac{\partial^2 \phi}{\partial t^2}$ and rearranging, we get

$$\nabla^2\phi - \mu\varepsilon\frac{\partial^2\phi}{\partial t^2} + \frac{\partial}{\partial t}\left(\operatorname{div}\mathbf{A} + \mu\varepsilon\frac{\partial\phi}{\partial t}\right) = -\frac{\rho}{\varepsilon}$$

From (4), we have
As

$$\operatorname{curl}\mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}$$

$\mathbf{B} = \mu\mathbf{H}$ and $\mathbf{D} = \varepsilon\mathbf{E}$, we have

$$\operatorname{curl}\mathbf{B} = \mu\mathbf{J} + \mu\varepsilon\frac{\partial \mathbf{E}}{\partial t}$$

Using (5) and (6), we get

$$\text{grad div } \mathbf{A} - \nabla^2 \mathbf{A} = \mu \mathbf{J} - \mu\varepsilon \frac{\partial^2 \mathbf{A}}{\partial t^2} - \mu\varepsilon \frac{\partial}{\partial t}(\text{grad } \phi)$$

Rearranging we get

$$\nabla^2 \mathbf{A} - \mu\varepsilon \frac{\partial^2 \mathbf{A}}{\partial t} - \text{grad}\left(\text{div } \mathbf{A} + \mu\varepsilon \frac{\partial \phi}{\partial t}\right) = -\mu \mathbf{J}$$

Generally $\mathbf{A}$ and ϕ are chosen subject to the condition

$$\text{div } A + \mu\varepsilon \frac{\partial \phi}{\partial t} = 0$$

Since div A is so far arbitrary, we can do so. This condition is known as Lorentz condition. Then equations (8) and (9) for electromagnetic potentials take the form

$$\nabla^2 \phi - \mu\varepsilon \frac{\partial^2 \phi}{\partial t^2} = -\frac{p}{\varepsilon}$$

and

$$\nabla^2 \mathbf{A} - \mu\varepsilon \frac{\partial^2 \phi}{\partial t^2} = -\mu J$$

If **A** and ϕ satisfy these equations, then the fields **B** and **E** determined by equations (5) and (6) satisfy Maxwell's equations. Equations (10), (11) and (12) form a set of equations equivalent in all respects to Maxwell's equations.

Introducing D' Alembert's
operator

$$\Box^2 = \nabla^2 - \mu\varepsilon \frac{\partial^2}{\partial t^2}$$

equations (11) and (12) take the form

$$\Box^2 \phi = -\frac{\rho}{\varepsilon}$$
$$\Box^2 \mathbf{A} = -\mu \mathbf{J}$$

and

These equations represent an extension of Poisson's equation.

Non-uniqueness of Electromagnetic Potentials and Concept of Gauge: For a given set of **A** and ϕ. equations (5) and (6) uniquely determine **B** and **E**. But the converse is not true, i.e., if **B** and **E** are given, the potentials **A** and ϕ are not unique. This may be seen as follows:

Since **A** defined by (5) is arbitrary to the extent that the gradient of some scalar function **S** can be added to **A** without affecting **B** (since curl grad S = 0 always), i.e.

$$\mathbf{A} \to \mathbf{A}' = \mathbf{A} + \operatorname{grad} S$$

Then equation (3) takes the form

$$\begin{aligned}\mathbf{E} &= -\operatorname{grad}\phi - \frac{\partial}{\partial t}\left(\mathbf{A}' - \operatorname{grad} S\right) \\ &= -\operatorname{grad}\left(\phi - \frac{\partial S}{\partial t}\right) - \frac{\partial \mathbf{A}'}{\partial t}\end{aligned}$$

This implies that if we adopt the transformation (15), then in order that the electric field (3) be unchanged as well, the scalar potentials ϕ must be simultaneously transformed as

$$\phi \to \phi' = \phi - \frac{\partial S}{\partial t}$$

Then expression for $\mathbf{B}$ and $\mathbf{E}$ remain unchanged under transformations (15) and (16), viz.

$$\mathbf{B} = \operatorname{curl}\mathbf{A} = \operatorname{curl}\left(\mathbf{A}' - \operatorname{grad} S\right) = \operatorname{curl}\mathbf{A}'$$

$$\begin{aligned}\mathbf{E} &= -\operatorname{grad}\phi - \frac{\partial \mathbf{A}}{\partial t} \\ &= -\operatorname{grad}\left(\phi' - \frac{\partial S}{\partial t}\right) - \frac{\partial}{\partial t}\left(\mathbf{A}' - \operatorname{grad} S\right) \\ &= -\operatorname{grad}\phi' - \frac{\partial \mathbf{A}'}{\partial t}\end{aligned}$$

Equations (17) indicate that we get the same field vectors **B** and **E** whether we use the set (A, ϕ) or (A′, ϕ′). Thus, we conclude that the electromagnetic potentials **A** and ϕ define the field vectors uniquely, while they themselves are not unique. The transformations given by equations (15) and (16) are known as the gauge transformations and the arbitrary scalar function S is called the gauge function. Since electromagnetic potentials **A** and ϕ have been introduced for convenience, it is the field vectors and not the electromagnetic potentials that have physical meaning. Thus, we can say that though **A** and ϕ are not unique, the field vectors **E** and **B** are invariant under gauge transformations. The invariance of fields under gauge transformations is known as gauge invariance. The property of gauge invariance is helpful in field formulation of interactions of charges and currents. The scalar potential ϕ (r, t) is given by

$$\phi(\boldsymbol{r},t)=\frac{1}{4\pi\epsilon}\int\frac{\rho(\mathbf{r}',t)}{|\mathbf{r}-\mathbf{r}'|}dr'$$

where $\rho(\mathbf{r}',t)$ is the charge density function at $(\mathbf{r}',t)$.
If $\rho=0,\phi=0$ and if $\rho=0$ and $\mathbf{J}=0$, then (14) gives
and

$$\Box^2\mathbf{A}=0$$

$$\mathbf{E}=-\frac{\partial\mathbf{A}}{\partial t}\text{ and }\mathbf{B}=\text{ curl }\mathbf{A}=\nabla\times\mathbf{A}$$

These equations define the radiation field classically.

7.7 SCHWINGER'S ACTION PRINCIPLE

In Dirac's view of quantum mechanics, the state of a system is associated with a vector in a complex vector space **V**. The knowledge of the values for a complete set of mutually compatible observables gives the most information about a state. It can then be assumed that {|a⟩}, where | a⟩ = | $a_1, \cdots, a_n$⟩, the set of all possible states, forms a basis for **V**. Associated with any vector space **V** is the dual space V^* whose elements are referred to as bras in Dirac's terminology. A basis for V^* is denoted by {⟨a|} and is dual to {| a ⟩}. The quantities satisfy

$$\langle a' \mid a'' \rangle = \delta(a', a''), \qquad \ldots (5)$$

where $\delta(a', a'')$ is the Kronecker delta if a' is a discrete set, and the Dirac delta if it is continuous. The choice of a complete set of mutually compatible observables is not unique. Suppose $\{| b \rangle\}$ also provides a basis for **V** relevant to another set of mutually compatible observables

B1, B2, ⋯. Since $\{| a \rangle\}$ and $\{| b \rangle\}$ are both bases for **V**, this means that one set of basis vectors can be expressed in terms of the other set

$$|b\rangle = \sum_a |a\rangle\langle a \mid b\rangle, \qquad \ldots (6)$$

and the $\langle a \mid b\rangle$ coefficients are some set of complex numbers, so that $\langle b \mid a\rangle^* = \langle a \mid b\rangle$. If there is a third basis for V provided by $\{|c\rangle\}$, then these complex numbers are related by means of

$$\langle a \mid c\rangle = \sum_b \langle a \mid b\rangle\langle b \mid c\rangle. \qquad \ldots (7)$$

Schwinger's action principle is based on the types of transformation properties of the transformation functions which can be constructed from this basis set [4].

Suppose the transformation function is subjected to, as Schwinger asserted, any conceivable infinitesimal variation. Then, by performing an arbitrary variation of (7), it follows that

$$\delta\langle a \mid c\rangle = \sum_b [(\delta\langle a \mid b\rangle)\langle b \mid c\rangle + \langle a \mid b\rangle(\delta\langle b \mid c\rangle)], \qquad \ldots (8)$$

and moreover, $\delta \langle a \mid b \rangle = \delta \langle b \mid a \rangle^*$.

Now a new operator can be defined which evaluates this actual variation when it is placed between the relevant state vectors. Define this operator to be δW_{ab}, so that it has the following action between states

$$\delta\langle a \mid b\rangle = \frac{i}{\hbar}\langle a|\delta W_{ab}|b\rangle. \qquad \ldots(10)$$

Including the factor of $\hbar$ gives the operator units of action. Using (10) in (8) produces,

$$\langle a|\delta W_{ac}|c\rangle = \sum_b [\langle a|\delta W_{ab}|b\rangle\langle b \mid c\rangle + \langle a \mid b\rangle\langle b|\delta W_{bc}|c\rangle] = \langle a|\delta W_{ab} + \delta W_{bc}|c\rangle \qquad \ldots(11)$$

using the completeness relation (7). Now it follows from (11) that

$$\delta W_{ac} = \delta W_{ab} + \delta W_{bc}. \qquad \ldots(12)$$

In the case in which the a and b descriptions are identified then using $\delta\langle a \mid a'\rangle = 0$, there results

$$\delta W_{aa} = 0. \qquad \ldots(13)$$

Identifying the a and c pictures in (11) gives,

$$\delta W_{ba} = -\delta W_{ab}. \qquad \ldots(14)$$

The complex conjugate of (10) with a and b descriptions reversed implies

$$-\frac{i}{\hbar}\langle b|\delta W_{ba}|a\rangle^* = \frac{i}{\hbar}\langle a|\delta W_{ab}|b\rangle. \qquad \ldots(15)$$

This has the equivalent form

$$-\left\langle a\middle|\delta W_{ba}^\dagger\middle|b\right\rangle = \langle a|\delta W_{ab}|b\rangle. \qquad \ldots(16)$$

Using (14), this yields the property

$$\delta W_{ba}^\dagger = \delta W_{ab}. \qquad \ldots(17)$$

The basic properties of the transformation function and the definition (10) have produced all of these additional properties [5,6].

In the Heisenberg picture, the basis kets become time dependent. The transformation function relates states which are Eigen-states of different complete sets of commuting observables at different times. Instead of using different letters, different subscripts 1, 2 can be used to denote different complete sets of commuting observables. In this event, (10) takes the form

$$\delta\langle a_2', t_2 \mid a_1', t_1\rangle = \frac{i}{\hbar}\langle a_2', t_2|\delta W_{21}|a_1', t_1\rangle. \qquad \ldots(18)$$

The assumption at the heart of this approach is that the operator δW_{21} in (18) is obtained from the variation of a single operator W_{21}. This is referred to as the action operator.

To adapt the results of the previous notation to the case with subscripts, we should have

$$W_{31} = W_{32} + W_{21}, \quad W_{11} = 0, \quad W_{21} = -W_{12} = W_{21}^{\dagger}. \qquad \ldots(19)$$

At this point, a correspondence between the Schwinger action principle and the classical principle of stationary action can be made. Suppose the members of a complete set of commuting observables A_1 which have eigenvectors $|a1, t\rangle$ in the Heisenberg picture are deformed in some fashion at time t_1. For example, take the alteration in the observables to correspond to a unitary transformation $\boldsymbol{A \rightarrow U^{\dagger}AU}$ such that $\boldsymbol{U^{\dagger} = U^{-1}}$. To remain eigenstates of the transformed operator, can be written U=I+iħ G, where G is Hermitian. It is then possible to define a variation it must be that states transform as $|\,\mathbf{a}\,\rangle \rightarrow \mathbf{U}^{\dagger}\,|\,\mathbf{a}\,\rangle$. Thinking of the transformation as being infinitesimal in nature, the operator **U** can be written $\boldsymbol{U = I + \frac{i}{\hbar}G}$, where G is Hermitian. It is then possible to define a variation:

$$\delta|a_1, t_1\rangle = -\frac{i}{\hbar} G_1 |a_1, t_1\rangle. \qquad \ldots (20)$$

Here operator G is a Hermitian operator and depends only on the observables A_1 at the time t_1. Similarly, if observables A_2 are altered at t_2, it is the case that

$$\delta\langle a_2, t_2| = \frac{i}{\hbar} \langle a_2, t_2| G_2, \qquad \ldots (21)$$

and the operator G_2 depends only on observables A_2 at time t_2. If both sets A_1, A_2 are altered infinitesimally, then the change in the transformation function is given by

$$\delta\langle a_2, t_2 \mid a_1, t_1\rangle = \frac{i}{\hbar} \langle a_2, t_2| G_2 - G_1 |a_1, t_1\rangle. \qquad \ldots (22)$$

Comparing this with (18), it is concluded that

$$\delta W_{21} = G_2 - G_1. \qquad \ldots (23)$$

If the time evolution from state $|a_1, t_1\rangle$ to $|a_2, t_2\rangle$ can be thought of as occurring continuously in time, then W_{21} can be expressed as

$$W_{21} = \int_{t_1}^{t_2} L(t) dt, \qquad \ldots (24)$$

where L(t) is called the Lagrange operator. As a consequence of (23), it follows that if the dynamical variables which enter L(t) are altered during an arbitrary infinitesimal change between t_1 and t_2, then it must be that

$$\delta W_{21} = 0 \qquad \ldots (25)$$

The operator equations of motion are implied in this result. The usual form for the Lagrange operator is

$$L(t) = \frac{1}{2}\left(p_i \dot{x}^i + \dot{x}^i p_i\right) - H(\mathbf{x}, \mathbf{p}, t). \qquad \ldots (26)$$

It is assumed that the Hamiltonian H is a Hermitian operator. The action operator (24) is used to calculate the variation δW_{21}. In order to vary the endpoints t_1, t_2, we follow Schwinger exactly and change the variable of integration from t to τ such that t = t (τ). This allows for the variation of the functional dependence of t to depend on τ with the variable of integration τ held fixed. Then W_{21} takes the form,

$$W_{21} = \int_{\tau_1}^{\tau_2} d\tau \left[\frac{1}{2} \left(P_i \frac{dy^i}{d\tau} + \frac{dy^i}{d\tau} P_i \right) - \tilde{H}(\mathbf{y}, \mathbf{P}, \tau) \frac{dt}{d\tau} \right], \qquad \dots (27)$$

where in (27),

$$\tilde{H}(\mathbf{y}, \mathbf{P}, \tau) = H(\mathbf{x}, \mathbf{p}, t) \qquad \dots (28)$$

Thus $y^i(\tau) = x^i(t)$ and $P_i(\tau) = p_i(t)$ when the transformation $t = t(\tau)$ is implemented. Evaluating the infinitesimal variation of (27), it is found that

$$\delta W_{21} = \int_{\tau_1}^{\tau_2} d\tau \left[\frac{1}{2} \delta P_i \frac{dy^i}{d\tau} + \frac{1}{2} P_i \delta \left(\frac{dy^i}{d\tau} \right) + \frac{1}{2} \delta \left(\frac{dy^i}{d\tau} \right) P_i + \frac{1}{2} \frac{dy^i}{d\tau} \delta P_i - \delta \tilde{H} \frac{dt}{d\tau} - \tilde{H} \delta \left(\frac{dt}{d\tau} \right) \right]. \qquad \dots (29)$$

Moving the operator δ through the derivative, this becomes

$$\delta W_{21} = \int_{t_1}^{t_2} d\tau \left\{ \frac{1}{2} \left(\delta P_i \frac{dy^i}{d\tau} + \frac{dy^i}{d\tau} \delta P_i - \frac{dP_i}{d\tau} \delta y^i - \delta y^i \frac{dP_i}{d\tau} \right) - \delta \tilde{H} \frac{dt}{d\tau} + \frac{d\tilde{H}}{d\tau} \delta t \right.$$
$$\left. + \frac{d}{d\tau} \left[\frac{1}{2} \left(P_i \delta x^i + \delta x^i P_i \right) - \tilde{H} \delta t \right] \right\}. \qquad \dots (30)$$

No assumptions with regard to the commutation properties of the variations with the dynamical variables have been made yet. It may be assumed that the variations are multiples of the identity operator, which commutes with everything. After returning to the variable t in the integral in δW_{21}, the result is

$$\delta W_{21} = \int_{t_1}^{t_2} dt \left(\delta p_i \dot{x}^i - \dot{p}_i \delta x^i + \frac{dH}{dt} \delta t - \delta H \right) + G_2 - G_1. \qquad \ldots (31)$$

Here G_1 and G_2 denote the quantity

$$G = p_i \delta x^i - H \delta t \qquad \ldots (32)$$

when it is evaluated at the two endpoints $t = t_1$ and $t = t_2$. If we define,

$$\delta H = \delta x^i \frac{\partial H}{\partial x^i} + \delta p_i \frac{\partial H}{\partial p_i} + \delta t \frac{\partial H}{\partial t}, \qquad \ldots (33)$$

then δW_{21} can be expressed in the form,

$$\delta W_{21} = \int_{t_1}^{t_2} dt \left\{ \delta p_i \left(\dot{x}^i - \frac{\partial H}{\partial p_i} \right) - \delta x^i \left(\dot{p}_i + \frac{\partial H}{\partial x^i} \right) + \left(\frac{dH}{dt} - \frac{\partial H}{\partial t} \right) \delta t \right\} + G_2 - G_1. \qquad \ldots (34)$$

Taking the variations with endpoints fixed, it follows that $G_1 = G_2 = 0$. Consequently, the operator equations of motion which follow from equating δW_{21} in (34) to zero are then

$$\dot{x}^i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial x^i}, \quad \frac{dH}{dt} = \frac{\partial H}{\partial t}. \qquad \ldots (35)$$

The results produced in this way are exactly of the form of the classical Hamilton equations of motion, and the derivatives in the first two equations of (35) are with respect to operators.

7.8 LAGRANGIAN AND HAMILTONIAN DENSITIES AND FIELD EQUATION

As discussed previously, a physical system with infinite (uncountable) degrees of freedom is referred to as a field. As the field has infinite degrees of freedom, it is analogous to a system consisting of an infinite number of particles. Just as a system of particles is specified by position coordinates q_i and their dependence on time t; a field is specified by its amplitudes ψ *(r, t)* at all points of space and the dependence of these amplitudes on time t. the amplitudes ψ *(r, t)* are known as field functions and may be considered as the degrees of freedom for the corresponding field. The variable ***r*** is continuous and must be considered as a continuous index. In analogy, with any physical system the field is the carrier of energy, momentum, angular momentum and other observable dynamical quantities.

The field equations, which represent relations between all the field functions $\psi(r, t)$ and their derivatives, play the role of mechanical equations of motion. The field propagates in accordance with field equations and carries with itself the dynamical variable.

Lagrangian Formulation: In classical mechanics the Hamilton's principle (necessary and sufficient condition for formulating equations of motion is

$$\delta \int_{t_1}^{t_2} L dt = 0; \delta q_i(t_1) = 0 \qquad \ldots (1)$$

where the last condition specifies that the virtual displacements at end points are zero. Let us expect that the field Lagrangian to depend on field amplitude ψ (**r**, t) and its first derivatives only. If ***L*** denotes the Lagrangian density, then the field Lagrangian is expressed as

$$L = \int \mathbf{L}(\psi, \nabla\psi, \dot{\psi}, t) d\tau \qquad \ldots (2)$$

This does not represent the most general case ; but covers all the cases of practical interest. The Hamilton's variational principle (1) gives

$$\delta \int_{t_1}^{t_2} L dt = \delta \int_{t_1}^{t_2} \int \mathbf{L}(\psi, \nabla\psi; \dot{\psi}, t) dt d\tau = 0 \qquad \ldots (3)$$

with the conditions

$$\delta\psi(\mathbf{r}, t_1) = \delta\psi(\mathbf{r}, t_2) = 0 \qquad \ldots (4)$$

As $\mathbf{L} = \mathbf{L}(\psi, \nabla\psi, \dot{\psi}, t)$ therefore we may write

$$\delta\mathbf{L} = \frac{\partial \mathbf{L}}{\partial \psi}\partial\psi + \sum_{k=1}^{3} \frac{\partial \mathbf{L}}{\partial\left(\frac{\partial\psi}{\partial x_k}\right)} \partial\left(\frac{\partial\psi}{\partial x_k}\right) + \frac{\partial \mathbf{L}}{\partial \dot{\psi}}\delta\dot{\psi} \qquad \ldots (5)$$

where we have replaced *x, y, z* by x_1, x_2, x_3 for convenience. As arbitrary variations δ are independent of the differentiation process, we have

$$\delta\left(\frac{\partial\psi}{\partial x_k}\right) = \frac{\partial}{\partial x_k}(\delta\psi) \text{ and } \delta\dot{\psi} = \frac{\partial}{\partial t}(\partial\dot{\psi}) \qquad \ldots(6)$$

Substituting these values in (5), we get

$$\delta\mathbf{L} = \frac{\partial\mathbf{L}}{\partial\psi}\delta\psi + \sum_{k=1}^{3}\frac{\partial\mathbf{L}}{\partial\left(\frac{\partial\psi}{\partial x_k}\right)}\frac{\partial}{\partial x_k}\left((\delta\psi) + \frac{\partial\mathbf{L}}{\partial\dot{\psi}}\frac{\partial}{\partial t}(\delta\psi)\right)$$

and hence equation (3) becomes

$$\int_{t_1}^{t_2}\iiint\left[\frac{\partial\mathbf{L}}{\partial\psi}\delta\psi + \sum_{k=1}^{3}\frac{\partial\mathbf{L}}{(\partial\psi/\partial x_k)}\frac{\partial}{\partial x_k}(\delta\psi) + \frac{\partial\mathbf{L}}{\partial\dot{\psi}}\frac{\partial}{\partial t}(\delta\psi)\right]dtdx_1dx_2dx_3 = 0 \qquad \ldots(7)$$

where we have used $d\tau = dx_1dx_2dx_3$.

Now let us consider the integration of the second term in the summation viz.

$$\int\frac{\partial\mathbf{L}}{\partial\left(\frac{\partial\psi}{\partial x_k}\right)}\frac{\partial}{\partial x_k}(\partial\psi)dx_k$$

Integration by parts, we obtain

$$\int\frac{\partial\mathbf{L}}{\partial\left(\frac{\partial\psi}{\partial x_k}\right)}\frac{\partial}{\partial x_k}(\delta\psi)dx_k = \left[\frac{\partial\mathbf{L}}{\partial\left(\frac{\partial\psi}{\partial x_k}\right)}\delta\psi\right] - \int\frac{\partial}{\partial x_k}\cdot\left[\frac{\partial\mathbf{L}}{\partial\left(\frac{\partial\psi}{\partial x_k}\right)}\right]\delta\psi dx_k \qquad \ldots(8)$$

The integrated term on RHS of (8) vanishes because ψ falls off rapidly at infinite distance (or because ψ obeys periodic boundary conditions at the walls of a large but finite box).
Therefore

$$\int\frac{\partial\mathbf{L}}{\partial\left(\frac{\partial\psi}{\partial x_k}\right)}\frac{\partial}{\partial x_k}(\delta\psi)dx_k = -\int\frac{\partial}{\partial x_k}\left[\frac{\partial\mathbf{L}}{\partial\left(\frac{\partial\psi}{\partial x_k}\right)}\right]\delta\psi dx_k. \qquad \ldots(9)$$

Now considering the integration of last term in (7), we get

$$\int_{t_1}^{t_2} \frac{\partial \mathbf{L}}{\partial \dot{\psi}} \frac{\partial}{\partial t}(\delta\psi)dt = \left[\frac{\partial \mathbf{L}}{\partial \dot{\psi}}\delta\psi\right]_{t_1}^{t_2} - \int_{t_1}^{t_2} \frac{\partial}{\partial t}\left(\frac{\partial \mathbf{L}}{\partial \psi}\right)(\delta\psi)dt$$

But $\left[\frac{\partial \mathbf{L}}{\partial \dot{\psi}}\delta\psi\right]_{t_1}^{t_2} = 0$ because of (4)

(integrating by parts)

$\int_{t_1}^{t_2} \frac{\partial \mathbf{L}}{\partial \dot{\psi}} \frac{\partial}{\partial t}(\delta\psi)dt = -\int_{t_1}^{t_2} \frac{\partial}{\partial t}\left(\frac{\partial \mathbf{L}}{\partial \psi}\right)\delta\psi dt \quad \ldots(10)$

Using (9) and (10) equation (7) takes the form

$$\int_{t_1}^{t_2} \iiint \left[\frac{\partial \mathbf{L}}{\partial \psi} - \sum_{k=1}^{3} \frac{\partial}{\partial x_k}\left\{\frac{\partial \mathbf{L}}{\partial(\partial\psi/\partial x_k)}\right\} - \frac{\partial}{\partial t}\left(\frac{\partial \mathbf{L}}{\partial \psi}\right)\right]\delta\psi dt dx_1 dx_2 dx_3 = 0 \quad \ldots(11)$$

Since $\delta\psi'$ ' s are arbitrary, equation (11) is equivalent to the differential equation

$$\frac{\partial \mathbf{L}}{\partial \psi} - \sum_{k=1}^{3} \frac{\partial}{\partial x_k}\left\{\frac{\partial \mathbf{L}}{\partial\left(\frac{\partial \psi}{\partial x_k}\right)}\right\} - \frac{\partial}{\partial t}\left(\frac{\partial \mathbf{L}}{\partial \psi}\right) = 0 \quad \ldots(12)$$

This is the classical field equation called the Euler's equation and corresponds to the Lagrangian equation in Classical Mechanics.

In order to have an analogy with Classical Mechanics it is desirable to rewrite equation (12) in terms of $\boldsymbol{L}$ rather than L. Since the aggregate of values of ψ and $\dot{\psi}$ at all points is analogous to q_i and q_i of particle theory, we require derivatives of L with respect to ψ and $\dot{\psi}$ at particular points. These are called the functional derivatives and are denoted by:

$$\frac{\bar{\partial}\mathbf{L}}{\bar{\partial}\psi} \text{ and } \frac{\bar{\partial}\mathbf{L}}{\bar{\partial}\dot{\psi}}$$

Expressions for these can be obtained by dividing up all space into small cells and replacing volume integral by summation over these cells. The average values of quantities such as ψ, $\nabla\psi$ and $\dot{\psi}$ and t in the i^{th} cell are denoted by subscripts i and the volume of the cell by $\delta\tau_i$ then

$$L = \mathrm{Lim}_{\delta\tau_i \to 0} \sum_i \mathbf{L}[\psi_i, (\nabla\psi)_i, \psi_i, \mathbf{t}]d\tau_i.$$

Similarly, the t-integrand in equation (11) can be replaced by:

$$\sum_i \left\{ \frac{\partial \mathbf{L}}{\partial \psi} - \sum_{k=1}^{3} \frac{\partial}{\partial x_k} \left[\frac{\partial \mathbf{L}}{\partial \left(\frac{\partial \psi}{\partial x_k} \right)} \right] \right\} \delta\psi_i \delta\tau_i - \sum_i \left(\frac{\partial \mathbf{L}}{\partial \dot{\psi}} \right)_i \delta\dot{\psi}_i \delta\tau_i$$

where the variation in ***L*** is now produced by independent variations in ψ_i and $\dot{\psi}_i$. Let us now assume that the $\delta\psi_i$ and $\delta\dot{\psi}_i$ are zero except for particular $\delta\psi_j$. Let us now assume that the $\delta\psi_i$ and $\partial\dot{\psi}_i$ are zero except for particular $\delta\psi_j$. It is natural to relate the functional derivative of ***L*** with respect to ψ for a point in jth cell to the ratio of δL to $\delta\psi_j$; we therefore define derivative of ***L*** with respect to $\dot{\psi}$ is defined by setting.

$$\frac{\bar{\partial}\mathbf{L}}{\bar{\partial}\psi} = \mathrm{Lim}_{\delta\tau\to 0} \frac{\partial \mathbf{L}}{\delta\psi_j \delta\tau_j} = \frac{\partial \mathbf{L}}{\partial \psi} - \sum_{k=1}^{3} \frac{\partial}{\partial x_k} \left[\frac{\partial \mathbf{L}}{\partial \left(\frac{\partial \psi}{\partial x_k} \right)} \right] \qquad \ldots (13)$$

Similarly, the functional derivative of L with respect to $\dot{\psi}$ is defined by setting all the $\partial\psi_i$ and $\delta\dot{\psi}_i$ equal to zero except for a particular $\delta\psi_j$; which in the j_{th} cell is defined as:

$$\frac{\bar{\partial}\mathbf{L}}{\bar{\partial}\dot{\psi}} = \mathrm{Lim}_{\delta\psi_j\to 0} \frac{\partial \mathbf{L}}{\partial\dot{\psi}_j \delta\tau_j} = \frac{\partial \mathbf{L}}{\partial\dot{\psi}} \qquad \ldots (14)$$

Substituting (13) and (14) into (12) we get

$$\frac{\partial}{\partial t}\left(\frac{\bar{\partial}\mathbf{L}}{\bar{\partial}\dot{\psi}} \right) - \frac{\bar{\partial}\mathbf{L}}{\bar{\partial}\psi} = 0 \qquad \ldots (15)$$

which resembles the Lagrangian equation for a system of particles.

Hamiltonian Formulation: For quantisation of this classical field theory, we must first go over to Hamiltonian formulation, which is usually developed for systems having a countable number of degrees of freedom. We are here dealing with (uncountable) infinite number of degrees of freedom, corresponding to the values of the field $\psi\ (r, t)$ considered as functions of time at each point **r** of space. Therefore, we must use some limiting process. For the purpose let us consider a system at a fixed instant of time ***t*** and let the three-dimensional

space $\boldsymbol{\tau}$ be divided into small cells of volume $\delta\,\boldsymbol{\tau}_i$, $i = 1, 2, 3\ldots$, so that the system is now specified by countable degrees of freedom, viz.

$$q_i = \psi_i (i = 1, 2, 3, \ldots) \qquad \ldots (16)$$

giving values of the field in each cell which is suitably defined. Then Lagrangian of the system may be defined as

$$p_i = \frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial \dot{\psi}_i} = \frac{\partial \mathbf{L_i}}{\partial \dot{\psi}_i} \delta\tau_i. \qquad \ldots (18)$$

The simplified form of the last step is due to restricted form of the Lagrangian density which involves only ψ_i and not $(\nabla\psi)_i$ because this would overlap the neighbouring cells.

Taking the analogy from classical mechanics, the Hamiltonian function is defined as

$$H = \Sigma p_i \dot{q}_i - L. \qquad \ldots (19)$$

Let us define the conjugate field of $\psi(x)$ or momentum density by

$$\pi(x) = \frac{\bar{\delta} L}{\bar{\delta}\dot{\psi}} = \frac{\partial \mathbf{L}}{\partial \dot{\psi}} \qquad \ldots (20)$$

So that equation (14) takes the form

$$\begin{aligned} H &= \sum_i \pi_i \delta\tau_i \dot{\psi}_i - \Sigma \mathbf{L_i} \delta\tau_i \\ &= \sum_i \left(\pi_i \dot{\psi}_i - \mathbf{L_i}\right) \delta\tau_i \end{aligned} \qquad \ldots (22)$$

If we consider the cells to be infinitesimal, then ($\delta\boldsymbol{\tau}_i \rightarrow 0$); so that the cell summation may be replaced by volume integral, then equation (22) gives Hamiltonian as

$$H = \int (\pi\dot{\psi} - \mathbf{L}) d\tau \qquad \ldots (23)$$

where d$\boldsymbol{\tau}$ represents volume elements *dx1, dx2, dx3.*

or

$$H = \int \mathbf{H} d\tau \quad \ldots (24)$$

where the Hamiltonian density $\mathbf{H}$ is defined as

$$\mathbf{H} = \pi\psi - \mathbf{L}.; \quad \ldots (25)$$

Let us now derive classical Hamiltonian equations of motion. The variation of

L produced by variations of ψ and $\dot{\psi}$ can be written as

Using (15) and (20), we have

$$\delta L = \int \left(\frac{\bar{\partial} L}{\bar{\partial}\psi} \delta\psi + \frac{\bar{\partial} L}{\bar{\partial}\dot{\psi}} \delta\dot{\psi} \right) d\tau \quad \ldots (26)$$

so equation (26) takes the form

$$\frac{\bar{\partial}\mathbf{L}}{\bar{\partial}\psi} = \dot{\pi} \text{ and } \frac{\bar{\partial}\mathbf{L}}{\bar{\partial}\psi} = \pi,$$

$$\begin{aligned} \delta L &= \int (\dot{\pi}\delta\psi + \pi\delta\dot{\psi}) d\tau \\ &= \int [\delta(\pi\psi) + \dot{\pi}\delta\psi - \psi\delta\pi] d\tau \\ &= \delta H + \delta L + \int (\dot{\pi}\delta\psi - \dot{\psi}\dot{\delta}\pi) d\tau \quad \ldots (27) \end{aligned}$$

Similarly, the variation produced in H *(ψ, π)* by the corresponding variations of *ψ* and *π* can be written as

$$\delta H = \int \left(\frac{\bar{\partial} H}{\bar{\partial} \psi} \delta\psi + \frac{\bar{\partial} H}{\bar{\partial} \pi} \delta\pi \right) d\tau. \quad \ldots (28)$$

From (27), we have

$$\delta H = -\int (\pi \delta\psi - \dot{\psi}\delta\pi) d\tau \quad \ldots (29)$$

Comparing (28) and (29), we get

$$\dot{\psi} = \frac{\bar{\partial} H}{\bar{\partial} \pi} \text{ and } \dot{\pi} = \frac{\bar{\partial} H}{\bar{\partial} \psi} \quad \ldots (30)$$

Now to find the Hamiltonian equation for time rate of change of function F (Ψ, π, t) we express F as a volume integral of the corresponding functional density $\mathbf{F}(\psi, \pi, t)$, which for simplicity we assume not

$$\begin{aligned} \frac{d\mathbf{F}}{dt} &= \frac{\partial \mathbf{F}}{\partial t} + \int \left(\frac{\partial \mathbf{F}}{\partial t} \dot{\psi} + \frac{\partial \mathbf{F}}{\partial \pi} \dot{\pi} \right) d\tau \\ &= \frac{\partial \mathbf{F}}{\partial t} + \int \left(\frac{\bar{\partial} F}{\bar{\partial} \psi} \frac{\bar{\partial} H}{\bar{\partial} \pi} - \frac{\bar{\partial} F}{\bar{\partial} \psi} \frac{\bar{\partial} H}{\bar{\partial} \psi} \right) d\tau \\ &= \frac{\partial F}{\partial t} + \{F, H\} \quad \ldots (31) \end{aligned}$$

This equation defines the Poisson bracket expression for two functions of field variables. If ***H*** represents the total energy of the field. Up to now we have considered field described by a single real amplitude: but if the field has more than one component $\psi_1, \psi_2 \ldots, \psi_a \ldots$, then Lagrangian density has the form

$$\mathbf{L}\left(\psi_1, \nabla\psi_1, \dot{\psi}_1, \psi_2, \nabla\psi_2, \dot{\psi}_2, \ldots, \psi_f, \nabla\psi_f, \dot{\psi}_f, t \right)$$

If now each of the components is varied independently, the variational equation (3), leads to an equation of the form (12) for each of ψ_α ($\alpha = 1, 2, 3 \ldots,$). Thus

$$\frac{\partial \mathbf{L}}{\partial \psi_\alpha} - \sum_{k=1}^{3} \frac{\partial}{\partial x_k}\left(\frac{\partial \mathbf{L}}{\left(\frac{\partial \psi_\alpha}{\partial x_k}\right)}\right) - \frac{\partial}{\partial t}\frac{\partial \mathbf{L}}{\partial \psi_\alpha} = 0 \quad \ldots(32)$$

and the momentum density π_α and Hamiltonian density $\mathbf{H}_\alpha$ are given by

$$\pi_\alpha = \frac{\partial \mathbf{L}}{\partial \psi_\alpha}, \mathbf{H} = \sum_\alpha \pi \dot{\psi}_\alpha - \mathbf{L} \quad \ldots(33)$$

The example of fields with more than one component are electromagnetic fields described by four potential A_1, A_2, A_3, ϕ $(f = 4)$ or a single complex field ψ_c expressed in terms of real ψ_1, ψ_2 $(f = 2)$ as

$$\psi_c = \frac{1}{\sqrt{2}}(\psi_1 + i\psi_2), \psi_c^* = \frac{1}{\sqrt{2}}(\psi_1 - i\psi_2) \quad \ldots(34)$$

It should be noted that the Lagrangian density **L** depends only on the state of the fields in the cell under consideration i.e., on values of ψ_a and their derivative evaluated at given specific point. Therefore, we refer **L** as the local Lagrangian.

7.9 QUANTUM EQUATION FOR THE FIELD

The classical Hamiltonian field theory discussed earlier can be at once quantised by interpreting the conjugate coordinates (cell averages) a_i, p_i defined by (16) and (21) as operators satisfying the usual commutation relations of Quantum Mechanics

$$\left.\begin{array}{lll} [q_i, q_j] = 0 & \text{or} & \left[\hat{\psi}_i, \hat{\psi}_j\right] = 0 \\ [p_i, p_j] = 0 & \text{or} & [\hat{\pi}_i, \hat{\pi}_j] = 0 \\ [q_i, p_j] = i\hbar\delta_{ij} & \text{or} & \left[\hat{\psi}_i, \hat{\pi}_i\right] = i\hbar\frac{\partial_{ij}}{\partial \tau_j} \end{array}\right\} \quad \ldots(1)$$

This means that we have converted the wave-field from a real numerical function to a Hermitian operator in the Heisenberg picture.

If we assume that the cell volumes approach zero, $\delta\tau_i \to 0$, the commutation relations for the field variables at two points r and r′ at the same time are obtained. For the present we are concerned with one instant of time so let us employ the Schroedinger picture in which operators are time-independent. So, the commutation relations for the field take the form:

$$\left.\begin{aligned}\left[\hat{\psi}(\mathbf{r},t),\hat{\psi}(\mathbf{r}',t)\right] &= [\hat{\pi}(\mathbf{r},t),\hat{\pi}(\mathbf{r}',t)] = 0\\ \left[\hat{\psi}(\mathbf{r},t),\hat{\pi}(\mathbf{r}',t)\right] &= i\hbar\delta^3(\mathbf{r}-\mathbf{r}')\end{aligned}\right\} \quad \ldots(2)$$

Since in the limit $\delta\tau_j \to 0$, $\delta_{ij/\tau j}$, become the three-dimensional Dirac function $\delta^3(r - r')$, the points r and r' lying in the i_{th} and j_{th} cell respectively. For fields with more than one component, we have

$$\left.\begin{aligned}\left[\hat{\psi}_\alpha(\mathbf{r},t),\hat{\psi}_\beta(\mathbf{r}',t)\right] &= [\hat{\pi}_\alpha(\mathbf{r},t),\pi_\beta(\mathbf{r}',t)] = 0\\ \left[\hat{\psi}_\alpha(\mathbf{r},t),\hat{\pi}_\beta(r',t)\right] &= i\hbar\delta^3_{\alpha\beta}(\mathbf{r}-\mathbf{r}')\\ \alpha,\beta &= (1,2,3,\ldots f)\end{aligned}\right\} \quad \ldots(3)$$

Instead of specifying algebraic relation for $\hat{\Psi}$ and $\hat{\pi}$ directly, we may expand $\hat{\Psi}$ in terms of any complete orthonormal set functions $u_k(\underline{r})$ moves in the field i

$$\hat{\Psi}(\vec{r},t) = \sum_k \hat{a}_k(t)u_k(\mathbf{r}) \quad \ldots(4)$$

where $u_k(\mathbf{r})$ satisfy the relation $\int u_k^*(\mathbf{r})u_l(\mathbf{r}) = \delta_{kl}$ $\ldots(5)$

$$\sum_k u_k(\mathbf{r})u_k*(\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')$$

and the expansion coefficients $\hat{a}_k$ are quantised operators acting on the elements of the Hilbert space. The quantum mechanical properties of $\hat{\psi}$ will be fixed if $\hat{a}_k$ is allowed to satisfy suitable algebraic relations.

To complete the description, in analogy with quantum equation of motion, we assume that for any function ***F***

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \frac{1}{i\hbar}[F, H] \quad \ldots (6)$$

The commutator bracket can be evaluated with the help of (2) when explicit expressions for ***F*** and ***H*** in terms of $\hat{\psi}$ and $\hat{\pi}$ are given. Thus equations (2) and (6) completely describe the behaviour of the quantised field that is specified by the Hamiltonian ***H.***

7.10 SUMMARY

In this unit, you have studied about identical particles, symmetric and anti-symmetric wave functions for many particles system. Exchange degeneracy, classical fields and Schwinger's principle have been explained. Lagrangian and Hamiltonian densities and field equations are discussed. Quantum structure for free field is explained.

7.11 GLOSSARY

Identical- exactly the same, or very similar

Symmetry- the concept that the properties of particles such as atoms and molecules remain unchanged after being subjected to a variety of symmetry transformations or "operations.

Exchange- interchange

Explicit- clear

Distinguishable- able to be recognized as different

Indistinguishable- impossible to judge as being different when compared to another similar thing

7.12 REFERENCES

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3. Advanced Quantum Mechanics, J.J.Sakurai, Pearson

7.13 SUGGESTED READINGS

1. Advanced Quantum Mechanics, Franz Schwabl, Springer

2. Introduction to Quantum Mechanics, David J. Griffiths, Cambridge University Press

3. P.M. Mathews and K. Venkatesan, A Text book of Quantum Mechanics, Tata Mc Graw-Hill, New Delhi.

4. L.I. Schiff, Quantum Mechanics, McGraw-Hill

7.14 TERMINAL QUESTIONS

1. What are symmetric and anti-symmetric wave-functions? Construct anti-symmetric and symmetric functions from unsymmetrised wave-functions.

2. Show that the indistinguishability of similar particles implies that admissible wave-function must obey symmetry restrictions with respect to interchange of particles.

3. What are identical particles? How can the behaviour of particles be distinguished in systems having symmetric and anti-symmetric wave functions?

4. Derive the classical field equations.

5. Explain Schwinger's action principle.

6. Discuss the Lagrangian and Hamiltonian formulation. Also derive the field equations.

UNIT 8 QUANTISATION OF FIELDS

Structure

8.1 Introduction

8.2 Objectives

8.3 Second quantization and Quantization relations

8.4 Quantization of non-relativistic Schrödinger matter field

8.5 System of identical Bosons and Fermions

8.5.1 System of Bosons

8.5.2 System of Fermions

8.6 Creation and annihilation operators

8.7 Occupation number representation

8.8 Summary

8.9 Glossary

8.10 References

8.11 Suggested Readings

8.12 Terminal Questions

8.1 INTRODUCTION

Quantization is the systematic process used in physics to move from a classical to a quantum mechanical understanding of physical phenomena. It is a method for converting classical mechanics into quantum mechanics.

Field quantization is a generalization with unlimited degrees of freedom, as in "quantization of the electromagnetic field," where photons are referred to as field "quanta" (for instance as light quanta).

Quantum field theory (QFT) is a theoretical framework in theoretical physics that incorporates quantum mechanics, special relativity, and classical field theory.

The objective of quantizing fields is to calculate expectation values of observables and their behaviour with respect to time, energy, and momentum variations in order to describe experiments. These expectation values of quantum field combinations, may be used to describe cross-sections, in-depth probabilistic descriptions of scattering, decay rates and lifetimes, magnetic moments, particle masses and mixing, and other observables with scattering characteristics like the S matrix.

8.2 OBJECTIVES

After studying this unit, you should be able to-

- Define Quantization of fields
- Understand Second quantization and Quantization relations
- Explain Quantization of non-relativistic Schrödinger matter field and System of identical bosons and fermions
- Commutation and anti-commutation relations
- Occupation number representation
- Creation and annihilation operators

8.3 SECOND QUANTIZATION AND QUANTIZATION RELATIONS

Consider a one-particle system that is defined by an orthonormal set of fundamental vectors. The system's state ψ is then given by,

$$\psi = \sum_i a_i \phi_i \qquad \ldots\ldots (1)$$

The coefficients a_i satisfy the normalization condition

$$\sum_i a_i^* a_i = 1 \qquad \ldots\ldots (2)$$

These a_i are simply numbers. The second quantization is the formation that treats the coefficients a_i's as operators. Since the assumption of a_i's as operators implies the quantization of probability amplitudes along with the observables of the system, the term *"second quantization"* is appropriate. To describe the quantized or continuum states, respectively, the basic vectors may be discrete or continuous.

Let's briefly review the Hamiltonian formulation of quantum mechanics and its application to the single particle formulation before discussing the second quantization formalism.

If a system is described by generalised coordinates q_k and generalised momenta p_k and time *t* [i.e. (2*n*+1) independent variables in the phase space], then the Hamilton's equations are

$$\dot{q}_k = \frac{\partial H}{\partial p_k} \quad \text{and} \quad \dot{p}_k = -\frac{\partial H}{\partial q_k} \qquad \ldots\ldots (3)$$

and classical equation of motion of a function in Poisson bracket notation is

$$\frac{dF}{dt} = \{F, H\}_{\mathrm{q,p}} + \frac{\partial F}{\partial t} \qquad \ldots\ldots (4)$$

If *F* is replaced by q_k and p_k respectively, equation (4) immediately yields Hamilton's equation (3). The *(first quantized) quantum mechanical description of the system* is then

obtained by replacing the variables q_k and p_k by operators. Then the Poisson brackets are replaced by commutators such that,

$$\{F, H\} \to \frac{1}{i\hbar}[F, H] \qquad \ldots\ldots(5)$$

The *Hilbert space* state vectors also describe the different states of the system, and the time-dependent state vector can be represented as the time-dependent coefficients, *i.e.*,

$$\psi(\mathbf{r}, t) = \sum_i a_i(t)\phi_i(\mathbf{r})$$

Where the basis vectors $\phi_i(\mathbf{r})$ are time dependent.

Then the Schroedinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi$$

becomes an equation describing the time derivatives of the coefficients $a_i(t)$ as follows:

$$i\hbar\frac{\partial a_i}{\partial t} = \sum_i H_{ij}a_j \qquad \ldots\ldots(6)$$

H_{ij} being the matrix elements of H in the basis $\phi_i's$.

The equations of motion (6) must be quantized in order to quantize coefficients $a_i's$. We must treat equation (6) as the system's equation of motion with coefficients a_i acting as generalised coordinates q_i if we want to compare this quantization to Hamilton's equation (3).

Then using the techniques of Classical Mechanics the new Lagrangian, genralised momenta and the Hamiltonian may be constructed.

8.4 QUANTIZATION OF NON-RELATIVISTIC SCHRÖDINGER MATTER FIELD

First, consider the non-relativistic Schrodinger equation's quantization, which is

$$-\frac{\hbar^2}{2m}\nabla^2\psi + \psi(r,t)\psi = i\hbar\frac{\partial\psi}{\partial t} \qquad \ldots\ldots(1)$$

This equation can be obtained from Classical Hamiltonian by simply replacing the variables **q** and **p** by the corresponding operators that satisfy the standard commutation rules $[q_i, p_j] = i\hbar\delta_{ij}$. The is known as the first quantisation in quantum mechanics. If we approach the Schroedinger equation as though it were a classical equation describing motion of a certain kind of material, and again quantize it by substituting an operator for the commuting function (the wave function) by an operator then this is called the second quantization. However, it is clear that the wave-function and operator formulations are equivalent.
We must first determine the Lagrangian density, whose substitution into Euler's equation will result in the Schroedinger equation (1). It is clear that the Lagrangian density has the following form.

$$\mathbf{L} = i\hbar\psi^*\dot{\psi} - \frac{\hbar^2}{2m}\nabla\psi^*\cdot\nabla\psi - V(\mathbf{r},t)\psi^*\psi \qquad \ldots\ldots(2)$$

This gives,

$$\frac{\partial\mathbf{L}}{\partial\psi} = -V(\mathbf{r},t)\psi^*$$
$$\frac{\partial\mathbf{L}}{\partial\psi} = i\hbar\psi^*;\ \text{so}\ \frac{\partial}{\partial t}\left(\frac{\partial\mathbf{L}}{\partial\psi}\right) = i\hbar\psi^*$$

Also,

$$\sum_{k=1}^{\infty}\frac{\partial}{\partial x_k}\left(\frac{\partial\mathbf{L}}{\partial\left(\frac{\partial\psi}{\partial x_k}\right)} = \nabla\frac{\partial\mathbf{L}}{\partial(\nabla\psi)} = \nabla\left(-\frac{\hbar^2}{2m}\nabla\psi^*\right)\right.$$
$$= -\frac{\hbar^2}{2m}\nabla^2\psi^* \qquad \ldots\ldots(3)$$

The Euler's equation is,

$$\frac{\partial\mathbf{L}}{\partial\psi} - \sum_{k=1}^{3}\frac{\partial}{\partial x_k}\left[\frac{\partial\mathbf{L}}{\partial\left(\frac{\partial\psi}{\partial x_k}\right)}\right] - \frac{\partial}{\partial t}\left(\frac{\partial\mathbf{L}}{\partial\dot{\psi}}\right) = 0 \qquad \ldots\ldots(4)$$

By equation (3) and (4),

$$-V(r,t)\psi^* + \frac{\hbar^2}{2m}\nabla^2\psi^* - i\hbar\dot{\psi}^* = 0$$

or

$$-i\hbar\dot{\psi}^* = -\frac{\hbar^2}{2m}\nabla^2\psi^* + V(r,t)\psi^* \qquad .....(5)$$

Equation (5) is the complex conjugate of non-relativistic Schroedinger's equation

$$i\hbar\dot{\psi} = -\frac{\hbar^2}{2m}\nabla^2\psi + V(\mathbf{r},t)\psi \qquad .....(6)$$

The canonically conjugate momentum to ψ is,

$$\pi = \frac{\partial \mathrm{L}}{\partial\dot{\psi}} = i\hbar\psi^* \qquad .....(7)$$

As ψ^* does not appear in the Lagrangian density, the canonically conjugate momentum to ψ^* does not exist and is likewise zero. Under this condition the commutation relation,

$$\left[\psi^\dagger(\mathbf{r},t), \pi^\dagger(\mathbf{r},t)\right] = i\hbar\cdot\delta^3(\mathbf{r}-\mathbf{r}')$$

Can not be satisfied. We know ψ^*exists and π does not, hence they cannot be regarded as canonically conjugate variables. The *Hamiltonian density* is,

$$\begin{aligned} H &= \pi\dot{\psi} - \mathbf{L} = i\hbar\psi^*\dot{\psi} - \mathbf{L} \quad \text{using (7)} \\ &= i\hbar\psi^*\dot{\psi} - \left[i\hbar\psi^*\dot{\psi} - \frac{\hbar^2}{2m}\nabla\psi^*\cdot\nabla\psi - V(\mathbf{r},t)\psi^*\psi\right] \\ &= \frac{\hbar^2}{2m}\nabla\psi^*\cdot\nabla\psi + V(\mathbf{r},t)\psi^*\psi \qquad .....(8) \end{aligned}$$

From equation (7) for $\psi^* = \frac{\pi}{i\hbar}$, we obtain,

$$H = -\frac{i\hbar}{2m}\nabla\pi\cdot\nabla\psi - \frac{i}{\hbar}V(\mathbf{r},t)\pi\psi \qquad .....(9)$$

The volume integral of the Hamiltonian density is used to determine the Hamiltonian *i.e.*

$$\mathbf{H} = \int \mathbf{H}d^3r = \int\left(\frac{\hbar^2}{2m}\nabla\psi^*\cdot\nabla\psi + V(\mathbf{r},t)\psi^*\psi\right)d^3r \qquad .....(10)$$

Now $\mathbf{H}^\dagger = \mathbf{H}$. Consequently, $\mathbf{H}$, is a hermition. Instead of the energy operator for a single particle, the *quantised Hamiltonian* (10) is the operator that expresses the total energy of the real scalar field. In the Hamiltonian form of the clasical field equations are,

$$\dot{\psi} = \frac{\bar{\delta} H}{\bar{\delta} \pi}, \dot{\pi} = -\frac{\bar{\delta} H}{\bar{\delta} \psi} \qquad \ldots\ldots (11)$$

Where,

$$\frac{\bar{\delta} H}{\bar{\delta} \psi} = \frac{\bar{\delta} H}{\partial \psi} - \sum_{k=1}^{3} \frac{\partial}{\partial x} \left[\frac{\partial H}{\partial \left(\frac{\partial \psi}{\partial x_k} \right)} \right]$$

$$\frac{\bar{\delta} H}{\bar{\delta} \pi} = \frac{\partial H}{\partial \pi} - \sum_{k=1}^{3} \frac{\partial}{\partial x_k} \left[\frac{\partial H}{\partial \left(\frac{\partial \pi}{\partial x_k} \right)} \right] \qquad \ldots\ldots (12)$$

Consequently, using equation (9) for Hamiltonian density, the Hamiltonian equations found in this example are

$$\dot{\psi} = \frac{i}{\hbar} V \psi + \frac{i \hbar}{2m} \nabla^2 \psi \qquad \ldots\ldots (13a)$$

$$\dot{\pi} = \frac{i}{\hbar} V \pi + \frac{i \hbar}{2m} \nabla^2 \pi \qquad \ldots\ldots (13b)$$

Equation (13a) is identical to equation (6), and equation (13b) and equation (7) together are the complex conjugate of equation (6). Thus, according to classical field theory, the Lagrangian density, the canonical variables, and the Hamiltonian produced from it are in perfect agreement with the original Schroedinger's equation.

8.5 SYSTEM OF IDENTICAL BOSONS AND FERMIONS

Any observed elementary particle is either a fermion (with odd half-integer spin) or a boson with an integer spin. Elementary bosons play a unique role in particle physics, as opposed to leptons and quarks, which are fermions and make up ordinary matter. They either function as force carriers that generate forces between other particles or, in one case, as the source of the mass phenomena.

8.5.1 SYSTEM OF BOSONS

We use the following commutation relations using Jordan and Klein's method

$$\left.\begin{aligned} \left[a_k, a_l^+\right] &= \delta_{kl} \\ \left[a_k, a_l\right] &= \left[a_k^+, a_l^+\right] = 0 \end{aligned}\right\} \qquad \ldots\ldots (14)$$

where a_k and a_l refer to same time *t*.

We suppose the Hermitian operator

$$\hat{N}_k = a_k^+ a_k \qquad \ldots\ldots(15)$$

If ϕ_k is normalised eigen function, then eigen-value equation of $\hat{N}_k$ is

$$\hat{N}_k\phi_k = N_k\phi_k \Rightarrow \hat{N}_k|k>= N_k|k> \qquad \ldots\ldots(16)$$

where N_k is eigen-value of operator $\hat{N}_k$ multiplying this equation scalarly by $< k|$, we get

$$\left\langle k\middle|\hat{N}_k\middle|k>= N_k < k\middle|k>\right.$$

$$\left\langle k|a_k^+ a_k|k>= N_k \text{ since } \langle k \mid k\rangle = \int_{\phi_k}^{*} \phi_k d\tau = 1\right.$$

$$N_k = \left\langle ka_k|a_k k>=||a_k k>|^2 \geq 0 \right. \qquad \ldots\ldots(17)$$

This shows that the values of N_k are either zero or positive.

Now operating equation (16) by operator a_k^+ from the left, we get

$$a_k^+\left(\hat{N}_k\phi_k\right) = N_k\left(a_k^+\phi_k\right) \qquad \ldots\ldots(18)$$

As we know, $[a_k, a_k^+] = 1 \Rightarrow a_k a_k^+ - a_k^+ a_k = 1$

Using equation (15)

$$\hat{N}_k = a_k^+ a_k - 1$$

Therefore equation (18) gives

$$\begin{gathered} a_k^+\left(a_k a_k^+ - 1\right)\phi_k = N_k\left(a_k^+\phi_k\right) \\ \Rightarrow \left(a_k^+ a_k a_k^+ - a_k^+\right)\phi_k = N_k\left(a_k^+\phi_k\right) \\ a_k^+ a_k\left(a_k^+\phi_k\right) = (N_k+1)a_k^+\phi_k \\ \Rightarrow N_k\left(a_k^+\phi_k\right) = (N_k+1)a_k^+\phi_k \quad \ldots\ldots(19) \end{gathered}$$

This implies that if N_k is the eigen value of operator $\hat{N}_k$ in the state ϕ_k; then $(N_k + 1)$ is the eigen value of operator $\hat{N}_k$ in the state $(a_k^+\phi_k)$.

Likewise, we get

$$\hat{N}_k(a_k\phi_k) = (N_k - 1)(a_k\phi_k) \qquad \ldots\ldots(20)$$

This equation demonstrates that operator $\hat{N}_k$ also has an Eigen-function $(a_k\phi_k)$ with an Eigen-value $(N_k - 1)$. As a result, the operator a_k^+ raises the Eigen-value of $\hat{N}_k$ by 1 unit and operator a_k lowers the Eigen-value of $\hat{N}_k$ by 1 unit. As a result, $\hat{N}_k$ and N_k are referred to as raising and lowering operators, respectively. Additionally, since the eigenvalues of $\hat{N}_k$ are constrained to be either positive or zero, therefore a vector ϕ_0 or ket $|0>$ must exist and may be obtained by repeatedly applying a_k and ϕ_k in such a way that

$$a_k\phi_0 = 0 \qquad \ldots\ldots(21)$$
$$\hat{N}_k\phi_0 = 0$$

Then we may find,

$$\phi_r \propto \left(a_k^+\right)^r \phi_0 \qquad \ldots\ldots(22)$$

As an eigen-vector of $\hat{N}_k$ belonging to eigen-value $N_k = r$. The eigen-value equation being

$$\hat{N}_k\phi_r = r\phi_r$$

Thus, the eigen values of the operator produce an eigenvalue spectrum that includes all non-negative integral numbers, such as

$$N_k = 0, 1, 2, 3 \ldots, r, \ldots.$$

Hence the operator $\hat{N}_k$ is termed as **number operator**. This implies

$$\left[\hat{N}_k, \hat{N}_k\right] = 0 \qquad \ldots\ldots(23)$$

This shows the simultaneous diagonalization of the set of number operators. These Hermitian operators make up a complete set that encompasses the entire Hilbert space. Let this set have eigen values; $N_1, N_2 \ldots . N_k \ldots .$, so that one such eigen function will be

$$\phi N_1, N_2, \ldots, N_k \ldots\ldots = |N_1, N_2, \ldots N_k \ldots\rangle \qquad \ldots\ldots(24)$$

All of these eigen functions will be superimposed to get the most general eigen function ψ. The function for which all $N_k = 0$, is called the ground state (vacuum state) defined by equation (21).

Equation (22) allows us to generate the function $\phi N_1, N_2 \ldots . N_k \ldots .$, by repeatedly applying the operators a_k^+ as follows

$$\phi N_1, N_2 \ldots . N_k \ldots . = C\ (a_1^+)^{N_1} (a_2^+)^{N_2} \ldots\ldots (a_k^+)^{N_k} \ldots\ldots \phi_0$$

Or $$|N_1, N_2 \ldots . N_k \ldots . >= C\ (a_1^+)^{N_1} (a_2^+)^{N_2} \ldots\ldots (a_k^+)^{N_k} \ldots\ldots |0> \quad \ldots..(25)$$

Where C is normalization constant.

Alternatively, we may write,

$$\left.\begin{aligned} a_k^+ |N_1, N_2, \ldots, N_k \ldots > &= \alpha(N_k) |N_1, N_2, \ldots, (N_k + 1), \ldots > \\ \text{and} \quad a_k |N_1, N_2, \ldots, N_k \ldots > &= \beta(N_k) |N_1, N_2, \ldots, (N_k - 1), \ldots > \end{aligned}\right\} \qquad \ldots\ldots(26)$$

Where constants $\alpha(N_k)$ and $\beta(N_k)$ are to be determined combining these equations, we get

$$\begin{aligned} a_k^+ a_k \mid N_1, N_2 \ldots N_k \ldots > &= \beta(N_k)\alpha(N_k - 1) \mid N_1, N_2, \ldots N_k \ldots > \\ &= N_k \mid N_1, N_2, \ldots N_k \ldots > \end{aligned}$$

Or $$\beta(N_k)\alpha(N_k - 1) = N_k \quad \text{.....(27)}$$

Similarly, we get,

$$a_k a_k^+ |N_1, N_2 \ldots N_k \ldots > = \beta(N_k + 1)\ \alpha(N_k)\ |N_1, N_2 \ldots N_k \ldots >$$

Which gives, $$= (N_{k+1})\ |N_1, N_2 \ldots N_k \ldots > \quad \text{.....(28)}$$

$$\beta(N_k + 1)\ \alpha(N_k) = N_k + 1$$

Equations (27) and (28) give,

$$\alpha(N_k) = \sqrt{N_k + 1} \text{ and } \beta(N_k) = \sqrt{N_k} \quad \text{.....(29)}$$

Thus, we get,

$$(a_1^+)^{N_1}(a_2^+)^{N_2} \ldots\ldots (a_k^+)^{N_k} \ldots\ldots |0> = \sqrt{N_1! N_2! \ldots\ldots N_k! \ldots\ldots}\ \ N_1, N_2 \ldots N_k \ldots > \quad \text{..... (30)}$$

Comparing equation (25) and (30), we get

$$C = \frac{1}{\sqrt{N_1! N_2! \ldots\ldots N_k! \ldots\ldots}}$$

Then equation (25) may be expressed as,

$$|N_1, N_2 \ldots N_k \ldots > = \frac{1}{\sqrt{N_1! N_2! \ldots\ldots N_k! \ldots\ldots}}\ (a_1^+)^{N_1}(a_2^+)^{N_2} \ldots\ldots (a_k^+)^{N_k} \ldots\ldots |0> \quad \text{.....(31)}$$

Moreover, it can easily be seen

$$(a_k)^r (a_l^+)^N \Big| 0 > = \frac{N!}{(N-r)!} (a_k^+)^{N-r} \Big| 0 > \delta_{k,l} \quad \ldots\ldots (32)$$

So that,

$$(a_k)^N (a_l^+)^N |0> = N! \delta_{kl} |0> \quad \ldots\ldots (33)$$

Using these relations, we get,

$$< N_1', N_2' \ldots N_k' \ldots\ldots \mid N_1, N_2 \ldots N_k \ldots\ldots > = \delta_{N_1 N_1} \delta_{N_2 N_2'} \ldots \delta_{N_k}, N_k' \quad \ldots\ldots (34)$$

This equation shows that the base vectors are orthonormal. These vectors constitute a representation (called particle number representation) for the operators a_k, a_k^+ and $\widehat{N}_k$ such that,

$$\left.\begin{aligned} a_k^+|N_1,N_2\ldots N_k\ldots>&=\sqrt{N_k+1}|N_1,N_2\ldots N_k+1\ldots>>\\ a_k|N_1,N_2\ldots N_k\ldots>&=\sqrt{N_k}|N_1,N_2\ldots N_k-1,\ldots>\\ \hat{N}_k|N_1,N_2\ldots N_k\ldots>&=N_k|N_1,N_2\ldots N_k\ldots> \end{aligned}\right\} \quad \ldots..(35)$$

As such,

$$< N_1',N_2'\ldots N_k'|\hat{N}_k|N_1,N_2\ldots N_k>=N_k\delta_{N_1N_1'}\delta_{N_2N_2'}\ldots\delta N_kN_k' \quad \ldots..(36)$$

This shows that $\hat{N}_k$ are diagonal operators in this representation with the diagonal matrix elements N_k.

Using quantum field equation,

$$\psi(\mathbf{r},t)=\sum_k a_k(t)u_k(\mathbf{r}) \quad \ldots..(37)$$

With,

$$\int u_k^*(\mathbf{r})u_l(\mathbf{r})d\tau=\delta_{kl} \text{ and } \sum_k u_k(\mathbf{r})u_k^*(\mathbf{r}')=\delta(\mathbf{r}-\mathbf{r}') \quad \ldots..(38)$$

Substituting equation (37) into equation (10) and using (38) and single particle equation

$$\hat{H}_p u_k(\mathbf{r})=\varepsilon_k u_k(\mathbf{r})$$

$$\hat{H}_p=-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r}) \quad \ldots..(39)$$

We get,

$$H=\sum_k \hat{N}_k\varepsilon_k \quad \ldots..(40)$$

Hence the Eigen-values of the Hamiltonian for the quantized field are,

$$E=\sum_k N_k\varepsilon_k \quad \ldots..(41)$$

with the corresponding Eigen-vectors $|N_1,N_2\ldots N_k\ldots>$. This relation shows how the matter field can be conceptualised as an assembly of independently moving, non-interacting particles, each of which has an energy spectrum ϵ_k . The sum of individual particle energies and the total number of particles in the field makes up the total field energy

$$N=\sum_k N_k \quad \ldots..(42)$$

and any particle state may be occupied by any number of particles N_k. This is the condition of Bose-Einstein statistics. Thus, the field represents an assembly of bosons. Moreover, the particle number operator commutes with the field Hamiltonian $\hat{H}$ *i.e.*

$$\left[\hat{N}_k, \hat{H}\right] = \sum_{kl} \varepsilon_l \left[\hat{N}_k, \hat{N}_l\right] = 0 \qquad \ldots\ldots(43)$$

This implies that the total number of particles in the field is a constant of motion when potential function *V* does not depend on time. The creation a_k^+ and annihilation a_k operators are thus named because they, respectively, increase and decrease the particle number by 1.

8.5.2 SYSTEM OF FERMIONS

Fermions are half-integral spin particles that follow Fermi-Dirac statistics. Since the fermions follow the Pauli exclusion principle, hence any state can occupy either 0 or 1 particle, i.e., $N_k = 0 \; or \; 1$. According to Jordan and Winger, if the operators a_k and a_k^+ satisfy the anti-commutation relation instead of the commutation relation, this condition can be met i.e.

$$\{a_k, a_l^+\} = \{a_l^+, a_k\} = a_k a_l^+ + a_l a_k = \delta_{kl}$$

And

$$\{a_k, a_l\} = \{a_k^+, a_l^+\} = 0 \qquad \ldots\ldots(44)$$

These relations provide,

$$a_k a_k = a_k^+ a_k^+ = 0 \qquad \ldots\ldots(45)$$

All operators in these relations refer to same time using these relations it is readily seen that

$$\hat{N}_k^2 = \hat{N}_k \Rightarrow \left(\hat{N}_k^2 - \hat{N}_k\right) = 0$$
$$\hat{N}_k\left(\hat{N}_k - 1\right) = 0$$

Hence for any arbitrary state

$$\hat{N}_k\left(\hat{N}_k - 1\right)\phi_k = 0$$

This gives, $\hat{N}_k = 0 \; or \; 1$ for any *k*.

In view of commutation relation (43), we get $[\hat{N}_k, \hat{N}_1] = 0$

Hence the base vectors can be characterised as simultaneous Eigen-functions of number operators $\widehat{N}_k$,as in preceding case. Hence in this case equation (32) is satisfied and we may still choose the base vectors (31); but here $\widehat{N}_k! = 1$ (since $\widehat{N}_k = 0$ or 1 only). Thus

$$|N_1, N_2 \ldots . N_k \ldots . > = (a_1^+)^{N_1}(a_2^+)^{N_2} \ldots . . (a_k^+)^{N_k} \ldots . |0 > \qquad \ldots..(46)$$

As the operators a_k^+ anti-commute, a phase factor ± 1 is undertmined in this equation unless we specify the order in which these operators operate. We put (+) sign when the creation operators are arranged in equation (46) in order of increasing superscript. we get

$$a_k \, |N_1, N_2 \ldots . N_k \ldots . > = (-1)^{N_1 + N_1 + \ldots . + N_{k-1}} (a_1^+)^{N_1}(a_2^+)^{N_2} \ldots . . (a_k^+)^{N_k} \ldots . |0 >$$
$$= (-1)^{S_k} \, N_k \, |N_1, N_2 \ldots . N_{k-1} \ldots . > \qquad \ldots..(47)$$

Where, $S_k = \sum_{r=1}^{k-1} N_r$

Similarly for operators a_k^+, we have

$$a_k^+ \left| N_1, N_2 \ldots N_k \ldots > = (-1)^{S_k}(1 - N_k) \right| N_1, N_2 \ldots N_k + 1 \ldots > \qquad \ldots . . (48)$$

These equations show that still a_k^+ and a_k may be interpreted as creation and annihilation operators respectively. The factors N_k and $(1 - N_k)$ imply that an empty state $N_k = 0$ can not be further emptified, while an occupied state $(N_k = 1)$ cannot be further filled.

Combing equations, we get,

$$\hat{N}_k \mid N_1 N_2 \ldots N_k \ldots > = \hat{N}_k (N_1 N_2 \ldots N_k \ldots >$$
$$< N_1', N_2' \ldots N_k' \ldots , | \hat{N}_k \mid N_1, N_2 \ldots N_k \ldots >$$
$$= N_k \delta_{N_1 N'}, \delta_{N_2 N_2'} \ldots \delta_{N_k N_k'}$$

For operators $\hat{\psi}$ and $\hat{\pi}$, we also have

$$\left[\hat{\psi}(\mathbf{r}, t), \hat{\psi}'(\mathbf{r}', t) \right]_+ = \sum_{kl} \left[a_k, a_l^+ \right]_+ u_k(\mathbf{r}) u_k^*(\mathbf{r}')$$

And

$$\left[\hat{\psi}(\mathbf{r}, t), \hat{\pi}(\mathbf{r}', t) \right]_+ = i\hbar \delta(\mathbf{r} - \mathbf{r}')$$

These relations have no similarity with Hessenberg relations in contrast with the system for bosons.

8.6 CREATION AND ANNIHILATION OPERATORS

In quantum mechanics, creation and annihilation operators are mathematical operations that are often used, particularly in the study of many-particle systems. A creation operator (usually denoted as a_k^+) increases the number of particles in a given state by 1 and an annihilation operator (usually denoted as a_k) lowers the number of particles in a given state by 1. The use of these operators in place of wave-functions is referred to as *second quantization* in many branches of physics and chemistry. These operators were introduced by Paul Dirac.

Consider a number operator *N* defined by,

$$N = \int \psi^\dagger(\mathbf{r})\psi(\mathbf{r})d^3r \qquad \ldots\ldots(1)$$

where the operator $[\psi^\dagger(r)\ \psi'(r)]$ may be interpreted as the particle density; so that *N* represents the number of particles in the field.

We first note that operator *N* is *Hermitian*. Its time derivative is given by

$$i\hbar\frac{dN}{dt} = [N, H]$$

$$\left[\int \psi^\dagger\psi d^3r, \int\left(\frac{\hbar^2}{2m}\nabla'\psi'^\dagger\cdot\nabla'\psi' + V'\psi'^\dagger\psi'\right)d^3r'\right] \qquad \ldots\ldots(2)$$

The commutator of *N* with the *V* part of *H* can be expressed as,

$$\iint V'\left(\psi^\dagger\psi\psi'^\dagger\psi' - \psi'^\dagger\psi'\psi^\dagger\psi\right)d^3rd^3r' \qquad \ldots\ldots(3)$$

By means of the commutation relations,

$$\left.\begin{aligned}[\psi(\mathbf{r}),\psi(\mathbf{r})] = \left[\psi^\dagger(\mathbf{r}),\psi^\dagger(\mathbf{r})\right] = 0\\ \left[\psi(\mathbf{r}),\psi^\dagger(\mathbf{r}')\right] = \delta^3(\mathbf{r}-\mathbf{r}')\end{aligned}\right\} \qquad \ldots\ldots(4)$$

the bracketed term in (3) becomes

$$\begin{aligned}\psi^\dagger\psi\psi'^\dagger\psi' - \psi'^\dagger\psi'\psi^\dagger\psi &= \psi^\dagger\left[\psi'^\dagger\psi + \delta^3\left(\mathbf{r}-\mathbf{r}'\right)\right]\psi' - \psi'^\dagger\psi'\psi^\dagger\psi\\ &= \psi'^\dagger\psi^\dagger\psi'\psi + \psi^\dagger\psi'\delta^3\left(\mathbf{r}-\mathbf{r}'\right) - \psi'^\dagger\psi'\psi^\dagger\psi'\\ &= \psi'^\dagger\left[\psi'\psi^\dagger - \delta^3\left(\mathbf{r}-\mathbf{r}'\right)\right]\psi + \psi^\dagger\psi'\delta^3\left(\mathbf{r}-\mathbf{r}'\right) - \psi^\dagger\psi'\psi'^\dagger\psi\\ &= 0 \quad \text{since } \delta - \text{ function vanishes unless } \mathbf{r} = \mathbf{r}'\end{aligned}$$

It can also be demonstrated that,

$$\left[\psi^{\dagger}\psi, \nabla'\psi'^{\dagger}\cdot\nabla'\psi'\right] = \left[\psi^{\dagger}\nabla'\psi' - \left(\nabla'\psi'^{\dagger}\right)\psi\right]\cdot\nabla'\delta^{3}\left(\mathbf{r}-\mathbf{r}'\right)$$

The double integral of this over ***r*** and ***r***' is zero. Therefore R.H.S. of (2) is zero. Hence it is clear that *N is a constant of the motion*.

In order to find a diagonal representation of *N*, let us take a look. *N* has real eigenvalues since it is Hermitian. Let's use the expansion theorem to achieve our goals and express $\psi(r,t)$ in terms of a complete orthonormal set of functions $V_k(r)$, which we assume are discrete because of the assumption that definiteness exists. i.e.

$$\psi(\mathbf{r},\mathbf{t}) = \sum_{k} a_k\,(t)u_k(\mathbf{r})$$

$$\psi^{\dagger}(\mathbf{r},\mathbf{t}) = \textstyle\sum_k a_k^{\dagger}(t)\,u_k^{*}(\mathbf{r}) \qquad \text{…..(5)}$$

where u_k are numerical functions of space co-ordinates and the a_k are Heisenberg picture operators that depend on the time. Equation (5) can be solved for a_k:

$$\left.\begin{aligned} a_k(t) &= \int u_k^{*}(\mathbf{r})\psi(\mathbf{r},t)d^3r \\ \text{and } a_k^{\dagger}(t) &= \int u_k(\mathbf{r})\psi^{\dagger}(\mathbf{r},t)d^3r \end{aligned}\right\} \qquad \ldots\ldots(6)$$

Now multiplying the second commutation relation (4) by $u_k^{\dagger}(r)\;u_l(r)$on both sides and integrating over **r** and **r'**, we obtain

$$\left[a_k(t), a_l^{\dagger}(t)\right] = \iint u_k^{*}(\mathbf{r})u_l(\mathbf{r}')\delta^{3}\left(\mathbf{r}-\mathbf{r}'\right)d^3\mathbf{r}d^3\mathbf{r}' = \delta_{kl} \qquad \ldots\ldots(7)$$

because of orthonormality of u_k. Similarly, it is apparent that a_k and a_l commute and that $a_k^{\dagger}$ and $a_l^{\dagger}$ commute for all *k* and *l*.

Substituting equation (5) into equation (1), we get

$$N = \int \psi^{\dagger}(\mathbf{r})\,\psi(\mathbf{r})d^3\boldsymbol{r} = \int\left[\sum_k a_k^{\dagger}(t)\,u_k^{*}(\mathbf{r})\sum_l a_l(t)u_l(\mathbf{r})\right]d^3\boldsymbol{r}$$

$$= \textstyle\sum_k\sum_l \int a_k^{\dagger}(t)\,a_l(t)\,u_k^{*}(\mathbf{r})\,u_l(\mathbf{r})d^3\boldsymbol{r}$$

$$= \sum_k a_k^\dagger a_k$$

$$= \sum_k N_k \text{ where } N_k = a_k^\dagger a_k \qquad \text{.....(8)}$$

It may be easily verified that each N_k commutes with all the others, so that they can be diagonalized simultaneously.

To find a representation in which N and all the N_k are diagonal, let us write each of the a_k in the form,

$$a_k = \frac{1}{\sqrt{2}}(q_k + ip_k), a_k^\dagger = \frac{1}{\sqrt{2}}(q_k - ip_k) \qquad \ldots\ldots(9)$$

Where q_k and p_k are Hermitian. This is always possible since above equation leads to

$$q_k = \frac{1}{\sqrt{2}}\left(a_k + a_k^\dagger\right), p_k = -\frac{i}{\sqrt{2}}\left(a_k - a_k^\dagger\right) \qquad \ldots\ldots(10)$$

which are evidently Hermitian since

$$q_k^\dagger = q_k \text{ and } p_k^\dagger = p_k$$

$$\begin{aligned}
[q_k, p_l] &= \left[\frac{1}{\sqrt{2}}\left(a_k + a_k^\dagger\right), -\frac{i}{\sqrt{2}}\left(a_l - a_l^\dagger\right)\right] \\
&= -\frac{1}{2}\left\{[a_k, a_l] - \left[a_k, a_l^\dagger\right] + \left[a_k^\dagger, a_l\right] - \left[a_k^\dagger, a_l\right]\right\} \\
&= -\frac{i}{2}\left\{-\left[a_k, a_l^\dagger\right] + \left[a_k^\dagger, a_l\right]\right\} = \frac{i}{2} \cdot 2\left[a_k \cdot a_l^\dagger\right] \\
&= -i\delta_k^l \quad \{\text{ using (7) }\} \qquad \ldots\ldots(11)
\end{aligned}$$

Also

$$\left[q_k, q_l^\dagger\right] = \left[p_k, p_l^\dagger\right] = 0 \qquad \ldots\ldots(12)$$

By equation (9) and (11), we get

$$N_k = a_k^\dagger a_k = \frac{1}{\sqrt{2}}(q_k - ip_k) \cdot \left(\frac{1}{\sqrt{2}}(q_k + ip_k)\right) = \frac{1}{2}\left(q_k^2 + p_k^2\right) - \frac{1}{2} \qquad \ldots\ldots(13)$$

therefore, q and p are diagonal; they also make N_k diagonal. The solution of harmonic oscillator problem is equivalent to the diagonalization of the Hamiltonian matrix.

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

when the co-ordinate q and canonically conjugate momentum p obey the commutation rule $[q, p] = i\hbar$. The energy Eigen-values were obtained to be $E = \left(n + \frac{1}{2}\right)\hbar\omega$. Choosing an arbitrary system of units, let us put $\hbar = 1, K = m = 1$ so that $\omega = \sqrt{\frac{K}{m}} = 1$ and identify q with q_k and p_k; then we have

$$\left.\begin{aligned} &[q_k, p_k] = i, H = \tfrac{1}{2}\left(q_k^2 + p_k^2\right) \\ &E_n = \left(n + \tfrac{1}{2}\right) \end{aligned}\right] \quad \ldots\ldots(14)$$

These equations can be compared to (11) and (13) to show that $N_k + \frac{1}{2}$ has their eigenvalues $n_k + \frac{1}{2}$ and that can be identified with the oscillator's energy or Hamiltonian operator.

Where $n_k = 0,1,2,3\ldots..$

Analytically defined, the field corresponds to a system of harmonic oscillators where $K = m = 1$ and $\hbar = 1$. Here, we have noted the *second quantization* behaviour of Schroedinger equation describing matter field. Similar to the harmonic oscillator problem the non-vanishing matrix elements in non-vanishing matrix elements in Schroedinger picture*(t=0)* for q_k and p_k are

$$(q_k)_{n_k, n_k+1} = (q_k)_{n_k+1, n_k} = \sqrt{\left(\frac{n_k + 1}{2}\right)} \quad \ldots\ldots(15a)$$

$$(p_k)_{n_k, n_k+1} = (-p_k)_{n_k+1, n_k} = -i\sqrt{\left(\frac{n_k + 1}{2}\right)} \quad \ldots\ldots(15b)$$

So that the corresponding matrices are

$$q_k = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ \sqrt{2} & 0 & \sqrt{2} & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{bmatrix} \quad \ldots\ldots(16a)$$

$$p_k = -\frac{i}{\sqrt{2}} \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{bmatrix} \quad \ldots\ldots(16b)$$

Now the matrices for a_k and $a_k^\dagger$ may the obtained from equation (9) namely,

$$a_k = \frac{1}{\sqrt{2}}(q_k + ip_k), a_k^\dagger = \frac{1}{\sqrt{2}}(q_k - ip_k)$$

$$\therefore (a_k)_{n_k, n_k+1} = \frac{1}{\sqrt{2}}\{(q_k)_{n_k, n_k+1} + i\,(p_k)_{n_k, n_k+1}\}$$

$$= (n_k + 1)^{1/2}$$

And $(a_k^\dagger)_{n_k+1, n_k} = \frac{1}{\sqrt{2}}\{(q_k)_{n_k+1, n_k} - i\,(p_k)_{n_k+1, n_k}\}$

$$= (n_k + 1)^{1/2} \quad \ldots..(17)$$

$$(a_k^\dagger)_{n_k, n_k+1} = (a_k)_{n_k+1, n_k} = 0$$

So that the corresponding matrices are

$$a_k = \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & \ldots \\ 0 & 0 & \sqrt{2} & 0 & \ldots \\ 0 & 0 & 0 & \sqrt{3} & \ldots \\ 0 & 0 & 0 & 0 & \ldots \\ \ldots & \cdots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \end{bmatrix} \quad \ldots\ldots(18a)$$

$$a_k^\dagger = \begin{bmatrix} 0 & 0 & 0 & 0 & \ldots \\ \sqrt{1} & 0 & 0 & 0 & \ldots \\ 0 & \sqrt{2} & 0 & 0 & \ldots \\ 0 & 0 & \sqrt{3} & 0 & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \end{bmatrix} \quad \ldots\ldots(18b)$$

The matrix element $(a_k)_{n_k,n_k+1}$ means that in the kth state initially the number of particles was n_k+1 and finally it is n_k. Therefore a_k is interpreted as annihilation operator for particles in the state *k*. Similarly, $a_k^\dagger$ increases the number of particles in the kth state by unity: hence it is interpreted as a creation operator for the state *k*.

Thus, we may write

$$a_k\left|n_1,n_2\ldots n_k\ldots\right>=n_k^{1/2}\left|n_1,n_2\ldots.n_k-1,\ldots.\right> \quad \ldots..(19)$$

$$\text{and } a_k^\dagger\left|n_1,n_2\ldots.n_k\right>=(n_k+1)^{1/2}\left|n_1,n_2,\ldots..n_k+1,\ldots..\right> \quad \ldots..(20)$$

Where $|n_1,n_2,\ldots..n_k-1>$ are the kets. Obviously a_k decreases n_k to n_k-1 while $a_k^\dagger$ increases n_k to n_k+1 i.e a_k is the annihilation operator and $a_k^\dagger$ is creation operator.

Let's fully write the only non-vanishing matrix elements of a_k and $a_k^\dagger$ in order to define occupation number operator i.e.

$$\begin{aligned}(a_k)_{n_k,n_k+1} &=<\ldots n_l\ldots n_k\ldots|a_k|\ldots n_l'\ldots n_k+1\ldots> \\ &=\sqrt{(n_k+1)}\ldots\delta n_l,n_l' \quad \ldots..(21)\\ \left(a_k^\dagger\right)_{n_k,n_k+1} &=<\ldots n_l\ldots n_k+1\ldots\left|a_k^\dagger\right|\ldots n_l'\ldots n_k\ldots> \\ &=\sqrt{(n_k+1)}\ldots\delta n_l,n_l' \quad \ldots..(22)\end{aligned}$$

Matrix multiplication from right of (21) by (22) yields

$$<\ldots.n_k\ldots|a_k|\ldots n_k+1\ldots><\ldots n_k+1\ldots\left|a_k^\dagger\right|\ldots n_k\ldots>=(n_k+1)\ldots\delta_{n_l,n_l'}\ldots$$

$$<\ldots n_k\ldots\left|a_ka_k^\dagger\right|\ldots n_k\ldots>=(n_k+1)\ldots\delta_{n_l,n_i'}\ldots \quad \ldots..(23)$$

Similarly, multiplication from left gives,

$$\begin{aligned}&<\ldots n_k+1\ldots\left|a_k^\dagger a_k\right|\ldots n_k+1\ldots.>=(n_k+1)\ldots\delta_{n_in_l'}\ldots\\ &<\ldots n_k\ldots\left|a_k^\dagger a_k\right|\ldots n_k\ldots>=(n_k)\ldots\delta_{n_i}n_i'\ldots \quad \ldots..(24)\end{aligned}$$

The difference between (23) and (24) gives

$$\left[a_k,a_k^\dagger\right]=a_ka_k^\dagger-a_k^\dagger a_k=I.$$

In agreement with (7).

Equation (24) indicates that the operator $N_k=a_k^\dagger a_k$ when operating on $|\ldots n_l\ldots n_k>$ yields $n_k|\ldots n_l\ldots n_k>$ i.e.it tells us the number of particles in *k*th state of the field. Therefore $N_k=a_k^\dagger a_k$ is called the occupation number operator for the *k*th state. The total number

$N_k = \sum_k N_k$ operating on

$$|n_1, n_2 \ldots n_k >$$

Yields

$$\sum n_k \, |n_1, n_2 \ldots n_k >$$

the total number of particles being $n_k = \sum_k n_k$. Thus, the Eigen-values of operator *N* is *n*. Thus, we may say that the three operators $a_k^\dagger$, a_k and *N* are quantum mechanical analogs of three Gods, *Brahma* → $creator\ (a^\dagger)$, *Shiva* → $Destroyer\ (a)$ and Vishnu → preserver *N* of Hindu mythology.

After obtaining a representation in which all N_k^s are diagonal, the Hamiltonian *H* can be expressed in terms of a_k by substituting equation (5) into expression for Hamiltonian in equation (2) i.e.

$$H = \int \left(-\frac{\hbar^2}{2m} \nabla\psi^\dagger \cdot \nabla\psi + V\psi^\dagger\psi \right) d^3r \qquad \ldots\ldots (25)$$

We get,

$$H = \sum_{k,l} a_k^\dagger a_l \int \left(-\frac{\hbar^2}{2m} \nabla u_k^* \cdot \nabla u_l + V u_k^* u_l \right) d^3r \qquad \ldots\ldots (26)$$

applying a partial integration to $\int \nabla u_k^* \cdot \nabla u_l \, d^3r$ we obtain $-\int u_k^* \nabla^2 u_l \, d^3r$, the surface term vanishing as usual. Therefore

$$\begin{aligned} H &= \sum_{k,l} a_k^\dagger a_l \int u_k^* \left| -\frac{\hbar^2}{2m} \nabla^2 + V \right| u_l d^3r \\ &= \sum_{k,l} a_k^\dagger a_l E_l \delta_{kl} = \sum_k a_k^\dagger a_k E_k = \sum_k N_k E_k \qquad \ldots\ldots (27) \end{aligned}$$

Here, we've made the assumption that u_k are eigen function of $\left[-\frac{\hbar^2}{2m} \nabla^2 + V \right]$ with eigen values E_k. As *H* is diagonal in *N*-representation, the wave-function $\psi(\ldots n_k \ldots)$ has the eigen value for $\sum_k n_k E_k$ for *H*.

Since it is the product of an operator time its Hermitian adjoint, the eigenvalue of the operator $N_k = a_k^\dagger a_k$ can never be negative. In fact, for an arbitrary non-zero state ψ by which

$< \psi|\psi >$ is greater than zero, we have if we use definition of the scalar product in the Hilbert space.

$$(\psi, N_k\psi) = \left(\psi, a_k^\dagger a_k\psi\right) = (a_k\psi, a_k\psi) = |a_k\psi|^2 \geq 0 \qquad \ldots\ldots(28)$$

When the equality sign is holds in equation (28), it is obvious that the smallest possible eigen value of N_k is zero. Then there must exist a state ψ_0 for which,

$$a_k\psi_0 = 1,\ \psi_0^\dagger\psi_0 = 1$$

i.e. ψ_0 is the lowest normalized state with no particle to be destroyed; hence state ψ_0 is called no-particle or vacuum state.

$$N_k\psi_0 = a_k^\dagger a_k\psi_0 = 0 \text{ for all } k \qquad \ldots..(29)$$

However, all the basis vectors may be constructed by repeated applications of creation operators on $a_k^\dagger$ on $\psi_0 = | >$.

In this way, $$a_k^\dagger\psi_0 = a_k^\dagger|0> = |1> = \psi(1) \qquad \ldots..(30)$$

is a one particle state $[N_k|1>= 1|1>]$

$a_k^\dagger\, a_l^\dagger\psi_0 = |2> = \psi(2)$ is a two-particle state $[N_k|2>= 2|2>]$. Therefore, the Eigen-values of N_k are 0,1,2,3….

8.7 OCCUPATION NUMBER REPRESENTATION

There exists a formalism, called" second quantization" or the occupation-number representation, that is much more convenient. In this formalism the essential information of many-body states is incorporated in a very succinct way. This essential information consists of (i) the occupation number for each single-particle state (for fermions these numbers can only be 0 or 1), and (ii) the
symmetry/anti-symmetry of the state under particle exchange. Note that the wave-function formalism discussed earlier is often referred to as "first quantization" when it is compared and contrasted with the "second quantization" formalism.

An approach to deal with systems of many particles is provided by the *second quantization*. In this method, the Eigen-states are represented by the number of particles rather than the coordinates.

In other words, in this new approach the occupation numbers n_k's of the states play the role of independent variables. Because of this, the new formalism is known as *occupation number representation*. We shall now discuss the cases of Bose-Einstein and Fermi-Dirac statistics.

Second quantization corresponding to Bosons or Bose-Einstein case- The treatment given in above section 4.6 is applicable to *bosons.* Since in Bose- Einstein statistics each operator n_k may possess 0,1,2,3,4….. Eigen-values without any restriction.

Second quantization corresponding to Fermions or Fermi-Dirac case- Consider an assembly of particles that obey Fermi-Dirac statistics. In *Fermi-Dirac statistics*, a restriction is imposed by Pauli-exclusion principle that eigen-values of each operator are constrained to 0 or 1 and the function is antisymmetric. This restriction demands replacing the commutator bracket $[A, B] = AB - BA$ by anti-commutator bracket $[A, B]_+ = AB + BA$

Then the anticommutation relation for $\psi's$ are,

$$\left.\begin{aligned}[\psi(\mathbf{r}), \psi(\mathbf{r}')]_+ &= \left[\psi^\dagger(\mathbf{r}), \psi^\dagger(\mathbf{r}')\right]_+ = 0 \\ \left[\psi(\mathbf{r}), \psi^\dagger(\mathbf{r}')\right]_+ &= \left[\psi(\mathbf{r}), \psi^\dagger(\mathbf{r}') + \psi^\dagger(\mathbf{r}')\psi(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}')\right]\end{aligned}\right\} \quad \ldots\ldots(31)$$

It is evident from equations (5) and (7) that

$$\left.\begin{aligned}[a_k, a_l]_+ &= \left[a_k^\dagger, a_l^\dagger\right]_+ = 0 \\ \left[a_k, a_l^\dagger\right]_+ &= a_k a_l^\dagger + a_l^\dagger a_k = \delta_{k,l}\end{aligned}\right\} \quad \ldots\ldots(32)$$

We define $N_k = {a_k}^\dagger a_k$ as previously and interpret N_k as the number operator. Each N_k commutes with the all others so that they can be diagonalized at the same time. Evaluating the square of the number operator to find the eigen-values of N_k.

$$N_k^2 = a_k^\dagger a_k a_k^\dagger a_k = a_k^\dagger \left(1 - a_k^\dagger a_k\right) a_k = a_k^\dagger a_k = N_k \qquad \ldots\ldots(33)$$

$[since\ {a_k}^\dagger {a_k}^\dagger = a_k a_k = 0\ from\ equation\ (32)]$

As ${N_k}^2 = N_k$; the possible occupation numbers for states can only acceptably be 0 or 1 in agreement with Pauli exclusion principle. A further requirement of the commutation relations (32) is that no state can have occupation number greater than 1 since the application of two creation operators $({a_k}^\dagger {a_k}^\dagger = 0)$ for the same *k* for the same *k* on any state vector, makes it

vanish. The eigenvalues of $N = \sum_k N_k$ are positive integers or zero, as before. The total number of particles and energy eigenvalues are $\sum n_k$, E_k.

Let ψ_0 be the state for which,

$$N_k\psi_0 = 0;\ then\ a_k{}^\dagger\psi_0 = \psi(1)$$

$$N_k\ \psi(1) = N_k(a_k{}^\dagger\psi_0) = a_k{}^\dagger a_k a_k{}^\dagger\psi_0 = (1 - a_k a_k{}^\dagger)a_k{}^\dagger\psi_k{}^\dagger\psi_0 = a_k{}^\dagger\psi_0$$

i.e., there is just one particle in the state $\psi(1) = a_k{}^\dagger\psi_0$.

Similarly, it is observed,

$$N_k\ a_k\ \psi(1) = a_k{}^\dagger a_k a_k\psi(1) = 0$$

i.e., there are no particles in the state $a_k\psi(1) = \psi(0)$. Thus

$a_k\psi(1) = \psi_0$ and $a_k\psi_0 = 0$ for all *k*

In conclusion, we may say that by approaching the field as a mechanical system with an infinite number of degrees of freedom, we are able to develop a theory of the field by an analogy with classical mechanics of a particle. The field is described by field function that has an infinite number of degrees of freedom. A variational principle of stationary action can be used to find the equations for the system's *field function*. The appropriate differential equation, such as the Schrodinger equation for real scalar field, can then be obtained by substituting a suitable Lagrangian function into Euler's equation. Variational equations take on the form that is similar to classical mechanics equations. This gives us a strong tool for using a broad approach similar to classical mechanics to solve a variety of problems.

8.8 SUMMARY

In this unit, you have studied about *quantization of fields* or *second quantization*. To present the clear understanding of *second quantization*, some basic concepts have been discussed. You have studied about the *number operator*, *creation and annihilation operators*. In the unit, you have seen that occupation number system is a representation of second quantization or quantization of fields.

8.9 GLOSSARY

Operators – an operator is a function over a space of physical states onto another space of physical states

Relativistic - characterized by relativity

Creation operator - increases the number of particles in a given state by one

Annihilation operator - decreases the number of particles in a given state by one

Occupation number - The numerical extent to which a quantum state is filled (in a system of many, identical quantum particles)

Quantization - The concept that a physical quantity can have only certain discrete values

Simultaneously - happening or being done at exactly the same time

8.10 REFERENCES

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2. Advanced Quantum Mechanics, Satya Prakash, Kedar Nath Ram Nath, Meerut

3. Advanced Quantum Mechanics, J.J.Sakurai, Pearson

4. B.K. Agarwal, Quantum Mechanics and Field Theory, Lokbharti Publications, India

8.11 SUGGESTED READINGS

1. Advanced Quantum Mechanics, Franz Schwabl, Springer

2. Introduction to Quantum Mechanics, David J. Griffiths, Cambridge University Press

8.12 TERMINAL QUESTIONS

1. What do you mean by creation, annihilation and number operator? Hence describe occupation number representation in the case of Bose- Einstein and Fermi-Dirac statistics.

2. Explain the term second quantization. State the criterion for selection between commutators and anti-commutators when quantizing the given field.

3. What do you understand by creation and annihilation operators? If $a^\dagger$ and a are respectively the creation and annihilation operators and $|0>$ is the normalized particle state, evaluate the following

$$aa^\dagger|0>,\ a^{\dagger 4}a^4|0>,\ a^4a^{\dagger 4}|0>,\ (a^\dagger a)^4|0>,\ (aa^\dagger)^4|0>$$

4.Write short notes on:

(i) Second quantization

(ii) Creation, annihilation and number operators

(iii) Second quantization applied to bosons and fermions

(iv) Occupation number representation

5. Quantize the non-relativistic Schrodinger equation for bosons of mass (m) moving in a potential field.