Manonmaniam Sundaranar University,

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Tirunelveli - 627 012 Tamilnadu, India

OPEN AND DISTANCE LEARNING (ODL) PROGRAMMES

(FOR THOSE WHO JOINED THE PROGRAMMES FROM THE ACADEMIC YEAR 2023–2024)

II YEAR

M.Sc. Physics

Course Material

Quantum Mechanics - II

Prepared

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Tirunelveli - 12

Quantum Mechanics-II

Unit – I

SCATTERING THEORY

Scattering amplitude – Cross sections – Born approximation and its validity – Scattering by a screened coulomb potential – Yukawa potential – Partial wave analysis – Scattering length and Effective range theory for S wave – Optical theorem – Transformation from centre of mass to laboratory frame

Unit – II

PERTURBATION THEORY

Time dependent perturbation theory – Constant and harmonic perturbations – Fermi Golden rule – Transition probability - Einstein‘s A and B Coefficients – Adiabatic approximation – Sudden approximation – Semi – classical treatment of an atom with electromagnetic radiation – Selection rules for dipole radiation .

Unit – III

RELATIVISTIC QUANTUM MECHANICS

Klein – Gordon Equation – Charge and Current Densities – Dirac Matrices – Dirac Equation – Plane Wave Solutions – Interpretation of Negative Energy States – Antiparticles – Spin of Electron - Magnetic Moment of an Electron Due to Spin.

Unit – IV

DIRAC EQUATION

Covariant form of Dirac Equation – Properties of the gamma matrices – Traces – Relativistic invariance of Dirac equation – Probability Density – Current four vector – Bilinear covariant – Feynman ‘s theory of positron (Elementary ideas only without propagation formalism)

Unit – V

CLASSICAL FIELDS AND SECOND QUANTIZATION

Classical fields – Euler Lagrange equation – Hamiltonian formulation – Noether‘s theorem – Quantization of real and complex scalar fields – Creation, Annihilation and Number operators – Fock states – Second Quantization of K-G field.

TEXT BOOKS

1. P. M. Mathews and K. Venkatesan, A Text book of Quantum Mechanics,2nd Edition, Tata McGraw-Hill, New Delhi, 2010.
2. G. Aruldhas, Quantum Mechanics, 2nd Edition, Prentice-Hall of India, NewDelhi,2009
3. A L. I. Schiff, Quantum Mechanics, 3rd Edition, International Student Edition, McGraw-Hill Kogakusha, Tokyo, 1968
4. V. Devanathan, Quantum Mechanics, 1st Edition, Narosa Publishing House, New Delhi, 2005.
5. Nouredine Zettili, Quantum mechanics concepts and applications, 2nd Edition, Wiley, 2017

Unit – I

SCATTERING THEORY

Scattering amplitude – Cross sections – Born approximation and its validity – Scattering by a screened coulomb potential – Yukawa potential – Partial wave analysis – Scattering length and Effective range theory for S wave – Optical theorem – Transformation from centre of mass to laboratory frame

Scattering for particles moving in three spatial dimensions, with Hamiltonian

$$H = p^2 / 2m + V(r)$$

There are two distinct interpretations for such a Hamiltonian

We could think of this as the motion of a single particle, moving in a fixed background potential V (r). This would be appropriate, for example, in Rutherford's famous experiment where we fire an alpha particle at a gold nucleus.

Alternatively, we could think of this as the relative motion of two particles, separated by distance r, interacting through the force $F = -\nabla V(r)$. We could take V (r) to be the Coulomb force, to describe the scattering of electrons, or the Yukawa force to describe the scattering of neutrons.

1.1 Cross sections:

The simple reflection and transmission coefficients of the one-dimensional problem are no longer appropriate. We need to replace them by something a little more complicated.

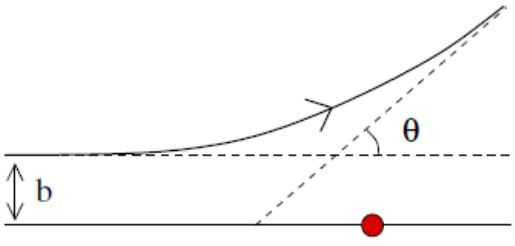


Figure 1.1 Initial trajectory is characterized by the impact parameter b

We throw a single particle with kinetic energy E. Its initial trajectory is characterized by the impact parameter b, defined as the closest the particle would get to the scattering centre at r = 0 if there were no potential.

The particle emerges with scattering angleθ, which is the angle between the asymptotic incoming and outgoing trajectories, as shown in the Fig. 1.2. By solving the classical equations of motion, we can compute θ (b; E) or, equivalently, b (θ;E).

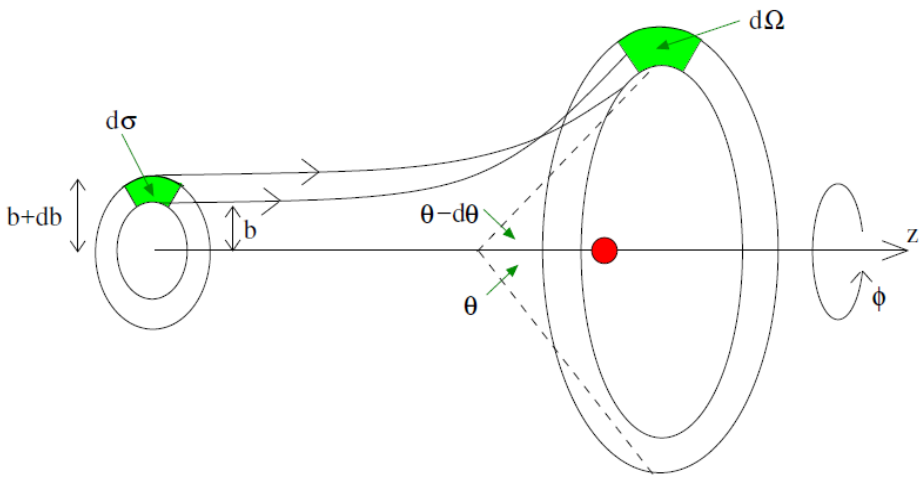


Figure 1.2 Scattering cross section

Now consider a uniform beam of particles, each with kinetic energy E. Consider the cross-sectional area, denoted dσ in Fig.1.2. We write this as

$$d\sigma = b\, d\varphi\ \ db$$

The particles within dσ will evolve to lie in a cone of solid angle dΩ, given by

$$d\Omega = \sin\theta\, d\varphi\ \ d\theta$$

where, for central potentials, the infinitesimal angles dφ, are the same in both these formulae. The differential cross-section is defined to be

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right|$$

The left-hand side should be $|\frac{d\sigma}{d\Omega}|$, but we'll usually drop the modulus. The differential cross-section is a function of incoming momentum k, together with the outgoing angle θ.

The differential cross-section can be thought of as

$$\frac{d\sigma}{d\Omega}\ d\Omega = \frac{\text{number of particles scattered into } d\Omega \text{ per unit time}}{\text{Number of incident particles per area } d\sigma \text{ per unit time}}$$

We write this in terms of flux, defined to be the number of particles per unit area per unit time.

$$\frac{d\sigma}{d\Omega} = \frac{\text{Scattered flux}}{\text{Incident flux}}$$

We can also define the total cross-section

$$\sigma_T = \int d\Omega \frac{d\sigma}{d\Omega}$$

Both the differential cross-section and the total cross-section have units of area. The usual unit used in particle physics, nuclear physics and atomic physics is the barn, with 1 barn = 10^{-28} m^2.

The total cross-section is the characterisation of the scattering power of the potential.

1.2 Scattering amplitude:

The language of cross-sections is also very natural when we look at scattering in quantum mechanics. we set up the scattering problem as a solution to the time-independent Schrodinger equation, which is

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \psi(r) = E\, \psi(r)$$

We will send in a plane wave with energy E which we choose to propagate along the z-direction. This is just

$$\psi_{\text{incident}}\,(r) = e^{ikz}$$

Where $E = \hbar^2 k^2 / 2m$. However, after scattering of the potential, the wave doesn't only bounce back in the z direction. Instead, it spreads out spherically, with a phase and amplitude which can vary around the sphere. It's hard to take photographs of quantum wavefunctions, but the water waves shown on the right give a good analogy for what's going on. Asymptotically, as $r \to \infty$, this scattered wave takes the form

$$\psi_{\text{incident}}(r) = f(\theta, \varphi)\frac{e^{ikr}}{r}$$

The 1/r fall-of follows from solving the free Schrodinger equation; However, there is a simple intuition for this behaviour which follows from thinking of $|\psi|^2$ as a probability, spreading over a sphere which grows as r^2 as $r \to \infty$. The 1/r fall-of ensures that this probability is conserved. Our final equation for the asymptotic wave function is then

$$\psi(r) = \psi_{\text{incident}}(r) + \psi_{\text{scattered}}(r)$$

The function $f(\theta, \varphi)$ is called the scattering amplitude.

For the central potentials considered here it is independent of φ, so $f = f(\theta)$. It is the 3d generalisation of the reflection and transmission coefficients. Our goal is to calculate it.

The scattering amplitude is very closely related to the differential cross-section. To see this, we can look at the probability current density

$$J = -i\frac{\hbar}{2m}(\psi^* \nabla\psi - (\nabla\psi^*)\psi)$$

which obeys $\nabla . J = 0$. For the incident wave, we have

$$J_{\text{incident}} = \frac{\hbar k}{m}\hat{z}$$

This is interpreted as a beam of particles with velocity $v = \frac{\hbar k}{m}$ travelling in the z-direction. Meanwhile, for the scattered wave we use the fact that

$$\nabla\psi_{\text{scattered}} = \frac{i k f(\theta) e^{ikr}}{r}\hat{r} + \vartheta\left(\frac{1}{r^3}\right)$$

$$J_{\text{scattered}} = \frac{\hbar k}{m} \frac{1}{r^2} |f(\theta)|^2 \hat{r} + \vartheta\left(\frac{1}{r^3}\right)$$

This means that, as $r \to \infty$, the flux of outgoing particles crossing an area dA subtended by the solid angle dΩ

$$J_{\text{scattered}} \hat{r}\, dA = \frac{\hbar k}{m} |f(\theta)|^2 \, d\Omega$$

The differential cross-section is defined to be the ratio of the scattered flux through dΩ, divided by the incident flux. In other words, it is

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

It means that if we can compute the scattering amplitude f (θ), it immediately tells us the differential cross-section. The total cross-section is defined, as before, as

$$\sigma_T = \int d\Omega \, |f(\theta)|^2$$

1.3 Born approximation and its validity

A perturbative solution to the Lippmann-Schwinger equation

$$\psi(k; r) = e^{ik.r} + \int d^3 r' \, G_0^+ (k; r - r') V(r') \psi(k; r') \qquad \text{-----(1)}$$

This solution is known as the Born series.

We write ψ as a series expansion

$$\psi(r) = \sum_{n=0}^{\infty} \varphi_n (r) \qquad \text{-------(2)}$$

where we take the leading term to be the plane wave

$$\varphi_0 (r) = e^{ik.r}$$

This series solves (1) if n obey the recursion relation

$$\varphi_{n+1}(r) = \int d^3\, r'\, G_0^+(k; r - r')V(r')\varphi_n(r')$$

Roughly speaking, things will work nicely if the potential V is small, so each successive term is smaller than those preceding it.

The Born approximation consists of taking just the leading order term, φ_1 in this expansion. (Strictly speaking this is the first Born approximation; the nth Born approximation consists of truncating the series at the nth term.) This

$$\psi(r) = e^{ik.r} - \frac{2m}{\hbar^2}\frac{1}{4\pi}\left[\int d^3\, r'\, e^{iq.r'}V(r')\right]\frac{e^{ikr}}{r} \qquad \text{----(3)}$$

$$q = k - k\,\hat{r}$$

can be thought of as the momentum transferred from the incoming wave to the outgoing wave. i to define the momentum of the outgoing wave to be

$$k' = k\,\hat{r}$$

so that q = k − k'. Comparing the Born approximation (3) to the asymptotic form (1), we see that the scattering amplitude is simply the Fourier transform of the potential,

$$f(\theta, \varphi) \approx f_0(\theta, \varphi)\frac{2m}{\hbar^2}\frac{1}{4\pi}\left[\int d^3\, r'\, e^{iq.r'}V(r')\right]$$

$$= \frac{m}{\hbar^2}\frac{1}{2\pi}\tilde{V}(q)$$

Note that the scattering amplitude is a function of $\theta$and φ , They're in the definition of q, with $k \cdot k' = k^2 \cos\theta$, and the variable , determining the relative orientation as shown in the Fig.1.3

For a central potential V (r) = V (r), the resulting scattering amplitude will be independent of φ.

The scattering amplitude is written as f (k, k') instead of f (θ, φ).

Finally, the cross-section in the Born approximation is

$$\frac{d\sigma}{d\Omega} \approx |f_0| = \left(\frac{m}{\hbar^2}\frac{1}{2\pi}\right)^2 \left|\tilde{V}(q)\right|^2 \qquad \text{------(5)}$$

There's so Suppose that your potential has some short distance structure on scales ~ L.

Then the Fourier transform $\tilde{V}(q)$ is only sensitive to this when the momentum transfer is of order q ~ 1/L. This is a manifestation of the uncertainty principle.

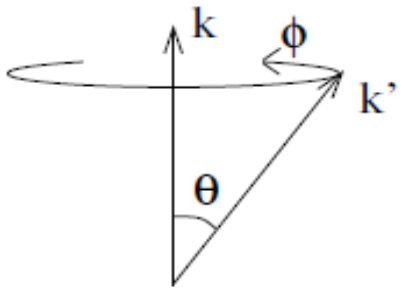


Figure 1.3

1.4 Coulomb potential -Yukawa potential:

At long distances, the strong nuclear force between, say, a proton and a neutron is well modelled by the Yukawa potential

$$V(r) = \frac{A\, e^{-\mu r}}{r}$$

where 1/μ is said to be the range of the force. We can compute the Fourier transform using the same kind of contour methods. We have

$$\tilde{V}(q) = \frac{4\,\pi\, A}{q^2 + \mu^2}$$

Writing this in terms of the scattering angle θ, we recall that q = k – k' with k' = k $\hat{r}$, so that

$$q^2 = 2\,k^2 - 2k\,.\,k'$$

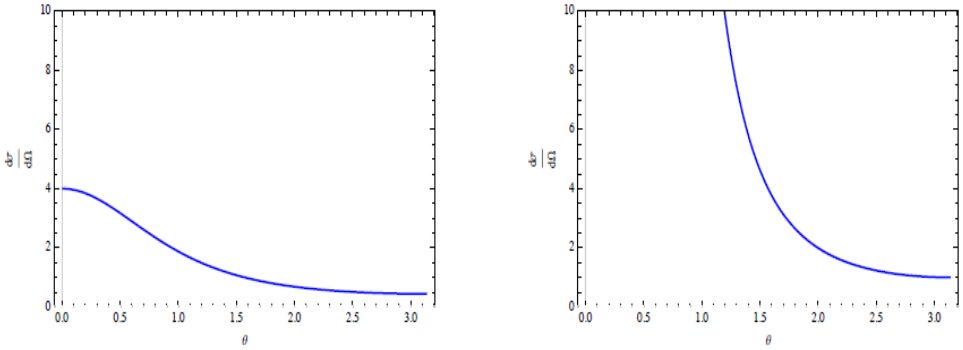
$$= 2\,k^2\,(1 - \cos\theta)$$

$$= 4k^2\,sin^2(\theta/2)$$

If we translate from momentum k to energy E = $\hbar^2k^2/2m$, we have the leading order contribution to the cross-section for the Yukawa potential given by

$$\frac{d\sigma}{d\Omega} = \left(\frac{2\,A\,m}{\hbar^2\,\mu^2 + 8\,m\,E\sin^2\left(\frac{\theta}{2}\right)}\right)^2 \qquad \text{---------(6)}$$

This is shown in the left-hand figure (for values A = m = ~μ = 1 and E = 1/4).



a. cross section for the yukawa potential b. for the coloumb potential

Figure 1.4 Yukawa potential

when $\mu \to 0$, so that the Yukawa force becomes the Coulomb force. For example, for electron-electron or proton-proton scattering, the strength of the Coulomb force is $A = e^2/4\,\pi\,\varepsilon_0$. In this case, the cross-section equation (6) become,

$$\frac{d\sigma}{d\Omega} = \left(\frac{A}{4\,E}\right)^2 \frac{1}{\sin^4\left(\frac{\theta}{2}\right)}$$

This is shown in the right-hand figure (with the same values). Note that there is an enhancement of the cross-section at all scattering angles, but a divergence at forward scattering.

1.5 Scattering length and Effective range theory for S wave:

To compute the amplitude for Rutherford scattering, we don't need any new conceptual ideas. But we do need to invoke some technical results about special functions. This is because the solution to the Schrodinger equation can be written as

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} e^{-\pi\gamma/2}\Gamma(1+i\gamma)\,{}_1F_1\left(-i\gamma;\,1;\,i(kr-\mathbf{k}\cdot\mathbf{r})\right)$$

where ${}_1F_1$ (a; b; w) is the confluent hypergeometric function, defined by the series expansion

$$ {}_1F_1(a;b;w) = 1 + \frac{a}{b}w + \frac{a(a+1)}{b(b+1)}\frac{w^2}{2!} + \frac{a(a+1)(a+2)}{b(b+1)(b+2)}\frac{w^3}{3!} + \dots $$

The only fact we'll need about the hypergeometric function is its expansion for large |w|. For our solution, this is an expansion in 1/(k r −k · r) and so is valid at large distance, but not along the direction of the incident beam k. If we take k = k $\hat{z}$, we have

$$ \psi(\mathbf{r}) \sim e^{ikz+i\gamma\log(k(r-z))} - \frac{\gamma}{k(r-z)}\frac{\Gamma(1+i\gamma)}{\Gamma(1-i\gamma)}e^{ikr-i\gamma\log(k(r-z))} + \dots $$

where the +. . . are corrections to both terms which are suppressed by 1/k(r − z). This is now very similar to our usual asymptotic, but with the corrected phases. The first term describes the ingoing wave, the second term the scattered outgoing wave. We can therefore write

$$ \psi(\mathbf{r}) \sim e^{ikz+i\gamma\log(k(r-z))} + f(\theta)\frac{e^{ikz-i\gamma\log(k(r-z))}}{r} $$

where the scattering amplitude is given by

$$ f(\theta) = -\frac{\gamma}{k}\frac{\Gamma(1+i\gamma)}{\Gamma(1-i\gamma)}\frac{r}{r-z} = -\frac{\gamma}{2k}\frac{\Gamma(1+i\gamma)}{\Gamma(1-i\gamma)}\frac{1}{\sin^2(\theta/2)} $$

the cross-section is

$$ \frac{d\sigma}{d\Omega} = \left(\frac{mA}{2\hbar^2 k^2}\right)^2 \frac{1}{\sin^4\left(\frac{\theta}{2}\right)} $$

This is the same result as using the Born approximation and the same result that we saw from a classical analysis. The Coulomb potential is an exception.

1.6 Optical theorem:

The scattering amplitude in partial waves as

$$f(\theta) = \sum_{l=0}^{\infty} \frac{2l+1}{k} f_l P_l \cos\theta \qquad \text{-------(1)}$$

The differential cross-section is $\frac{d\sigma}{d\Omega} = |f(\theta)|^2$.

Using the partial wave decomposition equation (1) we have

$$\frac{d\sigma}{d\Omega} = \frac{1}{k^2} \sum_{l,l'} (2l+1)(2l'+1)\, f_l\, f_{l'}\, P_l \cos\theta\, P_{l'} \cos\theta$$

The Legendre polynomials have orthogonality property

$$\int_{-1}^{+1} dw\, P_l(w)\, P_{l'}(w) = \frac{2}{2l+1}\, \delta_{lm} \qquad \text{-----(2)}$$

In computing the total cross-section σ_T, we can use the orthogonality of Legendre polynomials (2) to write

$$\sigma_T = 2\pi \int_{-1}^{+1} d(\cos\theta)\, \frac{d\sigma}{d\Omega}$$

$$= \frac{4\pi}{k^2} \sum_{l=0}^{\infty} 2l+1$$

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

We can compare this to our expansion. Using the fact that P (1) = 1, we have

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

The total cross-section is given by

$$\sigma_T = \frac{4\pi}{k}\, \mathrm{Im}\, f(0)$$

This is known as the optical theorem.

The potential causes scattering from the forward direction ($\theta = 0$) to other directions. Because total probability is conserved, clearly the amount of particles going in the forward direction must decrease. However, this decrease in the forward direction must be equal to the total increase in other directions – and this is what the total cross section σ_T measures. Finally, the amount of decrease in forward scattering is due to interference between the incoming wave and outgoing waves, and so is proportional to f (0).

Unit – II

PERTURBATION THEORY

Time dependent perturbation theory – Constant and harmonic perturbations – Fermi Golden rule – Transition probability - Einstein's A and B Coefficients – Adiabatic approximation – Sudden approximation – Semi – classical treatment of an atom with electromagnetic radiation – Selection rules for dipole radiation .

2.1 Time dependent perturbation theory:

In quantum mechanics, perturbation theory is a set of approximation schemes directly related to mathematical perturbation for describing a complicated quantum system in terms of a simpler one.

The basic notion is to use a simple system for which a mathematical solution is known, and then adding an additional 'Perturbing' Hamiltonian representing a weak disturbance to the system. If the disturbance is not too large, then the various physical quantities associated with the perturbed system, for example its energy levels and eigenstates, can be expressed as 'Corrections' to those of the simple system.

These corrections, being small compared to the size of the quantities themselves, can be calculated using approximate methods, such as asymptotic series. The complicated system can consequently be studied based on the simpler one.

Time dependent perturbation theory, developed by Paul Dirac, typically explains the effect of a time dependent perturbation V(t) applied to a time independent Hamiltonian, H_0. Since the perturbed Hamiltonian is time dependent accordingly are its energy levels and eigenstates. Thus, the goals of time dependent perturbation theory are slightly different from time independent perturbation theory.

Following are the two significant quantities of the time dependent perturbation:

1. The time dependent expectation value of some observable *A*, for a given initial state.

2. The time dependent amplitudes of those quantum states that are energy Eigen kets (eigenvectors) in the unperturbed system.

2.2 General Time Dependent Perturbations

Assume that the unperturbed energy eigenvalue problem is exactly of the form

$$H_0\phi_n = E_n\phi_n$$

To this is added a perturbation that depends on time, ν (t). To solve the time dependent problems we use the following time dependent Schrödinger equation.

$$(H_0 + \mathcal{V}(t))\,\psi(t) = i\hbar\frac{\partial\psi(t)}{\partial t}$$

Then we expand ψ in terms of the eigenfunctions as,

$$\psi(t) = \sum_k c_k(t)\phi_k e^{-iE_kt/\hbar} \text{ with } c_k(t)e^{-iE_kt/\hbar} = \langle\phi_k|\psi(t)\rangle$$

The time dependent Schrödinger equations is then given as,

$$\begin{aligned}
\sum_k (H_0 + \mathcal{V}(t))\, c_k(t)e^{-iE_kt/\hbar}\phi_k &= i\hbar\sum_k \frac{\partial c_k(t)e^{-iE_kt/\hbar}}{\partial t}\phi_k \\
\sum_k c_k(t)e^{-iE_kt/\hbar}\,(E_k + \mathcal{V}(t))\,\phi_k &= \sum_k \left(i\hbar\frac{\partial c_k(t)}{\partial t} + E_kc_k(t)\right)e^{-iE_kt/\hbar}\phi_k \\
\sum_k \mathcal{V}(t)c_k(t)e^{-iE_kt/\hbar}\phi_k &= i\hbar\sum_k \frac{\partial c_k(t)}{\partial t}e^{-iE_kt/\hbar}\phi_k
\end{aligned}$$

Now dot $\langle\phi_n|$ into this equation to get the time dependence of one coefficient.

$$\begin{aligned}
\sum_k \mathcal{V}_{nk}(t)c_k(t)e^{-iE_kt/\hbar} &= i\hbar\frac{\partial c_n(t)}{\partial t}e^{-iE_nt/\hbar} \\
\frac{\partial c_n(t)}{\partial t} &= \frac{1}{i\hbar}\sum \mathcal{V}_{nk}(t)c_k(t)e^{i(E_n \quad E_k)t/\hbar}
\end{aligned}$$

Assuming that at t = 0, we are in an initial state $\psi(t=0) = \phi_i$ and hence all the other c_k are equal to zero as $c_k = \delta_{ki}$

$$\frac{\partial c_n(t)}{\partial t} = \frac{1}{i\hbar}\left(\mathcal{V}_{ni}(t)e^{i\omega_{ni}t} + \sum_{k\neq i}\mathcal{V}_{nk}(t)c_k(t)e^{i\omega_{nk}t}\right)$$

Next we calculate the transition rates. Considering that for the first order, all the c_k (t) are small in comparison to c_i (t) = 1 , therefore the sum can be neglected.

$$\frac{\partial c_n^{(1)}(t)}{\partial t} = \frac{1}{i\hbar}\mathcal{V}_{ni}(t)e^{i\omega_{ni}t}$$

$$c_n^{(1)}(t) = \frac{1}{i\hbar}\int_0^t e^{i\omega_{ni}t'}\mathcal{V}_{ni}(t')dt'$$

This equation is used to calculate transition probabilities for a general time dependent perturbation. This can also be used as a basis to calculate the transition rates for the specific problem of harmonic potentials.

Assuming again'*t*' is small enough hence the c_i may not have changed much. Remember that, if there is a large energy difference between the initial and the final states, then a slowly varying perturbation can average to zero.

Subsequently we can find that the perturbation may require frequency components that are compatible with w_{ni} in order to cause transitions.

If the first order term is zero or higher accuracy is required, then the second order term can be calculated. In second order, first a transition is made to an intermediate state $\emptyset_k$ and then a transition to $\emptyset_n$. We simply put the first order into the sum.

$$\frac{\partial c_n(t)}{\partial t} = \frac{1}{i\hbar}\left(\mathcal{V}_{ni}(t)e^{i\omega_{ni}t} + \sum_{k\neq i}\mathcal{V}_{nk}(t)c_k^{(1)}(t)e^{i\omega_{nk}t}\right)$$

$$\frac{\partial c_n(t)}{\partial t} = \frac{1}{i\hbar}\left(\mathcal{V}_{ni}(l)e^{i\omega_{ni}t} + \sum_{k\neq i}\mathcal{V}_{nk}(l)\frac{1}{i\hbar}e^{i\omega_{nk}t}\int_0^t e^{i\omega_{ki}t'}\mathcal{V}_{ki}(l')dl'\right)$$

$$c_n^{(2)}(l) = \frac{-1}{\hbar^2}\sum_{k\neq i}\int_0^t dl''\mathcal{V}_{nk}(l'')e^{i\omega_{nk}t''}\int_0^{t''} dl'e^{i\omega_{ki}t'}\mathcal{V}_{ki}(l')$$

$$c_n^{(2)}(t) = \frac{-1}{\hbar^2}\sum_{k\neq i}\int_0^t dt''\mathcal{V}_{nk}(t'')e^{i\omega_{nk}t''}\int_0^{t''} dt'e^{i\omega_{ki}t'}\mathcal{V}_{ki}(t')$$

2.3 Einstein's A and B Coefficients:

Let us consider $E(v)$ as the energy density at equilibrium, where v is the frequency of photon. If N_1 and N_2 are the number of atoms in the lower energy state (ground state) and higher energy state (excited state) respectively, then we can write,

$$N_1 P_{12} = N_1 B_{12} E(v) \qquad \text{----------(1)}$$

where P_{12} is the probability of absorption proportional to energy density $E(v)$ and B_{12} is the Einstein's coefficient of absorption.

Therefore, we can express the energy state of N_2 as follows:

$$N_2 P_{21} = N_2 [A_{21} + B_{21} E(v)] \qquad \text{---------(2)}$$

Where P_{21} is the probability (stimulated) proportional to energy density $E(v)$ with addition to A_{21}, A_{21} is the Einstein's coefficient of spontaneous and B_{21} is the Einstein's coefficient of stimulated emission.

When thermal equilibrium exists, we can say that the total absorption probability is equal to the total emission probability.

So, from Equations (1) and (2), we have

$$N_1 B_{12} E(v) = N_2 [A_{21} + B_{21} E(v)]$$

$$E(v) = \frac{\frac{A_{21}}{B_{21}}}{\left(\frac{N_1}{N_2}\right)\left(\frac{B_{12}}{B_{21}}\right) - 1} \qquad \text{------(3)}$$

According to Einstein's assumption, coefficient of stimulated absorption and coefficient of stimulated emission are equal, i.e., $B_{12} = B_{21} = B$ (say) and if we consider $A_{21} = A$ (say), then the Equation (3) reduces to,

$$E(v) = \frac{\frac{A}{B}}{\left(\frac{N_1}{N_2}\right) - 1} \qquad \text{---------(4)}$$

A and B in the above equation are called Einstein's 'A' and 'B' coefficients.

According to Planck's radiation law, we know that

$$E(v) = \frac{8\pi h v^3}{c^3 e^{\frac{hv}{KT}} - 1}$$

$$\frac{A}{B} = \frac{8\pi h v^3}{c^3}$$

(Ratio of coefficients of spontaneous and stimulated emission, i.e., ratio of Einstein's 'A' and 'B' Coefficient)

Where h is the Planck's Constant.

K is the Boltzman's Constant.

c is the Velocity of Light.

T is the Temperature in Kelvin.

2.4 Semi – Classical treatment of an atom with electromagnetic radiation:

Semi-classical physics refers to a theory in which one part of a system is described quantum-mechanically whereas the other is treated classically.

For example, external fields will be constant, or when changing will be classically described.

In general, it incorporates a development in powers of Planck's constant, resulting in the classical physics of power 0, and the first nontrivial approximation to the power of (–1).

Thus, there is a clear link between the quantum mechanical system and the associated semi-classical and classical approximations, as it is similar in appearance to the transition from physical optics to geometric optics.

Four examples of a semi-classical approximations include:

WKB approximation: electrons in classical external electromagnetic fields.

Semi-classical gravity: quantum field theory within a classical curved gravitational background (see general relativity).

Quantum chaos: quantization of classical chaotic systems.

Quantum field theory: only Feynman diagrams with at most a single closed loop are considered, which corresponds to the powers of Planck's constant.

The semi-classical radiation theory consists of two elements: the classical Maxwell equations that is satisfied by the electric 'E' and the magnetic 'B' fields, and the ordinary quantum mechanics that is based on the Schrodinger equation of a single charged matter particle interacting with the electromagnetic field.

The single particle Schrodinger quantum mechanics can be modified to take into account spin or be replaced by the nonrelativistic quantum mechanics of many particles.

The distribution of energy in the spectrum of radiations of a hot body cannot be explained by applying the classical concepts of physics. Max Planck gave an explanation to this observation by his '**Quantum Theory of Radiation**'. His theory states that,

1. The 'Radiant Energy' is always in the form of tiny bundles of light called 'quanta', i.e., the energy is absorbed or emitted discontinuously.

2. Each quantum has some definite energy 'E', which depends upon the frequency of the radiations as,

$$E = h\gamma$$

Here, *E* is the energy of each quantum in Joules,

γ is the frequency of the radiations in s^{-1},

h is known as Planck's constant (a fundamental constant), whose value is,

$h = 6.626 \times 10^{-34}$ J-s.

Also, $E = hc\omega$

where w is known as wave number.

$$\omega = (1/\lambda) \quad m^{-1}.$$

From these equations, it is evident that

$$\gamma = c/\lambda$$
$$= c.\ \omega$$

The energy emitted or absorbed by a body is a multiple of a quantum, i.e., a body cannot absorb or emit energy in fractions of quantum. This concept is known as quantization of energy.

Unit – III

RELATIVISTIC QUANTUM MECHANICS

Klein – Gordon Equation – Charge and Current Densities – Dirac Matrices – Dirac Equation – Plane Wave Solutions – Interpretation of Negative Energy States – Antiparticles – Spin of Electron - Magnetic Moment of an Electron Due to Spin.

3.1 Klein – Gordon Equation:

Schrodinger proposed a relativistic form of his non-relativistic equation (at the same time when he developed his non-relativistic (NR) equation). Klein and Gordon developed this equation at a later time and is known as Klein-Gordon (KG) equation. Schrodinger used the NR energy momentum dispersion relation

$$E = p^2 / 2m .$$

Using the correspondence principle

$$E \rightarrow \hat{E} = i\hbar \frac{\partial}{\partial t}$$

$$\vec{p} = \hat{\vec{p}} = -i \vec{\nabla} \hbar \qquad \text{------(1)}$$

In $$E \varphi(\vec{r}, t) = \frac{p^2}{2m} \varphi(\vec{r}, t)$$

we arrive at the Schrodinger equation for free particle. Now extend the same algorithm for relativistic particle with energy-momentum relation

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

So we get the relativistic wave equation

$$E^2 \varphi(x) = (p^2c^2 + m^2c^4)\varphi(x) \qquad \text{-------(2)}$$

$$-\hbar^2 \frac{\partial^2}{\partial t^2} \varphi(x) = \left(-\hbar^2 c^2 \overrightarrow{\nabla^2} + m^2c^4\right) \varphi(x) \qquad \text{------(3)}$$

$$\left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \overrightarrow{\nabla^2}\right) \varphi(x) = -\frac{m^2c^2}{\hbar^2} \varphi(x) \qquad \text{-------(4)}$$

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \overrightarrow{\nabla^2}\right) + \frac{m^2c^2}{\hbar^2}\ )\ \varphi(x) = 0 \qquad \text{------(5)}$$

This equation is known as Klein-Gordon equation.

The Klein-Gordon equation describes the relativistic dynamics of a scalar particle.

The plane wave solution of the KG equation is

$$\varphi(x) = N\, e^{-i(Et - \vec{p}.\vec{x})} \qquad \text{-----(6)}$$

where N is the normalization constant and energy

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

i.e., energy can be both positive and negative.

Pre-multiply Eq. (4) by $\varphi*(x)$ to get

$$\varphi*(x)\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \overrightarrow{\nabla^2}\right)\varphi(x) = -\frac{m^2c^2}{\hbar^2}\varphi(x) \qquad \text{-----(7)}$$

Now take the complex conjugate of Eq.(4) and post-multiply with φ(x), which gives

$$\left(\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\varphi*\right)\varphi - \left(\overrightarrow{\nabla^2}\varphi*\right)\varphi\right) = -\frac{m^2c^2}{\hbar^2}\varphi*(x)\ \varphi(x) \qquad \text{------(8)}$$

Eq (7) - Eq (8) gives:

$$\varphi*\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\varphi - \frac{1}{c^2}\frac{\partial^2\varphi*}{\partial t^2}\varphi - (\varphi*\nabla^2\varphi - \varphi\nabla^2\varphi*) = 0 \qquad \text{-----(9)}$$

$$\frac{1}{c}\frac{\partial}{\partial t}\left[\frac{i\hbar}{2mc}\left(\varphi*\frac{\partial\varphi}{\partial t} - \frac{\partial\varphi*}{\partial t}\varphi\right)\right] + \vec{\nabla}\left[\frac{\hbar}{2mi}\left(\varphi*\overrightarrow{\nabla}\varphi - (\vec{\nabla}\varphi*)\varphi\right)\frac{\hbar}{2mi}\right.$$

$$\left.\varphi*\overrightarrow{\nabla}\varphi - (\vec{\nabla}\varphi*)\varphi\right)\Big] \qquad \text{----(10)}$$

$$\frac{1}{c}\frac{\partial}{\partial t}\rho + \overrightarrow{\nabla}\vec{j} = 0 \qquad \text{------(11)}$$

$$\partial_\mu\,\partial^\mu = 0 \qquad \text{------(12)}$$

This is the continuity equation for the Klein- Gordon equation, where

$$j^0 = \rho = \frac{i\hbar}{2mc}\left(\varphi*\frac{\partial\varphi}{\partial t} - \frac{\partial\varphi*}{\partial t}\varphi\right) \qquad \text{----(13)}$$

$$\vec{J} = \frac{\hbar}{2mi}\left(\varphi * \vec{\nabla}\varphi - (\vec{\nabla}\varphi *)\varphi\right) \qquad \text{----(14)}$$

The continuity equation for Schrodinger equation, ρ is the probability density and $\vec{J}$ is the probability current density. 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 equation also satisfies the same continuity equation, it is natural to interpret ρ as the probability density and $\vec{J}$ as the probability current.

3.2 Dirac Equation:

The probability density in KG equation depends on energy and becomes negative for negative energy. The energy in the expression of ρ appears due to the time derivative in Eq.(12). Dirac realised that this is due to the fact that KG equation involves second order time derivative. Notice that Schrodinger equation involves first order time derivative, and ρ does not involve any time derivative..

So, if we want to write a relativistic wave equation with positive definite probability density, the equation should be first order in time derivative. To be consistent with the Lorentz transformations in special theory of relativity, the wave equation with first order time derivative must also be first order in space derivatives. So, Dirac wrote the Hamiltonian as

$$H = \alpha_1 p_1 c + \alpha_2 p_2 c + \alpha_3 p_3 c + \beta mc^2.$$

Writing the momentum in differential operator form in the position space, we must have the wave equation

$$\begin{aligned} i\hbar\frac{\partial\psi(x)}{\partial t} &= \left(-i\hbar c(\alpha_1\frac{\partial}{\partial x^1} + \alpha_2\frac{\partial}{\partial x^2} + \alpha_3\frac{\partial}{\partial x^3}) + +\beta mc^2\right)\psi(x) \\ &= (-i\hbar c\vec{\alpha}\cdot\vec{\nabla} + \beta mc^2)\psi(x) \end{aligned}$$

------(15)

Since the above Hamiltonian has to describe a free particle, α_i and β cannot depend on space and time, since such terms would have the properties of space-time dependent energies and give rise to forces.

Also α_i and β cannot have space or time derivatives, the derivatives should appear only in p_i and E , since the equation is to be linear in all these derivatives. Thus α_i , β are some constants. For relativistic particle, it must satisfy the relativistic energy momentum relation

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

i.e., it must satisfy the Klein-Gordon equation.

Squaring both sides of Eq. (15), we get

$$\begin{aligned}(i\hbar\frac{\partial}{\partial t})^2\psi &= \left(-i\hbar c(\alpha_1\frac{\partial}{\partial x^1}+\alpha_2\frac{\partial}{\partial x^2}+\alpha_3\frac{\partial}{\partial x^3})++\beta mc^2\right)\\ &\quad\left(-i\hbar c(\alpha_1\frac{\partial}{\partial x^1}+\alpha_2\frac{\partial}{\partial x^2}+\alpha_3\frac{\partial}{\partial x^3})++\beta mc^2\right)\psi\\ &= \Big[-\hbar^2c^2\left(\alpha_1^2\frac{\partial^2}{\partial x^{1^2}}+\alpha_2^2\frac{\partial^2}{\partial x^{2^2}}+\alpha_3^2\frac{\partial^2}{\partial x^{3^2}}\right)+\beta^2m^2c^4\\ &\quad-\hbar^2c^2\left((\alpha_1\alpha_2+\alpha_2\alpha_1)\frac{\partial}{\partial x^1}\frac{\partial}{\partial x^2}+(\alpha_1\alpha_3+\alpha_3\alpha_1)\frac{\partial}{\partial x^1}\frac{\partial}{\partial x^3}+(\alpha_2\alpha_3+\alpha_3\alpha_2)\frac{\partial}{\partial x^2}\frac{\partial}{\partial x^3}\right)\\ &\quad-imc^3\hbar\left((\alpha_1\beta+\beta\alpha_1)\frac{\partial}{\partial x^1}+(\alpha_2\beta+\beta\alpha_2)\frac{\partial}{\partial x^2}+(\alpha_3\beta+\beta\alpha_3)\frac{\partial}{\partial x^3}\right]\psi \qquad (36)\end{aligned}$$

---(16)

To satisfy

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

the above equation must satisfy

$$-\hbar^2(\frac{\partial}{\partial t})^2\psi = -\hbar^2c^2\left(\frac{\partial^2}{\partial x^{1^2}}+\frac{\partial^2}{\partial x^{2^2}}+\frac{\partial^2}{\partial x^{3^2}}\right)\psi + m^2c^4\psi$$

-----(17)

Now if Eq.(16) has to satisfy Eq.(17), then α_i (i = 1, 2, 3) and β must satisfy

$$\alpha_i\alpha_j + \alpha_j\alpha_i = 0, \quad (i \neq j)$$
$$\alpha_i\beta + \beta\alpha_i = 0$$
$$\alpha_i^2 = 1, \quad \beta^2 = 1$$

-----(18)

Clearly, α_i and β cannot be ordinary classical numbers, rather they anti commute with each other. So, Dirac proposed that they are matrices. The above anticommutation relations can be written in the short forms as

$$\{ \alpha_i , \alpha_j \} = 0$$
$$\{ \alpha_i , \beta \} = 0$$

(The notation { , } is called the anticommutator.) Combining with the fact that $\alpha_i^2 = 1$ we can write

$$\{ \alpha_i , \alpha_j \} = 2\,\delta_{ij}\, I$$

If αi and β are matrices, ψ cannot be a single component wave function, it must have more than one components that can be written as a vector on which the matrices should operate.

For Dirac equation, we need four linearly independent matrices satisfying the anticommutation relations.

Since the Hamiltonian is Hermitian, each of the four matrices α_i , β must be Hermitian and hence they are square matrices (n × n). Since squares of all four matrices are unity, their eigenvalues are +1 and −1.

If we choose β to be diagonal, then αi cannot be diagonal as they anti commute with β. In two dimensions, we have three Pauli matrices which anti commute with each other but the fourth linearly independent matrix that we can have in 2D is the identity matrix which commutes with all other matrices.

So, we cannot find a linearly independent fourth matrix to anti commute with the Pauli matrices. Similarly, we fail to find four 3 × 3 matrices to satisfy all the above conditions. The smallest possible dimension to have four such matrices is 4 × 4. One such set of matrices are:

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$$

where σ_i are the Pauli matrices and I is 2 × 2 identity matrix.

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix};$$

α_i and β are not unique. All matrices related to these matrices by any unitary 4 × 4 matrix are equally valid i.e.,

$$\alpha_i' = U\alpha_i U^{-1}, \quad \beta' = U\beta U^{-1}$$

3.3 Plane Wave Solutions:

The space-time behaviour is of plane wave form:

$$\psi(x) = \omega\, e^{-i\frac{p.x}{\hbar}} = \omega\, e^{-i\frac{p.x}{\hbar}+i\frac{\vec{p}.\vec{x}}{\hbar}} \qquad \text{-----(1)}$$

where ω is a 4-component vector, independent of x and is called the Dirac spinor. Let us write ω in 2-component notation

$$\omega = \begin{pmatrix} \phi \\ \chi \end{pmatrix} \qquad \text{----(2)}$$

Where φ and χ are 2 - component spinors. Putting the solution in the Dirac equation we get

$$\begin{aligned} E\begin{pmatrix} \phi \\ \chi \end{pmatrix} &= c\vec{\alpha}\cdot\vec{p}\begin{pmatrix} \phi \\ \chi \end{pmatrix} + \beta mc^2\begin{pmatrix} \phi \\ \chi \end{pmatrix} \\ &= \begin{pmatrix} 0 & c\vec{\sigma}\cdot\vec{p} \\ c\vec{\sigma}\cdot\vec{p} & 0 \end{pmatrix}\begin{pmatrix} \phi \\ \chi \end{pmatrix} + mc^2\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\begin{pmatrix} \phi \\ \chi \end{pmatrix} \\ &= \begin{pmatrix} mc^2 I & c\vec{\sigma}\cdot\vec{p} \\ c\vec{\sigma}\cdot\vec{p} & -mc^2 I \end{pmatrix}\begin{pmatrix} \phi \\ \chi \end{pmatrix}. \end{aligned} \qquad \text{-----(3)}$$

The matrix equation can be written as two coupled equations:

$$E\phi = mc^2\phi + c\vec{\sigma}\cdot\vec{p}\chi \quad \Rightarrow (E - mc^2)\phi = c\vec{\sigma}\cdot\vec{p}\chi \qquad \textbf{----(4)}$$

$$E\chi = -mc^2\chi + c\vec{\sigma}\cdot\vec{p}\phi \Rightarrow (E+mc^2)\chi = c\vec{\sigma}\cdot\vec{p}\phi$$
$$\Rightarrow \chi = \frac{c\vec{\sigma}\cdot\vec{p}}{E+mc^2}\phi. \qquad \text{-----(5)}$$

Putting Eq.(5) in Eq.(4) we have

$$(E-mc^2)\phi = c\vec{\sigma}\cdot\vec{p}\frac{c\vec{\sigma}\cdot\vec{p}}{E+mc^2}\phi$$
$$= \frac{c^2(\vec{\sigma}\cdot\vec{p})^2}{E+mc^2}\phi = \frac{\vec{p}^2c^2}{E+mc^2}\phi$$

where we have used

$$(\vec{\sigma}.\vec{A})(\vec{\sigma}.\vec{B}) = \vec{A}.\vec{B}\,I + I\,\vec{\sigma}.(\vec{A}\times\vec{B})$$

$$(\vec{\sigma}.\vec{p})\text{^}2 = (\vec{p})^2.$$

So finally we get,

$$(E - mc^2)(E + mc^2)\varphi = p^2c^2\,\varphi = E^2 = p^2c^2 + m^2c^4$$

i.e., $E = \pm\sqrt{p^2c^2 + m^2c^4}$ which means negative energy solutions are still admitted. Dirac's prescription cannot get rid of the negative energy solutions.

3.4 Interpretation of Negative Energy States:

The physical interpretation of positive energy solutions is straight forward. They describe spin- 1 / 2 particles with 4-momentum.

The probability density ρ and the probability current $\vec{j}$ both are positive definite. But since the negative energy solutions are also allowed, like KG equation, a particle with +ve energy can cascade down through the -ve energy levels without limit.

Hence +ve energy states cannot be stable! To make any sense of Dirac equation, one then needs to make the +ve energy states stable, preventing them to make transition to -ve energy states. Here comes the masterclass of Dirac.

Dirac postulated that the normal empty or vacuum state corresponds to the state with no positive energy particle and all the negative energy states are completely filled up.

The state with completely filled up negative energy levels is called the Dirac sea. Since Dirac equation describes fermions, according to Pauli exclusion principle only two electrons(one spin up and one spin down) can occupy an energy level and once they are occupied any +ve energy particle is forbidden to fall in the -ve energy levels.

Let us assume that the spin 1/2 particle we are talking about is an electron. So, the vacuum is the state where all negative energy levels are filled up by electrons i.e., has infinite negative charge and energy.

But since all observations represent finite fluctuations of charge and energy with respect to the vacuum, it leads to an acceptable theory and we rescale the vacuum to be without any charge and energy (charge of the vacuum=0, energy of the vacuum=0, spin of the vacuum=0). Assume an electron with energy −E and spin up is removed from the Dirac sea.

It will create a "hole" relative to the normal vacuum:

energy of the "hole" = −(−E) = +E → positive

charge of the "hole" = −(−e) = e → positive charge.

spin of the "hole"=-(up)= down

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.

3.5 Antiparticles:

Antiparticle, subatomic particle having the same mass as one of the particles of ordinary matter but opposite electric charge and magnetic moment.

Thus, the positron (positively charged electron) is the antiparticle of the negatively charged electron. The spinning antineutron, like the ordinary neutron, has a net electric charge of zero, but its magnetic polarity is opposite to that of a similarly spinning neutron. Neutrino, an

uncharged particle that travels very close to the speed of light, spins counterclockwise as viewed from behind, whereas the antineutrino spins clockwise as viewed from behind. A particle and its antiparticle mutually react to produce energy by annihilation.

3.6 Spin of Electron:

The electron spin is one of the three inherent properties of the electrons; the others are the mass and charge of the electron. The electron spin is described as the electron spinning around its axis.

It is articulated as:

$$\|S\|=s(s+1)h$$

Where,

- **s** is equivalent to a quantized spin vector.
- The spin vector is articulated as **||s||.**
- The spin quantum number **(s)** is associated with the spin angular momentum and h is Planck's constant.

A total of four quantum numbers were developed to better understand the movement and pathway of electrons in its designated orbital within an atom.

1. Principal quantum number (*n*): energy level *n* = 1, 2, 3, 4, ...
2. Orbital Angular Momentum Quantum Number (*L*): shape (of orbital) *L* = 0, 1, 2, 3, ...*n*-1
3. Magnetic Quantum Number (m_L): orientation m_L = interval of (-*L*, +*L*)
4. Electron Spin Quantum Number (m_s): independent of other three quantum numbers because m_s *is always* = –½ *or* +½

3.7 Magnetic Moment of an Electron Due to Spin:

We consider the magnetic moment that arises from the spin of the electron. By analogy with the orbital magnetic moment, we might expect the spin magnetic moment to be related to the spin angular momentum by $\mu_s = \gamma S$, but this turns out not to be the case. T

his should not be too surprising however, because spin has no classical analogue, yet here we are trying to argue by analogy with orbital angular momentum, which does have a classical analogue.

The relation between the spin and its magnetic moment can be derived from the relativistic Dirac equation, which gives $\mu_s = 2\,\gamma S$: the magnetic moment due to spin is twice the value expected on the basis of a classical analogy.

The experimental value of the magnetic moment can be determined by observing the effect of a magnetic field on the motion of an electron beam, and it is found that

$$\mu_s = g\,\gamma\,S$$

where g = 2.002319

The factor g is called the g-factor of the electron. The small discrepancy between the experimental value and the Dirac value of exactly 2 is accounted for by the more sophisticated theory of quantum electrodynamics, in which charged particles are allowed to interact with the quantized electromagnetic field. Thus, the magnetic moment due to electron spin can be written as

$$\mu_s = -g\,\frac{e}{2\,m}\,S$$

The magnitude of S is equal to $\sqrt{S(S+1)}\,\hbar$. here s is called spin quantum number. Therefore, the absolute value the spin magnetic moment is

$$\mu_s = g\,\mu_B\,\sqrt{S(S+1)} = \sqrt{3}\,\mu_B$$

Thus, the spin magnetic moment of electron is nearly equal to $\sqrt{3}$ times the Bohr magneton. As for the orbital magnetic moment, the spin magnetic moment has quantized components on the z axis, and we write

$$\mu_s = -g\,\frac{e}{2\,m}\,S = -g\,\mu_B\,m_s$$

Where $m_s = \pm\,\frac{1}{2}$

Unit – IV

DIRAC EQUATION

Covariant form of Dirac Equation – Properties of the gamma matrices – Traces – Relativistic invariance of Dirac equation – Probability Density – Current four vector – Bilinear covariant – Feynman 's theory of positron (Elementary ideas only without propagation formalism)

4.1 Covariant form of Dirac Equation:

In accordance with the principle of relativity, physics must "look the same" in all Lorentz frames. This means that physical theories that are consistent with the principle of relativity must have the same form in all Lorentz frames, that is, they must be covariant.

In this, we examine the covariance of the Dirac equation. In these notes we mainly deal with the Dirac wave function ψ, which is understood to be a four-component spinor. But occasional reference is made to the scalar Klein-Gordon wave function, which will be denoted by ψ_{KG}.

The Dirac equation is,

$$i \hbar \ \partial\psi / \partial t = -I \ \ h \ c \ \alpha \cdot \nabla\psi + m \ c^2 \ \beta \ \psi. \qquad \text{------(1)}$$

The operator $\partial/\partial t$ on the left-hand side is not a Lorentz scalar, because the time t represents just one component of the 4-vector x^{μ} = (ct, x). The Dirac equation, as written, is not manifestly Lorentz covariant.

Let us bring all the derivatives over to one side, and write the Dirac equation as

$$I \ h \ c \ (\ \partial\psi / \ \partial(ct) \ \ + \alpha \cdot \nabla\psi \ ) \ = m \ c^2 \ \beta \ \ \psi. \qquad \text{-------(2)}$$

To put this into covariant form, we multiply through by β, using $\beta^2 = 1$, to obtain

$$i \hbar c \left(\beta \frac{\partial \psi}{\partial (ct)} + \beta \alpha . \nabla \psi \right) = m c^2 \psi \qquad \text{------(3)}$$

The constant operator on the right-hand side, mc^2 , is a Lorentz scalar, while the operators

$$\partial_\mu = \frac{\partial}{\partial x^\mu} = \left(\frac{\partial \psi}{\partial (ct)}, \nabla\right) \qquad \text{----(4)}$$

that appear on the left-hand side transform as a covariant vector .

Therefore we guess that the coefficients that multiply $\partial\mu$ on the left-hand side must transform as a contravariant 4-vector, so that the entire operator on the left-hand side will be a Lorentz scalar.

To bring this out notationally, we define

$$\gamma^0 = \beta, \quad \gamma^i = \beta \alpha_i \qquad \text{------(5)}$$

for i = 1, 2, 3, so that the free particle Dirac equation can be written,

$$i \hbar \gamma^\mu \frac{\partial \psi}{\partial x^\mu} = m c \psi \qquad \text{-------(6)}$$

after cancelling a factor of c. We have written the four matrices defined in Eq. (5) as $\gamma \mu$, $\mu = 0$, 1, 2, 3, which we can think of as a 4-vector of Dirac matrices, much as the Pauli matrices σ constitute a 3-vector of matrices. If we introduce the covariant momentum operators,

$$p_\mu = I \hbar \frac{\partial}{\partial x^\mu}$$

$$= i \hbar \left(\frac{\partial \psi}{\partial (ct)}, \nabla\right) \qquad \text{-----(7)}$$

then the free particle Dirac equation takes on the suggestive form,

$$(\gamma^\mu p_\mu - m c) \psi = 0 \qquad \text{---(8)}$$

The notation suggests that $\gamma^\mu p^\mu$ is a Lorentz scalar, but we will not have proven that until we see how and in what sense $\gamma \mu$ constitutes a 4-vector.

To do that, we will have to show that it transforms as a 4-vector under Lorentz transformations.

Moreover, since $\gamma \mu$ is a 4-vector of 4×4 matrices, not ordinary numbers, its transformation law will not be the same as that of the 4-vectors encountered in classical relativity

theory. Instead, as we shall see, it transforms by a four-dimensional generalization of the definition of a vector operator in quantum mechanics.

4.2 Properties of the gamma matrices:

The matrices γ^{μ}, defined by Eq. (5), constitute an alternative version of the Dirac matrices α and β, useful when we wish to reveal the covariant aspects of the Dirac equation.

All the properties of the α and β matrices can be converted into properties of the matrices γ^{μ}. Here we list some of them. First, there are the values of the matrices.

In the usual Dirac-Pauli representation, they are

$$\gamma^0 = \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \gamma^i = \beta\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix}, \qquad \text{(Dirac-Pauli)}$$

while in the Weyl representation they are

$$\gamma^0 = \beta = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}, \qquad \gamma^i = \beta\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix}. \qquad \text{(Weyl)}$$

Next there are the Hermiticity properties. Recall that α and β are Hermitian. This implies that γ^0 is Hermitian, while γ^i, i = 1, 2, 3, are anti-Hermitian.

This is easily proved using the properties of the α and β matrices, for example,

$$(\gamma^0)^\dagger = \beta^\dagger = \beta = \gamma^0,$$
$$(\gamma^i)^\dagger = (\beta\alpha_i)^\dagger = \alpha_i\beta = -\beta\alpha_i = -\gamma^i,$$

where we have used the anticommutation relation, $\{\alpha_i, \beta\} = 0$ and $\beta^2 = 1$.

Finally, there are the anticommutation properties of the γ^{μ}, which are easily derived from those of α and β. Explicitly, we have

$$\{\gamma^0, \gamma^0\} = \{\beta, \beta\} = 2,$$
$$\{\gamma^0, \gamma^i\} = \{\beta, \beta\alpha_i\} = \beta^2\alpha_i + \beta\alpha_i\beta = \alpha_i - \alpha_i = 0,$$
$$\{\gamma^i, \gamma^j\} = \{\beta\alpha_i, \beta\alpha_j\} = \beta\alpha_i\beta\alpha_j + \beta\alpha_j\beta\alpha_i = -\alpha_i\alpha_j - \alpha_j\alpha_i = -2\delta_{ij},$$

4.3 Current four vector:

In special and general relativity, the **four-current** (technically the **four-current density**) is the four-dimensional analogue of the current density, with units of charge per unit time per unit area.

Also known as **vector current**, it is used in the geometric context of *four-dimensional spacetime*, rather than separating time from three-dimensional space. Mathematically it is a four-vector and is Lorentz covariant.

Using the Minkowski metric of metric signature (+ − − −), the four-current components are given by:

$$J^{\alpha} = \left(c\rho, j^1, j^2, j^3\right) = (c\rho, \mathbf{j})$$

where:

- c is the speed of light;
- ρ is the volume charge density;
- $\mathbf{j}$ is the conventional current density;
- The dummy index α labels the spacetime dimensions.
-

4.4 Bilinear covariant:

The bilinear form

$$\bar{\psi}\gamma^{\mu}\psi$$

One can construct other bilinear forms $\psi\ \Gamma_i\ \psi$, i = 1, 2, . . . 16, which are scalars (V), tensors (T), axial vectors (A) and pseudoscalars (P):

matrix Γ^i	1	γ^μ	$\sigma^{\mu\nu}$	$\gamma^5\gamma^\mu$	γ^5
$\bar{\psi}\Gamma^i\psi$	S	V	T	A	P

Here

$$\sigma^{\mu\nu} = \frac{1}{2}\left(\gamma^{\mu}\gamma^{\nu} - \gamma^{\nu}\gamma^{\mu}\right) \text{ and } \gamma^{5} = i\gamma^{0}\gamma^{1}\gamma^{2}\gamma^{3}.$$

The matrix γ^5 plays an important role especially in the theory of weak interactions. The main properties of γ^5 are the following:

$$\begin{aligned} \gamma^{5}\gamma^{\mu} + \gamma^{\mu}\gamma^{5} &= 0 \\ \gamma^{5\dagger} &= \gamma^{5}, \qquad (\gamma^{5})^{2} = 1 \end{aligned}$$

These properties can be checked by direct calculations. In standard representation γ^5 is of the form

$$\gamma^{5} = \begin{pmatrix} 0 & \sigma_0 \\ \sigma_0 & 0 \end{pmatrix}$$

4.5 Feynman ‘s theory of positron:

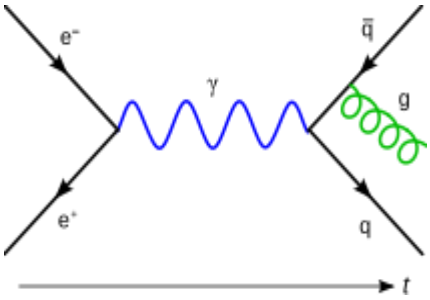
Feynman used Ernst Stueckelberg's interpretation of the positron as if it were an electron moving backward in time.[3] Thus, antiparticles are represented as moving backward along the time axis in Feynman diagrams.

The calculation of probability amplitudes in theoretical particle physics requires the use of rather large and complicated integrals over a large number of variables. Feynman diagrams can represent these integrals graphically.

A Feynman diagram is a graphical representation of a perturbative contribution to the transition amplitude or correlation function of a quantum mechanical or statistical field theory. Within the canonical formulation of quantum field theory, a Feynman diagram represents a term in the Wick's expansion of the perturbative *S*-matrix.

Alternatively, the path integral formulation of quantum field theory represents the transition amplitude as a weighted sum of all possible histories of the system from the initial to

the final state, in terms of either particles or fields. The transition amplitude is then given as the matrix element of the *S*-matrix between the initial and final states of the quantum system.



Unit – V

CLASSICAL FIELDS AND SECOND QUANTIZATION

Classical fields – Euler Lagrange equation – Hamiltonian formulation – Noether's theorem – Quantization of real and complex scalar fields – Creation, Annihilation and Number operators – Fock states – Second Quantization of K-G field.

5.1 Classical fields – Euler Lagrange equation:

Considering a field or set of fields φ(x), where x is the space time position. The Lagrangian is a functional of φ(x) and its derivatives

$$\frac{\partial \varphi(x)}{\partial x^{\mu}} = \partial_{\mu} \varphi(x) \qquad \text{----(1)}$$

Here φ(x) can be a set of fields with an internal index i, such that

$$\varphi(x) = \{ \varphi_i(x) \} \qquad \text{----(2)}$$

We will start with the Lagrangian formulation.

We define the Lagrangian density $L(\varphi(x), \partial\mu\varphi(x))$ by

$$L = \int d^{3}x L(\varphi(x), \partial\mu\varphi(x)) \qquad \text{------(3)}$$

In this way the action is

$$S = \int dt \; L$$

$$= \int d^{4} x \; L (\varphi(x), \; \partial_{\mu} \varphi(x) \;) \qquad \text{----(4)}$$

where we are again using the Lorentz invariant spacetime volume element

$$d^{4} x = dt \, d^{3}x . \qquad \text{-----(5)}$$

From (4) is clear that L must be Lorentz invariant.

In addition, L might also be invariant under other symmetries of the particular theory we are studying. These are generally called internal symmetries and we will study them in more detail later in this lecture, and a lot more in the rest of the course.

We now wish to vary the action in (4) in order to find the extremal solutions and obtain the equations of motion, just as we did in the case of a system of N particles. Here we get

$$\delta S = \int d^4x \left\{ \frac{\partial \mathcal{L}}{\partial \phi} \delta\phi + \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \delta(\partial_\mu \phi) \right\}$$

But, analogously to what we did in the previous section, we have that

$$\delta(\partial_\mu \phi) = \partial_\mu(\delta\phi)$$

Then, the variation of the action is

$$\begin{aligned} \delta S &= \int d^4x \left\{ \frac{\partial \mathcal{L}}{\partial \phi} \delta\phi + \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \partial_\mu(\delta\phi) \right\} , \\ &= \int d^4x \left\{ \left(\frac{\partial \mathcal{L}}{\partial \phi} - \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \right) \right) \delta\phi + \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \delta\phi \right) \right\} \end{aligned}$$

In the second line, we have integrated by parts.

The last term is a four-divergence, i.e. a total derivative. Since the integral is over the volume of all of spacetime, the resulting (hyper-) surface term must be evaluated at infinity.

But just as in the case of N particle dynamics, the value of the field variation at these extremes is $\delta\varphi = 0$. Thus, the (hyper-) surface term in (above equation) does not contribute. Then imposing $\delta S = 0$, we see that the first term in (above equation) multiplying $\delta\varphi$ must vanish for all possible values of $\delta\varphi$. We obtain

$$\frac{\partial \mathcal{L}}{\partial \phi} - \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \right) = 0$$

which are the Euler-Lagrange equations, one for each of the $\varphi_i(x)$, also known as equations of motion

5.2 Hamiltonian formulation:

If now we want to go to the Hamiltonian formulation, we start by defining the canonically conjugated momentum by

$$p(x) = \frac{\partial L}{\partial \dot{\phi}(x)} = \frac{\partial}{\partial \dot{\phi}(x)} \int d^3y \, \mathcal{L}(\phi(y), \partial_\mu \phi(y))$$

which results in the momentum density

$$\pi(x) = \frac{\partial \mathcal{L}}{\partial \dot{\phi}(x)}$$

Here π(x) is the momentum density canonically conjugated to φ(x). Then the Hamiltonian is given by

$$H = \int d^3x \, \pi(x) \, \dot{\phi}(x) - L$$

which leads to the Hamiltonian density

$$\mathcal{H}(x) = \pi(x) \, \dot{\phi}(x) - \mathcal{L}(x)$$

where we must remember that we evaluate at a fixed time t, i.e. x = (t, x) for fixed t. The Lagrangian formulation allows for a Lorentz invariant treatment. On the other hand, the Hamiltonian formulation might have some advantages. For instance, it allows us to impose canonical quantization rules.

5.3 Noether‘s theorem:

In addition to being invariant under Lorentz transformations, the Lagrangian density L can be a scalar under other symmetry transformations.

In particular, when the symmetry transformation is continuous, we can express it as an infinitesimal variation of the field φ(x) that leaves the equations of motion invariant. Let us consider the infinitesimal transformation

$$\phi(x) \longrightarrow \phi'(x) = \phi(x) + \epsilon\,\Delta\phi$$

where ϵ is an infinitesimal parameter. The change induced in the Lagrangian density is

$$\mathcal{L} \longrightarrow \mathcal{L} + \epsilon\,\Delta\mathcal{L}$$

where we factorized ϵ for convenience in the second term. This term can be written as

$$\begin{aligned} \epsilon\,\Delta\mathcal{L} &= \frac{\partial\mathcal{L}}{\partial\phi}\,(\epsilon\,\Delta\phi) + \frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)}\,\partial_\mu(\epsilon\,\Delta\phi) \\ &= \epsilon\,\Delta\phi\left\{\frac{\partial\mathcal{L}}{\partial\phi} - \partial_\mu\left(\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)}\right)\right\} + \epsilon\,\partial_\mu\left(\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)}\,\Delta\phi\right) \end{aligned}$$

The first term is vanishes when we use the equations of motion. The last term is a total derivative so it does not affect the equations of motion when we minimize the action. We can take advantage of this fact and define

$$j^\mu \equiv \frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)}\,\Delta\phi$$

such that its four-divergence

$$\partial_\mu\, j^\mu = 0$$

up to terms that are total derivatives in the action, and therefore do not contribute if we use the equations of motion. We call this object the conserved current associated with the symmetry transformation.

5.4 Quantization of real and complex scalar fields:

The strategy to quantize a classical field theory is to interpret the fields Φ(x) and Π(x) = Φ(˙ x) as operators which satisfy canonical commutation relations. This is completely analogous to the transition from classical to quantum mechanics for discrete systems, where q_i and p_i are promoted to self-adjoint operators that satisfy

$$[q_i, p_j] = i\delta_{ij}, \qquad [q_i, q_j] = [p_i, p_j] = 0\,.$$

These relations hold in the Schrodinger picture where the time dependence is carried by the states alone; in the Heisenberg picture the operators are time-dependent and the commutation relations are imposed at equal times. In the following we will always work in the Heisenberg picture, so we demand that for equal times

$$\begin{aligned}\big[\,\Phi(x), \Pi(y)\,\big]_{x^0=y^0} &= i\delta^{(3)}(\boldsymbol{x}-\boldsymbol{y})\,,\\ \big[\,\Phi(x), \Phi(y)\,\big]_{x^0=y^0} &= \big[\,\Pi(x), \Pi(y)\,\big]_{x^0=y^0} = 0\end{aligned}$$

Despite appearances, this does not destroy Lorentz covariance because x and y are separated by a spacelike distance $(x - y)^2 < 0$ which is preserved under a Lorentz transformation. By virtue of the Dirac delta function, Φ(x) and Π(x) are now operator valued distributions; to arrive at well-defined expressions one should in principle 'smear' them with smooth test functions.

5.5 Creation, Annihilation and Number operators:

In quantum mechanics the number of particles is fixed. We may work with 1 particle. Or with 2 particles. Or with 3. When say something like "consider a system of N spins", the number of particles was fixed at N. The jump to second quantization is quite simple: we lift this constraint and assume that the number of particles may fluctuate.

To describe this, we introduce creation and annihilation operators, similarly to what we do in the case of the harmonic oscillator, but which create or annihilate actual particles. This is the reason why we need single-particle states: these operators create and annihilate particles in single-particle states.

5.6 Bosons and Fermions:

Things become more interesting when we create multiple particles. Second quantization is specifically designed to describe identical particles. In 1940 Wolfgang Pauli published a paper entitled "The connection between spin and statistics" where he shows that, as a consequence of the Lorentz group of special relativity, identical particles can behave in one of two ways. Bosons are symmetric with respect to creation of two particles:

$$a_\beta^\dagger a_\alpha^\dagger |0\rangle = a_\alpha^\dagger a_\beta^\dagger |0\rangle := |1_\beta, 1_\alpha\rangle, \quad \text{-------(1)}$$

whereas Fermions are anti-symmetric:

$$a_\beta^\dagger a_\alpha^\dagger |0\rangle = -a_\alpha^\dagger a_\beta^\dagger |0\rangle := |1_\beta, 1_\alpha\rangle. \quad \text{-----(2)}$$

In the case of Bosons, due to (1), we can move the states around at will:

$$|1_\beta, 1_\alpha| = |1_\alpha, 1_\beta|.$$

For Fermions, however, every time we move the states around we get a minus sign:

$$|1_\beta, 1_\alpha| = -|1_\alpha, 1_\beta|.$$

Pauli also showed that Bosons and Fermions have different spin values: Bosons' spins are integer valued (0,1,2,. . .) whereas Fermions' spins are half-integers (1/2, 3/2, . . .). In the case of Fermions, in particular, if we set $\beta = \alpha$ in Eq. (2) we see that

$$(a_\alpha^\dagger)^2 |0\rangle = -(a_\alpha^\dagger)^2 |0\rangle. \quad \text{----(3)}$$

This is the Pauli exclusion principle: it is forbidden to create two fermions on the same single-particle state | α |. Eq. (3) implies that bosonic creation and annihilation operators should commute:

$$(a_\alpha^\dagger)^2 = 0 \qquad \text{(for Fermions)}.$$

fermionic operators should anti-commute:

$$\{a_\alpha, a_\beta\} = \{a_\alpha^\dagger, a_\beta^\dagger\} = 0,$$

5.7 Fock states:

We have found that the quantized free electromagnetic field is an infinite collection of uncoupled harmonic oscillators, each of which is described by a Hamiltonian

$$\hat{H}_\lambda = \hbar\omega_\lambda(\hat{n}_\lambda + 1/2).$$

We will now concentrate on the quantum states of light. The eigen value problem for

$$\hat{H} = \hbar\omega(\hat{n} + 1/2)$$

is solved by considering the eigenvalue problem for the number operator since

$$[\hat{H}, \hat{n}] = 0.$$

The solution is known from quantum mechanics, and we will briefly review it here. The eigenvalue equation reads

$$\hat{n}|\psi_n\rangle = n|\psi_n\rangle$$

where n is the eigenvalue of ˆn and the corresponding eigenvector. The number operator

$$\hat{n} = \hat{a}^\dagger\hat{a}$$

is an Hermitian operator, therefore its eigenvalues n are real and its eigenvectors form a complete set of orthogonal states. Writing

$$\langle\psi_n|\hat{n}|\psi_n\rangle = \langle\psi_n|\hat{a}^\dagger\hat{a}|\psi_n\rangle = n\langle\psi_n|\psi_n\rangle\,,$$

If we apply the commutation relation, we find that

$$[\hat{a},\hat{n}] = [\hat{a},\hat{a}^\dagger\hat{a}] = \hat{a}[\hat{a},\hat{a}^\dagger] = \hat{a},$$

This state will be called the ground state. It contains no excitation, and thus no quantum can be further annihilated. Similarly, we find that

$$\hat{n}\hat{a}|\psi_n\rangle = (\hat{a}\hat{n} - [\hat{a},\hat{n}])\,|\psi_n\rangle = (n-1)\hat{a}|\psi_n\rangle$$

$$\hat{n}\hat{a}^\dagger|\psi_n\rangle = (n+1)\hat{a}^\dagger|\psi_n\rangle$$

We assume that the ground state (or vacuum state) is already normalized. Then, we create the nth Fock state by

$$|n\rangle = c_n\left(\hat{a}^\dagger\right)^n|0\rangle$$

where we have yet to determine the normalization constants c_n. This is done by looking at the normalization condition

$$\langle n|n\rangle = |c_n|^2\langle 0|\hat{a}^n\left(\hat{a}^\dagger\right)^n|0\rangle = 1$$

We then calculate

$$\langle 0|\hat{a}^n\left(\hat{a}^\dagger\right)^n|0\rangle = \langle 0|\hat{a}^{n-1}\hat{a}\hat{a}^\dagger\left(\hat{a}^\dagger\right)^{n-1}|0\rangle = \langle 0|\hat{a}^{n-1}\left(\hat{a}^\dagger\right)^{n-1}|0\rangle + \langle 0|\hat{a}^{n-1}\hat{n}\left(\hat{a}^\dagger\right)^{n-1}|0\rangle$$

and use the commutation rule

$$[\hat{n},(\hat{a}^\dagger)^k] = k(\hat{a}^\dagger)^k$$

to obtain

$$\langle 0|\hat{a}^n \left(\hat{a}^\dagger\right)^n |0\rangle = n\langle 0|\hat{a}^{n-1} \left(\hat{a}^\dagger\right)^{n-1} |0\rangle = n(n-1)\langle 0|\hat{a}^{n-2} \left(\hat{a}^\dagger\right)^{n-2} |0\rangle = \ldots = n!\langle 0|0\rangle$$

from which it follows that

$$c_n = 1/\sqrt{n!}.$$

Collecting all the results, we find that

$$\boxed{|n\rangle = \frac{1}{\sqrt{n!}} \left(\hat{a}^\dagger\right)^n |0\rangle}.$$

Similarly, we find that

$$\boxed{\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle\,, \qquad \hat{a}|n\rangle = \sqrt{n}|n-1\rangle}$$

As mentioned before, the eigenvectors of the number operator are mutually orthogonal, hence

$$\langle m|n\rangle = \delta_{mn}$$

and they form a complete set of orthonormal vectors, hence

$$\sum_{n=0}^{\infty} |n\rangle\langle n| = \hat{I}$$

where ˆI is the identity operator in the Hilbert space of the single-mode system.

5.8 Second Quantization of K-G field:

We can write the Klein-Gordon field operator as

$$\phi(\mathbf{x}) = C \int \mathrm{d}^3k \ \left(e^{(-i\mathbf{k}\cdot\mathbf{x})} a(\mathbf{k}) + e^{(i\mathbf{k}\cdot\mathbf{x})} a^\dagger(\mathbf{k}) \right)$$

where

$$C = \frac{1}{\sqrt{2k^0(2\pi)^3}} \qquad (2)$$

and $k_0 = E_k$. The field operator satisfies the Klein-Gordon equation, i.e.

$$(\partial_\mu \partial^\mu + m^2)\phi = 0 \qquad (3)$$

This can be split into positive and negative energy components as follows:

$$\begin{aligned} \phi(\mathbf{x}) &= \phi^{(+)}(\mathbf{x}) + \phi^{(-)}(\mathbf{x}) \\ \phi^{(+)}(\mathbf{x}) &= C \int \mathrm{d}^3k \ e^{(-i\mathbf{k}\cdot\mathbf{x})} a(\mathbf{k}) \\ \phi^{(-)}(\mathbf{x}) &= C \int \mathrm{d}^3k \ e^{(i\mathbf{k}\cdot\mathbf{x})} a^\dagger(\mathbf{k}) \end{aligned} \qquad (4)$$

The conjugate momentum for the field operator is therefore

$$\begin{aligned} \Pi(\mathbf{x}) &= \dot{\phi}(\mathbf{x}) \\ &= -ik^0 C \int \mathrm{d}^3k \ \left(\exp(-i\mathbf{k}\cdot\mathbf{x}) a(\mathbf{k}) - \exp(i\mathbf{k}\cdot\mathbf{x}) a^\dagger(\mathbf{k}) \right) \end{aligned} \qquad (5)$$

Inverting equations 1 and 5 and solving for the annihilation and creation operators a and a† :

$$a(\mathbf{k}) = C \int \mathrm{d}^3x \; e^{i\mathbf{k}\cdot\mathbf{x}} \Big(k^0\phi(\mathbf{x}) + i\Pi(\mathbf{x}) \Big)$$
$$= iC \int \mathrm{d}^3x \; \Big(e^{i\mathbf{k}\cdot\mathbf{x}} \partial_t \phi(\mathbf{x}) - \partial_t e^{i\mathbf{k}\cdot\mathbf{x}} \phi(\mathbf{x}) \Big) \qquad (6)$$

$$a^\dagger(\mathbf{k}) = C \int \mathrm{d}^3x \; e^{-i\mathbf{k}\cdot\mathbf{x}} \Big(k^0\phi(\mathbf{x}) - i\Pi(\mathbf{x}) \Big)$$
$$= -iC \int \mathrm{d}^3x \; \Big(e^{-i\mathbf{k}\cdot\mathbf{x}} \partial_t \phi(\mathbf{x}) - \partial_t e^{-i\mathbf{k}\cdot\mathbf{x}} \phi(\mathbf{x}) \Big) \qquad (7)$$

Taking the time derivative of equation 6:

$$\partial_t a(\mathbf{k}) = iC\partial_t \int \mathrm{d}^3x \; \Big(e^{i\mathbf{k}\cdot\mathbf{x}} \partial_t \phi(\mathbf{x}) - \partial_t e^{i\mathbf{k}\cdot\mathbf{x}} \phi(\mathbf{x}) \Big)$$
$$= iC \int \mathrm{d}^3x \; \Big(\partial_t e^{i\mathbf{k}\cdot\mathbf{x}} \partial_t \phi(\mathbf{x}) + e^{i\mathbf{k}\cdot\mathbf{x}} \partial_t^2 \phi(\mathbf{x}) - \partial_t e^{i\mathbf{k}\cdot\mathbf{x}} \partial_t \phi(\mathbf{x}) - \partial_t^2 e^{i\mathbf{k}\cdot\mathbf{x}} \phi(\mathbf{x}) \Big)$$
$$= iC \int \mathrm{d}^3x \; \Big(e^{i\mathbf{k}\cdot\mathbf{x}} \partial_t^2 \phi(\mathbf{x}) - \partial_t^2 e^{i\mathbf{k}\cdot\mathbf{x}} \phi(\mathbf{x}) \Big)$$

must satisfy the Klein-Gordon equation, so

$$\partial_t a(\mathbf{k}) = iC \int \mathrm{d}^3x \; \Big(e^{i\mathbf{k}\cdot\mathbf{x}} (\nabla^2 - m^2)\phi(\mathbf{x}) + (k^0)^2 e^{i\mathbf{k}\cdot\mathbf{x}} \phi(\mathbf{x}) \Big)$$
$$= iC \int \mathrm{d}^3x \; \Big((k^0)^2 - k^2 - m^2 \Big) e^{i\mathbf{k}\cdot\mathbf{x}} \phi(\mathbf{x})$$
$$= 0$$

To reduce clutter, we define

$$C' \equiv C \Big|_{k^0 \to k'^0}$$

$$
\begin{aligned}
[\phi(\mathbf{x}),\phi(\mathbf{y})] = CC' \iint \mathrm{d}^3k \;\; \mathrm{d}^3k' \;\; \Big(& e^{-i(\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}[a(\mathbf{k}),a(\mathbf{k}')] \\
& + e^{-i(\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{y})}\big[a(\mathbf{k}),a^\dagger(\mathbf{k}')\big] + e^{-i(-\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}\big[a^\dagger(\mathbf{k}),a(\mathbf{k}')\big] \\
& + e^{-i(-\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{y})}\big[a^\dagger(\mathbf{k}),a^\dagger(\mathbf{k}')\big]\Big) \\
= 0 & \qquad (8)
\end{aligned}
$$

$$
\begin{aligned}
[\Pi(\mathbf{x}),\Pi(\mathbf{y})] = -k^0k'^0CC' \iint \mathrm{d}^3k \;\; \mathrm{d}^3k' \;\; \Big(& e^{-i(\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}[a(\mathbf{k}),a(\mathbf{k}')] \\
& - e^{-i(\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{y})}\big[a(\mathbf{k}),a^\dagger(\mathbf{k}')\big] - e^{-i(-\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}\big[a^\dagger(\mathbf{k}),a(\mathbf{k}')\big] \\
& + e^{-i(-\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{y})}\big[a^\dagger(\mathbf{k}),a^\dagger(\mathbf{k}')\big]\Big) \\
= 0 & \qquad (9)
\end{aligned}
$$

$$
\begin{aligned}
[\phi(\mathbf{x}),\Pi(\mathbf{y})] = -ik'^0CC' \iint \mathrm{d}^3k \;\; \mathrm{d}^3k' \;\; \Big(& e^{-i(\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}[a(\mathbf{k}),a(\mathbf{k}')] \\
& - e^{-i(\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{y})}\big[a(\mathbf{k}),a^\dagger(\mathbf{k}')\big] + e^{-i(-\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}\big[a^\dagger(\mathbf{k}),a(\mathbf{k}')\big] \\
& - e^{-i(-\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{y})}\big[a^\dagger(\mathbf{k}),a^\dagger(\mathbf{k}')\big]\Big) \\
= i\delta^3(\mathbf{x}-\mathbf{v}) & \qquad (10)
\end{aligned}
$$

The commutation relations between the annihilation and creation operators can be calculated from equations 6 and 7,

$$
\begin{aligned}
[a(\mathbf{k}),a(\mathbf{k}')] &= CC' \iint \mathrm{d}^3x \;\; \mathrm{d}^3y e^{i(\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}\Big(k^0k'^0[\phi(\mathbf{x}),\phi(\mathbf{y})] \\
&\quad + ik^0[\phi(\mathbf{x}),\Pi(\mathbf{y})] + ik'^0[\Pi(\mathbf{x}),\phi(\mathbf{y})] - [\Pi(\mathbf{x}),\Pi(\mathbf{y})]\Big) \\
&= CC' \iint \mathrm{d}^3x \;\; \mathrm{d}^3y e^{i(\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}\Big(ik^0[\phi(\mathbf{x}),\Pi(\mathbf{y})]+ik'^0[\Pi(\mathbf{x}),\phi(\mathbf{y})]\Big) \\
&= -CC'(k^0-k'^0) \iint \mathrm{d}^3x \;\; \mathrm{d}^3y e^{i(\mathbf{k}\cdot\mathbf{x}+\mathbf{k}'\cdot\mathbf{y})}\delta^3(\mathbf{x}-\mathbf{y}) \\
&= -CC'(k^0-k'^0) \int \mathrm{d}^3x e^{i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{x}} \\
&= -CC'(k^0-k'^0)e^{i(k^0+k'^0)\cdot\mathbf{x}}\delta^3(\mathbf{k}-\mathbf{k}') \\
&= 0 \qquad (11)
\end{aligned}
$$

In the last step, we use the fact that $k_0 = k_0$. Similarly, we find that

$$\left[a^\dagger(\mathbf{k}), a^\dagger(\mathbf{k}')\right] = 0 \qquad (12)$$

$$\left[a(\mathbf{k}), a^\dagger(\mathbf{k}')\right] = \delta^3(\mathbf{k} - \mathbf{k}') \qquad (13)$$

So the creation and annihilation operators commute with themselves for any two k and k0 , but do not commute with each other.