❖ Relativistic Quantum Mechanics

Introduction: The basis of both Schrodinger and Pauli are nonrelativistic. They ignore the fact that no mass point can move in space and no action can propagate in space at a velocity greater than the speed of light. A relativistic generalization of quantum mechanics requires introducing new physical concepts and even modifying the interpretation of the wave function. This modification is necessary because we need to introduce, besides spin, a new degree of freedom for the electron and because we cannot interpret this degree of freedom within the limits of the one body problem.

Introducing the Lorentz transformation condition

$$\overline{x}^{\mu} = g^{\mu}_{\upsilon} x^{\upsilon}$$

along with the relativistic Hamiltonian

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

into the non-relativistic form of the Schrodinger equation led to an equation which is difficult to interpret. This difficulty was, however, overcome by **Klein-Gordon and Fock**. They modified the Schrodinger equation into relativistic form ingenious way.

❖ Klein-Gordon and Fock equation:

We know that the time dependent Schrodinger equation is

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

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

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

$$H^2\psi = i\hbar \frac{\partial}{\partial t}\left(i\hbar \frac{\partial \psi}{\partial t}\right)$$

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

Equation (2) represents the relativistic Schrodinger equation or Klein Gordon-Fock equation for a massless relativistic particle.

For free particle of mass ‘m’ moving with velocity ‘c’ and momentum ‘p’, the Hamiltonian is

$$H^2 = p^2c^2 + m^2c^4 \qquad (3)$$

Using (3) in (2), we get

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

Introducing the operator, $p \to \frac{\hbar}{i}\nabla$

We obtain

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

This is the Klein-Gordon-Fock equation for a free particle. This equation may also be written as

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{m^2c^2}{\hbar^2}\right)\psi = 0 \qquad (5)$$

Or, $\left[\Box^2 - \frac{m^2c^2}{\hbar^2}\right]\psi = 0$ (6)

where $\Box^2 = \nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}$ is called the D’Alembertian operator.

In natural unit, $\hbar$ =1, c=1, and the Klein-Gordon equation takes the form

$$\left[\Box^2 - m^2\right]\psi = 0. \qquad (7)$$

❖ Charge and current densities from KG equation:

The Klein-Gordon equation for a free particle is

$$\left[\Box^2 - \frac{m^2c^2}{\hbar^2}\right]\psi = 0$$

Or, $\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{m^2c^2}{\hbar^2}\right)\psi = 0$

Or, $\nabla^2\psi - \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} - \frac{m^2c^2}{\hbar^2}\psi = 0$ (8)

Taking the complex conjugate of (8), we get

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

Premultiplying (8) by ψ^* and (9) by ψ, we get

$$\psi^*\nabla^2\psi - \frac{1}{c^2}\psi^*\frac{\partial^2\psi}{\partial t^2} - \frac{m^2c^2}{\hbar^2}\psi^*\psi = 0 \quad (10)$$

and $\psi\nabla^2\psi^* - \frac{1}{c^2}\psi\frac{\partial^2\psi^*}{\partial t^2} - \frac{m^2c^2}{\hbar^2}\psi\psi^* = 0$ (11)

Subtracting (11) from (10), we get

$$\psi^*\nabla^2\psi - \psi\nabla^2\psi^* + \frac{1}{c^2}\left(\psi\frac{\partial^2\psi^*}{\partial t^2} - \psi^*\frac{\partial^2\psi}{\partial t^2}\right) = 0$$

$$\nabla\bullet\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) + \frac{1}{c^2}\left(\psi\frac{\partial^2\psi^*}{\partial t^2} - \psi^*\frac{\partial^2\psi}{\partial t^2}\right) = 0$$

Multiplying by $\frac{\hbar}{2im}$, we get

$$\nabla\bullet\left[\frac{\hbar}{2im}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)\right] + \frac{\hbar}{2imc^2}\left(\psi\frac{\partial^2\psi^*}{\partial t^2} - \psi^*\frac{\partial^2\psi}{\partial t^2}\right) = 0$$

$$\nabla\bullet\left[\frac{\hbar}{2im}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)\right] + \frac{\partial}{\partial t}\left[\frac{\hbar}{2imc^2}\left(\psi\frac{\partial\psi^*}{\partial t} - \psi^*\frac{\partial\psi}{\partial t}\right)\right] = 0 \quad (12)$$

This is similar to the continuity equation

$$\nabla\bullet J + \frac{\partial\rho}{\partial t} = 0 \quad (13)$$

where ρ is the probability charge density and J is the current density given by

$$\rho = \left[\frac{\hbar}{2imc^2}\left(\psi\frac{\partial\psi^*}{\partial t} - \psi^*\frac{\partial\psi}{\partial t}\right)\right] \quad (14)$$

and $J = \left[\frac{\hbar}{2im}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)\right]$ (15)

The current density J has the same form as in the non-relativistic case, but ρ cannot be interpreted as the position probability density in analogy with the non-relativistic case. It is called the probability charge density due to the following reason.

Since

$$\rho = \left[\frac{\hbar}{2imc^2}\left(\psi \frac{\partial \psi^*}{\partial t} - \psi^* \frac{\partial \psi}{\partial t}\right)\right]$$

$$\rho = \frac{1}{2mc^2}\left[\psi\left(\frac{\hbar}{i}\frac{\partial \psi^*}{\partial t}\right) - \psi^*\left(\frac{\hbar}{i}\frac{\partial \psi}{\partial t}\right)\right]$$

$$\rho = \frac{1}{2mc^2}\left[\psi\left(H\psi^*\right) - \psi^*\left(-H\psi\right)\right]$$

$$\rho = \frac{1}{2mc^2}\left[\psi\left(E\psi^*\right) + \psi^*\left(E\psi\right)\right]$$

$$\rho = \frac{1}{2mc^2}\left[2E\psi^*\psi\right]$$

Or, $\rho = \frac{E}{mc^2}\left[\psi^*\psi\right]$ (16)

Since $E = \pm\sqrt{p^2c^2 + m^2c^4}$, the energy of a particle may be either positive or negative. So, 'ρ' is not definitely positive, i.e., it is not the conventional position probability density. Pauli and Weisskopf interpreted 'eρ' as the charge density where 'e' is the charge of the particle. As e may be either positive or negative, so 'eρ' may be either positive or negative. Accordingly 'eJ' may be regarded as the probability current dnsity.

❖ <u>**Short comings of Klein-Gordon equation:**</u>

The Klein-Gordon equation

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

does not give the correct interpretation of the probability charge density ρ(r.t).

The equation also does not account for the spinning motion of the particles since in this equation it is assumed that ψ has only one component, i.e., it is a scalar. Thus the Klein-Gordon equation describe particles of zero spin (spinless) like π and K-mesons which are strongly interacting (and not for electrons).

❖ Klein-Gordon-Fock equation in an electromagnetic field:

Let us consider a particle of mass 'm' and charge 'e' with a velocity 'c' in an electromagnetic field characterized by the vector and the scalar potentials A and φ respectively.
We know that the energy of a particle in field free space is given as

$$E^2=p^2c^2+m^2c^4 \tag{1}$$

In the presence of an electromagnetic field, the energy E and the momentum p are replaced by $\left(E-e\phi\right)$ and $\left(p-\frac{e\mathrm{A}}{c}\right)$ respectively, so that (1) becomes

$$\left(E-e\phi\right)^2=\left(p-\frac{e\mathrm{A}}{c}\right)^2c^2+m^2c^4$$

Or, $\left(E-e\phi\right)^2=\left(pc-e\mathrm{A}\right)^2+m^2c^4$

Using the operators, $E\rightarrow i\hbar\frac{\partial}{\partial t},\;\; p\rightarrow -i\hbar\nabla,$

we get the K.G. equation as

$$\left(i\hbar\frac{\partial}{\partial t}-e\phi\right)^2\psi=\left[\left(-i\hbar c\nabla-e\mathrm{A}\right)^2+m^2c^4\right]\psi \tag{2}$$

$$\left[\left(i\hbar\frac{\partial}{\partial t}-e\phi\right)\left(i\hbar\frac{\partial}{\partial t}-e\phi\right)\right]\psi=\left[\left(-i\hbar c\nabla-e\mathrm{A}\right)\left(-i\hbar c\nabla-e\mathrm{A}\right)+m^2c^4\right]\psi$$

$$\left[-\hbar^2\frac{\partial^2}{\partial t^2}-i\hbar e\frac{\partial\phi}{\partial t}-ie\hbar\phi\frac{\partial}{\partial t}+e^2\phi^2\right]\psi=\left[-c^2\hbar^2\nabla^2+iec\hbar\nabla\bullet\mathrm{A}+iec\hbar\mathrm{A}\nabla+e^2\mathrm{A}^2+m^2c^4\right]\psi$$

$$-\hbar^2\frac{\partial^2\psi}{\partial t^2}-i\hbar e\frac{\partial}{\partial t}\left(\phi\psi\right)-ie\hbar\phi\frac{\partial\psi}{\partial t}+e^2\phi^2\psi=-c^2\hbar^2\nabla^2\psi+iec\hbar\nabla\bullet\left(\mathrm{A}\psi\right)+iec\hbar\mathrm{A}\nabla\psi+e^2\mathrm{A}^2\psi+m^2c^4\psi \tag{3}$$

This is the K.G. equation in an electromagnetic field.
To find the connection between (3) and similar non-relativistic equation, let

$$\psi=\psi^{/}e^{-\frac{imc^2t}{\hbar}} \tag{4}$$

where mc^2 is the rest energy.

$$\frac{\partial\psi}{\partial t}=\frac{\partial\psi^{/}}{\partial t}e^{-\frac{imc^2t}{\hbar}}-\frac{imc^2}{\hbar^2}\psi^{/}e^{-\frac{imc^2t}{\hbar}}$$

$$\frac{\partial\psi}{\partial t}=\left[\frac{\partial\psi^{/}}{\partial t}-\frac{imc^2}{\hbar^2}\psi^{/}\right]e^{-\frac{imc^2t}{\hbar}} \tag{5}$$

$$\frac{\partial^2\psi}{\partial t^2}=\frac{\partial^2\psi'}{\partial t^2}e^{-\frac{imc^2t}{\hbar}}-\frac{imc^2}{\hbar}\frac{\partial\psi'}{\partial t}e^{-\frac{imc^2t}{\hbar}}+\left(\frac{imc^2}{\hbar}\right)^2\psi' e^{-\frac{imc^2t}{\hbar}}-\frac{imc^2}{\hbar}\frac{\partial\psi'}{\partial t}e^{-\frac{imc^2t}{\hbar}}$$

$$\frac{\partial^2\psi}{\partial t^2}=\left[\frac{\partial^2\psi'}{\partial t^2}-\frac{2imc^2}{\hbar}\frac{\partial\psi'}{\partial t}-\frac{m^2c^4}{\hbar^2}\psi'\right]e^{-\frac{imc^2t}{\hbar}} \qquad (6)$$

Substituting these values in (3), we get

$$\left[-\hbar^2\frac{\partial^2\psi'}{\partial t^2}+2imc^2\hbar\frac{\partial\psi'}{\partial t}+m^2c^4\psi'-ie\hbar\frac{\partial\phi}{\partial t}\psi'-2ie\hbar\phi\left(\frac{\partial\psi'}{\partial t}-\frac{imc^2}{\hbar}\psi'\right)+e^2\phi^2\psi'\right]e^{-\frac{imc^2t}{\hbar}}=\left[-c^2\hbar^2\nabla^2+iec\hbar\nabla\bullet\mathrm{A}+2iec\hbar\mathrm{A}\bullet\nabla+e^2\mathrm{A}^2+m^2c^4\right]\psi' e^{-\frac{imc^2t}{\hbar}}$$

$$\left[-\hbar^2\frac{\partial^2\psi'}{\partial t^2}+2imc^2\hbar\frac{\partial\psi'}{\partial t}-ie\hbar\psi'\frac{\partial\phi}{\partial t}-2ie\hbar\phi\left(\frac{\partial\psi'}{\partial t}-\frac{imc^2}{\hbar}\right)+e^2\phi^2\psi'\right]=\left[-c^2\hbar^2\nabla^2+iec\hbar\nabla\bullet\mathrm{A}+2iec\hbar\mathrm{A}\bullet\nabla+e^2\mathrm{A}^2\right]\psi' \qquad (7)$$

Dividing throughout by $2mc^2$, we get

$$-\frac{\hbar^2}{2mc^2}\frac{\partial^2\psi'}{\partial t^2}+i\hbar\frac{\partial\psi'}{\partial t}-\frac{ie\hbar}{2mc^2}\psi'\frac{\partial\phi}{\partial t}-\frac{ie\hbar}{mc^2}\phi\frac{\partial\psi'}{\partial t}-e\phi\psi'+\frac{e^2}{2mc^2}\phi^2\psi'=-\frac{\hbar^2}{2m}\nabla^2\psi'+\frac{ie\hbar}{2mc}\psi'\nabla\bullet\mathrm{A}+\frac{ie\hbar}{mc}\mathrm{A}\nabla\bullet\psi'+\frac{e^2}{2mc^2}\mathrm{A}^2\psi' \qquad (8)$$

In non-relativistic case, $mc^2 >> E$ and $mc^2 >> e\varphi$, so we may neglect the terms containing the denominator ~ mc^2 and ~mc.

$$i\hbar\frac{\partial\psi'}{\partial t}-e\phi\psi'=-\frac{\hbar^2}{2m}\nabla^2\psi'+\frac{ie\hbar}{2mc}\psi'\nabla\bullet\mathrm{A}+\frac{ie\hbar}{mc}\mathrm{A}\bullet\nabla\psi'+\frac{e^2}{2mc^2}\mathrm{A}^2\psi'$$

$$\left(i\hbar\frac{\partial}{\partial t}-e\phi\right)\psi'=\left[\left(-i\hbar\nabla\right)^2\frac{1}{2m}+\frac{ie\hbar}{2mc}\nabla\bullet\mathrm{A}+\frac{ie\hbar}{mc}\mathrm{A}\bullet\nabla+\frac{e^2\mathrm{A}^2}{2mc^2}\right]\psi'$$

Rearranging, we get

$$\left(E-e\phi\right)\psi'=\frac{\left(p-\frac{e\mathrm{A}}{c}\right)^2}{2m}\psi' \qquad (9)$$

This is the non-relativistic Schrodinger equation in an electromagnetic field. Thus K.G. equation in electromagnetic field reduces to correct non-relativistic limit with appropriate approximations.

Note.

K.G. equation results that probability density have positive and negative values. But probability density cannot have negative values. This is the fundamental drawback of this equation.
