Relativistic Quantum Mechanics

by

Dr. R. S. Singh

Prof. (Physics)

Govt. V.Y.T.PG Autonomous College, Durg (C.G.)-491001

Relativistic Quantum Mechanics

Notations

In the four dimensional space-time manifold, commonly known as the Minkowski space, the four vectors are defined by

$$x^\mu = (ct, \mathbf{x}),$$
$$x_\mu = (ct, -\mathbf{x}). \qquad (\mu = 0, 1, 2, 3)$$

The contravariant and the covariant vectors are related to each other through the metric tensor of the four dimensional manifold, namely,

$$x_\mu = \eta_{\mu\nu} x^\nu,$$
$$x^\mu = \eta^{\mu\nu} x_\nu.$$

$$\eta^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$\eta_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

The operator implying differentiation with respect to a contravariant (covariant) coordinate vector component transforms as a component of a covariant (contravariant) vector,

$$\left.\begin{aligned} \partial^\mu &\equiv \frac{\partial}{\partial x_\mu} = \left(\partial^0, \partial^1, \partial^2, \partial^3\right) = \left(\frac{\partial}{\partial x_0}, -\vec{\nabla}\right) \\ \partial_\mu &\equiv \frac{\partial}{\partial x^\mu} = \left(\partial_0, \partial_1, \partial_2, \partial_3\right) = \left(\frac{\partial}{\partial x^0}, \vec{\nabla}\right) \end{aligned}\right\}$$

where $\vec{\nabla} = \left(\frac{\partial}{\partial x^1}, \frac{\partial}{\partial x^2}, \frac{\partial}{\partial x^3}\right) = \left(\partial_1, \partial_2, \partial_3\right) = \left(-\partial^1, -\partial^2, -\partial^3\right)$ is the 3-divergence.

(thus $\vec{\nabla}.\vec{A} = \partial_k A^k$).

We may then define a 4-divergence of a 4-vector A^μ by

$$\partial_\mu A^\mu = \partial^\mu A_\mu = \frac{\partial A^0}{\partial x^0} + \vec{\nabla}.\vec{A} = \frac{\partial A^0}{\partial x^0} + \vec{\nabla}_i . A^i$$

In this notation the 4-dimensional d'Alembertian operator is the contraction

$$\Box^2 \equiv \partial_\mu \partial^\mu = \frac{\partial^2}{\partial x^0 \partial x_0} - \nabla^2 = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2$$

and is a scalar under Lorentz transformations.

Klein-Gordon equation

The relativistic relation between the energy and momentum of a free particle is

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

Substituting $E = i\hbar \frac{\partial}{\partial t}$; $\vec{p} = -i\hbar\vec{\nabla}$, we have

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

Simplifying the above equation we get $\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 + \frac{m^2 c^2}{\hbar^2}\right)\psi = 0$

$$\left(\Box^2 + \frac{m^2 c^2}{\hbar^2}\right)\psi = 0, \qquad \text{where } \Box^2 \equiv \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2$$

This equation is known as Klein-Gordon equation.

There is no way in which the Pauli spin matrices can be included in Klein-Gordon equation without destroying the invariance of the theory. This is because the spin matrices transform like the components of three dimensional vector, rather than a four dimensional vector.

Thus the Klein-Gordon relativistic equation represents a particle that has no spin.

Solution of Klein-Gordon equation is of the form

$$\psi = N \exp\left(i(\vec{p}\cdot\vec{x} - Et)\right)$$

where N is the normalization constant and

$$E = \pm\left(p^2 c^2 + m^2 c^4\right)^{1/2}$$

In addition to the acceptable $E > 0$ solutions, we also have negative energy solution. A second problem is that $E < 0$ solutions are associated with a negative probability density. The negative energy solutions cannot be simply discarded as these correspond to *antiparticles*.

Plane wave solutions

Klein-Gordon equation also has plane wave solutions which are characteristic of free particle solutions. In fact, the functions

$$e^{\mp ik\cdot x} = e^{\mp ik_\mu x^\mu} = e^{\mp ik^\mu x_\mu} = e^{\mp i(k_0 t - \mathbf{k}\cdot\mathbf{x})}$$

with $k^\mu = (k^0, \mathbf{k})$ are eigenfunctions of the energy-momentum operator,

$$p^\mu e^{\mp ik\cdot x} = i\partial^\mu e^{\mp ik\cdot x} = i\frac{\partial}{\partial x_\mu} e^{\mp ik\cdot x} = \pm\ \hbar k^\mu e^{\mp ik\cdot x}$$

so that $\pm k^\mu$ are the eigenvalues of the energy-momentum operator. This shows that the plane waves define a solution of the Klein-Gordon equation provided

$$k^2 - m^2\mathbf{c}^2 = (k^0)^2 - \mathbf{k}^2 - m^2\mathbf{c}^2 = 0$$

$$k^0 = \pm E = \pm\sqrt{\mathbf{k}^2 + m^2\mathbf{c}^2}$$

Klein-Gordon equation and its complex conjugate

$$(\Box^2 + \frac{m^2\mathbf{c}^2}{\mathbf{h}^2})\Psi = 0$$

$$(\Box^2 + \frac{m^2\mathbf{c}^2}{\mathbf{h}^2})\Psi^* = 0$$

would imply

$$\Psi^*\Box^2\Psi - \Psi\Box^2\Psi^* = 0$$

$$\partial_\mu\left(\Psi^*\partial^\mu\Psi - \Psi\,\partial^\mu\Psi^*\right) = 0$$

$$\frac{\partial}{\partial t}\left(\Psi^*\frac{\partial\Psi}{\partial t} - \Psi\ \frac{\partial\Psi^*}{\partial t}\right) - \nabla\cdot\left(\Psi^*\nabla\Psi - \Psi\ \nabla\Psi^*\right) = 0$$

Defining the probability current density four vector as

$$J^\mu = (j^0, \mathbf{J}) = (\rho, \mathbf{J})$$

where

$$\begin{aligned} \mathbf{J} &= \frac{1}{2im}\left(\Psi^* \boldsymbol{\nabla} \Psi - \Psi \ \boldsymbol{\nabla} \Psi^*\right) \\ \rho &= \frac{i}{2m}\left(\Psi^* \frac{\partial \Psi}{\partial t} - \Psi \quad \frac{\partial \Psi^*}{\partial t}\right) \end{aligned}$$

This shows that the continuity equation for the probability current is

$$\partial_\mu J^\mu = \frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot \mathbf{J} = 0$$

The probability current density

$$\mathbf{J} = \frac{1}{2im}\left(\Psi^* \boldsymbol{\nabla} \Psi - \Psi \ \boldsymbol{\nabla} \Psi^*\right)$$

of course, has the same form as in non-relativistic quantum mechanics. However, we note that the form of the probability density (which results from the requirement of covariance)

$$\rho = \frac{i}{2m}\left(\Psi^* \frac{\partial \Psi}{\partial t} - \Psi \quad \frac{\partial \Psi^*}{\partial t}\right)$$

is quite different from that in non-relativistic quantum mechanics and it is here that the problem of the negative energy states shows up. For example, even for the simplest of solutions, namely, plane waves of the form

$$\phi(x) = e^{-ik\cdot x}$$

we obtain

$$\rho = \frac{i}{2m}(-ik^0 - ik^0) = \frac{k^0}{m} = \pm\frac{E}{m}$$

Since energy can take both positive and negative values, it follows that ρ cannot truly represent the probability density which, by definition, has to be positive semi-definite. Klein-Gordon equation is second order in time derivatives. This has the consequence that the probability involves a first order time derivative and that is how the problem of the negative energy states enters.

The positive energy solutions alone do not define a complete set of states (basis) in the Hilbert space and, consequently, even if we restrict the states to be of positive energy to begin with, negative energy states may be generated through quantum mechanical corrections.

It is for these reasons that the Klein-Gordon equation was abandoned as a quantum mechanical equation for a single relativistic particle.

Dirac equation

The origin of negative probability density is the second order derivative $\frac{\partial}{\partial t}$ in the Klein-Gordon equation. In order to avoid these problems, Dirac in the year 1927, derived a relativistic wave equation linear in $\frac{\partial}{\partial t}$ and ∇. He succeeded in overcoming the problem of the negative probability density, with the unexpected bonus that the equation described spin-1/2 particles.

Dirac approached the problem of finding a relativistic wave equation by starting from the Hamiltonian of the form

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = H\psi(\vec{r},t) \qquad or \qquad E\psi = H\psi$$

The simplest Hamiltonian that is linear in the momentum and mass term is

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

Substituting H, we have

$$\left(E - c\vec{\alpha}.\vec{p} - \beta mc^2\right)\psi = 0$$

or

$$\left(i\hbar\frac{\partial}{\partial t} + i\hbar c\vec{\alpha}.\vec{\nabla} - \beta mc^2\right)\psi = 0$$

where $\vec{\alpha}$ has three components α_x, α_y and α_z.

Multiplying by $\left[E + c\vec{\alpha}.\vec{p} + \beta mc^2\right]$ from left, we have

$$\left[E + \left(c\vec{\alpha}.\vec{p} + \beta mc^2\right)\right]\left[E - \left(c\vec{\alpha}.\vec{p} + \beta mc^2\right)\right]\psi = 0$$

$$\left[E^2 - \left(c\vec{\alpha}.\vec{p} + \beta mc^2\right)\left(c\vec{\alpha}.\vec{p} + \beta mc^2\right)\right]\psi = 0$$

Using $\quad \vec{\alpha}.\vec{p} = \left(\hat{i}\alpha_x + \hat{j}\alpha_y + \hat{k}\alpha_z\right)\cdot\left(\hat{i}p_x + \hat{j}p_y + \hat{k}p_z\right) = \alpha_x p_x + \alpha_y p_y + \alpha_z p_z$

the term $\left(c\vec{\alpha}.\vec{p} + \beta mc^2\right)\left(c\vec{\alpha}.\vec{p} + \beta mc^2\right)$ can be simplified as follows:

$$\begin{aligned}
&\left(c\vec{\alpha}.\vec{p} + \beta mc^2\right)\left(c\vec{\alpha}.\vec{p} + \beta mc^2\right) \\
&= \left[c\left(\alpha_x p_x + \alpha_y p_y + \alpha_z p_z\right) + \beta mc^2\right]\cdot\left[c\left(\alpha_x p_x + \alpha_y p_y + \alpha_z p_z\right) + \beta mc^2\right] \\
&= c^2\left[\left(\alpha_x^2 p_x^2 + \alpha_y^2 p_y^2 + \alpha_z^2 p_z^2\right) + \alpha_x p_x \alpha_y p_y + \alpha_x p_x \alpha_z p_z + \alpha_y p_y \alpha_x p_x + \alpha_y p_y \alpha_z p_z + \right. \\
&\quad \left. \alpha_z p_z \alpha_x p_x + \alpha_z p_z \alpha_y p_y\right] + m^2c^4\beta^2 + mc^3\left(\alpha_x p_x \beta + \alpha_y p_y \beta + \alpha_z p_z \beta\right) + \\
&\quad mc^3\left(\beta\alpha_x p_x + \beta\alpha_y p_y + \beta\alpha_z p_z\right) \\
&= c^2\left[\alpha_x^2 p_x^2 + \alpha_y^2 p_y^2 + \alpha_z^2 p_z^2 + \left(\alpha_x\alpha_y + \alpha_y\alpha_x\right)p_x p_y + \left(\alpha_y\alpha_z + \alpha_z\alpha_y\right)p_y p_z + \right. \\
&\quad \left. \left(\alpha_z\alpha_x + \alpha_x\alpha_z\right)p_z p_x\right] + m^2c^4\beta^2 + mc^3\left[\left(\alpha_x\beta + \beta\alpha_x\right)p_x + \left(\alpha_y\beta + \beta\alpha_y\right)p_y + \left(\alpha_z\beta + \beta\alpha_z\right)p_z\right]
\end{aligned}$$

Using above relation, the above eq. becomes

$$\begin{aligned}
&\left\{E^2 - c^2\left[\alpha_x^2 p_x^2 + \alpha_y^2 p_y^2 + \alpha_z^2 p_z^2 + \left(\alpha_x\alpha_y + \alpha_y\alpha_x\right)p_x p_y + \left(\alpha_y\alpha_z + \alpha_z\alpha_y\right)p_y p_z + \right.\right. \\
&\left.\left. \left(\alpha_z\alpha_x + \alpha_x\alpha_z\right)p_z p_x\right] - mc^3\left[\left(\alpha_x\beta + \beta\alpha_x\right)p_x + \left(\alpha_y\beta + \beta\alpha_y\right)p_y + \left(\alpha_z\beta + \beta\alpha_z\right)p_z\right] - m^2c^4\beta^2\right\}\psi = 0
\end{aligned}$$

This equation agrees with free particle equation

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

when $\vec{\alpha}, \beta$ satisfy the relations

$$\left.\begin{array}{c} \alpha_x^2 = \alpha_y^2 = \alpha_z^2 = 1 \\ \beta^2 = 1 \\ \alpha_x \alpha_y + \alpha_y \alpha_x = \alpha_y \alpha_z + \alpha_z \alpha_y = \alpha_z \alpha_x + \alpha_x \alpha_z = 0 \\ \alpha_x \beta + \beta \alpha_x = \alpha_y \beta + \beta \alpha_y = \alpha_z \beta + \beta \alpha_z = 0 \end{array}\right\}$$

The four quantities α_x, α_y, α_z and β anticommute (anticommutator of two operators A and B is defined as {A,B}=AB+BA) in pairs, and their squares are unity. Further,

$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}, \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$$

with $I \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $0 \equiv \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$

and $\vec{\sigma}$ are the Pauli spin matrices given by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

More precisely

$$\alpha_x = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}; \qquad \alpha_y = \begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}$$

$$\alpha_z = \begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}; \qquad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Covariant form of the Dirac equation

The relativistic Dirac equation is given as

$$i\hbar \frac{\partial \psi}{\partial t} = -i\hbar c \vec{\alpha}.\vec{\nabla} \psi + \beta m c^2 \psi$$

Multiplying by β from left, we have

$$i\hbar \beta \frac{\partial \psi}{\partial t} = -i\hbar c \beta \vec{\alpha}.\vec{\nabla} \psi + \beta^2 m c^2 \psi$$

$\beta^2 = 1$, therefore

$$i\hbar \beta \frac{\partial \psi}{\partial t} = -i\hbar c \beta \vec{\alpha}.\vec{\nabla} \psi + m c^2 \psi \qquad (1)$$

Now we introduce Dirac γ-matrices $\gamma^{\mu} \equiv (\beta, \beta\vec{\alpha})$ where μ=0, 1, 2, 3, i.e.

$$\gamma^0 = \beta$$
$$\gamma^i = \beta\alpha^k = \gamma^0\alpha^k \qquad k = 1, 2, 3$$

Using Dirac γ-matrices, eq. (1) may be written as

$$\left(i\hbar\gamma^{\mu}\frac{\partial}{\partial x^{\mu}} - mc\right)\psi = 0$$

$$or \qquad (i\hbar\gamma^{\mu}\partial_{\mu} - mc)\psi = 0$$

This eq. is the known as the covariant form of the Dirac equation.

Properties of Dirac matrices

The Dirac γ matrices satisfy the following anti commutation relations

$$\gamma^{\mu}\gamma^{\nu} + \gamma^{\nu}\gamma^{\mu} = 2g^{\mu\nu}$$

where $g^{\mu\nu}$ is metric tensor given by

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Further, since $\gamma^0 = \beta$, we have

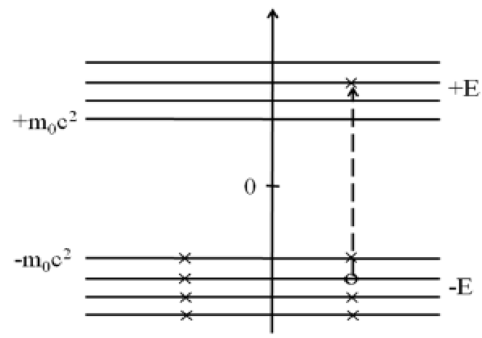
$$\gamma^{0\dagger} = \gamma^0, \quad (\gamma^0)^2 = I$$
$$\gamma^{k\dagger} = (\beta\alpha k)^{\dagger} = \alpha^k\beta = -\gamma^k$$
$$(\gamma^k)^2 = \beta\alpha^k\beta\alpha^k = -I$$

where k=1,2,3 and the superscript † denotes the Hermitian conjugate of a matrix which is obtained by interchanging the rows and columns and taking complex conjugate of each element. The Hermitian conjugation results can be summarized by

$$\gamma^{\mu\dagger} = \gamma^0\gamma^{\mu}\gamma^0$$

Positron theory

Dirac proposed that the negative energy states are occupied and the exclusion principle prevents transition into such occupied states. The normal states of the vacuum then consists of an infinite density of negative energy electrons called as negative energy sea. It is assumed that there are no electromagnetic or gravitational effects of these electrons but that deviations from the norm produced by emptying one or more of the negative energy states can be observed.



Schematic diagram showing transition from negative energy to positive energy.

The absence of a negatively charged electron that has negative mass and kinetic energy would then be expected to manifest itself as a positively charged particle that has an equal positive mass and kinetic energy. In this way, a "hole" theory or positrons can be developed without recourse to holes.

When an energy $E > 2m_0c^2$ is supplied to an electron of negative energy, it can be excited into a states of positive energy, as shown in figure . The absence of an electron of charge $-e$ and energy *-E* is interpreted as the presence of an antiparticle (a positron) of charge $+e$ and energy *+E*. Thus the net effect of this excitation is the production of pair e^--e^+.

Dirac's equation with electromagnetic potentials

Terms involving electromagnetic potentials can be added to the Dirac's relativistic in a relativistic way by making the replacements

$$c\vec{p} \to c\vec{p} - e\vec{A}$$
$$E \to E - e\phi$$

where $\vec{A}$ and ϕ are the vector and scalar potentials, respectively. Substituting in eq. Dirac equation, we get

$$\left[E - e\phi - \vec{\alpha}\cdot\left(c\vec{p} - e\vec{A}\right) - \beta mc^2\right]\psi = 0$$

Multiplying above equation by $\left[E - e\phi + \vec{\alpha}\cdot\left(c\vec{p} - e\vec{A}\right) + \beta mc^2\right]$ from the left, we get

$$\left\{(E - e\phi)^2 - \left[\vec{\alpha}\cdot\left(c\vec{p} - e\vec{A}\right)\right]^2 - m^2c^4 - (E - e\phi)\vec{\alpha}\cdot\left(c\vec{p} - e\vec{A}\right) + \vec{\alpha}\cdot\left(c\vec{p} - e\vec{A}\right)(E - e\phi)\right\}\psi = 0$$

Consider the identity

$$\left(\vec{\alpha}\cdot\vec{\beta}\right)\left(\vec{\alpha}\cdot\vec{C}\right) = \vec{B}\cdot\vec{C} + i\vec{\sigma}'\cdot\left(\vec{B}\times\vec{C}\right)$$

Replacing $\vec{B}$ and $\vec{C}$ with $\left(c\vec{p} - e\vec{A}\right)$, we get

$$\left[\vec{\alpha}\cdot\left(c\vec{p} - e\vec{A}\right)\right]^2 = \left(c\vec{p} - e\vec{A}\right)^2 + i\vec{\sigma}'\cdot\left(c\vec{p} - e\vec{A}\right)\times\left(c\vec{p} - e\vec{A}\right)$$

Now $\quad \left(c\vec{p} - e\vec{A}\right)\times\left(c\vec{p} - e\vec{A}\right) = -ce\left(\vec{A}\times\vec{p} + \vec{p}\times\vec{A}\right)$

The term $\vec{A}\times\vec{p} + \vec{p}\times\vec{A}$ can be evaluated as follows

$$\begin{aligned}
\left(\vec{A}\times\vec{p} + \vec{p}\times\vec{A}\right)\psi &= \vec{A}\times\vec{p}\,\psi + \vec{p}\times\left(\vec{A}\,\psi\right) \\
&= -i\hbar\left[\vec{A}\times\vec{\nabla}\,\psi + \vec{\nabla}\times\left(\vec{A}\,\psi\right)\right] \\
&= -i\hbar\left[\vec{A}\times\vec{\nabla}\,\psi + \vec{\nabla}\times\left(\psi\vec{A}\right)\right] \\
&= -i\hbar\left[\vec{A}\times\vec{\nabla}\,\psi + \psi\vec{\nabla}\times\vec{A} + \vec{\nabla}\,\psi\times\vec{A}\right] \\
&= -i\hbar\left(\vec{\nabla}\times\vec{A}\right)\psi \\
\left(\vec{A}\times\vec{p} + \vec{p}\times\vec{A}\right) &= -i\hbar\left(\vec{\nabla}\times\vec{A}\right)
\end{aligned}$$

Substituting, we have $\quad \left(c\vec{p} - e\vec{A}\right)\times\left(c\vec{p} - e\vec{A}\right) = ie\hbar c\vec{\nabla}\times\vec{A} = ie\hbar c\vec{B}$

where $\vec{B}$ is the magnetic field.

$$\begin{aligned}
\left[\vec{\alpha}\cdot\left(c\vec{p} - e\vec{A}\right)\right]^2 &= \left(c\vec{p} - e\vec{A}\right)^2 + i\vec{\sigma}'\cdot\left(ie\hbar c\vec{B}\right) \\
&= \left(c\vec{p} - e\vec{A}\right)^2 - e\hbar c\,\vec{\sigma}'.\vec{B}
\end{aligned}$$

Now we consider the last two terms

$$\begin{aligned}
&\left[-(E - e\phi)\vec{\alpha}\cdot\left(c\vec{p} - e\vec{A}\right) + \vec{\alpha}\cdot\left(c\vec{p} - e\vec{A}\right)(E - e\phi)\right]\psi \\
&= \left[-E\vec{\alpha}\cdot\left(c\vec{p} - e\vec{A}\right) + e\phi\vec{\alpha}\cdot\left(c\vec{p} - e\vec{A}\right) + \vec{\alpha}\cdot\left(c\vec{p} - e\vec{A}\right)E - \vec{\alpha}\cdot\left(c\vec{p} - e\vec{A}\right)e\phi\right]\psi \\
&= \left[-E\vec{\alpha}\cdot c\vec{p} + E\vec{\alpha}\cdot e\vec{A} + e\phi\vec{\alpha}\cdot c\vec{p} - e\phi\vec{\alpha}\cdot e\vec{A} + \vec{\alpha}\cdot c\vec{p}E - \vec{\alpha}\cdot e\vec{A}E - \vec{\alpha}\cdot c\vec{p}e\phi + \vec{\alpha}\cdot e\vec{A}e\phi\right]\psi \\
&= \left[e\vec{\alpha}\cdot\left(E\vec{A} - \vec{A}E\right) + ce\vec{\alpha}\cdot\left(\phi\vec{p} - \vec{p}\phi\right)\right]\psi
\end{aligned}$$

Now
$$\begin{aligned}(E\vec{A}-\vec{A}E)\psi &= E\vec{A}\psi-\vec{A}E\psi\\ &= i\hbar\frac{\partial}{\partial t}(\vec{A}\psi)-\vec{A}i\hbar\frac{\partial\psi}{\partial t}\\ &= \vec{A}i\hbar\frac{\partial\psi}{\partial t}+\left(i\hbar\frac{\partial\vec{A}}{\partial t}\right)\psi-\vec{A}i\hbar\frac{\partial\psi}{\partial t}\\ &= \left(i\hbar\frac{\partial\vec{A}}{\partial t}\right)\psi\end{aligned}$$

Further,
$$\begin{aligned}(\phi\vec{p}-\vec{p}\phi)\psi &= -\phi i\hbar\vec{\nabla}\psi+i\hbar\vec{\nabla}(\phi\psi)\\ &= -i\hbar\phi\vec{\nabla}\psi+i\hbar(\vec{\nabla}\phi)\psi+i\hbar\phi\vec{\nabla}\psi = (i\hbar\vec{\nabla}\phi)\psi\end{aligned}$$

eq. takes the form
$$\begin{aligned}-(E-e\phi)\vec{\alpha}\cdot(c\vec{p}-e\vec{A})+\vec{\alpha}\cdot(c\vec{p}-e\vec{A})(E-e\phi) &= e\vec{\alpha}\cdot\left(i\hbar\frac{\partial\vec{A}}{\partial t}\right)+ce\vec{\alpha}\cdot(i\hbar\vec{\nabla}\phi)\\ &= ie\hbar c\vec{\alpha}\cdot\left(\frac{1}{c}\frac{\partial\vec{A}}{\partial t}+\vec{\nabla}\phi\right)\\ &= -ie\hbar c\vec{\alpha}\cdot\vec{E}\end{aligned}$$

where $\vec{E}=-\frac{1}{c}\frac{\partial\vec{A}}{\partial t}-\vec{\nabla}\phi$.

Finally, substituting , we get
$$\left[(E-e\phi)^2-(c\vec{p}-e\vec{A})^2-m^2c^4+e\hbar c\vec{\sigma}'\cdot\vec{B}-ie\hbar c\vec{\alpha}\cdot\vec{E}\right]\psi=0$$

Non relativistic limit

In order to obtain the non-relativistic limit we substitute
$$E\to E'+mc^2$$
Further, we assume $E'<<mc^2$ and $e\phi<<mc^2$. Now
$$\begin{aligned}(E-e\phi)^2 &= (E'+mc^2-e\phi)^2\\ &= m^2c^4\left[1+\frac{E'-e\phi}{mc^2}\right]^2\\ &= m^2c^4\left[1+\frac{2(E'-e\phi)}{mc^2}+\text{higher order terms}\right]\end{aligned}$$
Neglecting higher order terms, we get
$$(E-e\phi)^2\approx m^2c^4+2(E'-e\phi)mc^2$$
Substituting, we get
$$\left[2(E'-e\phi)mc^2-(c\vec{p}-e\vec{A})^2+e\hbar c\vec{\sigma}'\cdot\vec{B}-ie\hbar c\vec{\alpha}\cdot\vec{E}\right]\psi=0$$
or
$$E'\psi=\left[\frac{1}{2m}\left(\vec{p}-\frac{e}{c}\vec{A}\right)^2+e\phi-\frac{e\hbar}{2mc}\vec{\sigma}'\cdot\vec{B}+\frac{ie\hbar}{2mc}\vec{\alpha}\cdot\vec{E}\right]\psi$$
Here E' is equivalent to the time derivative operator $i\hbar\frac{\partial}{\partial t}$ if a factor $\exp(-imc^2t/\hbar)$ is taken out of ψ. The term containing $\vec{B}$ has the form associated with the energy of a magnetic dipole of moment $\vec{\mu}=\frac{e\hbar}{2mc}\vec{\sigma}'$. In practical cases the term containing $\vec{E}$ is of order of $(v/c)^2$ times the $e\phi$ term and hence may be neglected in the non relativistic limit.

Dirac's equation in a central field

The electron spin carries no energy in itself. Therefore, it can be observed only through its coupling with the orbital motion of the electron. This coupling can be made visible either *through conservation of total angular momentum* or *through the spin-orbit energy*. In both cases we work with such potentials $\vec{A}$, ϕ that there is no transfer of angular momentum to the electron. This implies that we have a central field ($\vec{A}=0$ and ϕ spherically symmetric).

Spin angular momentum

Dirac's equation with electromagnetic potentials is given as

$$\left[E - e\phi - \vec{\alpha}.\left(c\vec{p} - e\vec{A}\right) - \beta mc^2\right]\psi = 0$$

With $\vec{A}(\vec{r},t)=0$ and $\phi(\vec{r},t)=\phi(r)$, we have

$$\left(E - V - c\vec{\alpha}\cdot\vec{p} - \beta mc^2\right)\psi = 0$$

$$E\psi = \left(c\vec{\alpha}\cdot\vec{p} + \beta mc^2 + V\right)\psi$$

where $V = e\phi$.

It might be expected that the orbital angular momentum $\vec{L}=\vec{r}\times\vec{p}$ is a constant of motion in such a central field. Let us investigate this point by calculating the time rate of change of $\vec{L}$ in the Heisenberg picture.

$$i\hbar\frac{dL_x}{dt} = [L_x, H] = \left[L_x, \left\{c\vec{\alpha}.\vec{p} + \beta mc^2 + V\right\}\right]$$

$$= \left[L_x, \left\{c\left(\alpha_x p_x + \alpha_y p_y + \alpha_z p_z\right) + \beta mc^2 + V\right\}\right]$$

Using commutation relations

$$[L_x, c\alpha_x p_x] = \left[L_x, \beta mc^2\right] = [L_x, V(r)] = 0$$

the above **eq. becomes**

$$i\hbar\frac{dL_x}{dt} = [L_x, c\alpha_y p_y] + [L_x, c\alpha_z p_z]$$

Now

$$\begin{aligned}
[L_x, c\alpha_y p_y] &= c\alpha_y [L_x, p_y] \\
&= c\alpha_y \left[yp_z - zp_y, p_y\right] \\
&= c\alpha_y \left\{\left[yp_z, p_y\right] - \left[zp_y, p_y\right]\right\} \\
&= c\alpha_y \left\{\left[y, p_y\right]p_z + y\left[p_z, p_y\right] - \left[z, p_y\right]p_y - z\left[p_y, p_y\right]\right\} \\
&= i\hbar c\alpha_y p_z
\end{aligned}$$

Similarly

$$\begin{aligned}
[L_x, c\alpha_z p_z] &= c\alpha_z [L_x, p_z] \\
&= c\alpha_z \left[yp_z - zp_y, p_z\right] \\
&= c\alpha_z \left\{-[z, p_z]p_y\right\}
\end{aligned}$$

$$i\hbar\frac{dL_x}{dt} = [L_x, H] = [L_x, \{c\vec{\alpha}.\vec{p} + \beta mc^2 + V\}]$$
$$= [L_x, \{c(\alpha_x p_x + \alpha_y p_y + \alpha_z p_z) + \beta mc^2 + V\}]$$

Using commutation relations $[L_x, c\alpha_x p_x] = [L_x, \beta mc^2] = [L_x, V(r)] = 0$

$$i\hbar\frac{dL_x}{dt} = [L_x, c\alpha_y p_y] + [L_x, c\alpha_z p_z]$$

Now
$$\begin{aligned}[L_x, c\alpha_y p_y] &= c\alpha_y [L_x, p_y] \\ &= c\alpha_y [yp_z - zp_y, p_y] \\ &= c\alpha_y \{[yp_z, p_y] - [zp_y, p_y]\} \\ &= c\alpha_y \{[y, p_y]p_z + y[p_z, p_y] - [z, p_y]p_y - z[p_y, p_y]\} \\ &= i\hbar c\alpha_y p_z\end{aligned}$$

Similarly
$$\begin{aligned}[L_x, c\alpha_z p_z] &= c\alpha_z [L_x, p_z] \\ &= c\alpha_z [yp_z - zp_y, p_z] \\ &= c\alpha_z \{-[z, p_z]p_y\} \\ &= -i\hbar c\alpha_z p_y\end{aligned}$$

$$i\hbar\frac{dL_x}{dt} = -i\hbar c(\alpha_z p_y - \alpha_y p_z)$$

Thus, L_x is not constant of motion.

However, on physical grounds it is possible to define total angular momentum that it is constant in a central field of force.

$$\begin{aligned}i\hbar\frac{d\sigma'_x}{dt} &= [\sigma'_x H] \\ &= [\sigma'_x, \{c\vec{\alpha}.\vec{p} + \beta mc^2 + V(r)\}] \\ &= [\sigma'_x, \{c(\alpha_x p_x + \alpha_y p_y + \alpha_z p_z) + \beta mc^2 + V(r)\}]\end{aligned}$$

Using commutation relations $[\vec{\sigma}'_x, \alpha_y] = 2i\alpha_z; [\vec{\sigma}'_x, \alpha_z] = -2i\alpha_y; [\sigma'_x, \beta] = 0; [\sigma'_x, \alpha_x] = 0$

and the fact that σ'_x commutes with p_x, p_y and p_z as $\vec{p}$ is differential operator and $\vec{\sigma}'$ are numbers, the above eq. becomes

$$\begin{aligned}i\hbar\frac{d\sigma'_x}{dt} &= [\sigma'_x, c\alpha_y p_y + c\alpha_z p_z] \\ &= c[\vec{\sigma}'_x, \alpha_y]p_y + c[\vec{\sigma}'_x, \alpha_z]p_z \\ &= 2ic(\alpha_z p_y - \alpha_y p_z)\end{aligned}$$

Multiplying by $\hbar/2$ and adding to $i\hbar\frac{d\sigma'_x}{dt}$, we have

$$i\hbar\frac{d}{dt}\left(L_x + \frac{1}{2}\hbar\sigma'_x\right) = 0$$

Defining $\vec{J} = \vec{L} + \frac{1}{2}\hbar\vec{\sigma}'$ and $\vec{S} = \frac{1}{2}\hbar\vec{\sigma}'$ we have $\vec{J} = \text{constant}$ or $[\vec{J}, H] = 0$

where $\vec{J}$ can be taken as total angular momentum and $\vec{S}$ is the spin angular momentum of electron.

References used :

1. Relativistic Quantum Mechanics by J. D. Bjorken and S. D. Drell, Mc-Graw Hill, New York,
2. Advanced Quantum Mechanics by J. J. Sakurai, Addison-Wesley New York , &
3. Quantum Mechanics by L. I. Schiff, Mc-Graw Hill, Kogakusha.

Questions

1. Obtain the Klein-Gordon equation. What were its limitations?
2. Derive the Dirac equation for a free particle and obtain its solutions.
3. Develop the Dirac equation with the inclusion of electromagnetic vector and scalar potentials and obtain its non-relativistic limit.
4. Deduce the covariant form of Dirac equation and discuss the properties of Dirac γ-matrices.
5. Derive the Dirac equation under influence of a central potential and show that spin-orbit energy appears as an automatic consequence of the Dirac equation.
6. Apply Dirac equation for a central field to study the hydrogen atom and obtain the relation for energy along with total spread in energy of fine-structure levels for a given quantum number n.
7. Discuss the positron theory and its limitations.
8. What are the identical particles and particle exchange operator? Obtain the eigenvalues of particle exchange operator.