Relativistic Quantum Mechanics

The Schrödinger eqn. for a non-relativistic particle as such cannot be applied in the case of relativistic particles. One way of arriving at the wave eqn. is to start with the relativistic expression

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

and replace the variables by operators. On using operators the above equation is transformed into

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

In this equation space and time operators appear in very different ways. In relativity theory space and time have identical role. Hence they should be appearing in a similar form in the wave equation. More over the meaning of the operator $\left(-\hbar^2 c^2\nabla^2+m^2 c^4\right)^{1/2}$ is itself unclear. Therefore the method to arrive at the wave equation is to make the operator replacing in the expression for E^2

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

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

Rearranging

$$-\hbar^2\frac{\partial^2\psi}{\partial t^2}+\hbar^2 c^2\nabla^2\psi-m^2 c^4\psi=0$$

dividing by $\hbar^2 c^2$ we get $\left[\nabla^2-\frac{1}{c^2}\frac{\partial^2}{\partial t^1}\right]\psi-\frac{m^2 c^2}{\hbar^2}\psi=0$

ie

$$\left[\Box^2-\left(\frac{mc}{\hbar}\right)^2\right]\psi=0$$

where $\square^2=\nabla^2-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}$ and is called the de-Alembertian operator.

This is known as Klein – Gordon equation.

Let $\psi(r,t)$ is a solution of Klein Gordon

$\psi(r,t)=f(t)\,e^{i\vec{k}.\vec{r}}$ $\Rightarrow$ Plane were solution.

Substituting in Klein – Gorden equation.

$$-k^2 f(t)e^{i\,k.r}-\frac{1}{c^2}f''(t)e^{i\,k.r}-\left(\frac{mc}{\hbar}\right)^2 f(t)\,e^{i\,k.r}=0$$

$$-\frac{1}{c^2}f''(t)-\left[k^2+\left(\frac{mc}{\hbar}\right)^2\right]f(t)=0$$

multiplying by -c^2

$$f''(t)+\left[c^2k^2+\frac{m^2c^4}{\hbar^2}\right]f(t)=0$$

This equation is similar to the equation of simple Harmonic motion.

The solution of this equation is

$$f(t)=A\,e^{\pm i\omega t}$$

If $A=1,\quad f(t)=e^{\pm i\omega t}$

$$\therefore\ \psi(r,t)=e^{i(k.r\pm\omega t)}$$

Where $\omega=\left[c^2k^2+\frac{m^2c^4}{\hbar^2}\right]^{1/2}$

$$p=\hbar k \qquad E=\hbar\omega$$

$$\therefore\ \psi(r,t)=e^{i\left(\frac{\vec{p}.r\pm Et}{\hbar}\right)}$$

$$E=\pm\hbar\omega=\pm\hbar\left[c^2k^2+\frac{m^2c^4}{\hbar^2}\right]^{1/2}$$

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

Hence –ve energies are also possible. One main difficulty of Klein-Gordon equation is $\psi^*\psi$ can not be interpreted as the probability density. Hence the expectation value of a dynamical variable is also not defined. H is not defined in the case of Klein – Gordan equation. If H were defined it might have been possible to write

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

Which is 1st order equation.

Dirac assumed that such a first order equation is necessary to overcome the difficulties experienced with Klein – Gordon equation. Dirac suggested such a first order equation in which time and space enter in a symmetric fashion.

Probability and current density

$$\left[\Box^2-\left(\frac{mc}{\hbar}\right)^2\right]\psi=0 \qquad \ldots\ldots\ldots(1)$$

multiplying from left by ψ^* in (1)

$$\psi^*\left(\Box^2-\frac{m^2c^2}{\hbar^2}\right)\psi=0 \qquad \ldots\ldots\ldots\ldots(2)$$

Taking complex conjugate of eqn (1) and then multiplying by ψ from the right

$$\left(\Box^2\psi^*\right)\psi-\left(\frac{m^2c^2}{\hbar^2}\psi^*\right)\psi=0 \qquad \ldots\ldots\ldots(3)$$

Subtracting (3) from (2)

$$\psi^*\left(\Box^2\psi\right)-\left(\Box^2\psi^*\right)\psi=0$$

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

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

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

or $\nabla.S+\frac{\partial p}{\partial t}=0 \qquad \ldots\ldots\ldots.(4)$

where $S=\frac{\hbar}{2im}\{\psi^*(\nabla\psi)-(\nabla\psi^*)\psi\}$, current density and

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

Eqn (4) in known as equation of continuity

Probability density p

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

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

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

$$p=\left(\frac{E}{mc^2}\right)\psi^*\psi$$

The expression for S coincides exactly with the corresponding non-relativistic expression. But p is different. It vanishes identically if ψ is real and in the case of complex wave functions, p can even be made negative by choosing $\frac{\partial\psi}{\partial t}$ appropriately. Clearly p cannot be a probability density. If we multiply p by charge e, we interpret it as a charge density, which can be positive or negative and S as the corresponding electric current density.

Dirac equation

1. Dirac Hamiltonian

The Dirac Hamiltonian for the relativistic particle is

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

Where β *and* $\vec{\alpha}$ are defined in the manner given below.

$$H^2=\left[c(\alpha_x p_x+\alpha_y p_y+\alpha_z p_z)+\beta mc^2\right]\times\left[c(\alpha_x p_x+\alpha_y p_y+\alpha_z p_z)+\beta mc^2\right]$$

They are not joint numbers otherwise the expression for H^2 will contain terms like $p_x p_y,\ p_x\beta mc^2$ ……etc. But no such term appear in the relativistic expression for

E^2. Dirac assumed that $\alpha_x, \alpha_y, \alpha_z \; and \; \beta$ do not commute among themselves. But they commute with r and p. The commutation relation of $\alpha_x, \alpha_y, \alpha_z \; and \; \beta$ were determined by requiring that H^2 should reduce of $p^2c^2+m^2c^4$ form.

$$H^2=c^2(\alpha_x p_x+\alpha_y p_y+\alpha_z p_z+Bmc) \quad (\alpha_x p_x+\alpha_y p_y+\alpha_z p_z+\beta mc)$$

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

Comparing H^2 and E^2 we get

$$\alpha^2=I \; and \; \beta^2=I$$

In the expression for E^2 there are no terms containing cross terms $\alpha_x\alpha_y, \alpha_y\alpha_z$ so on.

$$\therefore \; \alpha_x\alpha_y+\alpha_y\alpha_x=0$$

Also $\alpha_x\beta+\beta\;\alpha_x=0$

$$\alpha_y\beta+\beta\;\alpha_y=0$$

$$\alpha_z\beta+\beta\;\alpha_z=0$$

Thus $\alpha_x \; and \; \beta$ are anti commuting.

Ie $\alpha_x, \alpha_y \; and \; \alpha_z$ do not commute with β. The simplest non-commuting quantities are matrices

$\therefore \; \alpha_x, \alpha_y, \alpha_z \; and \; \beta$ are taken to be matrices with properties $\alpha_x\alpha_y=-\alpha_y\alpha_x$ etc.

Also each matrix should be Hermitian for the Hamiltonian to be hermitian

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

But $\hat{H}=c\vec{\alpha}\,p+\beta cm^2$

$$\therefore i\hbar\frac{\partial\psi}{\partial t}=[c\vec{\alpha}\,p+\beta mc^2]\psi$$

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

$$(AB)^\dagger=B^\dagger A^\dagger$$

$$-i\hbar\frac{\partial\psi^{\dagger}}{\partial t}-i\hbar c\ \nabla\psi^{\dagger}\alpha+mc^{2}\psi^{2}\beta$$

$$i\hbar\frac{\partial\psi^{\dagger}}{\partial t}=i\hbar c\ \nabla\psi^{\dagger}.\alpha-mc^{2}\psi^{\dagger}\beta \qquad \ldots\ldots\ldots\ldots(2)$$

$$i\hbar\frac{\partial}{\partial t}(\psi^{\dagger}\psi)=i\hbar\frac{\partial\psi^{\dagger}}{\partial t}.\psi+i\hbar\ \psi^{\dagger}\frac{\partial\psi}{\partial t}$$

To obtain expression for $i\hbar\frac{\partial}{\partial t}(\psi^{\dagger}\psi)$ we have to pre-multiply eqn(1) by $\psi^{\dagger}$ and post multiply eqn. (2) by ψ and add the resulting eqns.

Eqn (1) $\Rightarrow i\hbar\psi^{\dagger}\frac{\partial\psi}{\partial t}=i\hbar c\ \psi\alpha^{\dagger}.\nabla\psi+\beta mc^{2}\psi^{\dagger}\psi$

Eqn (2) $\Rightarrow i\hbar\frac{\partial\psi^{\dagger}}{\partial t}\psi=-i\hbar c\ \nabla\psi^{\dagger}\psi.\alpha=mc^{2}\psi^{\dagger}\psi\beta$

$$\therefore\ i\hbar\ \frac{\partial}{\partial t}(\psi^{\dagger}\psi)=-i\hbar c\psi^{\dagger}\alpha.\nabla\psi-i\hbar c\alpha.\nabla\psi^{\dagger}\psi$$

$$=-i\hbar c\ \psi^{\dagger}\alpha\nabla\alpha-i\hbar\ c\ \nabla\psi^{\dagger}\alpha.\psi$$

$$\frac{\partial}{\partial t}(\psi^{\dagger}\psi)=-c(\psi^{\dagger}\alpha.\nabla\psi+\nabla\psi^{\dagger}\alpha\psi)$$

$$-c\ \nabla.(\psi^{\dagger}\alpha\psi)$$

$$\frac{\partial p}{\partial t}=-\nabla.s$$

where $p=\psi^{\dagger}\psi$ $\qquad s=c(\psi^{\dagger}\alpha\psi)$

$$\frac{\partial p}{\partial t}+div\ s=0$$

So the Dirac eqn. satisfies the eqn. of continuity $p=\psi^{\dagger}\psi$ is probability density $s=c(\psi^{\dagger}\alpha\psi)$ is the probability current density.

Dirac Matrices

The eigen values of matrices obey the same algebraic equations as there obeyed by the matrix themselves. It is already shown that

$$\alpha_{x}^{2}=\alpha_{y}^{2}=\alpha_{z}^{2}=\beta^{2}=1$$

The eigen values of these matrices should be ± 1.

Also $\alpha_x = \alpha_x \beta^2 = \alpha_x \beta\beta = -\beta\alpha_x \beta$ $\quad \because \alpha_x \beta = -\beta\alpha_x$

Since the trace of a product matrix is unaltered by transferring the first matrix to the last position.

ie trace,

$$(\alpha_x) = trace\ (-\beta\alpha_x \beta) = -trace\ (\alpha_x \beta^2)$$

$$= -trace\ (\alpha_x)$$

ie

$$trace\ \ of\ \ (\alpha_x) = -trace\ \ of\ \ (\alpha_x)$$

ie

$$trace\ (\alpha_x) = 0$$

similarly,

$$trace(\alpha_y) = 0$$

$$trace(\alpha_z) = 0$$

$\therefore \alpha_x$ must have the sane number of +1 or -1 along the diagonal. If the matrices are in diagonalized form, the diagonal elements are eigen values. Since the trace is zero, the number of elements along the diagonal must be even (1 + -1= 0, 1 + -1 + 1 - 1 = 0). The simple even order non-zero matrices are 2 × 2 matrices. We can find three anti commuting matrices satisfying all the conditions described alone. They are the Pauli's spin matrices.

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

They have the property $\sigma_x \sigma_y = -\sigma_y\ \sigma_x$

$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I,$ unit matrix and trace = 0.

But if we try to find a fourth matrix satisfying the above conditions all the elements in that matrix will be zero. Hence we cannot get four different 2 × 2 matrices satisfying all the conditions. The next probability is taking 4 × 4 matrices. We can see that the following four matrices satisfy all the conditions.

$$\alpha_x=\begin{pmatrix}0&0&0&1\\0&0&1&0\\0&1&0&0\\1&0&0&0\end{pmatrix},\quad \alpha_y=\begin{pmatrix}0&0&0&-1\\0&0&i&0\\0&-i&0&0\\i&0&0&0\end{pmatrix},\quad \alpha_z=\begin{pmatrix}0&0&1&0\\0&0&0&-1\\1&0&0&0\\1&-1&0&0\end{pmatrix}$$

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

ie

$$\alpha_x=\begin{pmatrix}0&\sigma_x\\\sigma_x&0\end{pmatrix},\quad \alpha_y=\begin{pmatrix}0&\sigma_y\\\sigma_y&0\end{pmatrix},\quad \alpha_z=\begin{pmatrix}0&\sigma_z\\\sigma_z&0\end{pmatrix}\text{ and }\beta_x=\begin{pmatrix}I&0\\0&-I\end{pmatrix}$$

Where ”0” is a null matrix of order 2 × 2

$$\alpha_x^2=\begin{pmatrix}0&\sigma_x\\\sigma_x&0\end{pmatrix}\begin{pmatrix}0&\sigma_x\\\sigma_x&0\end{pmatrix}=\begin{pmatrix}\sigma_x^2&0\\0&\sigma_x^2\end{pmatrix}=\begin{pmatrix}I&0\\0&I\end{pmatrix}$$

ie, $\sigma_x^2=I$

$$\alpha_y\alpha_x=\begin{pmatrix}0&\sigma_y\\\sigma_y&0\end{pmatrix}\begin{pmatrix}0&\sigma_x\\\sigma_x&0\end{pmatrix}=\begin{pmatrix}\sigma_x\sigma_y&0\\0&\sigma_x\sigma_y\end{pmatrix}$$

$$\alpha_x\alpha_y=\begin{pmatrix}0&\sigma_y\\\sigma_y&0\end{pmatrix}\begin{pmatrix}0&\sigma_y\\\sigma_y&0\end{pmatrix}=\begin{pmatrix}\sigma_y\sigma_x&0\\0&\sigma_y\sigma_x\end{pmatrix}$$

$$\alpha_x\alpha_y-\alpha_y\alpha_x=\begin{pmatrix}\sigma_y\sigma_x&0\\0&\sigma_y\sigma_x\end{pmatrix}-\begin{pmatrix}\sigma_x\sigma_y&0\\0&\sigma_x\sigma_y\end{pmatrix}$$

Now $$\sigma_x\sigma_y=\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}0&-i\\i&0\end{pmatrix}=\begin{pmatrix}i&0\\0&-i\end{pmatrix}$$

$$=i\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}=i\sigma_x$$

$$\sigma_x\sigma_y=i\sigma_z$$

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

$$\sigma_y\sigma_x=-i\ \sigma_z$$

$$\alpha_x\alpha_y-\alpha_y\alpha_x=\begin{bmatrix}\sigma_x\sigma_y-\sigma_y\sigma_x & O\\ 0 & \sigma_x\sigma_y-\sigma_y\sigma_x\end{bmatrix}$$

$$=\begin{pmatrix}2i\sigma_z & 0\\ 0 & 2i\sigma_z\end{pmatrix}=2i\begin{pmatrix}\sigma_z & 0\\ 0 & \sigma_z\end{pmatrix}$$

$$\alpha_x\alpha_y-\alpha_y\alpha_x=2i\sum_z$$

So $[\alpha_x,\ \alpha_y]=2i\sum_z$

$$\alpha_x\alpha_y+\alpha_y\alpha_x=\begin{bmatrix}\sigma_x\sigma_y+\sigma_y\sigma_x & O\\ 0 & \sigma_x\sigma_y+\sigma_y\sigma_x\end{bmatrix}$$

$$=\begin{pmatrix}0 & 0\\ 0 & 0\end{pmatrix}$$

$[\alpha_x,\ \alpha_y]_+=0$ anti-commutator.

Any other set of 4 × 4 matrices satisfying the above equation can be brought to above form by similarity transformation. So all other 4 × 4 matrices are equivalent to above 4 matrices Higher order matrices of order 8, 16………. Can be found for α and β.

Plane wave solution for Dirac Equation:

The dirac equation is

$$i\hbar\frac{\partial\psi}{\partial t}=\left[-i\hbar c.\vec{\alpha}.\nabla+\beta mc^2\right]\psi \qquad \text{…………(1)}$$

Let the solution be

$$\psi(r,t)=U(p)\, e^{i\left(\frac{p.r-Et}{\hbar}\right)} \qquad \text{…………..(2)}$$

$$\frac{d\psi}{dt}=\frac{-iE}{\hbar}u(p)\; e^{i\left(\frac{p.r-Et}{\hbar}\right)} \qquad \text{…………….(3)}$$

and $\nabla\psi=\frac{ip}{\hbar}u(p)\; e^{i\left(\frac{p.r-Et}{\hbar}\right)}$

Substitute (2) and (3) in (1) and canceling $e^{-\left(\frac{p.r-Et}{\hbar}\right)}$

$$E\; u(p)=(c\vec{\alpha}.\hat{p}+\beta mc^2)u(p) \qquad \text{……………….(4)}$$

Since $\vec{\alpha}$ *and* β are 4 × 4 matrices the wave function u(p) on which these matrices operate must be have four element column.

Let u(p) be represented by

$$u(p)\rightarrow\begin{bmatrix}u_1\\u_2\\u_3\\u_4\end{bmatrix}\rightarrow\begin{bmatrix}u\\w\end{bmatrix} \quad \text{where} \quad u=\begin{bmatrix}u_1\\u_2\end{bmatrix},\; w=\begin{bmatrix}u_3\\u_4\end{bmatrix}$$

$$\alpha.p=\begin{bmatrix}0 & \sigma.p\\ \sigma.p & 0\end{bmatrix}$$

Substituting there in eqn. (4) we get.

$$E\begin{bmatrix} u \\ w \end{bmatrix} = c\begin{bmatrix} 0 & \sigma . p \\ \sigma . p & 0 \end{bmatrix}\begin{bmatrix} u \\ w \end{bmatrix} + mc^2\begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix}\begin{bmatrix} u \\ w \end{bmatrix}$$

$$E\upsilon = C(\sigma . p)w + mc^2\upsilon \quad \ldots\ldots\ldots\ldots\ldots.(5)$$

$$E\omega = C(\sigma . p)\upsilon + mc^2\omega \quad \ldots\ldots\ldots\ldots\ldots.(6)$$

Eqn. (7) × (E + mc^2)

$$(E^2 - m^2c^4)\upsilon = c(\sigma . p)\omega(E + mc^2)$$

$$= c(\sigma . p)\omega . c(\sigma . p)\frac{\upsilon}{\omega} \quad \{sub\ from\ (8)$$

ie $$(E^2 - m^2c^4)\upsilon = c^2(\sigma . p)^2\upsilon \quad \ldots\ldots\ldots\ldots.(9)$$

$$(\sigma . p)^2 = (\sigma_n p_x + \sigma_y p_y + \sigma_z p_z)(\sigma_x p_x + \sigma_y p_y + \sigma_z p_z)$$

$$= p^2$$

ie $$(E^2 - m^2c^4)\upsilon = c^2p^2\upsilon$$

$$(E^2 - m^2c^4 - c^2p^2)\upsilon = 0 \quad \ldots\ldots\ldots\ldots\ldots\ldots.(10)$$

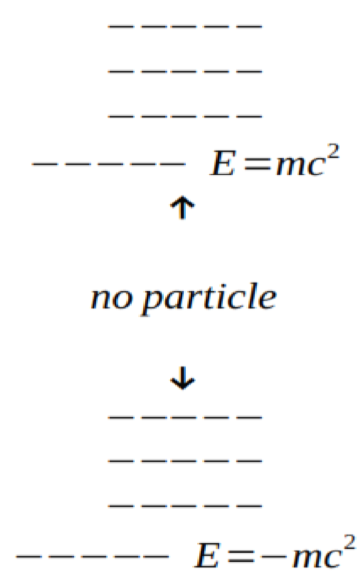
This is valid for any arbitrary column matrix

Then

$$E^2 - m^2c^4 - c^2p^2 = 0$$

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

$$\therefore\ E = \pm\sqrt{c^2p^2 + m^2c^4} \quad \ldots\ldots\ldots\ldots\ldots(11)$$



The energy spectrum of Dirac particle Consists of two branches corresponding To the two signs. The +ve branch And extends $to +\infty$ when $|p| \to \infty$ While the negative

Energy begins at E = -mc^2 and goes down $t-\infty$ as $|p|\to\infty$. There is a forbidden gap of width 2mc^2 between two branches with in which no energy level exists.

From (7) – (8)

$$[E-mc^2)\upsilon=c(\sigma,\ p)\ w \qquad \ldots\ldots\ldots\ldots(7)$$

$$[E+mc^2)]\omega=c(\sigma,\ p)\upsilon \qquad \ldots\ldots\ldots\ldots(8)$$

Either υ *or* ω can be arbitrary two component column. The simplest way is which two element arbitrary column can be selected in either as $\begin{bmatrix}0\\1\end{bmatrix}$ or $\begin{bmatrix}1\\0\end{bmatrix}$

Let $\upsilon=\begin{bmatrix}1\\0\end{bmatrix}$

To determine +ve energy solutions, the equation $(E+mc^2)\omega=c(\sigma.p)u$ is used the other equation is not useful because for E = mc^2 corresponding p = 0 the equation becomes in determinate. +ve energy levels are designated by E_+ and –ve energy states by E_-

ie $[E_- - mc^2)\upsilon=c(\sigma.p)\omega \qquad \ldots\ldots\ldots\ldots(12)$

$$(E_+ + mc^2]\omega=c(\sigma.p)\upsilon \qquad \ldots\ldots\ldots\ldots(13)$$

$$\therefore\ \omega=\frac{c(\sigma.p)\upsilon}{E_+ + mc^2} \qquad \ldots\ldots\ldots\ldots(14)$$

and $\upsilon=\dfrac{c(\sigma.p)\upsilon}{(E-mc^2)}$

$$\upsilon=-\frac{c(\sigma.p)\upsilon}{E_+ + mc^2} \qquad \to(16)$$

$$E_+=+(c^2p^2=m^2c^4)^{1/2}$$

$$E_-=-(c^2p^2+m^2c^3)^{1/2}$$

Since $E_+ = -E_-$

For eqn. (14) two independent solution are possible since there are two linearly independent possibilities for the two component column υ. The simplest forms for the two columns are $\begin{bmatrix}0\\1\end{bmatrix}$ or $\begin{bmatrix}1\\0\end{bmatrix}$

$$\sigma . p = \sigma_x p_x + \sigma_y p_y + \sigma_z p_z$$

$$\sigma . p = \begin{bmatrix}0 & 1\\1 & 0\end{bmatrix} p_x + \begin{bmatrix}0 & -1\\i & 0\end{bmatrix} p_y + \begin{bmatrix}1 & 0\\0 & -1\end{bmatrix} p_z$$

$$\sigma . p = \begin{bmatrix}p_z & p_x - ip_y\\p_x + ip_y & -p_z\end{bmatrix} \quad \ldots\ldots\ldots..(17)$$

Let $p_x + ip_y = p_+$ and $p_x - ip_y = p_-$

$$\sigma . p = \begin{bmatrix}p_z & p_-\\p_+ & -p_z\end{bmatrix} \quad \ldots\ldots\ldots\ldots(18)$$

Substituting (18) in eqn. (14) and taking $\upsilon \ as \begin{bmatrix}0\\1\end{bmatrix}$

$$\omega = \frac{c}{E_+ + mc^2} \times \begin{bmatrix}p_z & p_-\\p_+ & -p_z\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix}$$

$$\omega \rightarrow \begin{bmatrix}\frac{cp_z}{E_+ + mc^2}\\ \frac{cp_+}{E_+ + mc^2}\end{bmatrix}$$

$$\therefore \ u \rightarrow \begin{bmatrix}\upsilon\\ \omega\end{bmatrix} \qquad u_I \rightarrow \begin{bmatrix}1\\0\\ \frac{cp_z}{E_+ + mc^2}\\ \frac{cp_+}{E_+ + mc^2}\end{bmatrix}$$

If $u = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

$$\omega \rightarrow \begin{bmatrix} \frac{cp_-}{E_+ + mc^2} \\ \frac{-cp_z}{E_+ + mc^2} \end{bmatrix}$$

$$\therefore \; u \rightarrow \begin{bmatrix} \upsilon \\ \omega \end{bmatrix} \qquad u_{II} \rightarrow \begin{bmatrix} 1 \\ 0 \\ \frac{cp_-}{E_+ + mc^2} \\ \frac{cp_z}{E_+ + mc^2} \end{bmatrix}$$ There are for +ve energy states.

Using eqn. (16) and proceeding in same manner we get solutions for –ve energy states as

$$\therefore \; u_{III} \rightarrow \begin{bmatrix} \frac{-cp_z}{E_+ + mc^2} \\ \frac{-cp_+}{E_+ + mc^2} \\ 1 \\ 0 \end{bmatrix} \qquad \therefore \; u_{IV} \rightarrow \begin{bmatrix} \frac{-cp_-}{E_+ + mc^2} \\ \frac{cp_z}{E_+ + mc^2} \\ 0 \\ 1 \end{bmatrix}$$

To normalize u, taking u_I

$$Nu^\dagger Nu = 1$$

ie $N^2 u^\dagger u = 1$

$$N=\left[\frac{1}{2}\left[1+\frac{mc^2}{E_+}\right]\right]^{1/2}$$

$$N^2\begin{bmatrix}1 & 0 & \frac{c\ p_z}{E_++mc^2} & \frac{c\ p_-}{E_++mc^2}\end{bmatrix}\begin{bmatrix}1\\0\\\frac{cp_z}{E_++mc^2}\\\frac{cp_+}{E_++mc^2}\end{bmatrix}=1$$

$$N^2\left[1+0+\frac{c^2p_z^2}{(E_++mc^2)^2}+\frac{c^2p_-^2}{(E_++mc^2)^2}\right]=1$$

$$N^2\left[1+\frac{c^2(p_x^2+p_y^2+p_z^2)}{(E_++mc^2)^2}\right]=1$$

$$N^2.\left[1+\frac{c^2\boldsymbol{p}^2}{(E_++mc^2)^2}\right]=1$$

$$N^2\left[\frac{(E_++mc^2)^2+c^2\boldsymbol{p}^2}{(E_++mc^2)^2}\right]=1$$

$$N^2\left[\frac{2E_+^2+2E_+mc^2}{(E_++mc^2)^2}\right]=1$$

$$N^2\,2E_+\frac{(E_++mc^2)}{(E_++mc^2)^2}=1$$

$$\frac{N^2\ 2E_+}{E_++mc^2}=1 \qquad N^2\times\frac{1}{\frac{1}{2}\left[1+\frac{mc^2}{E_+}\right]}=1$$

$$\therefore\ N=\left[\frac{1}{2}\left(1+\frac{mc^2}{E_+}\right)\right]^{1/2}$$

The spin of the Dirac particle

For an isolated system angular momentum is to be a conserved quantity. We have to verify whether it is conserved in the case of Dirac's particle. In the Schrödinger picture for an operator $\hat{A}$

$$\frac{dA}{dt}=\frac{1}{i\hbar}[A.H]+\frac{\partial A}{\partial t}$$

$$\frac{d}{dt}L_z=\frac{1}{i\hbar}[L_z,\ H]$$

Where L_z is the z component of angular in momentum and is not a explicit function of time.

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

and $L_z=xp_y-y\ p_x$

$$i\hbar\frac{dL_z}{dt}=[x\ p_y-y\ p_x,\ c\alpha.p+\beta mc^2]$$

[α and β are not function of $p_x, p_y, p_z, x, y\ or\ z$

$$\therefore[xp_y-yp_x,\ \beta mc^2]=0$$

$$i\hbar\frac{dL_z}{dt}=[xp_y-y\ p_x,\ c(\alpha_x p_x+\alpha_y p_y+\alpha_z p_z)]$$

$$=[xp_y,c(\alpha_x p_x+\alpha_p p_y+\alpha_z p_z)]-[yp_x,\ c(\alpha_x p_x+\alpha_y p_y+\alpha_z p_z)]$$

$$[xp_y;\ c\ \alpha_x p_x]=c\alpha_x[x\ p_y.\ p_x]$$

$$[x\ p_y,\ p_x]=x[p_y,\ p_x]+[x,\ p_x]p_y$$

$$=i\hbar\ p_y$$

$$\therefore[x\ p_y,\ c\ \alpha_x p_x]=c\alpha_x\ i\hbar\ p_y$$

$$=i\hbar c\alpha_x p_y$$

$$-[y\ p_x\ ,\ c\alpha_y p_y] = ^{-} c\alpha_y [y\ p_x,\ p_y]$$

$$= -c\alpha_y .\ i\hbar\ p_x$$

$$= -i\hbar c\alpha_y p_x$$

$$[x,\ p_x] = [x,\ p_y] = [y,\ p_x] = [y,\ p_z] = 0$$

$$i\hbar \frac{d}{dt} L_z = i\hbar c\alpha_x p_y - i\hbar c\alpha_y p_x$$

$$i\hbar \frac{d}{dt} L_z = i\hbar c [\alpha_x p_y - \alpha_y p_x] \qquad \ldots\ldots\ldots\ldots(1)$$

The above equation shows that L_z is not a conserved quantity similar results hold good for L_x and L_y . Hence it can be concluded that L is not the complete angular momentum. There must be another part S such that L + S is conserved. It can be shown that if S_z is taken to be $\frac{1}{2}\hbar \Sigma_z$ where $\sum_z^1 = \begin{bmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{bmatrix}$ then $L_z + S_z$ commute with H

$$-i\alpha_x\alpha_y = -i \begin{bmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{bmatrix} \begin{bmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{bmatrix}$$

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

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

ie $\sigma_x\sigma_y = i\sigma_z$

$$i\alpha_x\alpha_y = -i \begin{bmatrix} i\sigma_z & 0 \\ 0 & i\sigma_z \end{bmatrix} = \begin{bmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{bmatrix} = \sum_z$$

ie $-i\alpha_x\alpha_y = \Sigma_z$ ……………………….(2) $\alpha_x\alpha_y = i\Sigma_z$

$$[\alpha_z,\ \Sigma_z] = \alpha_z\Sigma_z - \Sigma_z\alpha_z$$

$$\alpha_z \sum_z^1 = \begin{bmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{bmatrix} \begin{bmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{bmatrix} = 0$$

ie $[\alpha_z, \Sigma_z]=0$ ....(3)

similarly $[\beta, \Sigma_z]=0$ ....(4)

$[\alpha_x\alpha_y, \alpha_x]=-2\alpha_y$ ....(5)

$[\alpha_x\alpha_y, \alpha_y]=2\alpha_x$ ....(6)

$$i\hbar\frac{d}{dt}\left(\frac{1}{2}\hbar\Sigma_z\right)=\left[\frac{1}{2}\hbar\Sigma_z, H\right]=\frac{1}{2}\hbar[\Sigma_z, H]$$

$$[\Sigma_z, H]=[\Sigma_z^1, c\alpha.p+\beta mc^2]$$

$$=[\Sigma_z, \alpha.p]+mc^2[\Sigma_z, \beta]$$

$$[\Sigma_z, \beta]=0$$

$$[\Sigma_z, H]=c[\Sigma_z, \alpha_x p_x+\alpha_y p_y+\alpha_z p_z]$$

$$=c[\Sigma_z, \alpha_x p]+c[\Sigma_z, \alpha_y p_y]+c[\Sigma_z, \alpha_z p_z]$$

$$[\Sigma_z, p_z]=0$$

$$[\Sigma_z, H]=c[-\alpha_x\alpha_y, \alpha_x p_x]+c[-i\alpha_x\alpha_y, \alpha_y p_y]$$

$$=-ic\ p_x[\alpha_x\alpha_y, \alpha_x]-ic\ p_y[\alpha_x\alpha_y, \alpha_y]$$

$$=ic\ p_x(-2\alpha_y)-ic\ p_y z\alpha_x$$

$$=zic\ [\alpha_y p_x-\alpha_x p_y]$$

$$\therefore\ i\hbar\frac{d}{dt}\left[\frac{1}{2}\hbar\Sigma_z\right]=\frac{1}{2}\hbar.2ic[\alpha_y p_x-\alpha_x p_y]$$

$$=i\hbar c[\alpha_y p_x-\alpha_x p_y]$$

From eqn (1)

$$i\hbar\frac{d}{dt}L_z=i\hbar c(\alpha_x p_y-\alpha_y p_x)$$

ie $i\hbar\frac{d}{dt}\left[L_z+\frac{1}{2}\hbar\Sigma_z\right]=0$

ie $i\hbar\frac{d}{dt}(L_z+s_z)=0$

L_z+s_z is a conserved quantity.

Where $S_z = \frac{1}{2}\hbar\Sigma_z$ is the spin part.

Same properties of $\Sigma_x, \Sigma_y, \Sigma_z$

$\Sigma_x = -i\alpha_y\alpha_z$ $\quad$ $\Sigma_x\Sigma_y = -i\Sigma_z$

$\Sigma_y = -i\alpha_z\alpha_x$ $\quad$ $\Sigma_y\Sigma_z = -i\Sigma_x$

$\Sigma_z = -i\alpha_x\alpha_y$ $\quad$ $\Sigma_z\Sigma_x = -i\Sigma_y$

$\Sigma_x \pm \Sigma_y \pm \Sigma_z = 1$

The eigen values of Σ_x, Σ_y *and* Σ_z can be ± 1 $S_z = \frac{1}{2}\hbar\Sigma_z^1$. The eigen values of spin angular momentum is $\pm\frac{1}{2}\hbar$.

$$S^2 \Rightarrow \left(\frac{1}{4}\hbar^2 + \frac{1}{4}\hbar^2 + \frac{1}{4}\hbar^1\right) = \frac{3}{4}\hbar^2$$

Dirac's theory is applicable only in the case of spin half particle.

Significance of negative energy states

The –ve and +ve energy values according to Dirac's Hamiltonian are

$E_- = -(c^2p^2 + m^2c^4)^{1/2}$ and

$E_+ = +(c^2p^2 + m^2c^4)^{1/2}$ respectively

The two branches of energy extend to infinity in the negative and +ve directions. The minimum value of $E_+ = mc^2$, and the maximum value of $E_- = -mc^2$.

There is an energy gap of $2mc^2$. Even a weak electromagnetic perturbation can cause a particle in the +ve energy state to undergo a transition to $E = -\infty$ releasing infinite amount energy. But no such transition takes place in nature. To overcame this difficulty regarding –ve energy sates, Dirac postulated that all negative energy states are ordinarily occupied by electrons and that this sea of negative energy states would have no physically observable effects. Since e^- obey Fermi – Dirac statistics, these occupied states cannot accommodate any more electrons. Then transition of negative energy states is forbidden.

By Supplying enough energy to an e- in a –ve energy sate the e- can be made to jump to a +ve energy state a hole can be created in the –ve energy states. The amount of energy required for this purpose must be greater than the width $2mc^2$ of the energy gap. The creation of a hole means the removal of a certain amount of –ve energy and –ve change from the sea of –ve energy states. This is equivalent to the creation of an equal amount of +ve energy and charge. Thus the hole manifests itself as a partial of charge (+e) and the energy. the e- where expulsion created the hole also become observable since it gives to the energy states. The whole process may therefore be described as the disappearance of a quantum of energy with creation of a pair of observable particles a +ve energy e- and another particle differing from the e- only in the sign of its charge. No such particle was known at the time of Dirac's theory was formulated. But it was discovered in cosmic rays and named positron.

Problem:

$$(\sigma,\ A)(\sigma,\ B)=A.B+i\sigma.(A\times B)$$

Spin – orbit energy

The Dirac Hamiltonian in a electro magnetic field is given by

$$H=C\alpha.\left(p-\frac{eA}{c}\right)+\beta mc^2+V$$

ie $H=C(\alpha.\pi)+\beta mc^2+V$

where $\pi=p-\frac{eA}{c}$

$$Eu+Hu$$

$$E\begin{bmatrix} u \\ w \end{bmatrix} = c\begin{bmatrix} 0 & \sigma & \pi \\ \sigma & \pi & 0 \end{bmatrix}\begin{bmatrix} u \\ w \end{bmatrix} + \begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix} mc^2 \begin{bmatrix} u \\ w \end{bmatrix} + V\begin{bmatrix} u \\ w \end{bmatrix}$$

ie $Eu = C(\sigma.\pi)\omega + mc^2\mu + v\mu$

ie $[E - mc^2 - V]\mu = c(\sigma.\pi)\omega$

similarly $[E + mc^2 - V]\omega = c(\sigma.\pi)\mu$

$$\therefore\ \omega = \frac{c(\sigma.\pi)\mu}{E + mc^2 - V} \qquad \ldots\ldots\ldots..(3)$$

Sub (3) in (1)

$$[E - mc^2 - V)\mu = \frac{c(\sigma.\pi)c(\sigma.\pi)\mu}{[E_e + mc^2 - V]}$$

$$[E - mc^2]\mu = V\mu + \frac{c^2(\sigma.\pi)^2\mu}{[E + mc^2 - V]}$$

By using mathematical manipulations we can show that

$$E'u = \left[\frac{p^2}{2m} + V - \frac{(p)^2}{8m^3c^2} + \frac{\hbar^2}{4m^2c^2}\left\{\nabla^2 V + \frac{\partial V}{\partial r}\frac{\partial}{\partial r}\right\} + \frac{1}{2m^2c^2}\frac{1}{r}\frac{\partial V}{\partial r}S.L\right]\mu$$

Where $E' = E - mc^2$

First two terms give the non relativistic. Hamiltonian. The next term is the lowest under relativistic correction to the K.E, $\frac{p^2}{2m}$. The last term gives the spin orbit energy which emerges automatically from Dirac's equation.

Electron in a Magnetic field

(Spin magnetic moment)

The Hamiltonian of a charged particle in an electro-magnetic field is given

$$H=\frac{\left(p-\frac{eA}{c}\right)^2}{2m}+e\varphi$$

Where U(r) = 0 since we are considering a free particle.

When there is only magnetic field $\varphi=0$. Then Dirac Hamiltonian is

$$H=C\alpha.\left(P-\frac{eA}{c}\right)+\beta cm^2$$

The time dependent S.E is $i\hbar\frac{\partial\psi}{\partial t}=H\psi=\left[C\alpha.\left(P-\frac{eA}{c}\right)+\beta mc^2\right]\psi$

Assuming a solution for ψ

$$\psi(r,t)=U(r)e^{\frac{-iEt}{\hbar}}$$

$$\frac{-iE}{\hbar}\times i\hbar U(r)e^{\frac{-iEt}{\hbar}}=\left[C\alpha.\pi+\beta mc^2\right]U(r)e^{\frac{-iEt}{\hbar}}$$

Where $\pi=p-\frac{eA}{c}$

$$E\ u(r)=\left[c(\alpha.\pi)+\beta mc^2\right]u(r)$$

Substituting $U\rightarrow\begin{bmatrix}u\\w\end{bmatrix}$

$$E\begin{bmatrix}u\\w\end{bmatrix}=c\begin{bmatrix}0 & \sigma & \pi\\ \sigma & \pi & 0\end{bmatrix}\begin{bmatrix}u\\w\end{bmatrix}+\begin{bmatrix}I & 0\\0 & -I\end{bmatrix}mc^2\begin{bmatrix}u\\w\end{bmatrix}$$

$$E\mu=c(\sigma.\pi)w+mc^2\mu$$

$$E\omega=c(\sigma.\pi)u-mc^2\omega$$

$$[E=mc^2]\ u=c(\sigma.\pi)w \qquad \text{.....................(1)}$$

$$[E=mc^2]\ w=c(\sigma.\pi)u \qquad \text{.....................(2)}$$

multiplying eqn (1) by E + mc^2

$$[E^2-m^2c^4]\mu=c(\sigma.\pi)w.(E+mc^2)$$

$$=c(\sigma.\pi)\omega=\frac{c(\sigma.\pi)\mu}{\omega}$$

[Sub. From (2)]

$$[E^2-m^2c^4]\mu=c^2(\sigma.\pi)^2\mu \qquad \ldots\ldots\ldots\ldots\ldots\ldots(3)$$

Using identity

$$(\sigma.A)(\sigma.B)=(A.B)+i\sigma.(A\times B)$$

If $A=B=\pi$

$$(\sigma.\pi)^2=\pi^2+i\sigma(\pi\times\pi) \qquad \ldots\ldots\ldots\ldots\ldots(4)$$

Sub (4) in (3) for $(\sigma.\pi)^2$

$$[E^2-m^2c^4]\mu=c^2[\pi^2+i\sigma.(\pi\times\pi)]\mu$$

Assume $i\sigma(\pi\times\pi)=\frac{-e\hbar}{c}\sigma.H_m$

Where H_m is the magnetic field strength

$$\left[[E-mc^2][E+mc^2]-c^2\pi^2+e\hbar c\ \sigma.H_m\right]\mu=0$$

$$[E-mc^2][E+mc^2]=(E+2mc^2-mc^2)(E-mc^2)$$

If E = mc^2 = E'

$$[E^1+2mc^2]E^1=2mc^2E^1+E^1$$

E^{12} is very small for particles where energy is close to rest man energy hence E^{12} is neglected

$$[2mc^2E^1-c^2\pi^2+e\hbar c\ \ \sigma.H_m]\mu=0 \qquad ¿by\ 2mc^2$$

$$\left[E^1-\frac{\pi^2}{2m}+\frac{e\hbar}{2mc}\sigma.H_m\right]\mu=0$$

From the second equation, for the two element column ω also we can get a similar expression, combining these two expressions we can write

$$E'\,u(r)=\left[\frac{\left(p-\frac{eA}{c}\right)^2}{2m}=\frac{e\hbar}{2mc}\sigma.H_m\right]u(r)$$

The first term is the square bracket an the RHs is the non relativistic. Hamiltonian if a spin less particle in the presence of a vector potential. The presence of spin is manifested through the 2nd term which just interaction energy of a magnetic moment M_s

$$\overrightarrow{M}_s=\frac{e\hbar}{2mc}\vec{\sigma}$$

Then Dirac's theory requires a spin mag moment of one Bohr magneton $\frac{e\hbar}{2mc}$.

To find $i\sigma.(\pi\times\pi)$

$$\pi\times\pi=\begin{bmatrix} i & j & k \\ \pi_x & \pi_y & \pi_z \\ \pi_x & \pi_y & \pi_z \end{bmatrix}$$

$$=i[\pi_y,\pi_z]+\hat{j}[\pi_z,\pi_x]+\hat{k}[\pi_x,\pi_y]$$

Taking 2 component

$$[\pi_x,\pi_y]=\left[p_x-e\frac{Ax}{c},\ p_y-\frac{eA_y}{c}\right]$$

$$=[P_x,P_y]-\frac{e}{c}[P_x,A_y]-\frac{e}{c}[A_x,P_y]+\frac{e^2}{c^2}[A_x,A_y]$$

$$[P_x,P_y]=0\quad [A_x,P_y]=0$$

Because $P_x\ P_y$ are independent

$$\frac{-e}{c}[P_x,A_y]=\frac{-e}{c}[P_xA_y-A_yP_x]\psi$$

$$=\frac{ei\hbar}{c}\left(\frac{\partial A_y\psi}{\partial x}\right)\psi-\frac{ei\hbar}{c}A_y\frac{\partial\psi}{\partial x}$$

$$=\frac{ei\hbar}{c}\left(\frac{\partial A_y}{\partial_x}\right)\psi+\frac{ei\hbar}{c}Ay\frac{\partial\psi}{\partial n}-\frac{ei\hbar}{c}Ay\frac{\partial\psi}{\partial x}$$

$$\frac{-e}{c}[P_x, A_y]=\frac{ie\hbar}{c}\frac{dA_y}{d_x}$$

$$\frac{-e}{c}[A_x, P_y]=\frac{e}{c}[P_y, A_x]=\frac{-ie\hbar}{c}\frac{dA_x}{d_y}$$

$$\hat{k}[\pi_x, \pi_y]=\frac{+ie\hbar}{c}\left[\frac{dAx}{dy}-\frac{dAy}{dx}\right]$$

$$=\frac{ie\hbar}{c}\hat{k}H_z \qquad H=\nabla\times A$$

$$\pi\times\pi=\hat{i}\frac{ie\hbar}{c}H_x+\hat{j}\frac{ie\hbar}{c}H_y+\hat{k}\frac{ie\hbar}{c}H_z$$

$$=\frac{ie\hbar}{c}\vec{H}_m \qquad H_m=i\ H_x+j\ H_y+kH_z$$

$$i\sigma.(\pi\times\pi)=i\sigma.\frac{ie\hbar}{c}H_m$$

$$i\sigma.(\pi\times\pi)=-\frac{e\hbar}{c}\sigma.H_m$$

Hydrogen Atom

The Hamiltonian for a moving e- in a control potential is given by

$$H=C\alpha.p+\beta mc^2+V(r)$$

It can be shown that

$$\frac{dG}{d\rho}+\frac{kG}{\rho}-\left\{\frac{\alpha_2}{\sqrt{\alpha_1\alpha_2}}+\frac{V}{\hbar c\sqrt{\alpha_1\alpha_2}}\right\}F=0$$

and $\frac{dF}{d\rho}+\frac{kE}{\rho}-\left\{\frac{\alpha_1}{\sqrt{\alpha_1\alpha_2}}-\frac{V}{\hbar c\sqrt{\alpha_1\alpha_2}}\right\}G=0$ ....(1)

where $\alpha_1=\frac{mc^2+E}{\hbar c}$ $\alpha_2=\frac{mc^2-E}{\hbar c}$

$\rho=\sqrt{\alpha_1\alpha_2}$ $r=\sqrt{\frac{m^2c^4-E^2}{\hbar^2c^2}}$

and $R(r)=\begin{bmatrix}\frac{1}{r}F(r)\\ \frac{1}{r}G(r)\end{bmatrix}$

In the case of a bound electron.

$V(r)=\frac{-ze^2}{r}$

Then $\frac{V}{\hbar c\sqrt{\alpha_1\alpha_2}}=\frac{-Ze^2}{\hbar c\sqrt{\alpha_1\alpha_2 r}}=\frac{-r}{\rho}$

Where $r=+\frac{ze^2}{\hbar c}=z\times Fine\,structure\,contant.$

Sub. In (1)

$$\frac{dG}{d\rho}+\frac{kG}{\rho}-\left[\frac{\alpha_x}{\sqrt{\alpha_1\alpha_2}}-\frac{r}{\rho}\right]F=0$$

$$\frac{dF}{d\rho}-\frac{kF}{\rho}-\left[\sqrt{\frac{\alpha_1}{\alpha_2}}-\frac{r}{\rho}\right]G=0$$

As in non-relativistic case we seek solutions for eqn. (2) as

$F=e^{-\rho}\rho^2\sum_{V=0}^{\infty}a_0 p^v$ $G=e^{-p}\rho^s\sum_{V=0}^{\infty}b_u\rho^r$ ....(3)

Substituting in (2) and equating coefficients of $e^{-\rho}\rho^{s+v-1}$ we get recurrence relations.

$$(s+u+k)b_r - b_{v-1} + ra_u - \sqrt{\frac{\alpha_2}{\alpha_1}}\, a_{r-1} = 0$$

$$(s+u-k)a_v - a_{v-1} - r_{a_v} - \sqrt{\frac{\alpha_1}{\alpha_2}} a_{v-1} = 0$$

for u > 0

when u = 0 eqn. becomes

$$\left.\begin{matrix}(s+k)b_0 + ra_0 = 0 \\ (s-k)a_0 - rb_0 = 0\end{matrix}\right\} \quad \ldots\ldots\ldots\ldots(5)$$

Eqn. (5) are homogeneous equations in a_0 and b_0. They will have unique solutions only if the determinant of then coefficients varnish

ie $\begin{vmatrix} r & s+k \\ s-k & -V \end{vmatrix}$

ie $S = \pm\sqrt{k^2 - r^2}$

Comparing the energy value obtained from Schrödinger theory it can be shown that

$$n > j + \frac{1}{2} = |k|$$

The minimum value in can take in unit.

Then using Dirac's they energy equations are

$$E = mc^2\left[1 - \frac{r^2}{2n^2} - \frac{r^4}{2n^3}\left(\frac{1}{|k|} - \frac{3}{4}\right) - \ldots\ldots\right]$$

The total spread in energy of the fine structure leads for a given value of n can be calculated from the above equation.

In the Dirac's them each state of hydrogen atom can be completely characterized by n, k and j.

In 1947 WE.Lamb and RC.Rutherford observed splitting between $2S_{1/2}$ and $2P_{1/2}$ states of the hydrogen atom between $2S_{1/2}$ *and* $2P_{1/2}$ states. This Lamb shift is satisfactorily accounted, if we consider the interaction of e- with the quantized radiation field.

Covariance of Dirac's equation

Let us first consider the covariance under Lorentz transformation consider two observes associated Lorentz frames $\Sigma \; and \; \Sigma^1$. The requirement is that the scalar quantities should remain the same in to system while four vectors must transform like space-time coordinates. So we require that relativistic wave eqn. for e- is primed system should look like a Dirac equation. The eqn. is $\Sigma \; and \; \Sigma$ are to be

$$\left[\gamma_p \frac{\partial}{\partial xw} + \frac{m_o c}{\hbar}\right] \psi(x_p) = 0 \qquad \ldots\ldots\ldots\ldots\ldots\ldots(1)$$

$$\left[\gamma_p \frac{\partial}{\partial x^1 p} + \frac{m_o c}{\hbar}\right] \psi(x'p) = 0 \qquad \ldots\ldots\ldots\ldots\ldots\ldots(2)$$

$\therefore \gamma_p$ are the same in both frames $x_p \; and \; x_p$ are related though

$$x_\gamma = a_{p\gamma} x'^{p} \qquad \ldots\ldots\ldots\ldots\ldots\ldots(3)$$

$$\frac{\partial \psi}{\partial x^1 p} = \frac{\partial \psi}{\partial x_v} \frac{\partial x_v}{\partial x'_p} = a_{pv} \frac{\partial \psi}{\partial x_r} \qquad \ldots\ldots\ldots\ldots\ldots\ldots(4)$$

In analogy to the transformation of a four vector. We expect that $\psi(x_p) \; and \; \psi'(x'p)$ be related by a liman transformation.

$$\psi'(x'p) = s\psi(xp) \qquad \ldots\ldots\ldots\ldots\ldots\ldots(5)$$

When S is a 4 × 4 matrix which depends only on the nature of Lorentz transformation. Eqn. (2) can be written as

$$\left[\gamma_\omega a_{\omega\gamma} \frac{\partial}{\partial x_v} + \frac{m_x}{h}\right] s\psi(x\omega) = 0$$

multiplying by S^{-1} from left,

$$\left[S^{-1}\gamma_{\omega}a_{\omega v}\frac{S\partial}{\partial x_{v}}+\frac{m.c}{\hbar}\right]\psi(x_{p})=0 \qquad \ldots\ldots\ldots\ldots\ldots..(6)$$

This is equivalent to Dirac eqn. provided we can Sinda matrix S which satisfies

$$S^{-1}\gamma_{\omega}a_{\omega v}s=\gamma_{\omega}$$

The two matrices S and s^{-1} commutes because S rearrange the components of ψ under Lorentz transformation. Where S arranges the components of a four vector,

hence $S^{-1}\gamma_{\omega}Sa_{\omega v}=\gamma_{\omega}$

multiplying by $a\lambda_{v}$ and summing over V, we have

$$\sum_{1}S^{-1}\gamma_{p}Sa_{pv}a_{\lambda v}=V_{v}a_{\lambda v}$$

$$\sum_{1}S^{-1}\gamma_{p}S\,S_{p\lambda}=\gamma_{v}a_{\lambda v}$$

$$S^{-1}\gamma_{\lambda s}=\gamma_{v}a_{\lambda v} \qquad \ldots\ldots\ldots\ldots\ldots\ldots(7)$$

The problem now reduces to find S that satisfies eqn. (7)

(1) Now assuming that the frame Σ' is obtained by a simple rotation. Of Σ about the Z axis by an angle φ we shall show that following matrix S satisfies eqn. (7)

$$S^{-e}\exp.\left[\frac{i\varphi}{2}\sigma_{12}\right] \quad \text{when} \quad \sigma_{12}=\frac{i}{2}[\gamma,\gamma_{2}]=i\gamma,\gamma_{2}$$

Now $$S=1+\left(\frac{i\varphi}{2}\right)\sigma_{12}+\frac{1}{2i}\left(\frac{i\varphi}{2}\right)^{2}\sigma_{12}^{2}e\ldots\ldots\ldots$$

$$\sigma_{12}^{2}=(\iota)^{2}\gamma_{1}\gamma_{2}\gamma_{1}\gamma_{2}$$

$$=-(-\gamma_{1}\gamma_{2}\;\gamma_{2}\gamma_{1})=+1$$

It can easily be shown that

$$S=\cos\frac{\varphi}{2}+\gamma_{1}\gamma_{2}\frac{\varphi}{2} \qquad \ldots\ldots\ldots\ldots(8)$$

$$S^{-1}=\cos\frac{\varphi}{2}-\gamma_1\gamma_2\frac{\sin\varphi}{2} \qquad \ldots\ldots\ldots\ldots.(9)$$

Sub these values in eqn. (7) we get

$$\left(\cos\frac{\varphi}{2}-\gamma_1\gamma_2\sin\frac{\varphi}{2}\right)V_\lambda\left(\cos\frac{\varphi}{2}+\gamma_1\gamma_2\sin\frac{\varphi}{2}\right)=a_{\lambda v}\lambda_v \qquad \ldots\ldots\ldots\ldots(10)$$

Let us verify eqn. (10) for $\lambda=1$ *and* $\lambda=2$

For $\lambda=1$, considering LHS if eqn(10) we have

$$\left(\frac{\cos\varphi}{2}-\gamma_1\gamma_2\sin\frac{\varphi}{2}\right)\gamma_1\left(\cos\frac{\varphi}{2}+\gamma_1\gamma_2\sin\frac{\varphi}{2}\right)$$

$$=\gamma_1\cos^2\frac{\varphi}{2}+\gamma_1\gamma_2\gamma_1\cos\varphi/_2\sin\frac{\varphi}{2}.\gamma_1\gamma_2\gamma_1\sin\frac{\varphi}{2}.\cos\frac{\varphi}{2}- \quad \gamma_1\gamma_2\gamma_1\gamma_1\gamma_2\sin^2\frac{\varphi}{2}$$

$$=\gamma_1\left[\cos^2\frac{\varphi}{2}-\sin^2\frac{\varphi}{2}\right]+\gamma_2\gamma_1\gamma_1\cos\frac{\varphi}{2}\sin\frac{\varphi}{2}+\gamma_2\sin\frac{\varphi}{2}\cos\frac{\varphi}{2}$$

$$=\gamma_1\cos\varphi+\gamma_2\sin\frac{\varphi}{2}\cos\frac{\varphi}{2}+\gamma_2\sin\frac{\varphi}{2}\cos\frac{\varphi}{2}$$

$$=\gamma_1\cos\varphi+\gamma_2\sin\varphi$$

For pure rotation

$$\alpha_{\lambda v}=\begin{bmatrix}\cos\phi & \sin\phi & 0 & 0\\ -\sin\phi & \cos\phi & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{bmatrix}$$

$$a_{11}=\cos\varphi,\ a_{12}=\sin p,\ a_{13}=0,\ a_{14}=0,\ a_{21}=-\sin\varphi,\ a_{25}=\cos\varphi$$

$$a_{33}=1,\ a_{44}=1$$

$\therefore$ Lits of eqn.(10) $=a_{11}\gamma_1+a_{22}\lambda_2+a_{13}\gamma_3+a_{14}\gamma_4$ ………….(15)

$=a_v\gamma_v$

This St S given by eqn.(8) satisfies eqn. (1)

For $\lambda=2,$ the LHS of eqn.(10) can be written as

$$\left(\cos\frac{\varphi_0}{2}-\gamma_1\gamma_2\frac{\sin\varphi}{2}\right)\gamma_2\left(\cos\frac{\varphi}{2}+\gamma_1\gamma_2\sin\frac{\varphi}{2}\right)$$

$$=\gamma_2\cos^2\frac{\varphi}{2}-\gamma_1\gamma_2\gamma_2\cos\frac{\varphi}{2}\sin\frac{\varphi}{2}+\gamma_2\gamma_1\gamma_2\cos\frac{\varphi}{2}\sin\frac{\varphi}{2}-\gamma_1\gamma_2\gamma_2\gamma_1\gamma_2\sin^2\frac{\varphi}{2}$$

$$=\gamma_2\cos^2\frac{\varphi}{2}-\gamma_2\sin^2\frac{\varphi}{2}-\gamma_1\sin\frac{\varphi}{2}\cos\frac{\varphi}{2}-\gamma_1\sin\frac{\varphi}{2}\cos\frac{\varphi}{2}$$

$$=\gamma_2\left[\cos^2\frac{\varphi}{2}-\sin^2\frac{\varphi}{2}\right]-\gamma_1\left[\sin\frac{\varphi}{2}\cos\frac{\varphi}{2}+\sin\frac{\varphi}{2}\cos\frac{\varphi}{2}\right]$$

$$=\gamma_2\cos\varphi-\gamma_1\sin\varphi$$

$$=-\gamma_1\sin\varphi+\gamma_2\cos\varphi+\gamma_3(0)_e\gamma_a(0)$$

$$a_{21}\gamma_1+a_{22}\gamma_2+a_{23}\gamma_3+a_{34}\gamma_u$$

$$=a_{2v}\gamma_v \qquad \ldots\ldots\ldots\ldots\ldots\ldots(13)$$

Thus the relation is also true for $\gamma=2.$ In this way it can be shown that the result is also same for any value of γ .

(2) Now assuming the Lorentz transformation $u'\Sigma'$ moves along the X axis wrt Σ with a velocity BC we shall ST the matrix S is given by

$$S=\exp\left[\frac{i\varphi}{2}\sigma_{14}\right];\ \sigma_{14}=i\gamma_1\gamma_4 \qquad \ldots\ldots\ldots..(14)$$

Writing $i\varphi=0$

$$S=\cosh\left(\frac{\varphi}{2}\right)-i\gamma_1\gamma_4\sinh\frac{\varphi}{2} \qquad \ldots\ldots\ldots..(15)$$

And $S^{-1}=\cosh\frac{\theta}{2}+c\ \gamma_1\gamma_4\sin h\frac{\theta}{2}$ …………(16)

The eqn. (7) now becomes

$$\left(\cosh\frac{\theta}{2}-i\gamma_1\gamma_4\sinh\frac{\theta}{2}\right)\gamma_\lambda\left(\cosh\frac{\theta}{2}+i\gamma_1\gamma_4\sinh\frac{\theta}{2}\right)=a_{\lambda v}\gamma_v \qquad \ldots\ldots\ldots\ldots..(17)$$

We shall verify this eqn. for $\lambda=1.$

LHS of eqn. (17) is given by

$$\left(\cosh\frac{\theta}{2}-i\gamma_1\gamma_4\sinh\frac{\theta}{2}\right)\gamma_1\left(\cosh\frac{\theta}{2}+i\gamma_1\gamma_4\sin\frac{h}{2}\right)$$

$$=\gamma_1\cos\hbar^2\frac{\theta}{2}+\gamma_1\gamma_4\gamma_1\gamma_1\gamma_4\sinh^2\frac{\theta}{2}-i\gamma_1\gamma_4\gamma_1\sin\frac{h\theta}{2}\cos\frac{h\theta}{2}$$

$$+i\gamma_1\gamma_1\gamma_4\sinh\frac{\theta}{2}\cosh\frac{\theta}{2}$$

$$=\gamma_1\left(\cosh^2\frac{\theta}{2}+\sinh^2\frac{\theta}{2}\right)+i\gamma_1\gamma_1\gamma_4\sinh\frac{\theta}{2}\cosh\frac{\theta}{2}+c\gamma_4\sin\frac{h\theta}{2}\cos\frac{h\theta}{2}$$

$$=\gamma.\left(\cosh^2\frac{\theta}{2}+\sinh^2\frac{\theta}{2}\right)+i\gamma_n\left(2\sin\frac{h\theta}{2}\cos\frac{h\theta}{2}\right)$$

$$=\gamma_1\cosh\frac{\theta}{2}+i\gamma_4\sin\frac{h\theta}{2}$$

$$=a_{10}\gamma_v$$

So eqn. (1) is satisfied fully.

References:

1. W.Greiner – Relativistic Quantum Mechanics (Springer).
2. McGill-University course (Fall 2012. Introduction. Quantum Mechanics) (https://www.youtube.com/watch?v=AoJ8NGImz2A&list=PLrbYZnU7vahIbpIgN1YwOmpmlTh-cRJZ5)