Bound States in the Dirac Equation

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Melaku Ayenew

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Abstract

In this thesis the framework of Dirac equation has been exploited to make a detailed study on the relativistic bound state features of Hydrogen-like atoms. The relativistic energy eigenvalues calculated in this framework show the evidence of fine structure splitting for various levels. The origin of this feature can be traced to the relativistic calculations and the spin of the electron. The interesting features of these results are that the bound states are observed to lie in the forbidden gap between $-m_0c^2 \leq E \leq +m_0c^2$. For the attractive coulomb potential used in this work the bound states were observed to start from just below the positive energy continuum (E<0). The possibility of the existence of bound states even for repulsive potential was also observed provided we give up the single particle interpretation. Such bound sates for repulsive potential start from just above the lower negative energy continuum. The non-relativistic limit ($m_0c^2 >> |\vec{p}c|$) of the Dirac equation has also been investigated in this thesis. We observe that even in this approximation the Dirac equation is able to generate the exact form of the spin-orbit interaction term. We have also exploited the non-relativistic approximation of the Dirac equation to work out the value of the electron magnetic moment.

1. Introduction

In the Schrodinger wave mechanics we assign a complex valued wave function $\psi(\vec{x},t)$ to each particle. And this wave function is assumed to satisfy the wave equation known as the Schrodinger equation. $\psi(\vec{x},t)$ is not physically observable. But we interpret $|\psi|^2 d^3\vec{x}$ to be the probability of finding the particle in a volume element $d^3\vec{x}$ at some instant of time. Starting from the Schrodinger equation it is possible to define positive definite position probability density $P(\vec{x},t)$ and current density $\vec{j}(\vec{x},t)$ that satisfies the continuity equation.

The non-relativistic quantum mechanics based on the Schrodinger wave mechanics was capable of explaining numerous physical processes in atomic and molecular domains. But one can site a number of shortcomings [1-6], that the non-relativistic Schrodinger's equation fails to account. They are

i. The Schrodinger equation is totally inconsistent with special theory of relativity [7] since it does not treat space and time on an equal footing and hence this equation can not be applied for particles moving at relativistic speeds.
ii. It can not explain the spin of an electron.
iii. Non-relativistic quantum mechanics does not explain the creation /annihilation of matter and also the existence of anti matter – the leading discoveries of the 20^{th} century.
iv. It is a one-body theory and it can not account for processes like nuclear beta decay $(n \to p + e + \bar{\nu})$, pair creation $(\gamma \to e^- + e^+)$, etc.
v. Further it can not explain the fine structure of hydrogen like atoms, which is partly due to relativistic effect of mass and partly due to the spin of the electron.

Owing to the above facts, the need to have a new theory [1-5] that overcomes these difficulties became apparent. Schrodinger made the first attempt to relativize quantum mechanics and he proposed a relativistic form of his equation, which is now called the Klein-Gordon equation. The Klein-Gordon equation fails to arrive at a positive definite position probability density since it is second order in space and time

derivatives. Moreover this equation also gives both negative and positive energy eigenvalues for a free particle. But a free particle always has positive energy and negative energy eigenvalues seem unphysical. These difficulties with the K-G equation suggested that one would have to look for another relativistic wave equation that overcomes these difficulties. Then Dirac came up with a new-relativistic wave equation in 1928 which was linear in space and time derivative, so as to ensure a positive definite position probability density. The Dirac equation was successful in overcoming some of the difficulties of the Klein Gordon equation. But it was again confronted with the appearance of negative energy eigenvalues. This time Dirac gave an explanation for the appearance of the negative energy eigenvalues, by suggesting a hole theory [8] which predicted the existence of positron which were supposed to be the antiparticle of electrons even though antiparticles were not yet discovered at that time. A few years after the publication of Dirac's work the antiparticle of electron was discovered in the cosmic rays. Dirac equation was then applied to a number of quantum mechanical problems to study their relativistic properties. The investigation of bound state features has attracted many scholars.

Among the early works in this area the study of electrons confined to 1-dimensional square well potential was first done by O.Klein [9,10]. Klein reported a very interesting and unusual behavior of Dirac's relativistic theory. He found that if one tries to confine an electron to strong external static potential, he would find oscillatory solutions in the region of the potential where one expects an exponentially decaying behavior. And even more interesting is electrons incidents on a repulsive potential seem to have finite probability of penetrating the barrier. All these peculiar results are called Klein's paradox, which are paradoxes only in the context of a single particle theory. However this paradox can be explained if one involves the participation of negative energy electrons in such process. This is again a pointer to the fact that a single particle consistent relativistic theory is impossible, and one would have to look for a many particle relativistic theory [11,12].

In another work Schiff, Snyder and Weinber [11] investigated electron bound to a square potential well. They showed that when potential is increased the energy of the 1s state decreases and at some value of the potential called critical potential the 1s state

overlaps with the lower energy continuum. This is another example of the Klein's paradox. In another investigation in this area K.N.Case [12] showed that the Dirac equation becomes singular when the point nuclear charge is 137. The energy of the 1s state is a case in point which becomes imaginary if analytically continued beyond $Z\alpha=1$.

Pomeranchuk and Smrodinsky studied [13] the problem of an electron bound to an extended nuclear charge distribution. They found that the singular behavior observed in the case of point nuclei would not happen at $Z_{cr}=137$, rather they calculated the critical nuclear charge for extended nucleus to be equal to 200. Werner and Wheeler [15] considered the property of an electron bound to a uniformly charged sphere where they found Z_{cr} =170. This differs from that obtained by Pomerancuk and Smorodinsky. This disagreement between the two values is due to the difference in the nuclear charge distribution considered in each case. A more profound study of Dirac equation was done by Pieper and Greiner [14]. They found the critical value of Z to be 169. The difference between Pieper and Greiner's value for Z_{cr} and that of Werner and Wheeler's work is mainly due to the difference choice of the nuclear radius [9].

In the modern context the Dirac equation has also been applied to study the problem of Quark confinement in the hadrons in the MIT bag model [16,17,18] where the quarks are asymptotically free and move at relativistic speeds and are trapped inside the hadronic bag. This problem has attracted much attention and has been applied to calculate the mass spectrum of mesons and baryons. It is one of the most modern and successful applications of the Dirac equation.

In this thesis we intend to solve the hydrogen like atom problem by using the relativistic Dirac equation. We employ the most general coupled differential equation for spherically symmetric potentials. The power series method of solving differential equation will be applied to obtain the relativistic energy eigenvalues and wave functions. In addition we aim to investigate the non-relativistic limit of the Dirac equation by using degenerate first order perturbation theory. We extend this idea in determining the magnetic moment of the electron.

This thesis is organized as follows: in chapter 2 we study the relativistic feature of of Klein-Gordon equation and the Dirac equation. In chapter 3 we deal with hydrogen like atom problem by using the Dirac equation. We present the investigation of the non-

relativistic limit of the Dirac equation and calculation of the magnetic moment of the electron in chapter 4. Chapter 5 of this thesis is devoted to conclusion of the results obtained in the preceding two chapters.

2. Relativistic Wave Equations

Before we see the two different attempts made to relativise quantum mechanics, it is very important to answer the question, what are the general conditions a wave equation has to satisfy to be called a relativistic wave equation?. Above of all the position probability $P(\vec{x},t)d^3\vec{x}$ has to be invariant under Lorentz transformation equations, relating the co-ordinates of an event in S' frame to the co-ordinates of the same event in S frame moving with a constant velocity $\vec{v}$ along the $x-x'$ axis that can be written as

$$\begin{aligned} x_0' &= \gamma(x_0 - \beta x_1) \\ x_1' &= \gamma(x_1 - \beta x_0) \\ x_2' &= x_2 \\ x_3' &= x_3 \end{aligned} \qquad 2.1$$

where $\beta = \frac{|\vec{v}|}{c}$, $\gamma = \frac{1}{\sqrt{1-\beta^2}}$,and $x_0 = ct$, $x_1 = x\ x_2 = y, x_3 = z$

This is because it is necessary that $P(\vec{x},t)$ must transform like the fourth component of a four current density to satisfy the continuity equation written in covariant form

$$\frac{\partial j_\mu}{\partial x_\mu} = 0 \qquad 2.2$$

where $j_\mu = (\vec{j}, j_4) = (\vec{j}, icP)$

Therefore a complete relativistic wave equation must succeed in building bilinear forms [1-5], that can be interpreted as current density $\vec{j}(\vec{x},t)$ and positive definite position probability density $P(\vec{x},t)$ which are the space and time components of the four current density j_μ respectively. We define a four vector as,

$$A_\mu = (\vec{A}, A_4) = (\vec{A}, iA_0) \qquad 2.3$$

where $\vec{A}$ is the space part and A_0 is the time part. In this section we present the two relativistic wave equations separately. Much time has been devoted for discussion of the Dirac equation because it is with this equation later we are going to solve hydrogen atom problem

2.1 The Klein-Gordon Equation

The first attempt to formulate a relativistic wave equation started from the classical relation between energy and momentum

$$p^2 - \frac{E^2}{c^2} = -m_0^2 c^2 \qquad 2.4$$

Replacing p and E by their quantum operator

$$p = -i\hbar\vec{\nabla} = -i\hbar\frac{\partial}{\partial x_i}$$

$$E = i\hbar\frac{\partial}{\partial t} = -\hbar c\frac{\partial}{\partial ict} = -\hbar c\frac{\partial}{\partial x_4} \qquad 2.5$$

and defining $x_4 = ict$, we get

$$(\quad^2 - \frac{m_0^2 c^2}{\hbar^2})\psi = 0 \qquad 2.6$$

where $^2 = \frac{\partial}{\partial x_\mu}\frac{\partial}{\partial x_\mu} = \vec{\nabla}^2 - \frac{\partial^2}{\partial x_4^2}$ is the D 'Alembertian operator. This equation is called the Klein-Gordon equation. By defining the four- momentum as

$$p_\mu = (p_i, p_4) = (p_i, i\frac{E}{c})$$

the K-G equation now takes the more compact form

$$p_\mu p_\mu \psi = -m_0^2 c^2 \psi \qquad 2.7$$

Assuming a plane wave solution of the form

$$\psi = \exp(-\frac{i}{\hbar}p_\mu x_\mu) = \exp(-\frac{i}{\hbar}(\vec{p}.\vec{x} - Et)$$

we obtain from equation (2.6)

$$E = \pm\sqrt{p^2c^2 + m_0^2c^4} \qquad 2.8$$

This shows the K-G equation yields both positive and negative energy eigenvalues. The negative energy solution was considered as unphysical and ignored, since a free particle has only positive energies. Now we can construct the four current density from equation (2.7) in the same manner as in the Schrodinger equation, we get

$$\psi^*(p_\mu p_\mu)\psi - \psi(p_\mu p_\mu)\psi^* = 0 \qquad 2.9$$

Substituting

$$p_\mu = -i\hbar\frac{\partial}{\partial x_\mu}$$

in equation (2.9) we get

$$\frac{\partial}{\partial x_\mu}[\psi^*\frac{\partial\psi}{\partial x_\mu} - \psi\frac{\partial\psi^*}{\partial x_\mu}] = 0 \qquad 2.10$$

where we define the four current density as

$$j_\mu = \psi^*\frac{\partial\psi}{\partial x_\mu} - \psi\frac{\partial\psi^*}{\partial x_\mu} \qquad 2.11$$

Now equation (2.11) satisfies the continuity equation (2.2) with

$$j_\mu = (\vec{j}, j_4) = (\vec{j}, iP)$$

$$\vec{j}(\vec{x},t) = \psi^*\frac{\partial\psi}{\partial x_i} - \frac{\partial\psi^*}{\partial x_i}\psi \qquad 2.12a$$

$$P(\vec{x},t) = -\frac{1}{c^2}\{\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\} \qquad 2.12b$$

The position probability density $P(\vec{x},t)$ and the probability current density $\vec{j}(\vec{x},t)$ act as the time and space component respectively of the probability four current density, $j_\mu(x_\mu)$. But since ψ and $\frac{\partial\psi}{\partial t}$ may take arbitrary values at any given time, the expression for position probability $P(\vec{x},t)$ may assume both positive and negative values. Therefore the position probability density is not always positive definite. Thus it can not be interpreted as a physical position probability density. It can easily be seen that the appearance of negative probability is unavoidable as long as the wave equation is quadratic in the time derivative [1], which the Klein-Gordon equation is. This is a serious drawback of this equation. However the covariance of Klein-Gordon equation follows from the invariance of the relation between momentum p and energy E under Lorentz transformations.

2.2 The Dirac Equation

The second historical attempt to develop a relativistic wave equation, which overcomes the deficiencies of Klein-Gordon equation, was made by P.A.M. Dirac in 1928. Dirac succeeded in constructing a relativistic wave equation, by imposing the requirement that the wave equation be linear in $\frac{\partial}{\partial t}$. The Dirac equation is written as

$$H_D\psi = E\psi\,; \qquad E^2 = \vec{p}^2c^2 + m_0^2c^4 \tag{2.13}$$

where $H_D = c\vec{\alpha}.\vec{p} + \beta m_0c^2$ is the Dirac Hamilitonian (where momentum and energy of the Dirac particle appears on an equal footing) and $\alpha's$ and β are traceless and hermitian operators that operate in 4-dimensional spin space. Operating H_D from the left on both sides of eq. (2.13) and equating the coefficients of $\vec{p}^2c^2$ and $m_0^2c^4$ on both sides of eq. (2.13) we get,

$$\alpha_i^2 = \beta^2 = 1$$
$$\alpha_i\alpha_j + \alpha_j\alpha_i = 2\delta_{ij}$$
$$\alpha_i\beta + \beta\alpha_i = 0$$

The only possible forms which α_i and β can take are the 4x4 matrices

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

where σ_i's are the Pauli spin matrices and 1 represent 2x2 unit matrices . Note that the wave function ψ now becomes a 4-component column vector. The Dirc equation (2.13) is then linear in both space derivatives and time derivatives and hence treats space and time on perfectly equal footing, which Special Theory of Relativity demands. We will make use of the Dirac equation in section 3 to obtain the relativistic energy spectrum of hydrogen like atoms.

2.2.1 The covariant Form of Dirac Equation

Covariant form of Dirac equation means a form that is in accordance with the demands set by the Special Theory of Relativity which treats space and time on a perfectly equal footing without giving preferential treatment to either unlike the classical Newtonian mechanics which accords a preferential treatment to the time co-ordinate giving it a unique status. To see the perfect symmetry between time and space recall the Lorentz transformation equations given by equation (2.1). From the the Dirac equation (2.13), inserting $p_i = \frac{\hbar}{i}\frac{\partial}{\partial x_i}$ we get

$$\frac{\hbar c}{i}(\alpha_1 \frac{\partial \psi}{\partial x_1} + \alpha_2 \frac{\partial \psi}{\partial x_2} + \alpha_3 \frac{\partial \psi}{\partial x_3}) + \beta m_0 c^2 \psi = i\hbar \frac{\partial \psi}{\partial t} \qquad 2.14$$

Multiplying both sides of (2.14) by $\frac{\beta}{ic}$ yields

$$(\gamma_\mu \frac{\partial}{\partial x_\mu} + \frac{m_0 c}{\hbar})\psi = 0 \qquad \text{where } \mu = 1,2,3,4 \qquad 2.15$$

where $\gamma_\mu = (\gamma_i, \gamma_4)$ $\gamma_i = -i\beta\alpha_i$ and $\gamma_4 = \beta$

are the gamma matrices. This is the covariant form of the Dirac equation. The gamma matrices satisfy the following properties on account of hermiticity of the Dirac Hamiltonian:

$$\gamma_\mu^2 = 1$$
$$\gamma_\mu^+ = \gamma_\mu$$
$$\gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\mu = 2\delta_{\mu\nu} \qquad \mu,\nu = 1,2,3,4$$
$$tr(\gamma_\mu) = 0$$

They are written explicitly as

$$\gamma_i = \begin{pmatrix} 0 & -i\sigma_i \\ i\sigma_i & 0 \end{pmatrix} \qquad \gamma_4 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

2.2.2 Plane Wave solutions and Free Dirac Spinor

Multiplying the covariant form of Dirac equation from left by $\gamma_\nu \frac{\partial}{\partial x_\nu}$

$$\gamma_\nu \gamma_\mu \frac{\partial}{\partial x_\nu} \frac{\partial \psi}{\partial x_\mu} - (\frac{m_0 c}{\hbar})^2 \psi = 0$$

Adding to this equation the same equation written in the form in which the indices μ and ν are interchanged, we have

$$(\gamma_\nu \gamma_\mu + \gamma_\mu \gamma_\nu) \frac{\partial}{\partial x_\nu} \frac{\partial}{\partial x_\mu} \psi - 2(\frac{m_0 c}{\hbar})^2 \psi = 0$$

With $(\gamma_\nu \gamma_\mu + \gamma_\mu \gamma_\nu) = 2\delta_{\mu\nu}$ this equation reduces to

$$(\ ^2 - \frac{m_0^2 c^2}{\hbar^2})\psi = 0 \qquad 2.16$$

This shows the Dirac equation admits free particle plane wave solution of the form

$$\psi = u^{(r)}(\vec{p}) \exp[\frac{i}{\hbar}(\vec{p}.\vec{x} - Et)] \qquad r = 1,2,3,4 \qquad 2.17$$

where $u^{(r)}(\vec{p})$ is a four component spinor independent of $\vec{x}$ and t.

$$u^{(r)}(\vec{p}) = \begin{pmatrix} u^{(1)}(\vec{p}) \\ u^{(2)}(\vec{p}) \\ u^{(3)}(\vec{p}) \\ u^{(4)}(\vec{p}) \end{pmatrix} \equiv \begin{pmatrix} v \\ w \end{pmatrix} \qquad 2.18$$

where

$v = \begin{pmatrix} u^{(1)}(\vec{p}) \\ u^{(2)}(\vec{p}) \end{pmatrix}$ and $w = \begin{pmatrix} u^{(3)}(\vec{p}) \\ u^{(4)}(\vec{p}) \end{pmatrix}$ are the upper and lower two component sub spinors. Inserting the plane wave solution (2.17) into the Dirac equation (2.16), we get

$$(E - m_0 c^2)v = c\vec{\sigma}.\vec{p}w \qquad 2.19a$$

$$(E + m_0 c^2)w = c\vec{\sigma}.\vec{p}v \qquad 2.19b$$

Multiplying (2.19a) by $(E + m_0 c^2)$ and substitute for $(E + m_0 c^2)w$ from (2.19b) we get

$$E = \pm\sqrt{p^2 c^2 + m_0^2 c^4} \qquad 2.20$$

Note that like the Klein-Gordon equation the Dirac equation is satisfied for both positive and negative energy eigenvalues, which we cannot ignore at all. Dirac gave an explanation for the existence of negative energies, which led him to the prediction of anti-particles. The energy eigenvalue (2.20) can be written as

$$E = E_{\pm} = \pm\sqrt{p^2c^2 + m_0^2c^4}$$

and $$E_{-} = -E_{+} = -(\sqrt{p^2c^2 + m_0^2c^4})$$

Equation (2.19) has to be satisfied for a free particle at rest as well. Thus we must have

$$w = \frac{c\vec{\sigma}.\vec{p}}{E_{+} + m_0c^2} v \qquad \text{For} \quad E > 0 \qquad 2.21a$$

$$v = \frac{-c\vec{\sigma}.\vec{p}}{E_{+} + m_0c^2} w \qquad \text{For} \quad E < 0 \qquad 2.21b$$

We can write v and w as a linear combination of the Pauli spinors for spin up and down as

$$v = \begin{pmatrix} u^{(1)}(\vec{p}) \\ u^{(2)}(\vec{p}) \end{pmatrix} = u^{(1)}(\vec{p})\begin{pmatrix} 1 \\ 0 \end{pmatrix} + u^{(2)}(\vec{p})\begin{pmatrix} 0 \\ 1 \end{pmatrix} = u^{(1)}(\vec{p})v^{(1)} + u^{(2)}(\vec{p})v^{(2)}$$
$$w = \begin{pmatrix} u^{(3)}(\vec{p}) \\ u^{(4)}(\vec{p}) \end{pmatrix} = u^{(3)}(\vec{p})\begin{pmatrix} 1 \\ 0 \end{pmatrix} + u^{(4)}(\vec{p})\begin{pmatrix} 0 \\ 1 \end{pmatrix} = u^{(3)}(\vec{p})w^{(1)} + u^{(4)}(\vec{p})w^{(2)} \qquad 2.22$$

Thus we have for $E > 0$

$$w^{(i)} = \frac{c\vec{\sigma}.\vec{p}}{E_{+} + m_0c^2} v^{(i)} \qquad i = 1,2 \qquad 2.23$$

Now,

$$c\vec{\sigma}.\vec{p}v^{(1)} = c\begin{pmatrix} p_3 \\ p_{+} \end{pmatrix}$$
$$c\vec{\sigma}.\vec{p}v^{(2)} = c\begin{pmatrix} p_{-} \\ -p_3 \end{pmatrix} \qquad \text{where } p_{\pm} = p_1 \pm ip_2 .$$

This leads us to

$$w^{(1)} = \begin{pmatrix} \dfrac{cp_3}{E_+ + m_0c^2} \\ \dfrac{cp_1}{E_+ + m_0c^2} \end{pmatrix} \qquad w^{(2)} = \begin{pmatrix} \dfrac{cp_-}{E_+ + m_0c^2} \\ \dfrac{-cp_3}{E_+ + m_0c^2} \end{pmatrix}$$

Thus the complete Dirac Spinors of a free particle for $E > 0$ are written as

$$u^{(1)}(\vec{p}) = \begin{pmatrix} v^{(1)} \\ w^{(2)} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ \dfrac{cp_3}{E_+ + m_0c^2} \\ \dfrac{cp_+}{E_+ + m_0c^2} \end{pmatrix} \quad u^{(2)}(\vec{p}) = \begin{pmatrix} v^{(2)} \\ w^{(2)} \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ \dfrac{cp_-}{E_+ + m_0c^2} \\ \dfrac{-cp_3}{E_+ + m_0c^2} \end{pmatrix} \qquad 2.24$$

Similarly equation (2.21b) can be solved to yield the Dirac spinors for $E < 0$ to be

$$u^{(3)}(\vec{p}) = \begin{pmatrix} \dfrac{-cp_3}{E_+ + m_0c^2} \\ \dfrac{-cp_+}{E_+ + m_0c^2} \\ 1 \\ 0 \end{pmatrix} \qquad u^{(4)}(\vec{p}) = \begin{pmatrix} \dfrac{-cp_-}{E_+ + m_0c^2} \\ \dfrac{cp_3}{E_+ + m_0c^2} \\ 0 \\ 1 \end{pmatrix} \qquad 2.25$$

The complete wave function now takes the form

$$\psi(\vec{x},t) = Nu^{(r)}(\vec{p}) \exp \frac{i(\vec{p}.\vec{x} - E_+t)}{\hbar} \qquad \text{Where } r = 1,2 \text{ for } E > 0 \qquad 2.26a$$

$$\psi(\vec{x},t) = Nu^{(s)}(\vec{p}) \exp \frac{i(\vec{p}.\vec{x} + E_+t)}{\hbar} \qquad \text{Where } s = 3,4 \text{ for } E < 0 \qquad 2.26b$$

And N is the normalization constant, which can easily be verified to be equal to

$$N = \sqrt{\frac{E_+ + m_0c^2}{2E}} \qquad 2.26c$$

For a Dirac particle at rest (p_i=0) the above Dirac spinors reduce to the following form.

$$u^{(1)}(0) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \qquad u^{(2)}(0) = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad \text{For E>0} \qquad 2.27a$$

$$u^{(3)}(0) = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \qquad u^{(4)}(0) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \qquad \text{For E<0} \qquad 2.27b$$

2.2.1 Lorenz Covariance of Dirac Equation

The covariance of Dirac equation means that, if we have two frames S and S', S' moving with constant velocity relative to S' along a given direction, then an observer in the S' frame will write a relativistic Dirac equation for a Dirac particle in the S' frame with wave function $\psi'(x')$. And if $\psi(x)$ is the wave function of the same particle according to an observer who is at rest in the S frame then there must exist an explicit prescription [1], which relates the wave functions of the same particle in the two frames. Then we have to show that the Dirac equation written in the S' frame is actually equivalent to the Dirac equation in the S frame. The gamma matrices are not affected by the transformation, thus an observer in the S' frame would write the Dirac equation as,

$$\gamma_\mu \frac{\partial \psi'(x'_\mu)}{\partial x_\mu} + \frac{m_0 c}{\hbar} \psi'(x'_\mu) = 0 \qquad 2.28$$

We consider a prescription, which is linear

i.e. $\psi'(x'_\mu) = S\psi(x_\mu)$

since the Lorentz transformation and the Dirac equation are linear in space-time co-ordinates here S is a 4x4 matrix, which depends on the nature of Lorentz transformations and is independent of $\vec{x}$ and t. The four differential operator transforms as

$$\frac{\partial}{\partial x'_\mu} = a_{\mu\nu} \frac{\partial}{\partial x_\nu} \quad ;$$

where $a_{\mu\nu}$ is the transformation matrix. Multiplying equation (2.28) from left by S^{-1} we obtain

$$S^{-1}\gamma_\mu S a_{\mu\nu} \frac{\partial \psi}{\partial x_\nu} + \frac{m_0 c}{\hbar} \psi = 0 \qquad 2.29$$

This equation is equivalent to the Dirac equation, if we can find an S such that

$$S^{-1}\gamma_\mu S a_{\mu\nu} = \gamma_\nu$$

Multiplying (2.29) from right by $a_{\lambda\nu}$, we get

$$S^{-1}\gamma_\lambda S a_{\mu\nu} = \gamma_\nu a_{\lambda\nu} \qquad 2.30$$

Now the problem reduces to finding the form of S, which satisfies (2.30). If we can find S the covariance of Dirac equation is then guaranteed. We seek the form of S in both proper and improper Lorentz transformation.

a. S_{Lor} in proper Lorentz Transformations

In this case we have

$$\det(\ a_{\mu\nu}\ ) = 1$$

where $a_{\mu\nu}$ is the transformation matrix. In this category we find group of all transformations of coordinates from one coordinate system into another one which moves with constant velocity in an arbitrary direction. Ordinary three-dimensional rotation and translation belong to this group. We first consider the invariance of Dirac equation under 3-dimensional rotations. From non-relativistic quantum mechanics we recall that the generator of rotation, say about the x_3 axis is given by

$$S_{rot} = \cos\frac{\theta}{2} + i\sigma_3 \sin\frac{\theta}{2}$$

To generalize in to a four-dimensional space we introduce a 4-dimensional generalization of the Pauli spin matrices

$$\Sigma_3 = -i\gamma_1\gamma_2 = \begin{pmatrix} \sigma_3 & 0 \\ 0 & \sigma_3 \end{pmatrix}$$

Then

$$S_{rot} = \cos\frac{\theta}{2} + i\Sigma_3 \sin\frac{\theta}{2} = \cos\frac{\theta}{2} + \gamma_1\gamma_2 \sin\frac{\theta}{2} \qquad 2.31$$

is the operator, which generates rotation in the (1-2) plane in the 4-dimensional Minkowiski space. We can easily check that S_{rot} given in (2.31) satisfies the equation

(2.30) for $\mu = 1,2,3,4$. Now we know that the Lorentz transformation equation (2.1) can be written as

$$\begin{aligned} x_1^{'} &= x_1 \cos(i\theta) + x_4 \sin(i\theta) \\ x_2^{'} &= x_2 \\ x_3^{'} &= x_3 \\ x_4^{'} &= -x_1 \sin(i\theta) + x_4 \cos(i\theta) \end{aligned} \qquad 2.32$$

if we set $\beta = \tanh\theta$, $\gamma = \frac{1}{\sqrt{1-\beta^2}} = \cosh\theta$ and introduce $x_4 = ict$ which is the imaginary time co-ordinate. In matrix form the Lorentz transformation equation can be written as

$$\begin{pmatrix} x_1^{'} \\ x_2^{'} \\ x_3^{'} \\ x_4^{'} \end{pmatrix} = \begin{pmatrix} \cos(i\theta) & 0 & 0 & \sin(i\theta) \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -\sin(i\theta) & 0 & 0 & \cos(i\theta) \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}$$

From equation (2.32) one can visualize the Lorentz transformation equation as a rotation by an imaginary angle $i\theta$ in Minkowiski space in the 1-4 plane. By the same analogy as S_{rot}, S_{Lor} can be constructed as

$$S_{Lor} = \cosh\frac{\theta}{2} + i\gamma_1\gamma_4 \sinh\frac{\theta}{2} \qquad 2.33a$$

Thus

$$S_{Lor}^{-1} = \cosh\frac{\theta}{2} - i\gamma_1\gamma_4 \sinh\frac{\theta}{2} \qquad 2.33b$$

Now it can easily verified that S_{Lor} and S_{Lor}^{-1} expressed through the above equations satisfies equation (2.30) for $\mu = 1,2,3,4$. This shows the invariance of Dirac equation under 3-D rotation as well as Lorentz transformations, which constitute group of proper Lorentz transformation.

b. S_{Lor} in improper Lorentz Transformation

In this category of transformations

$$\det(a_{\mu\nu}) = -1$$

This group includes space and time inversion operation. We consider here inversion (parity operation) case only where the space co-ordinates of vectors are reflected through the origin while the time co-ordinate is left untouched. This transformation is defined as

$$\begin{aligned} x_i &\rightarrow -x_i \\ t &\rightarrow t \end{aligned} \qquad (i = 1,2,3) \qquad 2.34$$

The space –time 4-vector x_μ transforms under parity operation as

$$x'_\mu = a_{\mu\nu} x_\nu$$

where $a_{\mu\nu}$ is given as

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

Now we want a prescription for the transformation of the Dirac wave function $\psi(x)$ under this parity operation. We consider again a linear relationship between the parity-operated wave function $\psi'(x')$ and $\psi(x)$.

$$\psi'(x') = S_p \psi(x)$$

where S_p is a 4x4 matrix, with this relation the Dirac equation becomes

$$-S_p^{-1}\gamma_i S_p \frac{\partial \psi}{\partial x} + S_p^{-1}\gamma_4 S_P \frac{\partial \psi}{\partial x_4} + m_0 c\psi = 0 \qquad 2.35$$

The covariance of Dirac equation under this parity operation is guaranteed if we can find an S_p such that

$$\begin{aligned} \gamma_i &= -S_p^{-1}\gamma_i S_p \\ \gamma_4 &= S_p^{-1}\gamma_4 S_p \end{aligned} \qquad 2.36$$

If we choose $S_p = \gamma_4$, then the above conditions are satisfied. Thus the covariance of Dirc equation under parity transformation is guaranteed. We note the following

$$\begin{aligned} S_p u^{(1)}(0) &= u^{(1)}(0) \\ S_p u^{(2)}(0) &= u^{(2)}(0) \\ S_p u^{(3)}(0) &= -u^{(3)}(0) \\ S_p u^{(4)}(0) &= -u^{(4)}(0) \end{aligned} \qquad 2.37$$

This shows the upper and the lower component wave functions are of opposite parities. We will exploit this property in chapter 3 when we solve the hydrogen-like problem by using the Dirac Equation.

2.2.4 Probability and Current Density

We now try to calculate the position probability and probability current density in the Dirac theory to see whether the drawbacks of the Klein-Gordon theory are overcome. Take the hermitan adjoint of the Dirac equation (2.15). Multiplying it from right by γ_4 we get

$$-\frac{\partial \overline{\psi}}{\partial x_\mu}\gamma_\mu + \frac{m_0 c}{\hbar}\overline{\psi} = 0$$

where $\overline{\psi} = \psi^+ \gamma_4$ is the adjoint spinor. Now multiplying this equation by ψ from right and the Dirac equation by $\overline{\psi}$ from left, and subtracting we get,

$$\overline{\psi}\gamma_\mu \frac{\partial \psi}{\partial x_\mu} + \frac{\partial \overline{\psi}}{\partial x_\mu}\gamma_\mu \psi = 0$$

We can write this equation as,

$$\frac{\partial}{\partial x_\mu}(ic\,\overline{\psi}\gamma_\mu\psi) = 0$$

defining $S_\mu = ic\overline{\psi}\gamma_\mu\psi$ we get

$$\frac{\partial S_\mu}{\partial x_\mu} = 0 \qquad 2.38$$

where we interpret S_μ as the four current whose space and time components are given as

$$S_\mu = (c\psi^+\vec{\alpha}\psi, ic\psi^+\psi)$$

Here we interpret

$$\vec{j}(\vec{x},t) = c\psi^+\vec{\alpha}\psi \quad \text{as the probability Current density} \qquad 2.39a$$

$$P(\vec{x},t) = \psi^+\psi \quad \text{as the position probability density} \qquad 2.39b$$

We see that $P(\vec{x},t)$ in the Dirac theory is always positive definite unlike in the Klein – Gordon theory.

2.2.5 The Hole Theory and an Explanation for the Appearance of Negative Energies

The explanation for the appearance of negative energy states in the Dirac equation was given by Dirac in 1928. According to this theory, in nature we have two energy domains. The positive, and the negative energy domains. The positive domain begins with $E = m_0c^2$ (when $\vec{p} = 0$) and extends to $+\infty$ (when $|\vec{p}| \to +\infty$). The negative energy domain starts with $E = -m_0c^2$ and extends to $-\infty$. The two energy domains are separated from each other by a forbidden gap of energy $E = 2m_0c^2$ In his original paper Dirac suggested that the negative energy states are empty and the stable electron occupies the positive energy states. But any excited atomic state will return to the ground state by radative transitions. Thus an electron in the ground state of the positive energy domain can emit spontaneously a photon of energy $\geq 2m_0c^2$ and fall in to the negative energy state [1]. Once we get the electron in the negative energy domain it will keep on making radative transitions indefinitely and keep on lowering its energy because there is no lower bound for its energy in this domain. This would imply that an atom would not be stable. But all atoms in nature are stable. Thus existence of negative energy sates was a disaster for the stability of atoms.

The way out of this catastrophe was given by Dirac in 1930. He asserted that the negative energy states are completely filled, therefore by Pauli's exclusion principle

transitions from the positive energy states to the negative ener gy states are prohibited. What we normally call vacuum is interpreted as a sea of negative energy electrons, called the Dirac Sea, that has no observable effects under normal condition. Physically observable effects appear when a photon of energy $E \geq 2m_0c^2$ is absorbed by one of the electrons in the Dirac Sea and jumps to the positive energy continuum by crossing the forbidden gap. As a result a Hole is created in the Dirac Sea [2]. The hole is interpreted as the absence of a particle with energy $-|E|$ and charge $-|e|$ and hence as the appearance of a particle of energy $|E|$ and charge $|e|$. Dirac called this particle the anti-particle of electron.

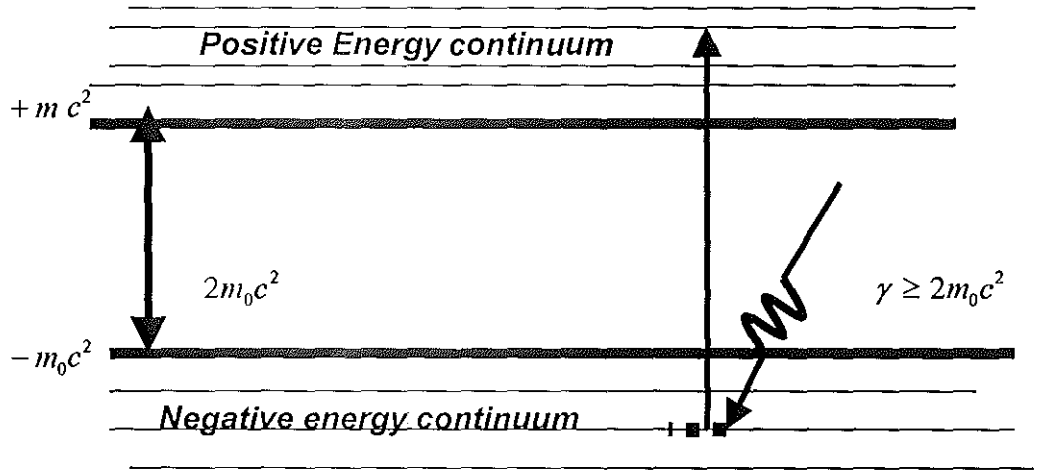

Fig.2.1 Energy spectrum of the Dirac Equation

In the beginning Dirac hoped the proton to be identified with anti particle of the electron. But this idea was not accepted, because J.R.Oppenheimer pointed it out if this interpretation was correct the hydrogen atom would undergo a self-annihilation in two photons. In addition the symmetry of Dirac equation requires the mass of the anti-particle to be the same as that of the electron. No particle was known at that time, which fit the Dirac's antiparticle description. So the hole theory seemed to be in trouble for some brief time. But in 1932 Anderson came to rescue this theory by discovering the positron, a particle with positive charge and the same mass as the electron, which is the anti particle of the electron in the cosmic rays particles. A few years later the anti-particles of proton, neutron, etc, were discovered subsequently. Now there is a strong

belief that for every particle in nature there is an anti particle. The prediction of antiparticles was one of the greatest successes of Theoretical Physics.

2.2.6 Charge Conjugation

We know from the hole theory that electrons have anti-particles called positrons. A positron is a hole in the filled Dirac Sea of electrons with negative energy. It has positive energy and the same mass as the electron. Equivalently positrons have all the properties of positively charged electrons. In this section we will try to show the complete correspondence between solutions of negative energy electrons and the positrons mathematically. We will see how the wave functions of positrons follow directly from the wave function of the negative energy electron.

For an electron interacting with an electromagnetic field the four momentum is written as

$$p_\mu \rightarrow p_\mu - \frac{e}{c} A_\mu$$

where A_μ is the four electromagnetic potentials. Replacing p_μ by its operator form we get the expression for the four differential operator in the presence of A_μ field, to be

$$\frac{\partial}{\partial x_\mu} \rightarrow \frac{\partial}{\partial x_\mu} - \frac{ie}{\hbar c} A_\mu$$

Thus the Dirac equation (2.15) for an electron of charge e, mass m_0 and wave function $\psi(\vec{x},t)$ in the presence of A_μ field takes the form,

$$\left(\frac{\partial}{\partial x_i} - \frac{ie}{\hbar c}\vec{A}\right)\gamma_i \psi(\vec{x},t) + \left(\frac{\partial}{\partial x_4} - \frac{ie}{\hbar c} A_4\right)\gamma_4 \psi(\vec{x},t) + \frac{m_0 c}{\hbar}\psi(\vec{x},t) = 0 \qquad 2.40$$

where we have separated the equation in to it's space and time components. Now let $\psi^{(c)}(\vec{x},t)$ be the wave function of a positron of mass m_0 and charge $|e|$ in same potential field A_μ. Then the Dirac equation (2.15) for positron reads,

$$\left(\frac{\partial}{\partial x_i}+\frac{ie}{\hbar c}\vec{A}\right)\gamma_i\psi^{(c)}(\vec{x},t)+\left(\frac{\partial}{\partial x_4}+\frac{ie}{\hbar c}A_4\right)\gamma_4\psi^{(c)}(\vec{x},t)+\frac{m_0c}{\hbar}\psi^{(c)}(\vec{x},t)=0 \qquad 2.41$$

There must exist a prescription that relates $\psi(\vec{x},t)$ and $\psi^{(c)}(\vec{x},t)$. Let us consider a prescription of the form.

$$\psi^{(c)}(\vec{x},t)=S_c\psi^*(\vec{x},t) \qquad 2.42$$

where S_c is a 4x4 matrix independent of $\vec{x}$ and t and $\psi^*(\vec{x},t)$ is the complex conjugate of $\psi(\vec{x},t)$. Inserting (2.42) in (2.41) and taking the complex conjugate, and multiplying it from left by S_c^{*-1} we obtain,

$$\left(\frac{\partial}{\partial x_i}-\frac{ie}{\hbar c}\vec{A}_i\right)S_c^{*-1}\gamma_iS_c^*\psi(\vec{x},t)+\left(-\frac{\partial}{\partial x_4}+\frac{ie}{\hbar c}A_4\right)S_c^{*-1}\gamma_4S_c^*\psi(\vec{x},t)+\frac{m_0c}{\hbar}\psi(\vec{x},t)=0 \qquad 2.43$$

For this equation to be equivalent to equation (2.40) one must have

$$S_{c1}^{*-1}\gamma_iS_c^*=\gamma_i \qquad (i=1,2,3)$$

And

$$S_c^{*-1}\gamma_4S_c^*=-\gamma_4$$

The above two conditions are satisfied only if S_c is chosen to be equal to γ_2 , thus we have

$$\psi^{(c)}(\vec{x},t)=\gamma_2\psi^*(\vec{x},t) \qquad 2.44$$

Now we have obtained the explicit form of the prescription that relates the wave function of the negative energy electrons and the positrons. So we can pick one of the negative energy wave functions we have obtained in section (2.2.3) for a free particle and apply (2.44) and observe the effect. Let us consider the spin down negative energy electron described by equation (2.26b) for $s=4$

$$\psi(\vec{x},t)=Nu^{(4)}(\vec{p})\exp\frac{i(\vec{p}.\vec{x}+E_+t)}{\hbar}$$

The positron wave function according to (2.44) now can be written as,

$$\psi^{(c)}(\vec{x},t)=N\gamma_2u^{(4)^*}(\vec{p})\exp\frac{-i(\vec{p}.\vec{x}+E_+t)}{\hbar}$$

$$\psi^{(e)}(\vec{x},t) = -\sqrt{\frac{E+m_0c^2}{2m_0c^2}}\begin{pmatrix} 1 \\ 0 \\ \dfrac{-cp_3}{E_+ + m_0c^2} \\ \dfrac{-cp_+}{E_+ + m_0c^2} \end{pmatrix} \exp\frac{i((-\vec{p}).\vec{x} - E_+t)}{\hbar} \qquad 2.45$$

where $u^{(4)}(\vec{p})$ has been replaced by (2.26b) and N by 2.26c. Apart from the minus sign (2.45) is just the complete wave function for positive energy electron with spin up where $\vec{p}$ is replaced by $-\vec{p}$, i.e.,

$$\psi^{(e)}(\vec{x},t) = -u^{(1)}(-\vec{p})\exp\frac{i(-\vec{p}.\vec{x} - E_+t)}{\hbar} \qquad 2.46$$

Therefore a positron is a particle of the same mass as the electron having positive energy but with opposite charge, opposite momentum and opposite spin to that of a negative energy electron in the Dirac Sea. The wave functions $\psi^{(e)}(\vec{x},t)$ and $\psi(\vec{x},t)$ are complex conjugates of each other. Thus we can interpret a negative energy electron propagating backward in time as a positron propagating forward in time. This prescription can also be applied to bosons. This prescription is made use of in devising the Feynman diagrams which are elegant tools for studying the interactions at the subatomic and subnuclear levels.

3. Relativistic Energy Spectrum of Hydrogen Like Atoms

In this section the Dirac equation would be employed to solve the hydrogen- like atom problem exactly and to study its bound state features and also to show the fine structure splitting of the spectrum more vividly. First a general problem of Dirac particle in a central Spherically symmetric potential will be considered and then we apply the results in solving the Hydrogen-like atom problem.

3.1 General Central Potential Problem

The Hamilitonian of a Dirac particle in a spherically symmetric potential $V(r)$ reads

$$H = c\vec{\alpha}.\vec{p} + \beta m_0 c^2 + V(r) \qquad 3.1$$

Investigation of the property of the orbital angular momentum of a Dirac particle is indispensable for the study of its behavior in a given potential. From the classical definition of orbital angular momentum we have,

$$\vec{L} = \vec{r} \times \vec{p} \qquad 3.2$$

whose different components take the form,

$$\begin{aligned} L_1 &= x_2 p_3 - x_3 p_2 \\ L_2 &= x_3 p_1 - x_1 p_3 \\ L_3 &= x_1 p_2 - x_2 p_1 \end{aligned} \qquad 3.3$$

If we work out the commutation of $\vec{L}$ with the Dirac Hamilitonian we find out that

$$[\vec{L}, H] = i\hbar c(\vec{\alpha} \times \vec{p}) \neq 0$$

Thus by the Heisenberg equation of motion

$$i\hbar \frac{d\vec{L}}{dt} = [L, H] = i\hbar c(\vec{\alpha} \times \vec{p}) \qquad \Rightarrow \frac{d\vec{L}}{dt} \neq 0 \qquad 3.4$$

Thus contrary to non-relativistic quantum mechanics, the orbital angular momentum of a Dirac Particle is not conserved and is no more a constant of motion. Now in equation (3.4), $\vec{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ are 4x4 matrices. Therefore if we define a 4-dimensional generalization $\vec{\Sigma}$ of the Pauli spin matrices as,

$$\vec{\Sigma} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix}$$

where $\vec{\Sigma}$ has the same properties as the 2x2 Pauli spin matrix $\vec{\sigma}$ and construct the spin angular momentum of the Dirac particle as

$$\vec{S} = \frac{\hbar}{2}\vec{\Sigma} \qquad 3.5$$

then one can easily verify that the commutator of $\vec{S}$ with H gives

$$[\vec{S}, H] = -i\hbar c(\vec{\alpha} \times \vec{p})$$

which is exactly the negative of $[\vec{L}, H]$. This actually leads to the conclusion that only if we construct the total angular momentum as a sum of the orbital angular momentum $\vec{L}$ and spin angular momentum $\vec{S}$ that we can have

$$[\vec{J}, H] = 0 \text{ and hence } \frac{d\vec{J}}{dt} = 0$$

where the total angular momentum $\vec{J}$ is defined as

$$\vec{J} = \vec{L} + \vec{S}. \qquad 3.6$$

In the non-relativistic Schrodinger-Pauli theory of the electron the spin of the electron is put into the theory by hand and there is no underlying dynamics in this theory which predicts the spin ½ nature of the electron. However here we can observe that the spin of the electron is brought out in the Dirac theory and this agrees fully with the experiment. We can thus have a meaningful relativistic theory of the electron by incorporating its spin angular momentum, $\vec{S} = \frac{1}{2}\hbar\vec{\Sigma}$. This is the inherent property of the Dirac equation.

In the non-relativistic quantum mechanics it is possible to separate the Schrodinger equation for any spherical symmetrical potential problem into radial and angular parts, and write the Hamilitonian as a function of the square of the orbital angular momentum $\vec{L}$, i.e., $H_{NR} = H(L^2)$. But in the relativistic case it is not possible to write the Hamilitonian as function of the square of the total angular momentum $\vec{J}^2$. This motivates us to define a new operator K^2. From the total angular momentum,

$$\vec{J} = \vec{L} + \frac{1}{2}\hbar\vec{\Sigma}$$

we write $\vec{J}^2$ as

$$J^2 = L^2 + \hbar\vec{\Sigma}.L + \frac{3}{4}\hbar^2 \qquad 3.7$$

We can solve for L^2 in terms of $\vec{\Sigma}.\vec{L}$, using the identity

$$(\vec{\Sigma}.\vec{A})(\vec{\Sigma}.\vec{B}) = \vec{A}.\vec{B} + i\vec{\Sigma}.(\vec{A}\times\vec{B})$$

$$(\vec{\Sigma}.\vec{L})(\vec{\Sigma}.\vec{L}) = \vec{L}.\vec{L} + i\vec{\Sigma}.(\vec{L}\times\vec{L}) \qquad 3.8$$

and $$\vec{L}\times\vec{L} = i\hbar\vec{L}$$

Solving for L^2 from (3.8), equation (3.7) can be written as

$$\vec{J}^2 + \frac{1}{4}\hbar^2 = (\vec{\Sigma}.\vec{L} + \hbar)^2 \qquad 3.9$$

Defining a new operator K such that

$$\mathrm{K}^2 = \vec{J}^2 + \frac{1}{4}\hbar^2 = (\vec{\Sigma}.\vec{L} + \hbar)^2$$

i.e., $$\mathrm{K} = \vec{\Sigma}.\vec{L} + \hbar$$

we see that this form of K does not commute with H, however if we modify K as

$$\mathrm{K} = \beta(\vec{\Sigma}.\vec{L} + \hbar) \qquad 3.10$$

we can show that K now commutes with H and K^2 is just equal to the RHS of (3.9). Therefore we can have simultaneous eigenfunctions of J^2, K^2 and H. The eigenvalue equation of J^2 is

$$J^2\psi = j(j+1)\hbar^2\psi \qquad 3.11$$

and that for K^2

$$\mathrm{K}^2\psi = (J^2 + \frac{1}{4}\hbar^2)\psi = \kappa^2\hbar^2\psi \qquad 3.12$$

where ψ are the eigenfunctions of J^2, K^2, H and κ is the eigenvalue of K, which is determined by combining (3.11) and (3.12) to yield

$$\kappa = \pm(j + \frac{1}{2}).$$

We can also write

$$\mathrm{K}\psi = \kappa\hbar\psi \qquad 3.13$$

We know that in the relativistic-quantum mechanics ψ is four component spinor, and we can split it up in to 2 two-component spinors ν and w

$$\psi = \begin{pmatrix} v \\ w \end{pmatrix} \qquad 3.14$$

where v represents the upper two components and w represents the lower two components and are (2x1) matrices. Equation (3.12) now assumes the form

$$\beta(\vec{\Sigma}.\vec{L} + \hbar)\begin{pmatrix} v \\ w \end{pmatrix} = \kappa\hbar\begin{pmatrix} v \\ w \end{pmatrix}$$

This leads to the following two important relations

$$\begin{aligned} (\vec{\sigma}.\vec{L})v &= (\kappa - 1)\hbar v \\ (\vec{\sigma}.\vec{L})w &= -(\kappa + 1)\hbar w \end{aligned} \qquad 3.15$$

Similarly equation (3.11) gives

$$\begin{aligned} \vec{L}^2 v &= \hbar^2(j(j+1) - (\kappa - 1) - \frac{3}{4})v \\ \vec{L}^2 w &= \hbar^2(j(j+1) + (\kappa + 1) - \frac{3}{4})w \end{aligned} \qquad 3.16$$

We observe that even though ψ is not an eigenfunction of $\vec{L}^2$ v and w are eigenfunctions of $\vec{L}^2$. Therefore we can write an eigenvalue equations for L^2 as

$$\begin{aligned} \vec{L}^2 v &= l_v(l_v + 1)\hbar^2 v \\ \vec{L}^2 w &= l_w(l_w + 1)\hbar^2 w \end{aligned} \qquad 3.17$$

where l_v is the eigenvalue of the orbital angular momentum for the upper wave function v and l_w is the eigenvalue of the orbital angular momentum for the lower component wave function. Equations (3.15) and (3.16) together give the table below that shows the different possible values of l_v and l_w for different eigenvalues of κ.

	$\kappa = j+\frac{1}{2}$	$\kappa = -j-\frac{1}{2}$
l_v	$j+\frac{1}{2}$	$j-\frac{1}{2}$
l_w	$j-\frac{1}{2}$	$j+\frac{1}{2}$

Table 3.1 Different eigenvalues of L_v and L_w

The Dirac equation together with the Dirac Hamilitonian (3.1) and (3.14) gives,

$$\begin{aligned}(E-V(r)-m_0c^2)v &= c\vec{\sigma}.\vec{p}w \\ (E-V(r)+m_0c^2)w &= c\vec{\sigma}.\vec{p}v\end{aligned} \qquad 3.18$$

Now we recall from equation (2.62) the parity of the upper and lower component wave functions is opposite. Thus equation (3.18) is satisfied only when v and w have opposite parities. Now let us see the effect of $\vec{\sigma}.\vec{p}$ on v and which are the two component spinors. The operator $\vec{\sigma}.\vec{p}$ can be written as

$$\vec{\sigma}.\vec{p} = \frac{(\vec{\sigma}.\vec{x})}{r^2}(\vec{\sigma}.\vec{x})\vec{\sigma}.\vec{p} = \frac{\vec{\sigma}.\vec{x}}{r^2}\left(\vec{x}.\vec{p}+i\vec{\sigma}.(\vec{x}\times\vec{p})\right)$$

where we have made use of the identity (3.8). Thus

$$\vec{\sigma}.\vec{p} = \frac{\vec{\sigma}.\vec{x}}{r^2}\left(-i\hbar r\frac{\partial}{\partial r}+i\vec{\sigma}.\vec{L}\right) \qquad 3.19$$

We separate the wave function into radial and angular parts as follows

$$\psi = \begin{pmatrix} v \\ w \end{pmatrix} = \begin{pmatrix} g(r)\Im^{j_3}_{j,l_v} \\ if(r)\Im^{j_3}_{j,l_w} \end{pmatrix}$$

where $\Im^{j_3}_{j,l}$ is the spin angular function. $\frac{\vec{\sigma}.\vec{x}}{r}$ is a pseudoscalar operator which changes only the parity of the wave function and it does not affect the quantum numbers j, j_3. of

the two component spinors v and w. Thus it only affects the angular part of the wave function. i.e.,

$$\frac{\vec{\sigma}.\vec{x}}{r}\left(\Im^{j_3}_{j,l_v}\right) = (-1)\Im^{j_3}_{j,l_w}$$

$$\frac{\vec{\sigma}.\vec{x}}{r}\left(\Im^{i_3}_{j,l_w}\right) = (-1)\Im^{i_3}_{j,l_v}$$

Putting (3.19) for $\vec{\sigma}.\vec{p}$ into the above equations, we obtain

$$\vec{\sigma}.\vec{p}g(r)\Im^{j_3}_{j,l_v} = i\hbar\frac{dg}{dr}\Im^{j_3}_{j,l_w} + i\frac{(\kappa+1)\hbar g(r)}{r}\Im^{j_3}_{j,l_w}$$

$$\vec{\sigma}.\vec{p}if(r)\Im^{j_3}_{j,l_w} = -\hbar\frac{df}{dr}\Im^{j_3}_{j,l_w} - \frac{(1-\kappa)}{\hbar}\hbar f(r)\Im^{j_3}_{j,l_v}$$

By making the substitutions

$$F(r) = rf(r) \qquad G(r) = rg(r)$$

finally we obtain the following coupled differential equations

$$\hbar c\left(\frac{dF}{dr} - \frac{\kappa}{r}F\right) = -(E - V(r) - m_0c^2)G$$

$$\hbar c\left(\frac{dG}{dr} + \frac{\kappa}{r}g\right) = (E - V(r) + m_0c^2)F \qquad 3.20$$

These coupled differential equations are the most general equations for the motion of a Dirac particle in any central potential $V(r)$ that have to be solved. We can tackle any central potential problem by using these equations. Thus our problem of solving for hydrogen like atom starts from the coupled differential equations (3.20).

3.2 The Hydrogen Like Atoms

For this particular case the central potential which is the coulomb potential between an electron and the nucleus is given by

$$V(r) = \frac{-Ze^2}{4\pi\varepsilon_0 r}$$

where Z is the atomic number. Let us make simple substitutions in (3.20)

$$\alpha_1 = \frac{m_0c^2 + E}{\hbar c} \qquad \alpha_2 = \frac{m_0c^2 - E}{\hbar c} \qquad \text{and } \beta = \frac{Ze^2}{4\pi\varepsilon_0\hbar c} = Z\alpha$$

where α is the fine structure splitting constant, thus (3.20) reduces to

$$\left(\frac{dG}{dr} + \frac{\kappa}{r}G\right) = \left(\alpha_1 + \frac{\beta}{r}\right)F$$
$$\left(\frac{dF}{dr} - \frac{\kappa}{r}F\right) = (\alpha_2 - \frac{\beta}{r})G \qquad 3.21$$

We start solving this coupled differential equation by studying its asymptotic behavior as $r \to 0$ and as $r \to \infty$. F and G must not diverge as $r \to 0$ and $r \to \infty$, with this in mind (3.21) reduces to

$$\frac{dG}{dr} = -\frac{\kappa}{r}G + \frac{\beta}{r}F$$
$$\frac{dF}{dr} = \frac{\kappa}{r}F - \frac{\beta}{r}G \qquad 3.22$$

as $r \to 0$. Let us make the following substitutions,

$$A = G + F$$
$$B = G - F$$

Then (3.22) becomes

$$\frac{dA}{dr} = -\left(\frac{\kappa}{r} + \frac{\beta}{r}\right)B$$
$$\frac{dB}{dr} = \left(-\frac{\kappa}{r} + \frac{\beta}{r}\right)A \qquad 3.23$$

Differentiating the first equation of (3.23) one more time substituting for B and $\frac{dB}{dr}$ from first and second equation of (3.23) respectively, we obtain

$$r^2\frac{d^2A}{dr^2}+r\frac{dA}{dr}+(\beta\ -\kappa^2)A=0 \qquad 3.24$$

This is Euler equation. Therefore we seek the solution in the form of

$$A\sim r^m$$

Equation (3.24) then yields

$$m=\pm\sqrt{\kappa^2-\beta^2} \qquad 3.25$$

We have to choose the positive root because the negative value of m makes the wave function divergent at $r=0$. Now we have known that G and F behaves like r^m near the origin. To study the asymptotic behavior as $r\to\infty$ we make the substitutions

$$\rho=2\sqrt{\alpha_1\alpha_2}r \qquad \sqrt{\alpha_1\alpha_2}=\sqrt{\frac{m_0^2c^4-E^2}{(\hbar c)^2}}=\lambda$$

We then obtain

$$\left(\frac{dG}{d\rho}+\frac{\kappa}{\rho}G\right)=\left(\frac{1}{2}\sqrt{\frac{\alpha_1}{\alpha_2}}+\frac{\beta}{\rho}\right)F$$
$$\left(\frac{dF}{d\rho}-\frac{\kappa}{\rho}F\right)=\left(\frac{1}{2}\sqrt{\frac{\alpha_2}{\alpha_1}}-\frac{\beta}{\rho}\right)G \qquad 3.26$$

Thus as $\rho\to\infty$ we have

$$\frac{dG}{d\rho}-\frac{1}{2}\sqrt{\frac{\alpha_1}{\alpha_2}}F=0$$
$$\frac{dF}{d\rho}-\frac{1}{2}\sqrt{\frac{\alpha_2}{\alpha_1}}G=0$$

and from these two equations it can easily be seen that F and G behave like

$$G\sim e^{\pm\frac{\rho}{2}} \qquad\qquad F\sim e^{\pm\frac{\rho}{2}}$$

as $\rho\to\infty$.We choose the negative sign because the other will make the wave function divergent as $\rho\to\infty$. The asymptotic behavior of F and G are known as $r\to 0$ and $r\to\infty$. Therefore here we are in the position to seek the complete solution in the form

$$G = \sqrt{\alpha_1}\, e^{-\frac{\rho}{2}} \left(\eta_1(\rho) + \eta_2(\rho)\right)$$
$$F = \sqrt{\alpha_2}\, e^{-\frac{\rho}{2}} \left(\eta_1(\rho) - \eta_2(\rho)\right) \qquad 3.27$$

where in this case $\eta_1(\rho)$ and $\eta_2(\rho)$ takes care of the solution as $\rho \to 0$. Inserting (3.27) in (3.26), dividing the first equation by $\sqrt{\alpha_1}$ and the second by $\sqrt{\alpha_2}$ we get

$$-\frac{1}{2}(\eta_1 + \eta_2) + \frac{d\eta_1}{d\rho} + \frac{d\eta_2}{d\rho} = -\frac{\kappa}{\rho}(\eta_1 + \eta_2) + \left(\frac{1}{2} + \sqrt{\frac{\alpha_2}{\alpha_1}}\frac{\beta}{\rho}\right)(\eta_1 - \eta_2)$$
$$-\frac{1}{2}(\eta_1 - \eta_2) + \frac{d\eta_1}{d\rho} - \frac{d\eta_2}{d\rho} = \frac{\kappa}{\rho}(\eta_1 - \eta_2) + \left(\frac{1}{2} - \sqrt{\frac{\alpha_1}{\alpha_2}}\frac{\beta}{\rho}\right)(\eta_1 + \eta_2)$$

Adding and subtracting the above two equations and making the simplification

$$\sqrt{\frac{\alpha_2}{\alpha_1}} - \sqrt{\frac{\alpha_1}{\alpha_2}} = -\frac{2E}{\hbar c\lambda}$$
$$\sqrt{\frac{\alpha_2}{\alpha_1}} + \sqrt{\frac{\alpha_1}{\alpha_2}} = \frac{2m_0c^2}{\hbar c\lambda}$$

we finally obtain two coupled differential equations in η_1 and η_2

$$\frac{d\eta_1}{d\rho} = \left(1 - \frac{E\beta}{\hbar c\lambda\rho}\right)\eta_1 - \left(\frac{\kappa}{\rho} + \frac{\beta m_0c^2}{\hbar c\lambda\rho}\right)\eta_2$$
$$\frac{d\eta_2}{d\rho} = \left(-\frac{\kappa}{\rho} + \frac{\beta m_0c^2}{\hbar c\lambda\rho}\right)\eta_1 + \frac{\beta E}{\hbar c\lambda\rho}\eta_2 \qquad 3.28$$

This coupled differential equation is singular at $\rho = 0$. Therefore we seek the solution of η_1 and η_2 in power series form as

$$\eta_1(\rho) = \rho^m \sum_{s=0}^{\infty} a_s \rho^s \qquad \eta_2(\rho) = \rho^m \sum_{s=0}^{\infty} b_s \rho^s$$

where in this case m is given by equation (3.25). Inserting this power series solution in (3.28) we get, two sets of equation that relates the coefficients of η_1 and η_2

$$a_s(m+s) = a_{s-1} - \frac{\beta E}{\hbar c\lambda} a_s - \left(\kappa + \frac{\beta m_0 c^2}{\hbar c\lambda}\right) b_s$$

$$b_s(m+s) = \left(-\kappa + \frac{\beta m_0 c^2}{\hbar c\lambda}\right) a_s + \frac{\beta E}{\hbar c\lambda} b_s \qquad 3.29$$

From the second equation of (3.29) we can solve for the relation between a_s and b_s as

$$\frac{b_s}{a_s} = \frac{\left(\kappa - \frac{\beta m_0 c^2}{\hbar c\lambda}\right)}{q-s} \qquad 3.30$$

where we have made the substitution

$$q = \frac{\beta E}{\hbar c\lambda} - m \qquad 3.31$$

Solving for b_s from (3.30) and putting it in the first equation of (3.29), leads to the recursion relation for η_1

$$a_s = \frac{-(q-s)}{s(2m+s)} a_{s-1} \qquad 3.33$$

If we choose a_0 arbitrarily, then we have

$$a_1 = \frac{-(q-1)}{1(2m+1)} a_0 = -\frac{(q-1)}{(2m+1)} a_0$$

$$a_2 = \frac{-(q-2)}{2(2m+2)} a_1 = \frac{(q-1)(q-2)}{2(2m+1)(2m+2)} a_0 \qquad 3.34$$

$$.a_s = \frac{(-1)^s (q-1)(q-2)...(q-s)}{s!(2m+1)(2m+2)...(2m+s)} a_0$$

Similarly from (3.30) we can solve for b_s

$$b_s = (-)^s \frac{q(q-1)...(q-s+1)}{s!(2m+1)....(2m+s)} b_0 \qquad 3.35$$

$$b_0 = \frac{\kappa - \frac{\beta m_0 c^2}{\hbar c\lambda}}{q} a_0$$

Now remember the Confluent Hypergeometric series defined as

$$F(a,c,x) = 1 + \frac{a}{c}x + \frac{a(a+1)}{c(c+1)}\frac{x^2}{2!} + \frac{a(a+1)(a+2)}{c(c+1)(c+2)}\frac{x^2}{3!} + \ldots$$

where

$$f_0 = 1$$

$$f_1 = \frac{a}{c}$$

$$f_2 = \frac{a(a+1)}{2!(c(c+1)}$$

.

$$f_s = \frac{a(a+1)(a+2)\ldots(a+s-1)}{s!c(c+1)(c+2)\ldots(c+s-1)}$$

Close examination of equation (3.33) and (3.34) reveals that for η_1 if we replace

$$a \to 1-q$$
$$c \to (2m+1)$$

and similarly for η_2 if we replace

$$a \to -q$$
$$c \to (2m+1)$$

then we have the following correspondence between η_1 and F(a,c,x)

$$f_0 = 1 = a_0$$
$$f_1 = \frac{(1-q)}{2m+1} = -\frac{(q-1)}{2m+1} = a_1$$
$$f_2 = \frac{(1-q)(1-q+1)}{2!(2m+1)2m+1+1)} = \frac{(q-1)(q-2)}{2(2m+1)(2m+2)} = a_2$$

and for η_2

$$f_0 = 1 = b_0$$
$$f_1 = \frac{-q}{2m+1} = b_1$$
$$f_2 = \frac{-q(-q+1)}{(2m+1)(2m+1+1)2} = \frac{q(q-1)}{2(2m+1)(2m+2)} = b_2$$

This clearly shows η_1 and η_2 can be represented by the known Confluent Hypergeometric series as

$$\eta_1(\rho) = a_0\rho^m F(1-q,2m+1,\rho)$$
$$\eta_2(\rho) = b_0\rho^m F(-q,2m+1,\rho) \qquad 3.36$$

However we must impose the condition that this series has to terminate and become a polynomial in order to have a non-divergent wave function as $\rho \to \infty$. From the properties of this series we know that the confluent Hypergeometric series breaks off and becomes a polynomial only when the argument a is zero or negative integer. Therefore we see that the condition we impose on the series now becomes a condition for q. Particularly we must have

$$1-q \le 0 \qquad \text{and } -q < 0$$

for our wave function to be finite as $\rho \to \infty$. In other words q must be positive integer greater than one. This condition helps us to determine the exact energy eigenvalues from equation (3.31). From this equation it follows that

$$E = \pm \frac{m_0c^2}{\sqrt{1+\dfrac{(Z\alpha)^2}{(q+\sqrt{(j+1/2)^2-(Z\alpha)^2})^2}}} \qquad 3.36$$

where β, κ and λ have been replaced by their explicit expressions. We choose the positive sign because equation (3.31) will not be satisfied for $E < 0$. But we know from section (2.2.1) that the Dirac equation is satisfied for positive and negative energy eigenvalues. Thus it seems unreasonable to discard the negative energy solutions at the moment. We will give an explanation for this later when we discuss the bound state features.

In order (3.36) to yield a similar expression to Bohr's result with n as a principal quantum number we define a principal quantum number n,

$$n = q + |\kappa| = q + \left|j + \frac{1}{2}\right|$$

Then (3.36) takes the form

$$E = m_0c^2\left(1+\frac{(Z\alpha)^2}{(n-(j+\frac{1}{2})+\sqrt{(j+\frac{1}{2})^2-(Z\alpha)^2})^2}\right)^{-\frac{1}{2}} \qquad 3.37$$

The fine structure splitting can be made more vivid by expanding (3.37) in power of ($Z\alpha$) for $Z\alpha << 1$ the expansion gives

$$E = m_0c^2\left(1-\frac{(Z\alpha)^2}{2n^2}-\frac{(Z\alpha)^4}{2n^3}\left(\frac{1}{(j+\frac{1}{2})}-\frac{3}{4n}\right)-\frac{(Z\alpha)^6}{8n^4}\left(\frac{n}{(j+\frac{1}{2})^3}-\frac{3(n+j+\frac{1}{2})}{n(j+\frac{1}{2})^2}\right)+\ldots\right) \qquad 3.38a$$

The relativistic wave function can be worked out from (3.27) and 3.35) as

$$\psi = Ne^{-\sqrt{\alpha_1\alpha_2}r}r^{m-1}\begin{pmatrix}\left(F(1-q,2m+1,2\sqrt{\alpha_1\alpha_2}r+\left(\frac{\kappa-\beta m_0c^2}{q}\right)F(-q,2m+1,2\sqrt{\alpha_1\alpha_2}r\right)\Im^{j_3}_{j,l_r}\\ i\left(F(1-q,2m+1,2\sqrt{\alpha_1\alpha_2}r-\left(\frac{\kappa-\beta m_0c^2}{q}\right)F(-q,2m+1,2\sqrt{\alpha_1\alpha_2}r\right)\Im^{j_3}_{j,l_w}\end{pmatrix} \qquad 3.38b$$

where $q = n-\left|j+\frac{1}{2}\right|$ and N is a normalization constant.

We note from (3.38) α the fine structure constant indeed controls the extent of fine structure splitting. A first glance at (3.38) shows the second term corresponds to the Bohr's formula for the energy eigenvalue calculated from the Schrodinger equation:

$$\frac{-\mu c^2}{2n^2}\left(\frac{Ze^2}{4\pi\varepsilon_0\hbar c}\right)^2 = \frac{-\mu}{2n^2}(Z\alpha)^2 \qquad 3.39$$

where μ is the reduced mass of the electron and the nucleus. The other terms are results that appear because of the relativistic feature of the problem. And we recall that in the non-relativistic quantum mechanics the energy eigenvalues depend only on the principal quantum number n and states with the same n but different $l's$ are degenerate. For a given principal quantum number n the degeneracy is given by

$$\sum_{l=0}^{n-1}(2l+1) = n^2$$

With the incorporation of the spin of the electron the degeneracy become $2n^2$. Since the electron in each state of a given n and l can exist in two spin states. Here the energy eigenvalues depend both on the principal quantum number n and the total angular momentum $j = l \pm \frac{1}{2}$. The degeneracy of energy levels of the atom for same n but different $l's$ is now lifted. But states like $2S_{1/2}$ and $2P_{1/2}$ with the same n but different $l's$ are still degenerate since they have the same j. In writing the spectroscopic notations for labeling the relativistic energy levels we used l to be the orbital angular momentum of the upper component spinor. Furthermore the numerical values calculated from (3.38) are a bit depressed than from that calculated from (3.39). This is because the spin of the electron depresses the energy of all the states compared to the energy of the non-relativistic spectrum. This depression is found to in increase with increase in j.

It is evident from (3.38) that the limit of ionization energy is m_0c^2 and therefore the ionization energy of the electron in nj state

$$E_{ion=} = m_0c^2 - E$$

$$E_{ion} = m_0c^2(Z\alpha)^2\left(\frac{1}{2n^2} + \frac{(Z\alpha)^2}{2n^3}\left(\frac{1}{j+\frac{1}{2}} - \frac{3}{4n}\right) + \ldots\right) \qquad 3.40$$

The binding energy is the negative of the ionization energy. We have calculated the binding energies of hydrogen atom for different levels up to eight decimal places. For comparison we present it along with the Schrodinger binding energy calculated from (3.39) in table (2).

Principal quantum number n	Relativistic		Non-Relativistic	
	Spectroscopic notation	Binding Energy (ev)	Spectroscopic notation	Binding Energy (ev)
1	$1S_{1/2}$	-13.6052223	$1S$	-13.59823902
2	$2S_{1/2}$	-3.40116985	$2P$	-3.39955975
	$2P_{1/2}$	-3.40116985		
	$2P_{3/2}$	-3.40120178		
3	$3S_{1/2}$	-1.511521038	3d	-1.50915477
	$3P_{1/2}$	-1.511521038		
	$3P_{3/2}$	-1.511530501		
	$3d_{3/2}$	-1.511530501		
	$3d_{5/2}$	-1.511533656		

Table 3.2 Relativistic and Non-Relativistic Binding Energies

3.3 Bound States Features in the Dirac Formulation

In this section we discuss bound state features in the Dirac formulation from the results we obtain from the pervious section. Equation (3.38) tells us if $Z = 0$ then the attractive coulomb potential $V = \frac{-Ze^2}{4\pi\varepsilon_0 r}$ vanishes. Thus the energy reduces to $E = m_0c^2$ which is the lower limit of the positive energy continuum. As Z increases the attractive potential increases and the energy of the electrons in the positive energy states gets pulled down below m_0c^2 becoming a bound state with energy

$$-m_0c^2 < E_{bound} < m_0c^2$$

In obtaining the expression for the total energy (3.36) we avoided the negative energy solutions. This is because if we look at (3.31) in the left-hand side we have q which is a positive integer. Therefore in order to have positive quantity in the right hand we must have $E > 0$. But we know that Dirac equation is satisfied for both positive and negative energy eigenvalues. So we must have included the negative solutions in our analysis. The reason why we did not so is according to the hole theory an electron in state of negative energy corresponds via charge conjugation to a state of particle of (i.e., positron) of positive energy and the same mass m_0 in the same attractive potential. Equivalently it is a state of electron in a repulsive potential. However the existence of bound states of an electron in a repulsive potential seems paradoxical. But it appears to be paradoxical only in the context of single particle theory. Bound states of an electron in a repulsive potential ($Z\alpha$)<0 are possible and this can be explained by the many particle theory as follows: When the repulsive potential is switched on the bound positron states emerge from the lower negative energy continuum just like bound states of electron appear below the upper positive energy continuum states when an attractive potential is applied. This is because the electrostatic potential that is repulsive for an electron is attractive for the positron and vice versa .The positive energy continuum in repulsive potential corresponds to the negative energy continuum in attractive potential. The energy spectrum of an electron in attractive potential shows a series of bound states which lie below the positive energy domain and the spectrum in a repulsive potential consists of bound states above the lower negative energy continuum.

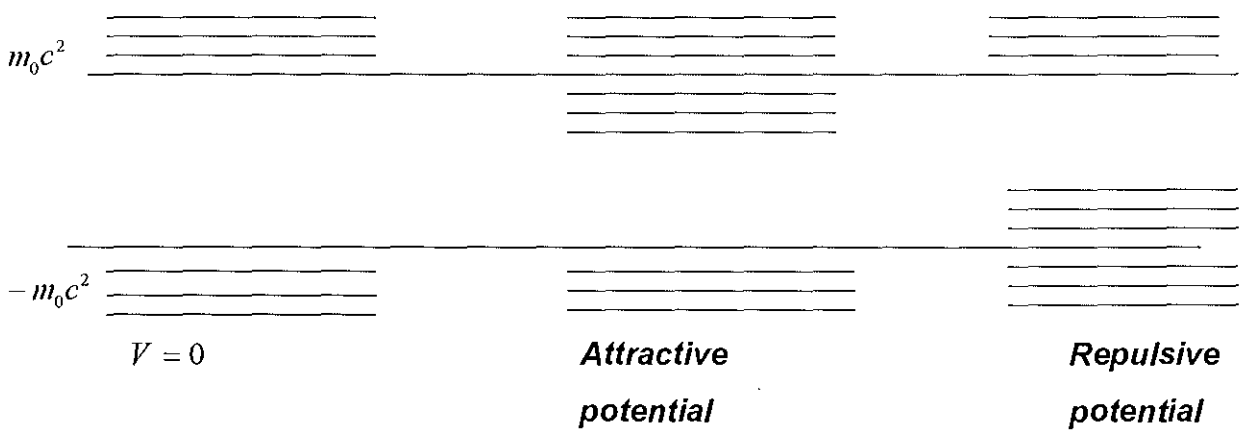

Fig. 3 Bound state spectrum in the Dirac equation

Conclusively the Dirac equation gives

I Positive energy continuum

$$m_0c^2 < E < \infty$$

II Discrete bound energy levels

$$-m_0c^2 < E_{bond} < m_0c^2$$

III Negative energy continuum

$$-\infty < E < -m_ec^2$$

Therefore the bound states of Dirac equation are the discrete energy levels between the forbidden gap $-m_0c^2$ and m_0c^2.

If we examine the expression for the total energy (3.37) closely, we notice a very interesting and unusual behavior for $j=\frac{1}{2}$ states. For $j=\frac{1}{2}$ states if $Z\alpha>1$ the total energy (3.37) becomes imaginary. This means there is no bound state for these states. Furthermore if we look at the expression for the wave function we observe that contrary to our expectation that it must vanish as $r\to\infty$, we have an oscillatory solution. This is because m given by (3.25) now becomes imaginary for $j=\frac{1}{2}$

$$\text{i.e,}\quad m=\sqrt{(j+\frac{1}{2})^2-(Z\alpha)^2}=\sqrt{1-(Z\alpha)^2}$$

and for Zα>1

$$m = i\sqrt{(Z\alpha)^2 - 1} = im'$$

where $m' = \sqrt{(Z\alpha)^2 - 1}$ .Thus the wave function assumes the form

$$\psi \sim r^m = r^{im'}$$

which is totally oscillatory.

This is the same condition as that of the Klein's Paradox we have in one-dimensional square well potential V_0 where we have the following: when electrons are incident on a square well potential they start to assume oscillatory solutions in the region of the potential after some value of the potential $V_0 > E + m_0c^2$. More interesting is that the amplitude of the reflected wave seems to be much greater than the amplitude of the incident wave as if the transmitted wave is coming from inside the barrier.

Here also the situation appears to be strange. But again this appears to be strange only in the context of single particle theory. We can understand this condition by the hole theory. When the attractive potential grows it further lowers the energy of the electron in the positive energy domain. Thus the positive energy domain gets stretched into the negative energy continuum and an overlap of the two energy domains happens. An electron from the positive domain will knock off the negative energy electron in the Dirac Sea, creating electron positron pairs. The oscillatory solution we have then is that of a positron coming from infinity. This condition is called an over critical condition and is referred to as the ***collapse of vacuum.*** This is because this over critical potential results in pair creation in which an electron-positron pair is generated from the vacuum. Therefore we note that the condition for collapse of vacuum for j=1/2 states in point nuclei atoms is given by

$$Z\alpha > 1$$

and by putting the fine structure constant $\alpha \sim \frac{1}{137}$ we determine the critical nuclea charge for pair creation or overlap of the two energy continuums to be equal to Z=13 for j=1/2 states

I.e., $Z_{cr} = 137$.

4. Energy Spectrum and Electron Magnetic Moment in the Non-Relativistic Limit

In section (3.1) we have solved the hydrogen atom problem exactly. In this section we would like to study it's non-relativistic limit by making some approximations. The Hamilitonian of the problem is given by (3.1).

4.1 The Non-Relativistic Limit of the Dirac Hamiltonian

In order to study the non-relativistic limit we replace E by

$$E = E' + m_0c^2$$

where E' is the non-relativistic energy and is very small compared to the rest energy m_0c^2. If we assume that the two component wave functions to be the non-relativistic Schrodinger Pauli wave functions

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

then the Dirac equation (2.13) yields

$$\begin{aligned} (E' - V)\psi_1 - c\vec{\sigma}.\vec{p}\psi_2 &= 0 \\ (E' + 2m_0c^2 - V)\psi_2 - c\vec{\sigma}.\vec{p}\psi_1 &= 0 \end{aligned} \qquad 4.1$$

Solving for ψ_2 from the second equation of (4.1) and inserting it in the first equation we get

$$E'\psi_1 = c^2\vec{\sigma}.\vec{p}(E' + 2m_0c^2 - V)^{-1}\vec{\sigma}.\vec{p}\psi_1 + V\psi_1 \qquad 4.2$$

In the non-relativistic limit we have $E' - V << m_0c^2$. Thus the term in the bracket can be expanded, keeping only first order terms as

$$(2m_0c^2 + E' - V)^{-1} \approx \frac{1}{2m_0c^2}(1 - \frac{E' - V}{2m_0c^2})$$

With this approximation (4.2) becomes

$$E'\psi_1 = \frac{1}{2m_0}\{p^2 - \frac{p^2E'}{2m_0c^2} + \frac{1}{2m_0c^2}(\vec{\sigma}.p V \vec{\sigma}.\vec{p})\}\psi_1 + V\psi_1 \qquad 4.3$$

where $(\vec{\sigma}.\vec{p})(\vec{\sigma}.\vec{p}) = p^2$ has been used. Making use of the commutation relation

$$[p,V] = -i\hbar\vec{\nabla}V$$

i.e. $$pV = Vp - i\hbar\vec{\nabla}V \qquad 4.4$$

equation (4.3) can be written as

$$E'\psi_1 = \frac{1}{2m_0}\{p^2 - \frac{p^2E'}{2m_0c^2} + \frac{1}{2m_0c^2}(\vec{\sigma}.Vp.\vec{\sigma}.\vec{p} - i\hbar(\vec{\sigma}.\vec{\nabla}V)\vec{\sigma}.p)\}\psi_1 + V\psi_1 \qquad 4.5$$

Inserting $(\vec{\sigma}.Vp.\vec{\sigma}.p) = V(\vec{\sigma}.\vec{p})(\vec{\sigma}.\vec{p}) = Vp^2$ equation (4.5) further reduces to

$$E'\psi_1 = \{(1 - \frac{E' - V}{2m_0c^2})\frac{p^2}{2m_0} - \frac{i\hbar}{2m_0^2c^2}[(\vec{\sigma}.\vec{\nabla}V)(\vec{\sigma}.p)]\}\psi_1 + V\psi_1 \qquad 4.6$$

Using the identity (3.8) we simplify the term in the square bracket as,

$$(\vec{\sigma}.\vec{\nabla}V)(\vec{\sigma}.\vec{p}) = (\vec{\nabla}V.\vec{p}) + i\vec{\sigma}.(\vec{\nabla}V \times \vec{p}$$

we get

$$E'\psi_1 = \{(1 - \frac{E' - V}{2m_0c^2})\frac{p^2}{2m_0} + V\}\psi_1 - \frac{i\hbar}{4m_0^2c^2}(\vec{\nabla}V.\vec{p} + i\vec{\sigma}.(\vec{\nabla}V \times \vec{p}))\psi_1 \qquad 4.7$$

Now for a spherically symmetric potential we have

$$\vec{\nabla}V.\vec{\nabla} = \frac{dV}{dr}\frac{\partial}{\partial r} \qquad \text{and} \qquad \vec{\nabla}V = \frac{\vec{r}}{r}\frac{dV}{dr}$$

where $\frac{\vec{r}}{r}$ is the unit vector along the direction of $\vec{r}$. Thus equation (4.7) reduces

$$E'\psi_1 = \{(1 - \frac{E' - V}{2m_0c^2})\frac{p^2}{2m_0} + V\}\psi_1 - \frac{\hbar^2}{4m_0^2}\{[\frac{dV}{dr}\frac{\partial}{\partial r}] + \frac{\hbar}{4m_0^2c^2}\vec{\sigma}.\frac{1}{r}\frac{dV}{dr}(\vec{r} \times \vec{p})\}\psi_1 \qquad 4.8$$

Replacing $\vec{r} \times \vec{p}$ by the orbital angular momentum $\vec{L}$ and $\frac{\hbar}{2}\vec{\sigma}$ by the spin angular momentum $\vec{S}$ and making the following approximation,

$$E' - V \approx \frac{p^2}{2m_0}$$

we eventually arrive at an equation, which has the same form as the Shrodinger equation

$$E'\psi_1 = (\frac{p^2}{2m_0} + V - \frac{p^4}{8m_0^3c^2} - \frac{\hbar^2}{4m_0^2c^2}\frac{dV}{dr}\frac{\partial}{\partial r} + \frac{1}{2m_0^2c^2}\frac{1}{r}\frac{dV}{dr}\vec{L}.\vec{S})\psi_1 \qquad 4.9$$

$$E'\psi_1 = H\psi_1$$

Hence we identify the Hamilitonian H to be

$$H = (\frac{p^2}{2m_0} + V - \frac{p^4}{8m_0^3c^2} - \frac{\hbar^2}{4m_0^2c^2}\frac{dV}{dr}\frac{\partial}{\partial r} + \frac{1}{2m_0^2c^2}\frac{1}{r}\frac{dV}{dr}\vec{L}.\vec{S})$$

The first two terms are the non relativistic part of the Hamilitonian, the third term corresponds to relativistic corrections to the kinetic energy, the fourth term shows relativistic correction to the potential energy, and the last term is the spin orbit interaction term. We note that this term is automatically included in the Dirac equation, where as we recall that in the non-relativistic Pauli Schrodinger theory the spin orbit (i.e., $\vec{L}.\vec{S}$ coupling) is put in the theory by hand.

4.2 The Energy Spectrum

Now from our exact solutions of hydrogen like atoms we obtained in section (3.1) we can observe that the relativistic corrections for atoms where Z is not too large is very small. Therefore we can apply the perturbation method treating the three extra terms we have in the Hamilitonian as a small perturbation .To begin with we write the Hamilitionain as

$$H = H_0 + H' \qquad 4.10$$

where

$H_0 = \frac{p^2}{2m_0} + V(r)$ is the unperturbed Hamilitonian

$H' = H_1 + H_2 + H_3$ is the perturbation term

Here

$$H_1 = \frac{-p^4}{8m_0^3c^2}$$

$$H_2 = \frac{1}{2m_0^2c^2}\frac{1}{r}\frac{dV}{dr}\vec{L}.\vec{S}$$

$$H_3 = -\frac{\hbar^2}{4m_0^2c^2}\frac{dV}{dr}\frac{\partial}{\partial r}$$

To calculate energy corrections we use the unperturbed modified two component Schrodinger-Pauli wave function,

$$\psi_{nlm_l m_s} = \psi_{nlm_l}(\vec{r})\chi_{\frac{1}{2},m_s} \qquad 4.11$$

where $\psi_{nlm_l}(\vec{r})$ is one-electron Schrodinger wave function and $\chi_{\frac{1}{2},m_s}$ the spin eigenfunction. They are simultaneous eigenfunctions of H_0 , L^2 , S^2 , L_Z , S_Z

$$H_0\psi_{nlm_l}(\vec{r}) = E_n\psi_{nlm_l} \qquad 4.12$$

Since H_0 does not act on the spin variable we have also

$$H_0\psi_{nlm_l m_s} = E_n\psi_{nlm_l m_s}$$

We have four quantum numbers (n,l,m_l,m_s) to describe a one electron atom. In this representation the introduction of spin dependent term in the Hamiltonian is to increase the degeneracy two fold. Therefore the degenerate perturbation method is employed. We now give the contribution up to first order energy shift resulting from various terms in the Hamiltonian in equation (4.10):

1. $H_1 = -\frac{p^4}{8m_0^3c^2}$ (relativistic correction to the kinetic energy)

H_1 does not act on the spin part of the wave function and it also commutes with L^2. This shows $\psi_{nlm_l m_s}$ is simultaneous eigenstate of H_1 and L^2, thus the task of digonalizing this perturbation matrix is now simplified, because H_1 is already diagonal in $\psi_{nlm_l m_s}$ basis The first order energy correction due to this perturbation is now given as,

$$[\Delta_n^{(1)}]_1 = \langle nlm_l m_s|H_1|nlm_l m_s\rangle = \frac{-1}{2m_0c^2}\langle nlm_l|(\frac{p^2}{2m_0})^2|nlm_l\rangle \qquad 4.13$$

$$\frac{p^2}{2m_0} = H_0 - V(r) = H_0 + \frac{Ze^2}{4\pi\varepsilon_0 r}$$

$$[\Delta_n^{(1)}]_1 = \frac{-1}{2m_0c^2}\{\langle nlm_l|H_0^2|nlm_l\rangle + \langle nlm_l|2H_0\frac{Ze^2}{4\pi\varepsilon_0 r}|nlm_l\rangle + \langle nlm_l|(\frac{Ze^2}{4\pi\varepsilon_0 r})^2|nlm_l\rangle\}$$

$$[\Delta_n^{(1)}]_1 = \frac{-1}{2m_0c^2}[E_n^2 + 2E_n \frac{Ze^2}{4\pi\varepsilon_0}\langle nlm_l|\frac{1}{r}|nlm_l\rangle + (\frac{Ze^2}{4\pi\varepsilon_0})\langle nlm_l|\frac{1}{r^2}|nlm_l\rangle \quad 4.14$$

In order to calculate the $\left\langle \frac{1}{r} \right\rangle_{nlm}$ and $\left\langle \frac{1}{r^2} \right\rangle_{nlm}$ we use the non-relativistic hydrogen atom wave functions. This is done in appendix A. Here we only present the final results

$$\left\langle \frac{1}{r} \right\rangle_{nlm} = (\frac{Z}{a_0})\frac{1}{n^2}$$

$$\left\langle \frac{1}{r^2} \right\rangle_{nlm_l} = (\frac{Z}{a_0})^2 \frac{1}{n^2(l+1/2)}$$

$$\left\langle \frac{1}{r^3} \right\rangle_{nlm_l} = (\frac{Z}{a_0})^3 \frac{1}{n^3 l(l+1/2)(l+1)}$$

We recall that the unperturbed energy eigenvalues of the hydrogen atom obtained from the Schrodinger equation is given by

$$E_n = \frac{-m}{2n^2}(\frac{Ze^2}{4\pi\varepsilon_0\hbar})^2 = \frac{-mc^2}{2n^2}(Z\alpha)^2 \qquad 4.15$$

Therefore with (4.15) the first order energy correction due to H_1 assumes

$$[\Delta_n^{(1)}]_1 = \frac{mc^2}{2}(\frac{Z\alpha}{n})^4(\frac{3}{4} - \frac{n}{l+1/2}) \qquad 4.16$$

2. $H_2 = \frac{1}{2m^2c^2}\frac{1}{r}\frac{dV}{dr}\vec{L}.\vec{S}$ (Spin-orbit interaction term):

Here the Coulomb potential is given by

$$V(r) = -\frac{Ze^2}{4\pi\varepsilon_0 r}.$$

Therefore

$$\frac{dV}{dr} = \frac{Ze^2}{4\pi\varepsilon_0 r^2}$$

Thus

$$H_2 = \frac{1}{2m_0^2c^2}(\frac{Ze^2}{4\pi\varepsilon_0 r^2})\vec{L}.\vec{S}.$$

Now we have to choose the unperturbed eigenfunctions which digonalize this interaction H_2. Here $\vec{L}.\vec{S}$ is not diagonal in Ψ_{nlmm_s} basis because it does not commute with L_z and S_z. Thus we introduce the total angular momentum operator.

$$\vec{J} = \vec{L} + \vec{S}$$

where now we can solve for $\vec{L}.\vec{S}$ from $\vec{J}^2$ as,

$$\vec{L}.\vec{S} = \frac{1}{2}(J^2 - L^2 - S^2).$$

Now if use the eigenfunctions ψ_{nljm_j}, which are the simultaneous eigenfunctions of J^2, L^2, S^2 and J_z the interaction H_2 will be diagonal. Here ψ_{nljm_j} are the linear combinations of $\psi_{nlm_lm_s}$. More explicitly

$$\psi_{nljm_j}(\vec{r}) = R_{nl}(r)\Im_l^{j=l\pm 1/2,m_j} \qquad 4.17$$

where $\Im_l^{j=l\pm 1/2,m_j}$ is the spin angular function and

$$\int \Im^+ \vec{L}.\vec{S}\Im d\Omega = \frac{1}{2}[j(i+1) - l(l+1) - 3/4]\hbar^2$$

The energy correction due to this perturbing term now takes the form.

$$[\Delta_n^{(1)}]_2 = \frac{1}{2m_0^2c^2}\left(\frac{Ze^2}{4\pi\varepsilon_0}\right)\left\langle\frac{1}{r^3}\right\rangle_{nljm_j}\frac{\hbar^2}{2}[j(i+1) - l(l+1) - 3/4]$$

$$[\Delta_n^{(1)}]_2 = \frac{m_0c^2}{4n^3}\frac{(Z\alpha)^4}{l(l+1/2)(l+1)}\begin{Bmatrix} l & for j = l+1/2 \\ -l-1 & for j = l-1/2 \end{Bmatrix}$$

If we consider the spin up state, finally we write

$$[\Delta_n^{(1)}]_2 = \frac{m_0c^2}{4n^3}\frac{(Z\alpha)^4}{j(j+1/2)} \qquad 4.18$$

where we have substituted $j = l + \frac{1}{2}$

2. $H_3 = \frac{-\hbar^2}{4m^2c^2}\frac{dV}{dr}\frac{\partial}{\partial r}$.

This term is called the Darwin term and in appendix B this term is shown to be equal to

$$H_3 = \frac{\pi^2\hbar^2}{2m_0^2c^2}\left(\frac{Ze^2}{4\pi\varepsilon_0}\right)\delta(\vec{r}).$$

where $\delta(\vec{r})$ is the three dimensional Dirac delta function.

This perturbation does not act on the spin variables and it is diagonal in ψ_{nlm} representation. It is effective only when $l = 0$. Therefore the energy correction due to this term becomes

$$[\Delta_n^{(1)}]_3 = \frac{\pi\hbar^2}{2m_0^2c^2}\left(\frac{Ze^2}{4\pi\varepsilon_0}\right)\langle\psi_{n00}|\delta(\vec{r})|\psi_{n00}\rangle = \int\psi_{n00}^*\delta(\vec{r})\psi_{n00}d^3r = |\psi_{n00}(0)|^2$$

$$\psi_{n00}(0) = R_{n0}(0)Y_0^0$$

where $R_{nl}(0)$ is the radial wave function at $r = 0$ and Y_0^0 is the spherical harmonic where

$$Y_0^0 = \frac{1}{\sqrt{4\pi}} \quad \text{and}$$

$$R_{n0}(0) = 2\left(\frac{Z}{na_0}\right)^{\frac{3}{2}}$$

where a_0 is the first Bohr radius.

Thus we have

$$|\psi_{n00}(0)|^2 = \frac{1}{\pi}\left(\frac{Zm_0e^2}{4n\pi\varepsilon_0\hbar^2}\right).$$

The first order energy correction due to the Darwin term now takes the form

$$[\Delta_n^{(1)}]_3 = \frac{m_0c^2}{2}\left(\frac{(Z\alpha)^4}{n^3}\right) \qquad \text{for } l = 0. \qquad 4.19$$

The total energy correction for $l \neq 0$ is the sum of individual correction due to each perturbing term. But H_3 does not contribute to this correction because it is effective only when $l = 0$. Therefore the total correction coming from H_1 and H_2 that are non-vanishing only for $l \neq 0$ is the sum of (4.16) and (4.18). i.e.,

$$\Delta_{nj}^{(1)} = -\frac{1}{2} m_0 c^2 \frac{(Z\alpha)^4}{n^4}\left(\frac{n}{j+1/2} - \frac{3}{4}\right) \qquad 4.20$$

The total energy is then the sum of the unperturbed zero order energy E_n given by (4.15) and the energy correction Δ_{nj} given by (4.20). With this correction the hydrogen like atom energy eigenvalues assume the form,

$$E_n = m_0 c^2\left(-\frac{(Z\alpha)^2}{2n^2} - \frac{(Z\alpha)^4}{n^4}\left(\frac{n}{j+1/2} - \frac{3}{4}\right)\right). \qquad 4.21$$

From this result we note that the non-relativistic limit of the Dirac equation does not exactly reduce to the non-relativistic Schrodinger wave equation. Even in its non-relativistic incarnation the solutions of the Dirac equation provides more information than the non-relativistic Schrodinger equation. The correction term in the energy eigenvalue in eq. (4.21) explains the fine structure splitting very well. Comparing the first order approximate solution (4.21) with the exact solution (3.38) we notice that except for an additional $m_0 c^2$ term in (3.38) they are exactly the same up to the fourth term.

4.3 The Electron Magnetic Moment

In this section we treat the interaction of an electron with an electromagnetic field to determine the magnetic moment of an electron. We make use of non-relativistic approximations exploited in the previous section. We start from the Dirac equation (2.13) where in this case we make the following replacements for a particle in an electromagnetic field.

$$\vec{p} \to \vec{p} - \frac{e}{c}\vec{A} \qquad \text{and} \qquad E \to E - e\phi$$

where $\vec{A}$ and ϕ are the vector and the scalar potential of the field respectively. With this replacement, the Dirac equation reads,

$$(E - e\phi)\psi = \left(c\vec{\alpha}.(\vec{p} - \frac{e}{c}\vec{A}) + \beta m_0 c^2 \right)\psi$$

Here $(E - e\phi)\psi$ and $(\vec{p} - \frac{e}{c}\vec{A})\psi$ are the gauge invariant combinations at the energy and the momentum levels respectively. By splitting the wave function in to upper and lower component as,

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

where ψ_1 and ψ_2 are the Schrodinger wave function, we get

$$\begin{aligned} E\psi_1 &= (m_0 c^2 + e\phi)\psi_1 + c\vec{\sigma}.(\vec{p} - \frac{e}{c}\vec{A})\psi_2 \\ E\psi_2 &= c\vec{\sigma}.(\vec{p} - \frac{e}{c}\vec{A})\psi_1 + (e\phi - m_0 c^2)\psi_2 \end{aligned} \qquad 4.21$$

To study its non-relativistic limit we write the energy as

$$E = E' + m_0 c^2$$

where E' is the non-relativistic energy. Then (4.21) reduces to

$$\begin{aligned} E'\psi_1 &= e\phi\psi_1 + c\vec{\sigma}.(\vec{p} - \frac{e}{c}\vec{A})\psi_2 \\ E'\psi_2 &= c\vec{\sigma}.(\vec{p} - \frac{e}{c}\vec{A})\psi_1 + (e\phi - 2m_0 c^2)\psi_2 \end{aligned} \qquad 4.22$$

We know that $|e\phi| << m_0c^2$ and $E' << m_0c^2$. Thus we can make the following approximation,

$$E' - e\phi + 2m_0c^2 \approx 2m_0c^2$$

With this approximation we can solve for ψ_2 from the second equation of (4.22) as

$$\psi_2 = \frac{1}{2m_0c}\vec{\sigma}.(\vec{p} - \frac{e}{c}\vec{A})\psi_1$$

Inserting this in the first equation of (4.22) we obtain

$$\frac{1}{2m_0}\left(\vec{\sigma}.(\vec{p} - \frac{e}{c}\vec{A})\vec{\sigma}.(\vec{p} - \frac{e}{c}\vec{A})\right)\psi_1 = (E' - e\phi)\psi_1 \qquad 4.23$$

Making use of identity (3.8) we make the following simplification

$$\vec{\sigma}.(\vec{p} - \frac{e}{c}\vec{A})\vec{\sigma}.(\vec{p} - \frac{e}{c}\vec{A}) = (\vec{p} - \frac{e}{c}\vec{A})^2 + i\vec{\sigma}.(\vec{p} - \frac{e}{c}\vec{A}) \times (\vec{p} - \frac{e}{c}\vec{A})$$

$$(\vec{p} - \frac{e}{c}\vec{A}) \times (\vec{p} - \frac{e}{c}\vec{A}) = \frac{-i\hbar e}{c}\left(\vec{\nabla} \times \vec{A} + \vec{A} \times \vec{\nabla}\right)$$

where the momentum $\vec{p}$ has been replaced by its operator $-i\hbar\vec{\nabla}$. And we know that the momentum operator acts on anything to the right of it. Therefore we have

$$\left(\vec{\nabla} \times \vec{A} + \vec{A} \times \vec{\nabla}\right)\psi_1 = \vec{\nabla} \times (\vec{A}\psi_1) + \vec{A} \times \vec{\nabla}\psi_1 = \psi_1\vec{\nabla} \times \vec{A} + \vec{\nabla}\psi_1 \times \vec{A} + \vec{A} \times \vec{\nabla}\psi_1$$
$$= \psi_1\vec{\nabla} \times \vec{A} = \vec{B}\psi_1$$

Thus equation (4.23) reduces to

$$E'\psi_1 = \left(\frac{1}{2m_0}(\vec{p} - \frac{e}{c}\vec{A})^2 + e\phi - \frac{e\hbar}{2m_0c}\vec{\sigma}.\vec{B}\right)\psi_1 \qquad 4.24$$

This equation has the same form as the Schrodinger equation

$$E'\psi_1 = H\psi_1$$

with a Hamilitonian H

$$H = \left(\frac{1}{2m_0}(\vec{p} - \frac{e}{c}\vec{A})^2 + e\phi - \frac{e\hbar}{2m_0c}\vec{\sigma}.\vec{B}\right). \qquad 4.21a$$

We can write the total Hamilitonian (4.21a) as,

$$H = H_1 + H_2$$

where

gyromagnetic ratio for the spin is double the gyromagnetic ratio for the orbital motion (i.e., $g_s = 2g_l$).

However the experimentally observed [1], gyromagnetic ratio of the electron is given by

$$g_s = 2\left(1+\frac{e^2}{4\pi\hbar c}\frac{1}{2\pi}+\ldots\right) \qquad 4.25$$

The origin of this correction to the electron magnetic moment is due to some quantum electrodynamic corrections which was explained by J.Schwinger [1], by taking account of the fact that a physical electron can emit and absorb a virtual photon.

Even though the Dirac equation does not account for this additional magnetic moment, we can make the Dirac's prediction consistent with the experimentally observed value by adding an additional interaction Hamilitonian

$$H'_{\text{int}} = -\frac{e\hbar}{2m_0c}\left(\frac{e^2}{4\pi\hbar c}\right)\frac{1}{2\pi}\vec{\sigma}.\vec{B}\ . \qquad 4.26$$

to (4.22).

Now with the value of g_s given by (4.25) and an additional interaction term given by (4.26) the total magnetic moment comes to be

$$\vec{\mu} = \frac{e}{m_0c}\left(1+\left(\frac{e^2}{4\pi\hbar c}\right)\frac{1}{2\pi}\right)\vec{S} \qquad 4.27$$

We can write this equation as

$$\vec{\mu} = \vec{\mu}_D + \kappa\mu_B$$

where $\kappa' = \left(\frac{e^2}{4\pi\hbar c}\right)\frac{1}{2\pi}$ is called the anomalous magnetic moment of the electron and μ_D is the Dirac magnetic moment.

The Dirac equation thus predicts the interaction of spin magnetic moment of the electron with the applied magnetic field. Further the magnetic moment of electron calculated by the Dirac equation gives the gyromagnetic ratio $g_s = 2$. But the correct value of magnetic moment of electron can be worked out in the framework of Quantum Electrodynamics and it agrees with experimental results to eighth place of decimal.

5. Conclusion

In the first part of this thesis we studied the properties of Dirac equation, where we have studied the covariant form of the Dirac equation, and the covariance of the Dirac equation was studied. We have also shown that Dirac equation is satisfied for both positive and negative energy eigenvalues. Moreover we have discussed the hole theory and charge conjugation in detail, which are the explanation given by Dirac for the existence of the negative energy eigenvalues and antiparticles.

In this thesis the hydrogen like atom problem was tackled by using the relativistic Dirac wave equation and its bound state features studied in detail. In the process we first showed how the spin of the electron is automatically brought out in the theory from the very outset. We obtained energy spectrum that vividly shows the fine structure splitting. The energy spectrum calculated from the Dirac theory is a bit depressed than that calculated from the non-relativistic Schrodinger equation. Some of the results for low lying energy levels are

$E(1S_{1/2}) = -13.6052223$ ev, $E(2S_{1/2}) = -3.40116985$ ev and $E(2P_{1/2}) = -3.40120178$ ev.

The existence of negative energy eigenvalues and bound states for both attractive and repulsive electrostatic potentials in this particular problem was pointed out and explained on the basis of hole theory and charge conjugation. We observed that generally bound states in the Dirac equation lie between $-m_0c^2$ and m_0c^2. Particularly we have shown that the bound states for attractive potential appear below the positive energy continuum and for repulsive potential they emerge above the lower energy continuum. The existence of bound states of an electron in repulsive potential seems a paradox. But it is only a paradox in a single particle context. It is observed that it no longer remains a paradox if the negative energy electrons are involved in this process. This is because by the hole theory and charge conjugation the absence of an electron with negative energy momentum $\vec{p}$ and spin up (down) is equivalent to presence of a particle of positive energy momentum $-\vec{p}$ and spin down (up). Thus a potential which is repulsive for an electron is attractive for positron and vice versa.

Appendix A

In this appendix we present the Calculation of the Expectation value of $\langle r^{\nu} \rangle$ where ν is any integer by using the normalized radial part of the wave function of hydrogen in non-relativistic quantum mechanics. The normalized radial wave function is given by

$$R_{nl}(r) = \left(\frac{Z}{na_0}\right)^{\frac{3}{2}} \sqrt{\frac{4}{n(n-l-1)!(n+l)!}} \left(\frac{Z}{na_0}\right)^{l} e^{\frac{-Zr}{na_0}} Q_{n-l-1}^{2l+1}\left(\frac{Zr}{na_0}\right) \qquad \text{A.1}$$

where $Q_{n-l-1}^{2l+1}(\frac{Zr}{na_0})$ are the Laguerre Polynomials that have the following form

$$Q_k^s(\rho) = \sum_{j=0}^{k} (-1)^{k+j} \frac{k!(k+s)!}{j!(k-j)!(k+s-j)!} \rho^{k-j} \qquad \text{A.2}$$

where

$$s = 2l+1$$
$$k = n-l-1$$
$$\rho = \frac{2Zr}{na_0}$$

Or in closed form

$$Q_k^{2l+1}(\rho) = e^{\rho} \rho^{-2l-1} \left(\frac{d^k}{d\rho^k} (e^{-\rho} \rho^{k+2l+1} \right) \qquad \text{A.3}$$

Thus

$$\left\langle \frac{1}{r^{\nu}} \right\rangle = \int \psi^*_{nlm}(\vec{r}) r^{-\nu} \psi_{nlm}(\vec{r}) d^3x = \int_0^{\infty} R_{nl}^2(r) r^{-\nu+2} dr \qquad \text{A.4}$$

or

$$\left\langle \frac{1}{r^{\nu}} \right\rangle = \left(\frac{na_0}{2Z}\right)^{-\nu+3} \int_0^{\infty} R_{nl}^2(\rho) \rho^{-\nu+2} d\rho$$

Equation (A.1) can be written in terms of ρ as

$$R_{nl}(\rho) = C_{nl}\rho^{l}e^{-\frac{\rho}{2}}Q_{n-l-1}^{2l+1}(\rho) \qquad \text{A.5}$$

where

$$C_{nl} = \left(\frac{Z}{na_0}\right)^{\frac{3}{2}}\sqrt{\frac{4}{n(n-l-1)!(n+l)!}}$$

now equation (A.4) becomes

$$\left\langle \frac{1}{r^{v}} \right\rangle = C_{nl}^{2}\left(\frac{na_0}{2Z}\right)^{-v+3}\int \rho^{-v+2}\rho^{2l}e^{-\rho}\left(Q_{n-l-1}^{2l+1}(\rho)\right)^{2}d\rho$$

express one of the Lagure polynomials $Q_{n-l-1}^{2l+1} = Q_{k}^{2l+1}$ in a series form given by (A.2) the other by closed form given by (A.3)

$$\left\langle \frac{1}{r^{v}} \right\rangle = C_{nl}^{2}\left(\frac{na_0}{2Z}\right)^{-v+3}\int_0^{\infty}\rho^{-v+1}\rho^{2l}\{-1)^{k}(\rho^{k} - k(k+2l+1)\rho^{k-1} + \ldots$$

$$\ldots + (-1)^{k-1}\frac{k(2l+k+1)!}{(2l+2)!}\rho + (-1)^{k}\frac{(2l+k+1)!}{}(2l+1)\}\left(\frac{d^{k}}{d\rho^{k}}(e^{-\rho}\rho^{k+2l+1}\right)d\rho$$

By using the identity

$$\int_{-\infty}^{\infty} U\frac{d^{n}V}{dx^{n}}dx = (-1)^{n}\int_{-\infty}^{\infty}\frac{d^{n}U}{dx^{n}}Vdx$$

For $v = 1$we will get

$$\left\langle \frac{1}{r} \right\rangle = C_{nl}^{2}\left(\frac{na_0}{2Z}\right)^{2}\int_0^{\infty}e^{-\rho}\rho^{k+2l+1}\frac{d^{k}}{d\rho^{k}}(\rho^{k})d\rho \qquad \text{A.6}$$

because the other terms vanish when differentiate k times

$$\frac{d^k}{d\rho^k}(\rho^k) = k!$$

making use of the relation

$$\int_0^\infty e^{-\rho}\rho^t d\rho = t! \qquad \text{A.7}$$

finally we obtain

$$\left\langle \frac{1}{r} \right\rangle = \left(\frac{Z}{a_0}\right)\frac{1}{n^2}$$

By the same procedure it can easily be proved that

$$\left\langle \frac{1}{r^2} \right\rangle = \left(\frac{Z}{a^0}\right)^2 \frac{1}{n^2(l+\frac{1}{2})}$$

$$\left\langle \frac{1}{r^3} \right\rangle = \left(\frac{Z}{a_0}\right)^3 \frac{1}{n^3 l(l+1)(l+\frac{1}{2})}$$

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