Introducing spin in Schrödinger dynamics of particle motion

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A non-perturbative relativistic atomic theory is presented. Spin is successfully introduced in Schrödinger dynamics of particle motion and the resulting energy levels of Hydrogen atom are shown to be exactly same as that of Dirac’s theory. The separation of new radial and angular wave equations in spherical polar coordinates is as simple as that of the Schrödinger theory. The solutions of the angular part of the wave equation for spin-0 particle are exactly same as that of the Schrödinger theory. The spherical harmonics for spin 1/2 particle are same as in Dirac’s theory. The radial wave function of the Schrödinger theory gets split into two spinor components. The new theory accounts for the energy due to spin-orbit interaction as well as for the additional potential energy due to spin and spin-orbit coupling. Spin angular momentum operator is as neatly integrated into the equation of motion as the orbital angular momentum operator. This requires modification to classical Laplacian operator. Consequently the Dirac matrices and the $k$ operator of Dirac’s theory are dispensed with. The theory also points out that the curvature of the orbit draws on certain amount of kinetic and potential energies affecting the momentum of electron and the spin-orbit interaction energy constitutes a part of this energy. It is shown that the correction introduced to the radial equation due to the modification of classical Laplacian is not the same as that of the Darwin and Pauli theory however, the resulting energy levels of Hydrogen atom are same as that of Darwin, Pauli and Dirac theories. This is because the new theory is not a perturbation theory. Probability current density for Hydrogen atom and for free particle is discussed. The main focus is on the spin 1/2 bound state single electron in Coulomb potential but the theory can also be extended to other spin values and potentials. The Pauli equation is obtained in the non-relativistic limit. The new wave equation is compared with the Klein-Gordon wave equation.

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1. INTRODUCTION

It has been more than three quarters of a century since the first publication of Schrödinger theory and apart from Dirac’s theory no other satisfactory solution to the fine structure problem of hydrogen has been found. Specifically, attempts at introducing spin in unperturbed Schrödinger formalism were unsuccessful. Inserting spin to Schrödinger formalism as a relativistic correction, as in case of the Pauli equation with two spinors is a subject of perturbation theories. Several other relativistic wave equations dealing with various aspects of spin have been put forth to address large variety of problems. For example, Klein-Gordon equation for spin-0 particles, wave equations for describing relativistic dynamics of a system of two interacting spin-1/2 particles, Breit equation for two electrons, also called two body Dirac equation, generalized Breit equation for two fermions, Duffin-Kemmer-Petiau (DKP) theory of scalar and vector fields for describing interactions of relativistic spin-0 and spin-1 bosons. Some of the other works include Poincaré invariant theory of classical spinning particles, quantum mechanical embedding of spinning particles and spin dependent gauge transformation between classical and quantum mechanics. All these theories fall under the class of perturbation theories and non of these theories include spin into the dynamics of motion.

In this paper I have argued that the classical Laplacian operator does not provide sufficient description for the total momentum of the particle and needs to be revised to include the effects of spin. This is because Laplacian is more of a mathematical operator based on geometry of particle motion which can very well account for the velocity but if there is increase or decrease of relativistic mass due to physical effect such as spin, the Laplacian cannot account for these changes. Secondly it is pointed out that the separation constant relating the time dependent and the time independent hamiltonian for a bound particle is not the same as the free particle which is commonly understood to be $E$. For the bound particle it is $(E + K)$ where $K$ is a function of orbit curvature. This additional term also affects the relativistic mass without affecting the velocity. In Dirac’s theory we provide correction to del operator from outside by introducing Dirac matrices, $k$ operator and by making a proper choice in selecting the the radial momentum operator. In this theory, the changes have been introduced from within the Laplacian. In other words the spin is included into the dynamics of motion. The resulting energy levels of Hydrogen atom are exactly same as that of Dirac’s
theory.

This section provides introduction to existing Schrödinger and Dirac formalisms. Sec. 2 introduces unified wave equation which can be reduced to both Schrödinger and Dirac type formalisms. Sec. 3 discusses energy levels and radial wave function of Hydrogen atom associated with improved Schrödinger formalism. Sec. 4 discusses current density associated with improved Schrödinger wave equation. Sec. 5 shows the derivation of the Pauli equation in the non relativistic limit. Sec. 6 provides concluding remarks.

A. Schrödinger wave equation

Schrödinger [1] based his wave equation on the classical one dimensional wave equation given by

$$\frac{\partial \psi}{\partial t} = i \frac{\hbar^2}{2m_o} \nabla^2 \psi. \quad (1.1)$$

requiring that the coefficient $\gamma$ be only a constant and should not involve any parameters of a particular kind of motion of the particle. With selection of $\gamma = \hbar/2m_o$ and generalizing to three dimension, the non-relativistic Schrödinger wave equation that would satisfy the expected wave function $\psi$ was obtained for a free particle.

$$i \hbar \frac{\partial \psi}{\partial t} = - \frac{\hbar^2}{2m_o} \nabla^2 \psi, \quad (1.2)$$

Inclusion of central potential $V$ brings it to the form,

$$i \hbar \frac{\partial \psi}{\partial t} = - \frac{\hbar^2}{2m_o} \nabla^2 \psi + V(r, t), \quad (1.3)$$

This classical form of wave equation could not account for the fine structure of the Hydrogen atom because it does not include spin of the electron. Later development of the relativistic Schrödinger wave equation [2] also had the same shortcoming because it could not include Pauli spin matrices without destroying the invariance of the theory.

B. Dirac’s relativistic wave equation

Dirac [8, 9] took another approach for addressing the spin problem and derived the Hydrogen energy levels that were in conformance with the fine structure of Hydrogen. However, certain finer effects such as Lamb shift [10, 65] are beyond the reach of Dirac’s theory and were later addressed by quantum electrodynamics. In discussing the relativistic wave equations we will not deal with the general case of the motion of electron in the presence of an external electromagnetic field but we will start with the free particle equation and add external fields as required. Dirac derived his wave equation by linearizing the energy-momentum invariant equation in space derivative.

$$E^2 = E_0^2 + (cp)^2. \quad (1.4)$$

where $E$ = total energy of the particle and $E_0 = m_0c^2$ is the rest energy of particle. Relativistic mass is little used by modern physicists. Notwithstanding the modern usage I have used $m$ for relativistic mass and $m_0$ for rest mass throughout the article. We can write Eq. (1.4) as,

$$E = \pm \sqrt{(m_0c^2)^2 + c^2(mv)^2}^{1/2}. \quad (1.5)$$

As usual, one can obtain Dirac’s wave equation by putting

$$(mv)^2 = (p_x^2 + p_y^2 + p_z^2) = \mathbf{p}^2. \quad (1.6)$$

The classical relativistic hamiltonian $H$ for a free particle is the right side of Eq. (1.5) with the positive sign. Dirac modified this hamiltonian to make it linear in the space derivative and is given by

$$H = \mathbf{p} \cdot \mathbf{A} + \beta m_0c^2, \quad (1.7)$$

where $\alpha$ and $\beta$ represent Dirac matrices. The relativistic wave equation is then given by

$$E\psi(r, t) = H\psi(r, t). \quad (1.8)$$

Substitution of $H$ from Eq. (1.7) and replacing $E$ by $i\hbar\partial/\partial t$ and $\mathbf{p}$ by $-i\hbar \nabla$ gives Dirac’s wave equation [11],

$$\left( i \hbar \frac{\partial}{\partial t} + i \hbar c \alpha \cdot \nabla - \beta m_0 c^2 \right) \psi = 0. \quad (1.9)$$

Dirac’s equation for a central potential $V$ is,

$$\left( i \hbar \frac{\partial}{\partial t} + i \hbar c \alpha \cdot \nabla - \beta m_0 c^2 - V \right) \psi(r, t) = 0. \quad (1.10)$$

From here on follows Dirac’s theory of Hydrogen atom which shall not be repeated here. Introduction of radial momentum, radial velocity and k operators yield familiar Dirac energy levels for Hydrogen atom.

In the presence of external electromagnetic field, Dirac’s wave equation takes the form

$$\left( i \hbar \frac{\partial}{\partial t} - e\phi - \alpha \cdot (-i \hbar \mathbf{e} \nabla - e \mathbf{A}) - \beta m_0 c^2 \right) \psi = 0. \quad (1.11)$$

where $\phi$ and $\mathbf{A}$ represent electric and magnetic potentials respectively. This is the basis for Dirac formalism in short.

2. IMPROVED SCHRÖDINGER FORMALISM

We can write de Broglie wavelength in squared form as,

$$\lambda^2 = V^2 T^2, \quad \left( \frac{\hbar}{p} \right)^2 = V^2 / \nu^2, \quad (2.1)$$
where $\lambda = \hbar / p$ is the associated de Broglie wavelength, $p$ momentum of particle, $\hbar$ Planck’s Constant, $V = c^2 / v$ the phase velocity, $v$ the particle velocity, $c$ velocity of light, $T$ the period of the wave and $\nu$ the frequency. Eqs. (2.1) can also be associated with the vanishing of the periodic invariant discussed in [58] and given by

$$s^2 = \lambda^2 - V^2 T^2.$$  

(2.2)

$$(h\nu)^2 = V^2 p^2, \quad E^2 = V^2 p^2.$$  

(2.3)

These relations can also be directly obtained from the fundamental relativistic mass energy equivalence expression

$$E = mc^2 \equiv (E - V).$$  

(2.4)

where $V$ on the r.h.s. can represent the central coulomb potential. If we square and multiply and divide r.h.s. by $v^2$, we get

$$(E - V)^2 = \frac{c^4}{v^2} (mv)^2 = \frac{c^4}{v^2} p^2.$$  

(2.5)

In following sections we will see that in case of Hydrogen atom, the energy $E$ appearing in Eq. (2.5) can be made to represent the Dirac energy levels with a proper choice of quantum mechanical operator for representing the momentum $p^2$. We can introduce the velocities corresponding to the stationary states in Eq. (2.5), and it will make no difference to this equation. Now keeping the velocity constant for a particular stationary state if we increase or decrease the relativistic mass to $m_+$ or $m_-$, it will change the momentum and energy levels to $p_+, p_-$ and $E_+, E_-$. What is suggested here is that the Laplacian operator for the angular momentum has sufficient provision for altering the velocity of the particle but it has no provision for altering the relativistic mass of the particle without altering the velocity. This deficiency can be removed by introducing the spin operator in the Laplacian which I propose can alter the relativistic mass of the particle without changing its velocity. Therefore the theory based on this concept discussed in following sections is perfectly invariant under Lorentz group. We use Lorentz transformation Eq. (2.6)

$$(E - V) = m_0 c^2 (1 - \beta^2)^{-\frac{1}{2}}.$$  

(2.6)

with Eq. (2.5) to obtain the energy momentum invariant

$$(E - V)^2 = [(c p)^2 + (m_0 c^2)^2].$$  

(2.7)

which is equivalent to Eq. (1.4). This allows us to write the wave equation in the form

$$E \psi = \pm [(c p)^2 + (m_0 c^2)^2]^{1/2} \psi + V \psi,$$  

(2.8)

where $\pm$ sign indicates positive and negative energies of Dirac’s theory. Here $E$ represents the total orbital energy of the particle consisting of kinetic energy $E'$, rest energy $m_0 c^2$ and the potential energy $V$,

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

(2.9)

In Eq. (2.5) we replace $E$ by $i\hbar \partial / \partial t$ and $p$ by an unconventional quantum mechanical operator $-i\hbar \nabla$. Assuming spherically symmetric potential, we define operator $\nabla_j^2$ in spherical polar coordinates as

$$\nabla_j^2 = \frac{1}{r^2} \left[ \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) - \frac{1}{r^2} (L + S)^2 \right],$$  

(2.10)

where $L$ is the orbital angular momentum operator given by,

$$L^2 = -\hbar^2 \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{2}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right].$$

(2.11)

$S$ is the spin angular momentum operator. For electron, $S = \frac{1}{2} \hbar \sigma$ where $\sigma$ are the Pauli spin matrices [11]. If we put $S = 0$ in Eq. (2.10), we get the classical Laplacian $\nabla^2$ of the Schrödinger theory. Operator $\nabla_j^2$ is associated with the total angular momentum of the particle and is capable of replacing Dirac matrices. Introduction of this operator in Eq. (2.5) yields four spinors. The rectangular coordinates in terms of the spherical polar coordinate system we are using, have been defined according to the scheme $x = r \sin \theta \cos \phi, y = r \sin \theta \sin \phi,$ and $z = r \cos \theta$.

The Laplacian in spherical coordinates contains the squared radial momentum operator $p_r^2$ which is Hermitian. However, as pointed out by several authors [14, 61–64] the radial momentum operator $p_r$ of Dirac theory is not Hermitian. The proposed momentum operator $\nabla_j^2$ also contains the squared radial momentum operator $p_r^2$ which is Hermitian. The angular momentum operator $L$, and the spin operator $S$ contributes nothing to the the squared radial momentum operator $p_r^2$. $S$ only change the relativistic mass of the particle. Therefore in this respect the theory has an advantage over Dirac theory.

The wave equation Eq. (2.8) can be written as

$$i\hbar \frac{\partial \psi}{\partial t} = \pm [-h^2 c^2 \nabla_j^2 + (m_0 c^2)^2]^{1/2} \psi + V \psi,$$  

(2.12)

The wave equation Eq. (2.12) can be considerably simplified if potential $V$ does not depend on time. It is then possible to express its general solution as a sum of products of functions of $r$ and $t$ separately. We consider a particular solution of Eq. (2.12) that can be written as a product $\psi(r, t) = z(r) f(t)$. A general solution can be written as a sum of such separated solutions. If we substitute the above product in Eq. (2.12) and divide thru by the product, we get

$$i\hbar \frac{1}{z} \frac{df}{dt} = \pm \frac{1}{z} [-h^2 c^2 \nabla_j^2 + (m_0 c^2)^2]^{1/2} z + V.$$  

(2.13)

If we define another function $u(r)$ such that

$$\frac{1}{z} \left[ 1 - \left( \frac{\hbar}{m_0 c} \right)^2 \nabla_j^2 \right]^{1/2} z = \left[ 1 - \left( \frac{\hbar}{m_0 c} \right)^2 \frac{1}{u} \nabla_j^2 u \right]^{1/2},$$

(2.14)
then we can write Eq. (2.13) as
\[
\frac{i\hbar}{f} \frac{df}{dt} = \pm \left[ -\frac{\hbar^2 c^2}{u} \nabla^2 u + (m_o c^2)^2 \right]^{1/2} + V. \tag{2.15}
\]

Since the left side depends only on \(t\) and right side only on \(r\), both side must be equal to a same separation constant which in this case is \((E + K)\) where
\[
K = (E - V) \left[ -1 + \left( 1 + \frac{\kappa \alpha \hbar^2 c^2}{2(E - V)^2} \right)^{1/2} \right]. \tag{2.16}
\]

\(K\) represents correction to the particle energy level due to the orbit curvature \(\kappa\). Energy levels of two particles having identical parameters (including velocity), and one having a straight trajectory of a free particle and another having a curvature of the bound orbit, cannot be the same. This results in different relativistic masses and therefore different energy levels. The curvature of the orbit can alter the relativistic mass without changing the velocity. \(\alpha\) is a function of the particle energy which we define as
\[
\alpha = \frac{2((m_o c^2)^2 - E^2)^{1/2}}{\hbar c}. \tag{2.17}
\]

In case of circular orbits \(\kappa = 1/r\), and for a free particle \(\kappa = 0\) and thus \(K = 0\). Then equation for \(f\) can be easily integrated to give,
\[
f(t) = C \exp(-i(E + K)t/\hbar), \tag{2.18}
\]
where \(C\) is an arbitrary constant and the equation for \(u\) becomes,
\[
\{(E - V)^2 - (m_o c^2)^2\}u(r) = -\hbar^2 c^2 (\nabla^2 + \kappa \alpha/2)u(r). \tag{2.19}
\]

If we expand both sides of Eq. (2.14), we find that for slow moving particles, \(z \approx u\).

1. Separation of angular and radial wave equations

Substitution of Eq. (2.10) in Eq. (2.19) gives Eq. (2.21). The radial and the angular parts are then separated by substituting
\[
u(r, \theta, \phi) = R(r)Y(\theta, \phi) \tag{2.20}
\]
in Eq. (2.21) and dividing thru by \(RY\). As is expected in the presence of spin, the radial and the angular wave functions do get split into two spinor components. These two components are sufficient to explain both positive and negative energies.

\[
\left[ \frac{1}{\hbar^2 c^2}((m_o c^2)^2 - (E - V)^2) - \frac{\alpha}{2r} \right] u(r) = \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) - \frac{i}{r^2} \sin \theta \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2} \sin^2 \theta \frac{\partial^2}{\partial \phi^2} \right]^{1/2} + \frac{S}{\hbar} \right]^2 u(r). \tag{2.21}
\]

\[
\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) - \frac{r^2}{\hbar^2 c^2}((m_o c^2)^2 - (E - V)^2) + \frac{\alpha r}{2} = \frac{1}{Y} \frac{1}{\hbar^2} \left[ i \hbar \left( \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} \right)^{1/2} + S \sqrt{Y} \right]^2. \tag{2.22}
\]

Since the left side of Eq. (2.22) depends only on \(r\) and the right side depends only on \(\theta\) and \(\phi\), both sides must be equal to a constant that we call \(\Gamma\). Thus Eq. (2.22) gives us a radial equation
\[
\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) - \frac{1}{\hbar^2 c^2}((m_o c^2)^2 - (E - V)^2) R + \frac{\alpha}{2r} R - \frac{\Gamma}{r^2} R = 0, \tag{2.23}
\]
and an angular equation
\[
\frac{1}{\hbar^2} \left[ i \hbar \left( \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} \right)^{1/2} + S \sqrt{Y} \right]^2 - \Gamma Y = 0. \tag{2.24}
\]

The angular equation can be further separated by substituting
\[
Y(\theta, \phi) = \Theta(\theta) \Phi(\phi) \tag{2.25}
\]
into it and dividing by \(\Theta \Phi\).

\[
\left[ \frac{1}{\Theta} \frac{1}{\sin \theta} \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta}{d\theta} \right) + \left( \sqrt{\Gamma - \left( \frac{S}{\hbar} \right)^2} \right) \sin^2 \theta \right] + \frac{1}{\Theta} \frac{d^2 \Phi}{d\phi^2} = \nu.
\]

(2.26)

From the theory of unitary groups and infinitesimal rotations \[11\], it follows that the spin angular momentum operator \(\mathbf{S}\) is strictly a constant of the motion and can be replaced by the number \(s(s+1)\hbar^2\) where \(s\) is an integer or half an odd integer and we have already defined \(\Gamma\) as a constant. Therefore the quantity \(\{\sqrt{\Gamma - \left( \frac{S}{\hbar} \right)^2}\}^2\) appearing in Eq. (2.23) can only be a constant which we shall call \(\lambda\). Hence we end up with two equations

\[
\frac{d^2 \Phi}{d\phi^2} + \nu \Phi = 0, \quad (2.27)
\]

\[
\frac{1}{\sin \theta} \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta}{d\theta} \right) + \left( \lambda - \frac{\nu}{\sin^2 \theta} \right) \Theta = 0. \quad (2.28)
\]

Eqs. (2.27) and (2.28) have exactly the same solutions as that given by Schrödinger theory where \(\nu\) is chosen to be equal to square of an integer \(m\) which takes on positive or negative integer values or zero. Therefore,

\[
\Phi_m(\phi) = (2\pi)^{-\frac{1}{2}} \exp(im\phi). \quad (2.29)
\]

The condition that the solution of Eq. (2.28) be finite at \(\cos \theta = \pm 1\) limits the values of \(\lambda\) to \(l(l+1)\) where \(l\) is a positive integer or zero. The physically acceptable solutions of Eq. (2.28) when \(m = 0\) are called Legendre polynomials and for \(m \leq l\) are called associated Legendre functions. Solution for \(\lambda\) gives us the new relationship

\[
\{\sqrt{\Gamma - \left( \frac{S}{\hbar} \right)^2}\}^2 = l(l+1) = \Lambda^2/\hbar^2. \quad (2.30)
\]

This can be written as

\[
\{\sqrt{\Gamma - \mathbf{S}^2}\}^2 = \Lambda^2. \quad (2.31)
\]

This condition can be satisfied if we substitute \(\sqrt{\Gamma \mathbf{h}} = \Lambda \mathbf{S}\) and this will also be consistent with Eq. (2.24) which can be written as

\[
(\mathbf{L} + \mathbf{S})^2 Y = \Gamma \hbar^2 Y. \quad (2.32)
\]

Furthermore, the theory of unitary groups and infinitesimal rotations \[11\] would require that we identify \(\Gamma \hbar^2\) with eigenvalues \(j(j+1)\hbar^2\) of the total angular momentum operator \(\mathbf{J}^2\), where \(j\) is zero or a positive integer or half an odd integer. This is good enough for the radial Eq. (2.23) and it is also good enough for Eq. (2.32) for integer \(j = l\), but this will not permit separation of variables in Eq. (2.23) in case of hydrogen atom with spin 1/2 electron. Therefore Eqs. (2.24) thru (2.32) are valid only for integer values of \(j\) and in a special case of \(\mathbf{S} = 0\) we get \(\Gamma = \lambda = l(l+1)\) The angular part \(Y_m(\theta, \phi)\) of the complete wave function which is a solution of Eq. (2.24) when \(\Gamma = \lambda = l(l+1)\) is called spherical harmonic. If we put \(\Gamma = \lambda = l(l+1)\) and \(\alpha/\hbar = 0\) in the radial equation Eq. (2.23), we get the energy eigenvalues of the relativistic Schrödinger theory. All these solutions of the Schrödinger theory remain unaltered in this theory.

2. Separation of angular wave equation for spin 1/2 electron

In case of hydrogen with spin 1/2 electron, the separation of angular wave equation \[50\] is carried out in the same manner as in Dirac’s theory. This can be done by redefining Eq. (2.20) and Eq. (2.32) as

\[
\psi(r, \theta, \phi) = e^{-iEt/\hbar} R_{\nu m}(r) \psi^{(2)}_{j, j, m}(\theta, \phi) = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}. \quad (2.33)
\]

\[
(\mathbf{L} + \mathbf{S})^2 \psi^{(2)}_{j, j, m} = \Gamma \hbar^2 \psi^{(2)}_{j, j, m}. \quad (2.34)
\]

Here common subscripts \(l, 1/2\) are omitted.

\[
\psi^{(2)}_{l+1/2, m+1/2} = \left( \frac{l + m + 1}{2l + 1} \right)^{1/2} \psi^{(1)}_{l, m+1/2} + \left( \frac{l - m}{2l + 1} \right)^{1/2} \psi^{(1)}_{l, m-1/2}. \quad (2.35)
\]

\[
\psi^{(2)}_{l-1/2, m+1/2} = \left( \frac{l - m + 1}{2l + 1} \right)^{1/2} \psi^{(1)}_{l, m+1/2} - \left( \frac{l + m + 1}{2l + 1} \right)^{1/2} \psi^{(1)}_{l, m-1/2}. \quad (2.36)
\]

Coefficients in Eqs. (2.35) and (2.36) are the Clebsch-Gordon coefficients \[60\]. Here simultaneous eigenstates of \(L^2, S^2, L_\theta\) and \(S_\phi\) are given by

\[
\psi^{(1)}_{m, \pm 1/2} = Y_{lm}(\theta, \phi) \chi_{\pm}, \quad (2.37)
\]

where \(Y_{lm}(\theta, \phi)\) are the spherical harmonics from Eq. (2.32) for \(S = 0\), and \(\chi_{\pm}\) are the unit spinors.

3. Orbit curvature affects momentum

The radial wave equation Eq. (2.23) may be rewritten in a form that resembles the classical Schrödinger wave equation \[13\]. If we put \(R(r) = \chi(r)/r\) and \(E^* = E' + V\) with reference to Eq. (2.29), then the equation for the modified radial wave function \(\chi\) may be written as

\[
-\frac{\hbar^2}{2m_0} \frac{d^2 \chi}{dr^2} + \left[ V(r) - \frac{\hbar c}{r} \left( \frac{E'}{2m_0 c^2} \right)^{1/2} - \frac{(E' - V)^2}{2m_0 c^2} \right] \chi = \frac{\hbar \sigma \cdot \mathbf{L}}{2m_0 r^2} \chi. \quad (2.38)
\]
Thus the radial motion is similar to the classical motion of a particle in a potential defined by the quantity within the large brackets. The first term is equivalent to the classical kinetic energy $\mathbf{p}^2/2m_0$. The first, second and the fifth terms are same as the classical Schrödinger theory. The fourth term is approximately equal to $\mathbf{p}^2/Sm_0c^2$ which has the form of the classical relativistic mass correction and is same as Dirac’s theory. The seventh term includes spin-orbit coupling. The sixth term is due to the spin itself. The third term is associated with the curvature of the circular orbit $\kappa = 1/r$ which originates from the separation constant $(E + K)$ given by Eq. (2.10). The magnitude of this term is dependent on the kinetic and potential energies in addition to the curvature. For very large $r$ this term becomes negligible. Therefore there is a certain amount of correction to the potential energy when a particle travels along an orbit having large curvature. There is a corresponding change in momentum. This curvature term contributes only to the relativistic mass of the particle. The same is the case with the term due to spin. The classical Laplacian part of the operator Eq. (2.10) contributes to both the relativistic mass as well as the orbital velocity of the particle. This curvature term can be conveniently analyzed by substituting $-E^* = m_0c^2 - E$. The effect of introducing the separation constant $(E + K)$ is equivalent to adding the term $\kappa \alpha/2$ to the operator $\nabla_j^2$, provided $f(t)$ is defined by Eq. (2.13).

In Dirac’s analysis, the third, fifth and sixth terms do not appear at all and the seventh spin orbit coupling term appear in the form of spin-orbit interaction energy associated with Larmor precession and Thomas precession. It also includes one more term as a correction to the potential energy and is declared difficult to demonstrate experimentally.

4. Spin-orbit interaction energy

In our case, the last term in brackets in Eq. (2.38) has nothing to do with the spin-orbit interaction energy but the last three terms together represent additional potential energy due to total angular momentum. Spin-orbit interaction energy term is hidden within the third term which is due to curvature effect and can be demonstrated as follows. It is to be noted that the parameter $1/r$ in this term does not have its origin in the classical Laplacian. $\gamma$ in following derivation is the fine structure constant.

$$\begin{align*}
-\frac{\hbar}{r} \left( -E^* \right)^{1/2} &= \frac{V}{\sqrt{2\gamma}} \left( \frac{-(E - m_0c^2)}{m_0c^2} \right)^{1/2} \\
&= \frac{V}{\sqrt{2\gamma}} \left( 1 - \frac{m}{m_0} - \frac{V}{m_0c^2} \right)^{1/2}.
\end{align*}$$

Using Eq. (2.12) we can write

$$(E - V)^2 = (mc^2)^2 = -\hbar^2 c^2 (\nabla_j^2 + \kappa \alpha/2) + (m_0c^2)^2,$$

(2.40)

$$\frac{m}{m_0} = \pm \left[ 1 - \left( \frac{\hbar}{m_0c} \right)^2 \left( \nabla_j^2 + \kappa \alpha/2 \right) \right]^{1/2}.$$  

(2.41)

Eq. (2.41) shows that the particles can have positive or negative relativistic mass but the rest mass is always positive. This is the difference between particle and anti-particle. Since the second term in the bracket is small we can have

$$\frac{m}{m_0} = \pm \left[ 1 - \frac{1}{2} \left( \frac{\hbar}{m_0c} \right)^2 \left( \nabla_j^2 + \kappa \alpha/2 \right) \right].$$

(2.42)

Using Eq. (2.10) we can write

$$\nabla_j^2 = \nabla^2 - \frac{1}{\hbar^2 r^2} (S^2 + 2L \cdot S).$$

(2.43)

Substitution of Eq. (2.43) in Eq. (2.42) gives

$$\frac{m}{m_0} = \pm \left[ 1 + \frac{p^2 r^2 + S^2 + 2L \cdot S - (\alpha rh^2/2)}{2m_0^2c^2 r^2} \right].$$

(2.44)

We have been using two different varieties of momentum $p$. One associated with $\nabla_j$ and another with $\nabla$. The later associates only with the relativistic mass due to Lorentz transformation where as the former associates with the relativistic mass which includes effect due to the Lorentz transformation plus the effect due to spin. For a free particle we can have $\kappa \alpha/2 = 0$ and in the absence of spin $S = 0$. This reduces Eq. (2.41) to

$$\frac{m}{m_0} = \pm \left[ 1 - \frac{v^2}{c^2} \right]^{-1/2},$$

(2.45)

which is the familiar Lorentz transformation equation of special relativity. Next we substitute Eq. (2.44) with positive sign for positive energy in Eq. (2.39) to obtain

$$\begin{align*}
-rac{\hbar c}{r} \left( -E^* \right)^{1/2} &\approx \gamma \left( \frac{V}{4} \left\{ -\frac{p^2 r^2 + S^2 - (\alpha rh^2/2)}{m_0^2 c^2 r^2} \right\} \right) \\
&= \frac{1}{2m_0^2 c^2 r} \frac{1}{V} \frac{dV}{dr} (L \cdot S - \frac{V^2}{2m_0c^2})^{1/2}.
\end{align*}$$

(2.46)

The middle term on the right has the form of the spin-orbit interaction energy associated with Larmor precession and Thomas precession. Now we have sufficient information to conclude that the term $\kappa \alpha/2$ appearing in Eq. (2.10) simulates the bound state of the electron and provides coupling between the momentum, orbit curvature, spin-orbit interaction and the central coulomb potential. Therefore in order to deal with the free particle, we have to put curvature $\kappa = 0$, but this does not eliminate the spin and so it makes its presence felt in the presence of an external electromagnetic field as in case of the Pauli equation.
3. THE HYDROGEN ATOM

A. Energy levels

The second term in radial equation (2.23) is,

\[- \frac{1}{\hbar^2 c^2} \left\{ (m_e c^2)^2 - (E - V)^2 \right\} R = - \frac{(m_e c^2 + E - V)}{\hbar c} \left( \frac{m_e c^2 - E + V}{\hbar c} \right) R.\]  

(3.1)

We will substitute

\[\alpha_1 = \frac{2(m_e c^2 + E)}{\hbar c}, \quad \text{and} \quad \alpha_2 = \frac{2(m_e c^2 - E)}{\hbar c}.\]  

(3.2)

Hence with respect to Eq. (2.17), \(\alpha^2 = \alpha_1 \alpha_2\). The attractive coulomb interaction between an atomic nucleus of charge +Ze and an electron of charge \(-e\) is represented by the potential energy \(V(r) = -Ze^2k'/r\) where \(k'\) is Coulomb’s constant. In case of hydrogen atom, \(Z = 1\). We introduce these hydrogen parameters into Eq. (3.1) with the fine structure constant \(\gamma\) defined as \(\gamma = (e^2kZ)/(\hbar c)\).

\[- \frac{1}{\hbar^2 c^2} \left\{ (m_e c^2)^2 - (E - V)^2 \right\} R = - \alpha^2 \left( \frac{\gamma}{r} \left( \frac{\alpha_2 - \alpha_1}{2 \alpha^2} \right) - \frac{\gamma^2}{r^2 \alpha^2} \right) R.\]  

(3.3)

We will rewrite the radial equation (2.23) in dimensionless form by introducing a unitless independent variable \(\rho = \alpha r\) which we have already defined earlier with Eq. (2.17). Substitution of Eqs. (3.3) and (3.2) gives,

\[\frac{1}{\rho^2} \frac{d}{d\rho} \left( \rho^2 \frac{dR}{d\rho} \right) - \frac{1}{4} \left( \frac{\gamma}{\rho} \left( \frac{\alpha_2 - \alpha_1}{2 \alpha^2} \right) - \frac{\gamma^2}{\rho^2} \right) R = \frac{1}{2\rho} R - j(j + 1) \frac{\rho^2}{R} = 0,\]  

(3.4)

As far as the leading terms are concerned, for sufficiently large \(\rho\) it is apparent that \(R(\rho) = \rho^s e^{\pm \lambda \rho}\) satisfies Eq. (3.3) when \(s\) has any finite value. This suggests that we look for an exact solution of Eq. (3.4) of the form

\[R(\rho) = F(\rho) e^{\pm \lambda \rho} \]  

(3.5)

where \(F(\rho)\) is a polynomial of finite order in \(\rho\). Substitution of Eq. (3.5) into Eq. (3.4) gives equation for \(F(\rho)\) as

\[F'' + \left( \frac{2}{\rho} - 1 \right) F' + \left[ \frac{\lambda - (1/2)}{\rho} - j(j + 1) - \gamma^2 \right] F = 0,\]  

(3.6)

where we have substituted

\[\lambda = -\gamma \left( \frac{\alpha_2 - \alpha_1}{2 \alpha} \right).\]  

(3.7)

Now we find a solution for \(F\) in the form

\[F(\rho) = \rho^s (a_0 + a_1 \rho + a_2 \rho^2 + \cdots) = \rho^s L(\rho).\]  

(3.8)

and \(a_0 \neq 0, \ s \geq 0.\)

Substitution of Eq. (3.3) into Eq. (3.6) gives us the equation for \(L\).

\[\rho^2 L'' + \rho \left( 2(s + 1) - \rho \right) L' + \rho \left[ \lambda - s - (1/2) \right] + s^2 + s + \gamma^2 - j(j + 1) = 0.\]  

(3.10)

If we set \(\rho = 0\) in Eq. (3.10), it follows from Eqs. (3.8) and (3.3) that

\[s^2 + s + \gamma^2 - j(j + 1) = 0.\]  

(3.11)

This quadratic equation in \(s\) has two solutions,

\[s = -\frac{1}{2} \pm \left( \frac{j + 1}{2} - \gamma^2 \right)^{1/2}.\]  

(3.12)

The boundary condition that \(R(\rho)\) be finite at \(\rho = 0\) requires that we choose upper sign for \(s\). It is to be noted here that both, Schrödinger’s relativistic theory as well as Dirac’s theory allow value of \(s\) which is very slightly less than the permissible value. This problem does not exist in this theory. The smallest value in this theory is \((1 - \gamma^2)/2\), well within the range \(s \geq 0\). With this, Eq. (3.10) reduces to

\[\rho L'' + \{2(s + 1) - \rho \} L' + \{ \lambda - s - (1/2) \} L = 0.\]  

(3.13)

Equation (3.13) can be solved by substituting Eq. (3.8). The recursion relation between the coefficients of successive terms of the series is observed to be

\[a_{\nu+1} = \frac{(\nu + s + (1/2) - \lambda)}{\nu(\nu + 1) + 2(\nu + 1)(s + 1)} a_{\nu}.\]  

(3.14)

If the series does not terminate, its dominant asymptotic behavior when \(\rho \to \infty\) can be inferred from the coefficients of its high terms:

\[\frac{a_{\nu+1}}{a_{\nu}} \to \frac{1}{\nu}.\]  

(3.15)

This means that the series has the asymptotic form \(e^\rho\) and regular solution is obtained only if it terminates. Suppose that this occurs at \(\nu = n'\), so that \(a_{n'+1} = 0\). Then Eq. (3.14) give the relation

\[n' + s + (1/2) - \lambda = 0, \quad n' = 0, 1, 2, \ldots\]  

(3.16)

Substituting for \(s\) and \(\lambda\) from Eqs. (3.14) and (3.15) respectively, we get the energy levels of hydrogen atom

\[E = m_0 c^2 \left( 1 + \frac{\gamma^2}{\left[ \left( j + \frac{1}{2} \right)^2 - \gamma^2 \right]^{1/2} + n'} \right)^{-1/2}.\]  

(3.17)
where the radial quantum number $n'$ is related to the total quantum number $n$ by the expression
\[
n = n' + (j + (1/2)).
\] (3.18)

These are exactly the same Dirac energy levels having the same total spread in energy of the fine-structure levels for a given $n$.

B. Radial wave function

It is clear that Eq. (3.13) has the form of associated Laguerre differential equation [11],
\[
\rho L_q'' + (p + 1 - \rho)L_q' + (q - p)L_q = 0.
\] (3.19)
The associated Laguerre polynomials $L_q^p$ can be constructed according to formula
\[
L_q^p(\rho) = \sum_{k=0}^{q-p} (-1)^{k+p} \frac{[q]!\rho^k}{(q-p-k)!(p+k)!k!}.
\] (3.20)

In case of Eq. (3.13), we have $p = 2s+1$, $(q-p) = \lambda - s - (1/2)$ and $q = \lambda + s + (1/2)$. Comparison with Eq. (3.19) shows that $(q-p)$ are integers but $p$ and $q$ are not integers. Therefore it is possible to solve Eq. (3.13) using Laguerre polynomials only if we introduce the approximations $p \approx 2j + 1$ and $q \approx \lambda - s + 2j + (1/2)$ by ignoring $\gamma^2$ term in $s$. Hence we get,
\[
L_{\lambda-s-2j+(1/2)}^{2j+1}(\rho) = \sum_{k=0}^{\lambda-s-(1/2)} (-1)^{k+2j+1} \frac{[(\lambda-s+2j+(1/2))]!\rho^k}{(\lambda-s-\lambda-2j-1)!(2j+1+k)!k!}.
\] (3.21)

This will yield two associated Laguerre polynomials $L_q^p$ corresponding to two values of $\lambda$ associated with two spinors which are applicable to positive energy as well as the negative energy solutions. The resulting approximate radial wave function is of the form $e^{-\lambda \rho}\rho^k L_{\lambda-s+2j+(1/2)}^{2j+1}$ and the normalization constant may be found by using the generating function to evaluate the integral
\[
\int_0^\infty e^{-\rho^2} [L_{\lambda-s+2j+(1/2)}^{2j+1}(\rho)]^2 \rho^2 d\rho.
\] (3.22)

C. Comparison with previous theories

We shall now compare the radial equation Eq. (3.13) with previous theories of Schrödinger [7], Darwin-Pauli [12, 19] and Dirac [8]. Integer eigenvalues of the $k$ operator in Dirac’s theory are same as the orbital angular momentum $k$ in Pauli-Darwin theory. If we substitute $k$ for $j + (1/2)$ in Eq. (3.14) we write
\[
\frac{1}{\rho^2} \frac{d}{d\rho} \left( \rho^2 \frac{dR}{d\rho} \right) + \left( \frac{\lambda}{\rho} - 1 - \frac{k(k+1) - \gamma^2}{\rho^2} \right) R = 0.
\] (3.23)
If one neglects the last term, the remaining two terms constitute the ordinary relativistic Schrödinger equation for particle that does not have spin. Therefore the third term represents the correction introduced by this theory. If we replace $(k+1)$ by $-k$ in Eq. (3.23), we do not alter the first two terms but the third term will change to
\[
\left( \frac{1}{2\rho} - \frac{k+(3/4)}{\rho^2} \right) R,
\] (3.24)
which is the second possible correction to the ordinary relativistic Schrödinger equation. Now, even by transforming the wave function $R$, it is not possible to relate these two correction terms with that of Pauli-Darwin and Dirac’s theories which are given by
\[
e^2 k'_{2m_0c^2 \gamma^2} k \quad \text{and} \quad -e^2 k'_{2m_0c^2 \gamma^2} (k+1).
\] (3.25)
At the same time the energy levels of the Hydrogen atom are exactly same as that of Dirac’s theory. The principle reason being that in present theory, the spin is included in the dynamics of motion where as in Pauli-Darwin and Dirac theories it is introduced as a perturbation. For the same reason the spin-orbit interaction energy appears in Dirac’s theory in a little different way than in this theory.

Next we compare wave equation of this theory with the Klein-Gordon wave equation which is the square of the Dirac equation and can be written as
\[
(\Box^2 + \mu^2) \psi = 0 \quad \text{where} \quad \mu = \frac{mc}{\hbar}.
\] (3.26)

\[
\Box^2 = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 = d’Alembert operator.
\] (3.27)

With respect to the wave equation Eq. (2.12), for a free particle we have $V = 0$ and $\kappa = 0$. Hence
\[
\left( \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 + \mu^2 \right) \psi = 0.
\] (3.28)
where the first two terms denote the modified d’Alembert operator $\Box^2$ which includes the spin operator and hence can account for all spin values.

\[
(\Box^2 + \mu^2) \psi = 0.
\] (3.29)

The Klein-Gordon wave equation (3.26) cannot account for spin 1/2 particles, it is beieved to account only for scalar spin 0 particles. The wave equation of this theory Eq. (3.28) can account for all spin values: 0, 1/2, 1 and 2. The spin is just a quantum number.
4. CURRENT DENSITY

The total angular momentum operator $\nabla_j^2$ given by Eq. (2.110) can be written as

$$\nabla_j^2 = \nabla^2 - \frac{S^2}{\hbar^2 r^2} - \frac{2L \cdot S}{\hbar^2 r^2}. \quad (4.1)$$

Substitution of Eq. (4.1) in Eq. (2.19) gives

$$\{ (E-V)^2 - (m_o c^2)^2 \} u(r) = -\hbar^2 c^2 \left[ \nabla^2 - \frac{S^2}{\hbar^2 r^2} - \frac{2L \cdot S}{\hbar^2 r^2} \right] u(r). \quad (4.2)$$

Therefore the spin-orbit coupling term in Eq. (4.5) can be verified using similar identity applicable

Substitution of Eq. (4.1) in Eq. (2.19) gives

$$(E + K)z(r) = i\hbar c \left[ \nabla^2 - \frac{S^2}{\hbar^2 r^2} - \frac{2L \cdot S}{\hbar^2 r^2} \right] \frac{1}{2} z(r) + V z(r). \quad (4.3)$$

Expanding this to first order accuracy we can write

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m_0} \left[ \nabla^2 - \frac{2L \cdot S}{\hbar^2 r^2} - \frac{S^2}{\hbar^2 r^2} \right] \psi + V \psi, \quad (4.5)$$

where $i\hbar (\partial / \partial t) = E^* = (E + K - m_o c^2)$. In order to evaluate the spin-orbit coupling term, we make use of the following identity applicable to Pauli matrices.

$$(\sigma \cdot B)(\sigma \cdot C) = (B \cdot C) + i\sigma' \cdot (B \times C). \quad (4.6)$$

Eq. (4.6) can be verified using similar identity applicable to Dirac matrices.

$$(\alpha \cdot B)(\alpha \cdot C) = (B \cdot C) + i\sigma' \cdot (B \times C). \quad (4.7)$$

If we replace vectors B and C in Eq. (4.6) by vectors $p$ and $r$, we get

$$(\sigma \cdot p)(\sigma \cdot r) = (p \cdot r) + i\sigma \cdot (p \times r). \quad (4.8)$$

$$i\sigma \cdot (p \times r) = (i\hbar \nabla \cdot r) - (\sigma \cdot i\hbar \nabla)(\sigma \cdot r). \quad (4.9)$$

$$\sigma \cdot (p \times r) = \hbar \left[ (\nabla \cdot r) - (\sigma \cdot \nabla)(\sigma \cdot r) \right]. \quad (4.10)$$

Therefore the spin-orbit coupling term in Eq. (4.5) can be written as

$$\frac{2L \cdot S}{\hbar^2 r^2} = \frac{\hbar \sigma \cdot (p \times r)}{\hbar^2 r^2},$$

Substitution of Eq. (4.11) in Eq. (4.5) gives

$$\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m_0} \left[ \nabla^2 - (\nabla \cdot \hat{r}) + (\nabla \cdot \sigma)(\hat{r} \cdot \sigma) \right. \quad (4.12)$$

The Hamiltonian adjoint of Eq. (4.12) is written as

$$\frac{\partial \psi^\dagger}{\partial t} = -\frac{i\hbar}{2m_0} \left[ \nabla^2 + (\nabla \cdot \hat{r}) - (\nabla \cdot \sigma)(\hat{r} \cdot \sigma) \right. \quad (4.13)$$

We multiply Eq. (4.12) on the left by $\psi^\dagger$ and Eq. (4.13) on the right by $\psi$ and add one to another.

$$\frac{\partial w}{\partial t} = \frac{i\hbar}{2m_0} \left[ \psi^\dagger \nabla \psi - \psi \nabla \psi^\dagger \right. \quad (4.14)$$

If we substitute $\sigma^2 = 3$ in Eq. (4.13), it reduces to

$$\frac{\partial w}{\partial t} + \nabla \cdot j = 0 \quad (4.16)$$

Eq. (4.14) has the form of continuity equation

provided we define the probability current density vector $j$ as

$$j = \frac{\hbar}{2m_0} \left[ \psi^\dagger \nabla \psi - \psi \nabla \psi^\dagger \right. \quad (4.17)$$

From Eqs. (4.14) and (4.17) it is clear that in case of a bound electron, the spin-orbit coupling term does contribute to the probability density and the current density. For a free particle we can assume a very large value for $r$ in these two equations and the last two terms become negligible, hence we get for two spinors

$$\frac{\partial w}{\partial t} = \frac{i\hbar}{2m_0} \left[ \psi^\dagger \nabla \psi - \psi \nabla \psi^\dagger \right. \quad (4.18)$$

$$j = \frac{\hbar}{2m_0} \left[ \psi^\dagger \nabla \psi - \psi \nabla \psi^\dagger \right. \quad (4.19)$$
This is same as the first term of the current density for Pauli equation. In comparison the free particle current density for spinless particle in Schrödinger theory is

\[ S(r, t) = \frac{\hbar}{2m_0}(\psi^* \nabla \psi - (\nabla \psi^*)\psi), \quad (4.20) \]

and Dirac’s theory with four spinors yields

\[ S(r, t) = c\psi^\dagger \alpha \psi. \quad (4.21) \]

In case of Schrödinger current density Eq. (4.20), the classical results for Hydrogen atom indicate nil value [20] when the quantum number \( m = 0 \). In case of Dirac current density Eq. (4.21), this value is not nil and corresponds to a circular rotation of probability [22]. A good approximation of the Dirac current is obtained when Gordon current [21] \( S_1 = (\hbar/2m_0)\text{rot}(\psi^*\sigma\psi) \) is added to Eq. (4.20) in the Pauli approximation [22] and \( S_1 = (1/m_0)\nabla P \times \mathbf{S} \) in the Schrödinger approximation [21, 22], where \( P \) is the probability density and \( \mathbf{S} \) the constant spin vector [20].

5. THE PAULI EQUATION

In the non-relativistic limit, for the motion of electron in the presence of an external electromagnetic field, the present theory can be shown to reduce to the Pauli equation. In the non-relativistic limit, we have \( \kappa \alpha/2 = 0 \) and \( \mathbf{S} = 0 \), and the equation of motion is given by Eq. (2.19) where \( V = e\phi \). We use the following standard quantization procedure in the presence of an external electromagnetic field. \( \nabla = (\partial_1, \partial_2, \partial_3) \),

\[ E \Rightarrow \left( i\hbar \frac{\partial}{\partial t} - e\phi \right), \quad \mathbf{p} \Rightarrow \left( -i\hbar \nabla - \frac{e}{c} \mathbf{A} \right), \quad (5.1) \]

where \( e \) is the charge on the particle and \( c \) is the speed of light. The electric and magnetic field strengths are given in terms of the respective potentials \( \phi \) and \( \mathbf{A} \) by

\[ E = -\frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} - \nabla \phi, \quad \mathbf{H} = \nabla \times \mathbf{A}. \quad (5.2) \]

Therefore Eq. (2.19) together with Eq. (2.10) reduces to

\[ (E - e\phi)^2 - (m_ec^2)^2 \psi = (cp - eA)^2 \psi, \quad (5.3) \]

Here we make use of the identity Eq. (4.6) and replace both vectors \( \mathbf{B} \) and \( \mathbf{C} \) with the vector \( (cp - eA) \). This gives

\[ \mathbf{σ} \cdot (cp - eA)^2 = (cp - eA)^2 + i\mathbf{σ} \cdot [(cp - eA) \times (cp - eA)]. \quad (5.4) \]

Using Eq. (5.2) we can derive the relation

\[ \mathbf{σ} \cdot (cp - eA) \times (cp - eA) = -e(eA \times \mathbf{p} + \mathbf{p} \times \mathbf{A}) = i\hbar e \mathbf{σ} \times \mathbf{A} = i\hbar e \mathbf{H}. \quad (5.5) \]

Substitution of Eq. (5.5) in Eq. (5.4) gives

\[ (cp - eA)^2 = |\mathbf{σ} \cdot (cp - eA)|^2 + e\hbar \mathbf{σ} \cdot \mathbf{H}. \quad (5.6) \]

In case of the motion of electron in an external electromagnetic field, Eq. (2.9) gets modified to

\[ E = E' + m_ec^2 + e\phi. \quad (5.7) \]

If we put \( E' = E' + e\phi \) and assume that \( E' \) and \( e\phi \) are small in comparison with \( m_ec^2 \), we can then make the replacement

\[ (E - e\phi)^2 - (m_ec^2)^2 \approx 2m_ec^2(E' - e\phi), \quad (5.8) \]

in Eq. (5.3) and substitute Eq. (5.6) to obtain

\[ E'\psi = \left[ \frac{1}{2m_0} \left( \sigma \cdot (p - eA) \right)^2 + c\phi + \frac{e\hbar}{2m_0c} \sigma \cdot \mathbf{H} \right] \psi \quad (5.9) \]

where \( \psi = \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} \). \quad (5.10)

Eq. (5.9) is a system of two coupled differential equations for \( \psi_1 \) and \( \psi_2 \), describing electrons with \( z \) component of their spin up or down respectively. Therefore we can replace \( \sigma^2 \) by \( \sigma_z^2 = 1 \) and in the non-relativistic limit, Eq. (5.9) reduces to the Pauli equation

\[ i\hbar \frac{\partial \psi}{\partial t} = \left[ \frac{1}{2m_0} \left( \mathbf{p} \cdot - \frac{e}{c} \mathbf{A} \right)^2 + c\phi + \frac{e\hbar}{2m_0c} \sigma \cdot \mathbf{H} \right] \psi, \quad (5.11) \]

where the \( \mathbf{H} \) term represents the magnetic moment of an electron.

6. CONCLUSION

Spin is successfully introduced in Schrödinger formalism. The resulting energy levels of Hydrogen atom in this theory are exactly same as that of Dirac’s theory. The separation of the new wave equation in spherical polar coordinates is as simple as that of the Schrödinger theory and the solution of the angular part of the wave equation for spin 1/2 electron is same as in Dirac’s theory. The separation constant relating the time dependent and the time independent hamiltonian for a bound particle is not the same as the free particle but has an additional term which accounts for the energy contribution in the formation of the orbit curvature. The radial wave function of the Schrödinger theory gets split into two spinor components. These two components are sufficient to explain both positive and negative energies. The new theory accounts for the energy due to spin-orbit interaction as well as for the additional potential energy due to spin and spin-orbit coupling. Spin angular momentum operator \( \mathbf{S} \) is as
neatly integrated into the equation of motion as the orbital angular momentum operator $\mathbf{L}$. Consequently the Dirac matrices and the k operator of Dirac’s theory are dispensed with. The theory also points out that the curvature of the orbit draws on certain amount of kinetic and potential energies affecting the momentum of electron and the spin-orbit interaction energy constitutes a part of this energy. A new relationship between the relativistic mass and the rest mass is discussed which reduces to the Lorentz transformation equation in the absence of the spin. It is shown that the correction introduced to the radial equation due to the modification of classical Laplacian is not the same as that of the Darwin and Pauli theory however, the resulting energy levels of Hydrogen atom are same as that of Darwin, Pauli and Dirac theories. This is because the new theory is not a perturbation theory. Both the spin and the curvature effect are assumed to affect only the relativistic mass of the particle and the Laplacian operator part of Eq. [2.10] contributes to both the relativistic mass as well as the orbital velocity of the particle. Dirac’s theory cannot detect the curvature effect because the spin in that theory is not part of the dynamics of motion but it gets introduced as a perturbation just like Darwin and Pauli theory. Also the selection of the radial momentum operator is somewhat arbitrary in that theory [14-18] and not hermitian as pointed out by several authors. The probability density and the current density for the hydrogen atom have been calculated. 

The probability density and the current density for a free particle is comparable to that of the Pauli equation for the motion of electron in an electromagnetic field with spin included. In the presence of the external electromagnetic field, the theory reduces to the Pauli equation in the non relativistic limit. Comparison of the new wave equation with the Klein-Gordon equation shows why the later cannot account for spin values other than zero.

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