CHAPTER I

THE RELATIVISTIC SYMMETRIC HAMILTONIAN
AND FOLDY-WOUTHUYSEN TRANSFORMATION*

INTRODUCTION

There are only a few cases of the exact solutions of the Dirac equation for a particle in an external field and the Coulomb problem is one of them. The non-relativistic Kepler problem has however received renewed attention in recent years, specially because of its relation to the \( O(4), O(4,1) \) and \( SL(2,\mathbb{R}) \) groups. Further the simplest bound atomic system, the hydrogen atom, has characteristic features similar to some distinguishing invariance properties of elementary particles. In view of these, one would like to have some insight into the relativistic Coulomb problem as well. Since the Dirac Coulomb problem spoils the \( O(4) \) symmetry, it is of interest to

* A paper by the author with this title has been published in Nuovo Cimento, 54A, 549 (1968).
look for a relativistic Coulomb Hamiltonian having the O(4) symmetry. By removing the symmetry breaking fine structure interaction from the relativistic Dirac Hamiltonian, Biedenharn and Swamy\textsuperscript{2} have shown the existence of a Hamiltonian, which retains the O(4) symmetry. While the latter model is approximate the degree of approximation is rather negligible being of the order \( \frac{\alpha Z}{\hbar} \) where \( \alpha \) is the fine structure constant and \( \hbar \) the Dirac angular momentum quantum number. It is of interest to know how the Hamiltonian itself differs from the Dirac model in the non-relativistic limit. This can be done by the well-known Foldy–Wouthuysen transformation\textsuperscript{3} and we discuss this particular aspect of the problem in this Chapter.

\* We will refer to this as R2.
SECTION — I

In this section we wish to review briefly the Foldy-Wouthuysen transformation* and its importance in the physical interpretation of the Dirac equation.

In the introduction of the free-field Dirac equation we note that the equation proposed differs mainly in its non-diagonal character when compared to the Schrodinger equation, although in both, the position operator is assumed to be diagonal. However, the Dirac equation provides us with almost all the requirements that are necessary to describe a spin \( \frac{1}{2} \) particle, but it involves the so-called negative energy problem. But in spite of this, one would like to examine the non-relativistic limit of the Dirac Hamiltonian and compare it with the Schrodinger-Pauli Hamiltonian which is

\[
\mathcal{H} = \frac{\left(\vec{p} - e\vec{A}\right)^2}{2m} + e\phi - \frac{e\hbar}{2mc} \vec{\sigma} \cdot \nabla \times \vec{A}
\]  

(1)

* Popularly the name of the transformation is given as above, since Foldy-Wouthuysen were the first to introduce it. However Tani and Pryce have also to be included.
in the presence of an electro-magnetic field with vector potential $\mathbf{A}$ and scalar potential $\phi$. It is quite evident that this has not even a superficial resemblance to the Dirac Hamiltonian. The usual procedure of getting the non-relativistic limit of the Dirac equation is to use the fact that the two of the four components of the Dirac wave function become small when the momentum of the particle is small compared to its mass. Now after writing all the corresponding equations satisfied by each of those components one finds an approximate solution for the small components, and then those approximate solutions are substituted in the equations of the large components. One thus gets a pair of equations for the large components, which yield the Schrödinger—Pauli equations in a suitable expansion where terms of the order of $1/c$ are retained. However, one is left with the following numerous difficulties:

(1) If one is interested in the higher orders of approximation the method leads to a non-Hermitian Hamiltonian (in the presence of the field).

(2) The expectation values of any operators are calculated
by using all the four components, whereas in the Pauli theory one needs only two components.

(3) The operator representing velocity is \( \mathbf{\not{v}} \) whose components have eigenvalues \( \pm 1 \), whereas in the Pauli theory one has the velocity operator as \( \mathbf{\not{p}}/m \), whose components have eigenvalues embracing all real numbers.

(4) The components of the velocity operator do not commute and hence are not measurable with arbitrary precision, whereas in Pauli theory these components do commute and obey the quantum conditions.

These difficulties have been overcome by casting the Dirac Hamiltonian in a representation in which the Hamiltonian is diagonal. In such a representation the Dirac equation for a free particle separates into two uncoupled equations, one describing the particle of positive energy, second the particle of negative energy. The transformation which accomplishes this was first shown by Foldy and Wouthuysen.
and almost simultaneously by Tani. If we define
an odd-operator as the one which anticommutes with \( \rho_3 \),
and the even-operator as the one which commutes with \( \rho_3 \), then we see that it is the odd operator that
couples the negative energy state with the positive ones. Hence a unitary transformation has been found
which eliminates these odd operators from the free-field Dirac equation. The existence of such a unitary
transformation which accomplishes this follows from the fact that if

\[
\hat{q}' = \rho_1 \hat{q}_1 + \rho_3 \hat{q}_3 \ldots
\]  

(2)

where \( \hat{q}_1, \hat{q}_3 \) are commuting operators which commute
with \( \rho_1 \) and \( \rho_3 \) (Note that \( \rho_i \), \( i=1,2,3 \) are the Pauli
matrices defined in the Dirac space), then there
exists a similarity transformation such that

\[
\hat{q}' = U^{-1} \hat{q} U = \rho_3 ( \hat{q}^2 )^{\frac{1}{2}} \ldots
\]  

(3)

Now the position operator which was earlier
chosen to be diagonal in the Dirac representation,
becomes a non-diagonal operator, having a non-local
characteristic. This leads to the definition of a
"mean position operator" in the Dirac representation.
having non-local characteristics and one obtains the 'velocity operator whose components now commute and have appropriate eigen-values. Further we note that the eigen-states of the mean position operator are wave packets of width $\hbar/mc$. This mean-position operator is to be interpreted as the position operator in the Pauli theory. However this mean position operator was also introduced by Pryce and later by Newton and Wigner in a different manner. Localised states and position operators can be defined by demanding certain nearly inevitable requirements prescribed by Newton and Wigner. According to Newton-Wigner formulation, the set $S_\vec{a}$ of states localized at a point $\vec{a}$ of the three dimensional space at a given time must satisfy the following axioms:

(a) $S_\vec{a}$ is linear manifold

(b) $S_\vec{a}$ is invariant under rotations about $\vec{a}$, reflections in $\vec{a}$ and time inversion.

(c) $S_\vec{a}$ is orthogonal to all its space translates.

(d) Certain regularity conditions, amounting essentially to the requirement that all the
infinitesimal operators of the Lorentz group be applicable to the localized states.

But as was pointed out by Wightman, it may be noted that the Newton-Wigner formulation is to be regarded as a limit of the notion of localizability in a region. However we note that a sharper localization of the "mean-position operator" than the packets of width \(\hbar/\rho_0\) brings in negative components and with this a new element into space-time behaviour; the Schrödinger "Zitterbewegung". This trembling motion is seen whenever one considers superposition of positive and negative energy states, since positive and negative energy parts have a time dependence given by \(\exp(\pm i\hbar t/\hbar)\) respectively and because of this the density contains now interference terms which shift the charge around with a frequency, at least \(2\rho_0^2/\hbar\).

Further this trembling motion is excited whenever the particle is subjected to a force whose potential varies significantly over a distance of order \(\hbar/\rho_0\). In a similar manner one defines "mean orbital angular momentum" and "mean spin angular momentum" whose z-components are separately constants of motion and it is those operators that are to be compared with the
corresponding operators of the non-relativistic theory. Hence one has operators in the Dirac theory representing physical quantities and have a one-to-one correspondence with the operators of the Schrödinger-Pauli theory.

So far we have dealt with the Foldy-Wouthuysen transformation applied to the free particle Dirac Hamiltonian. In the presence of the field it may not in general be possible to find a unitary transformation in closed form which rid the Hamiltonian of odd operators. This follows from the fact that the operators involved in Eqn. (2) do not satisfy the required conditions. Only in very special cases such as a time independent magnetic field it is possible to find a unitary transformation. However it has been shown by Foldy and Wouthuysen that in the presence of the external field it is always possible to make a sequence of transformations, each of which eliminates odd operators from the Hamiltonian to one higher order in the expansion parameter $1/m$. In this way one obtains a Hamiltonian free from odd operators which is an infinite power series in powers of $1/m$, and if the interaction is very weak compared to $m$, the series tends to be convergent. This procedure helps one to
give a physical interpretation of the additional terms that one gets in the non-relativistic limit of the Dirac equation in the presence of the interaction. Since the "Symmetric Hamiltonian", which we will discuss in the next section, differs from the Dirac Coulomb Hamiltonian by a "fine structure interaction", it is of interest to develop the procedure of getting a two component Hamiltonian. Hence we give the general procedure of doing this in the presence of the time independent field. In general the transformed Hamiltonian is given by

$$H' = e^{iS} H e^{-iS} \quad \ldots$$ \hspace{1cm} (4)

where $S = S_1 + S_2 + S_3 + \ldots$, is the unitary transformation. The transformed Hamiltonian can be made to be free from odd operators to the required order in the expansion parameter $\dfrac{1}{m}$. If we now write the Hamiltonian as

$$H = \mathcal{O} + \mathcal{K} + \beta m \quad \ldots$$ \hspace{1cm} (5)

where $\mathcal{O}$ is the odd operator and $\mathcal{K}$ is the even operator,

* We adopt units defined by $\hbar = c = 1$
we see that the odd operators can be removed through
order \(1/m^2\) by defining the transformation as

\[
S = S_1 + S_2 + S_3
\]

where

\[
S_1 = \frac{-i \beta \gamma_0}{2m}
\]

\[
S_2 = -\frac{i \beta}{2m} \left\{ \frac{\gamma_0}{2m} \left[ \gamma, \frac{\gamma_3}{2m} \right] \right\}
\]

\[
S_3 = -\frac{i \beta}{2m} \left\{ -\frac{\gamma_0^3}{8m^6} + \frac{1}{4m^2} \left[ \gamma, \frac{\gamma_3}{2m} \right] \right\}
\]

and the transformed Hamiltonian is given by

\[
H' = \beta \left( m + \frac{\gamma_0^2}{2m} - \frac{\gamma_0^4}{8m^3} \right) + \frac{\gamma_3}{2m} - \frac{1}{8m} \left[ \gamma, \left[ \gamma, \frac{\gamma_3}{2m} \right] \right]
\]

Now it is of interest to look for the physical interpretation of each of these terms. So for the sake of completeness we investigate the consequences of such a transformation as applied to the Dirac Hamiltonian in

* The details are given in the Appendix - I.
the presence of the Coulomb field. Now we write the Hamiltonian as

\[ H_D = Q + \mathcal{H} + \beta m \quad \ldots \quad (11) \]

where \( Q = \vec{J} \cdot \vec{p} \) and \( \mathcal{H} = -\kappa z/r \). The energies of the bound states are given by

\[ E_N = m \left[ 1 + \left( \frac{\kappa z}{N - |\kappa| + \gamma} \right)^2 \right]^{-\frac{1}{2}} \quad (12) \]

where the quantum number \( N = 1, 2, 3, \ldots \) etc. is the so-called principal quantum number and \( |\kappa| = \gamma + \frac{1}{2} \)

and \( \gamma = \sqrt{\kappa^2 - (\kappa z)^2} \)

Expanding in powers of \( (\kappa z)^2 \) we see that

\[ E_N = m \left\{ 1 - \frac{1}{2} \left( \frac{\kappa z}{N^2} \right)^2 + (\kappa z)^4 \left( \frac{3}{8N^4} - \frac{1}{2! |\kappa| N^3} \right) \right. \]

\[ \left. + O((\kappa z)^6) + \ldots \right\} \quad (13) \]

The first term is the non-relativistic energy exclusive of the rest energy. The terms in \( (\kappa z)^4 \) are exactly the terms obtained by including in the Pauli theory the sum of the following terms

(1) the additional energy due to the variation of mass with velocity.
(2) the spin orbit coupling

(3) the Darwin "fluctuation" term,

and the terms are evaluated to first order perturbation. However the inclusion of the last term physically cannot be explained and is often referred to as the "mysterious" Darwin term. Now using the equation (10) we transform the Hamiltonian and we get

\[
H' = \beta \left( m + \frac{\mathbf{p}^2}{2m} - \frac{\mathbf{p}^4}{8m^3} \right) + \frac{\kappa \mathbf{z}}{4m^2 \lambda^3} \mathbf{\nabla} \cdot \mathbf{\nabla} + \frac{\pi \kappa \mathbf{z}}{2m^2} \delta (\mathbf{x})
\]

(14)

as the non-relativistic limit of the Dirac-Coulomb-Hamiltonian. It is interesting to note that all the terms required accompanying \((\kappa x)\) of equation (13) are recovered. But now we can give a physical interpretation to the mysterious Darwin term. In the Dirac representation the interaction is local in the position of the particle. Hence it will be non-local in the mean position and so in the transformed Hamiltonian the interaction will be non-local or in other words the interaction will be like that of a spatially extended charge distribution. This spatial extension of the charge distribution of the order of the Compton
wave length of the electron $\frac{\hbar}{mc}$ gives in the first order a correction to the electrostatic interaction which is just the Darwin term. So it now clear that the Darwin term may be attributed to the Zitterbewegung.
In this section we wish to review briefly the Symmetric-Hamiltonian and some of its important features.

It was shown by Biedenharn that the iterated Dirac equation in the presence of the Coulomb field, which can be written as

\[
\left( \frac{1}{2} \frac{\partial}{\partial t} + \frac{1}{2} \frac{\partial^2}{\partial \mathbf{r}^2} - \frac{1}{2} \frac{m}{c^2} \right) \Phi = 0
\]

(15)

where \( \gamma = \gamma_0 + i \gamma_1 - \mathbf{\gamma} \cdot \mathbf{r} \), \( \gamma_0 = \frac{\mathbf{\gamma} \cdot \mathbf{p}}{\mathbf{K} \cdot \mathbf{c}} \), and \( \mathbf{K} = \mathbf{p} + \mathbf{r} \).

This can be thrown exactly into the non-relativistic form by defining a transformation

\[
S = \exp \left[ -\frac{1}{2} \mathbf{p} \cdot \mathbf{\sigma} \cdot \mathbf{J} \cdot \text{tanh}^{-1} \left( \frac{\mathbf{K} \cdot \mathbf{c}}{\mathbf{K} \cdot \mathbf{r}} \right) \right]
\]

(17)

which accomplishes the diagonalisation of \( \gamma \). Here \( \mathbf{K} = \mathbf{p} \cdot \mathbf{r} \), the familiar Dirac operator. However, this transformation leads to the definition of an irrational angular momentum \( \gamma \). The radial Coulomb functions are expressed in terms of this non-integral...
Further as a consequence of this it is shown that there exists a Coulomb helicity operator that happens to be a constant of the motion. Although we get some insight in the relativistic Coulomb problem in this representation, this is not convenient to work since the radial Coulomb functions are expressed in terms of $\ell(\gamma)$.

Later it was shown by Biedenharn and Swamy that the requirement that this irrational orbital angular momentum go to an integral orbital momentum,

\[ i.e. \quad \ell(\gamma) \rightarrow \ell(\kappa) \]

leads to the transformation,

\[ S_1 = \exp \left[ -\rho \vec{\sigma} \cdot \vec{\mathcal{A}} \omega n h^{-1} \left( \frac{\kappa \gamma}{\kappa} \right) \right] \tag{18} \]

This new transformation gives us the so-called "Symmetric Hamiltonian" defined by

\[ H_{\gamma m}^s = S_1 \ H \rho \ S_1^{-1} \]

\[ = \vec{z} \cdot \vec{p} + \beta \ m - \frac{\kappa \gamma}{\kappa} - \frac{\rho \vec{\sigma} \cdot \vec{\mathcal{A}}}{\kappa} \ K \left\{ 1 - \sqrt{1 + \left( \frac{\kappa \gamma}{\kappa} \right)^2} \right\} \tag{19} \]

where $\vec{p} = \vec{z} \cdot \vec{p} + \beta \ m$, the free-particle Dirac Hamiltonian. It is now seen that the Symmetric Hamiltonian differs from the Dirac Coulomb Hamiltonian.
by a fine structure interaction

\[ H_f = -\frac{p_{z}^{2}}{\epsilon_{p}} \quad \kappa \left\{ 1 - \sqrt{1 + \left(\frac{\kappa z}{\kappa} \right)^{2}} \right\} \]

(20)

which is of the order of \( \frac{(\kappa z)^{2}}{\kappa} \). The name given to the Hamiltonian is derived from the fact that this now Hamiltonian is having the symmetry group as \( O(4) \) whose operators have been explicitly worked out in their paper. Hence we see that this \( O(4) \) symmetry which is a well-known characteristic of the non-relativistic Coulomb Hamiltonian has been recovered in the relativistic case also, which in the Dirac case was lost.

The energies of the bound states are given by

\[ E_{N} = \frac{m}{\left[ 1 + \left( \frac{\kappa z}{N} \right)^{2} \right]^{\frac{1}{2}}} \]

\[ = m \left[ 1 - \frac{1}{2} \left( \frac{\kappa z}{N} \right)^{2} + \frac{3}{8} \left( \frac{\kappa z}{N} \right)^{4} + \cdots \right] \]

(21)

We note that the eigenvalues depend only on \( N \) the principal quantum number just as in the non-relativistic case, a well-known characteristic of the Hamiltonian related to its symmetry. We shall postpone
to another Chapter a discussion of the symmetry properties of this Hamiltonian. From the equation (21) we see that the first term in the expansion exclusive of the rest mass energy is the familiar non-relativistic energy and we need to interpret the terms accompanied by $(\alpha s)^{4}$ etc. We also note in passing that it is easy to take either non-relativistic or the free-field limit of the solutions of this Hamiltonian.
In this section we examine the non-relativistic limit of the Symmetric Hamiltonian by the Foldy-Wouthuysen transformation and study the physical significance of including the so-called fine structure interaction.

We write in our usual notation from eqn. (19)

$$H_{\text{sym}} = \frac{\mathbf{Q}}{2} + \frac{\mathbf{P}^2}{2m} + \mathbf{a} \cdot \mathbf{p}$$

where

$$\mathbf{Q} = \mathbf{Z} \cdot \mathbf{p} - \frac{i \hbar}{\alpha} \left( \mathbf{\sigma} \cdot \mathbf{\tau} + 1 \right) \left\{ 1 - \sqrt{1 + \left( \frac{\alpha Z}{\mathbf{Z}} \right)^2} \right\}$$

$$\mathbf{a} = - \frac{\alpha Z}{\hbar}$$

(22)

The basic expressions needed to transform the Hamiltonian are

$$[\mathbf{Q}, \mathbf{p}] = -i \hbar \mathbf{Z} \cdot \mathbf{a}$$

$$[\mathbf{Q}, [\mathbf{Q}, \mathbf{p}]] = -i \hbar \pi \alpha Z \delta(\mathbf{Z}) - \frac{2 \alpha Z}{\hbar} \mathbf{D} \cdot \mathbf{Z}$$

$$+ \frac{2 \alpha Z}{\hbar^3} \left( \mathbf{\sigma} \cdot \mathbf{\tau} + 1 \right) \left\{ \sqrt{1 + \left( \frac{\alpha Z}{\mathbf{Z}} \right)^2} - 1 \right\}$$

(23)

(24)

* See Appendix - II.
and the transformations defined by

\[ S_1 = -\frac{\mathbf{p}}{2m} \]

\[ S_2 = -\frac{\mathbf{k} \cdot \mathbf{\lambda}}{4m^2} \mathbf{k} \cdot \mathbf{\lambda} \]

\[ S_3 = \frac{\mathbf{p}^2}{12m^2} \left\{ \mathbf{k}^2 - \mathbf{\lambda} \cdot \mathbf{\lambda} + \frac{\mathbf{k} \cdot \mathbf{\lambda}}{4m^2} \left( \mathbf{k} \cdot \mathbf{\lambda} + 1 \right) \right\} \times \left\{ \frac{1}{\sqrt{1 + \left( \frac{\mathbf{k} \cdot \mathbf{\lambda}}{\mathbf{k}} \right)^2} - 1 \right\} \]

(27)

The transformed Hamiltonian, accurate to the order \((1/m)^2\), and with neglect of terms of the higher than the \((\kappa \cdot \mathbf{\lambda})^2\) reduces to,

\[ H' = e^{iS} H_{\text{sym}} e^{-iS} \]

\[ = \beta m - \mathbf{\lambda} \cdot \mathbf{\lambda} + \frac{\mathbf{p}}{2m} \left\{ \mathbf{\lambda}^2 - \left( \frac{\mathbf{k} \cdot \mathbf{\lambda}}{4m^2} \right) \left[ \frac{1}{2 \left( \mathbf{k} \cdot \mathbf{\lambda} + 1 \right)} - 1 \right] \right\} \]

\[ - 2m \delta(\mathbf{\lambda}) \left( \frac{\mathbf{k} \cdot \mathbf{\lambda}}{2 \left( \mathbf{k} \cdot \mathbf{\lambda} + 1 \right)} \right) \]

\[ - \frac{\beta \mathbf{p}^2}{8m^3} + \frac{\mathbf{k} \cdot \mathbf{\lambda}}{2} \]

\[ + \frac{\mathbf{k} \cdot \mathbf{\lambda}}{4m^3 \lambda^3} \mathbf{\lambda} \cdot \mathbf{\lambda} \]

(28)

where \( S = S_1 + S_2 + S_3 \)

We notice that all the terms in the exact Dirac case are recovered i.e. the first order
relativistic correction to the kinetic energy, the spin-orbit coupling term and the Darwin term. We also get a term involving $\mathcal{A}(\mathbf{r})$ which can be ignored because of its vanishing expectation value for all states. The important additional term which does not exist in the FW transformed Dirac Hamiltonian is

$$
- \frac{1}{2m} \left( \frac{\mathbf{A} \cdot \mathbf{r}}{\hbar} \right)^2 \left[ \frac{1}{2(\mathbf{A} \cdot \mathbf{r}^2 + 1)} - 1 \right]
$$

(39)

This can be interpreted as an additional kinetic energy due to vector potential which is of magnitude

$$
\frac{\mathbf{A} \cdot \mathbf{r}}{\hbar} \left[ \frac{1}{2(\mathbf{A} \cdot \mathbf{r}^2 + 1)} + 1 \right]^{1/2}
$$

and whose direction is parallel to the orbital angular momentum $\mathbf{L}$ and, therefore, perpendicular to $\mathbf{p}$. An estimate of this can be made as follows:

Now if we denote $\psi_i$ as the wave function corresponding to the eigenvalue problem

$$
\hat{H}_{sym} \psi_i = E_N \psi_i
$$

(30)
then we see that from R2,

\[ \psi_s = \left( A \left| \nu \mu \right\rangle + B F_{\nu \overline{\nu}} \chi^\mu \right) \]

\[ + C F_{n \ell} \chi^\ell - D \left| \nu - \mu \right\rangle \]

where

\[ \left| \nu \mu \right\rangle = F_{\nu \ell \left(\nu \mu \right)} \chi^\nu \chi^\mu \]

\[ \left| \nu - \mu \right\rangle = i F_{\nu \ell \left(-\nu \mu \right)} \chi^\nu - \chi^\mu \]

and

\[ \chi^\nu = \sum_{\ell} C_{\ell \left(\nu \mu \right)} \chi^\ell \]

and \( A, B, C, \) and \( D \) are the proper normalising factors\(^*\).

\( F_{\nu \ell \left(\nu \mu \right)} \) and \( F_{\nu \ell \left(-\nu \mu \right)} \) are the familiar radial Coulomb functions (see for example R2). Further we note that the constants \( B, C \) and \( D \) are small compared to \( A \) in the non-relativistic domain. Hence it is enough if we know the expectation values of the respective operators with \( \left| \nu \mu \right\rangle \) accurate to the order \( \frac{1}{\ell \mu 2 m} \). It is to be noted that one can just estimate the expectation values by taking non-relativistic Coulomb functions as the first order

\(^*\) All the details will be discussed in Chapter II, since these finer details are relevant in that chapter.
perturbation. These have been already worked out earlier in the non-relativistic calculations. Hence we have

$$\langle N \times \mu | - \frac{1}{2m} \left( \frac{k^2}{2} \right) \left[ \frac{1}{2} \left( \frac{1}{2} + 1 \right) \right] | N \times \mu \rangle$$

$$= \frac{m (k^2)}{2 N^3} \frac{1}{l + 1} + \frac{3m (k^2)}{2 N^3 (l + 1)}$$

(33)

$$\langle N \times \mu | - \frac{p^2}{2m^3} | N \times \mu \rangle$$

$$= - \frac{m}{2} \frac{(k^2)}{N^3} \frac{1}{l + 1} + 3m \frac{(k^2)}{N}$$

(34)

$$\langle N \times \mu | \frac{k^2}{4 N^2} \hat{\sigma} \cdot \hat{\tau} | N \times \mu \rangle$$

$$= \frac{m}{2} \frac{(k^2)}{N^3} \frac{1}{(l + 1)(2l + 1)}$$

for \( j = l + \frac{1}{2} \)

(35)

$$= - \frac{m}{2} \frac{(k^2)}{N^3} \frac{1}{(2l + 1)}$$

for \( j = l - \frac{1}{2} \)

(36)

Now we see that the first term in expression (33) exactly cancels the spin-orbit coupling term and the second term likewise cancels the angular momentum dependent term in the mass variation correction. This is as it should be. This probably confirms the assertion in Ref. 2 that the Symmetric model in a sense corresponds
to the existence of Sommerfeld's\textsuperscript{11} closed planar orbits in a suitably rotating coordinate system. The additional magnetic energy can be assumed to arise from this type of a field and the axis of rotation comes out consistently.
Appendix - 1

We have the eigenvalue problem as,

\[ H \psi = i \frac{\partial}{\partial t} \psi = E \psi \]  

(1a)

Assuming that the Hamiltonian is time independent any unitary transformation $S$ which transforms the Hamiltonian into a new representation is also time independent. The transformation is introduced by requiring that

\[ \psi' = e^{iS} \psi \]  

(1b)

so that the eqn. (1a) reduces to

\[ H e^{-iS} \psi' = E e^{-iS} \psi' \]

\[ i e^{iS} H e^{-iS} \psi' = E \psi' \]

or putting $e^{iS} H e^{-iS} = H'$ we have

\[ H' \psi' = E \psi' \]  

(1c)
It is easy to see that
\[ e^{iS} H e^{-iS} = H + i \left[ S, H \right] + \frac{i^2}{2!} \left[ S, \left[ S, H \right] \right] + \cdots + \frac{i^n}{n!} \left[ S, \left[ S, \cdots \left[ S, H \right] \cdots \right] \right] + \cdots \] (1d)

Now from the equation (5) it follows that for \( S_1 \)
defined by (7):
\[ H_1 = e^{iS_1} H e^{-iS_1} = \beta \left( m + \frac{Q^2}{2m} - \frac{Q^4}{8m^3} \right) + \beta \frac{Q^2}{2m} \left[ Q, [Q, \beta] \right] + \beta \frac{Q^4}{2m^3} \left[ Q, [Q, \beta] \right] - \frac{Q^3}{3m^2} \]
which is approximate to the order \( 1/n \).

Now defining \( S_2 \) as given by (8) we see that from (1d)
\[ H_2 = e^{iS_2} H e^{-iS_2} = \beta \left( m + \frac{Q^2}{2m} - \frac{Q^4}{8m^3} \right) + \beta \frac{Q^2}{2m} \left[ Q, [Q, \beta] \right] \]
\[ - \frac{Q^3}{8m^2} + \beta \frac{Q^4}{4m^3} \left[ Q, [Q, \beta] \right] + \beta \frac{Q^6}{6m^4} \]
This still contains the terms of the order $1/n$.

Finally defining $S_3$ as given by (9) we have

$$H' = H_3 = e^{iS_3} H_2 e^{-iS_3}$$

$$= \beta \left( m + \frac{Q^2}{2m} - \frac{Q^4}{8m^4} \right) + \varepsilon - \frac{1}{8m^2} \left[ \partial \times [\partial \times \varepsilon] \right]$$

which is accurate to the order $1/m^2$. However, this indefinitely procedure can be continued to get the Hamiltonian of the required accuracy.
Appendix - 2

We note the following anticommutation relations:

\[ \left[ \bar{\sigma}^2 \cdot \lambda , \sigma^2 \cdot \mathbf{I} + 1 \right]_+ = 0 \]  \hspace{1cm} (2a)

\[ \left[ \bar{\sigma}^2 \cdot \mathbf{P} , \sigma^2 \cdot \mathbf{I} + 1 \right]_+ = 0 \]  \hspace{1cm} (2b)

Also we have,

\[ \bar{\sigma}^2 \cdot \mathbf{A} \cdot \sigma^2 \cdot \mathbf{B} = \bar{\mathbf{A}} \cdot \mathbf{B} + \lambda \cdot \mathbf{A} \cdot \mathbf{B} \times \mathbf{A} \]

\[ = \mathbf{\lambda} \cdot \bar{\mathbf{A}} \times \mathbf{A} \]

where \( \mathbf{A} \) and \( \mathbf{B} \) are some vector operators commuting with \( \bar{\sigma}^2 \) but not commuting with each other.

We easily have

\[ \left[ \bar{\sigma}^2 \cdot \mathbf{P} , \lambda \cdot \mathbf{A} \right] = - \lambda \cdot \bar{\sigma}^2 \cdot \nabla \left( \frac{1}{\mathbf{A}} \right) \]

\[ = \frac{\lambda}{\mathbf{A}^2} \bar{\sigma}^2 \cdot \mathbf{A} \]  \hspace{1cm} (2c)

Hence we note that in general

\[ \left[ \bar{\sigma}^2 \cdot \mathbf{P} , \sigma^2 \cdot \mathbf{A} \right] = - \frac{2\lambda}{\mathbf{A}^2} (\bar{\sigma}^2 \cdot \mathbf{I} + 1) - 4 \pi \lambda \mathbf{A} \cdot \delta(\mathbf{A}) \]  \hspace{1cm} (2d)

where the fact \( \nabla^2 \left( \frac{1}{\mathbf{A}} \right) = -4\pi \delta(\mathbf{A}) \) has been used and \( \delta(\mathbf{A}) \) is the usual three dimensional Dirac delta.
function\(^\text{12}\). From (2d) it is quite evident that
the contribution from the \(\delta(x^3)\) function is always
vanishing, however had we started with the second
relation defined in (2o) then we will miss the
contribution due to the delta function even if the
commutation relation (2d) is accompanied by a
multiplying term \(1/r^2\) in the left.

So now the commutator

\[
\begin{align*}
\left[ \mathbf{\nabla} \cdot \mathbf{\hat{p}}, & \left[ \mathbf{\nabla} \cdot \mathbf{\hat{\mathbf{r}}}, \mathbf{\hat{\mathbf{r}}} \right] \right] \\
= -i \left[ \mathbf{\nabla} \cdot \mathbf{\hat{\mathbf{r}}}, \left[ \mathbf{\nabla} \cdot \mathbf{\hat{\mathbf{r}}}, \mathbf{\hat{\mathbf{r}}} \right] \right] \\
= -i \left[ \mathbf{\nabla} \cdot \mathbf{\hat{\mathbf{r}}}, \mathbf{\nabla} (\mathbf{\hat{\mathbf{r}}}) - \mathbf{\nabla} (\mathbf{\hat{\mathbf{r}}}) \cdot \mathbf{\hat{\mathbf{r}}} \\
+ i \mathbf{\nabla} \cdot \{ \mathbf{\nabla} (\mathbf{\hat{\mathbf{r}}}) - \mathbf{\nabla} (\mathbf{\hat{\mathbf{r}}}) \times \mathbf{\hat{\mathbf{r}}} \} \right] \\
= -i \left[ -i \mathbf{\nabla} \cdot (\mathbf{\hat{\mathbf{r}}}) + \frac{2i}{\lambda^2} \mathbf{\nabla} \cdot \mathbf{\hat{\mathbf{r}}} \right] \\
= 4 \pi \delta(x^3) + \frac{2}{\lambda^2} \mathbf{\nabla} \cdot \mathbf{\hat{\mathbf{r}}}
\end{align*}
\]

(2e)

\[
\begin{align*}
i \left[ \mathbf{\nabla} \cdot \mathbf{\hat{\mathbf{r}}}, \mathbf{\hat{\mathbf{r}}} \right] = & \left[ \mathbf{\nabla} \cdot \mathbf{\hat{p}}, \frac{1}{\lambda^2} \mathbf{\nabla} \cdot \mathbf{\hat{\mathbf{r}}} \right] + \mathbf{\sigma} \cdot \mathbf{\nabla} \cdot \left( \mathbf{\hat{\mathbf{r}}} + \lambda^3 \mathbf{\hat{\mathbf{r}}} \right) \left\{ \sqrt{1 + \left( \frac{\lambda^2}{\lambda^2} \right)^2} - 1 \right\} \\
- \frac{\alpha Z}{\lambda^2}
\end{align*}
\]
\[-\alpha z \left[ \mathbf{r} \cdot \mathbf{p}^\prime, \frac{1}{\mathbf{x}} \right] \]
\[-\alpha \mathbf{x} \left[ \frac{\mathbf{x} \cdot \mathbf{r}}{x^2} (\mathbf{p} \cdot \mathbf{x}^2 + 1) \left\{ \sqrt{1 + \left( \frac{\mathbf{z} \cdot \mathbf{x}}{x} \right)^2} - 1 \right\}, \frac{1}{2} \right] \]
\[-\alpha \mathbf{z} \left[ \mathbf{z} \cdot \mathbf{p}, \mathbf{p} \cdot \mathbf{r}, \frac{i}{\mathbf{c}} \right] \]
\[-\alpha \mathbf{x} \left[ \frac{i}{2} \mathbf{x} \cdot \mathbf{r} (\mathbf{p} \cdot \mathbf{x}^2 + 1) \left\{ \sqrt{1 + \left( \frac{\mathbf{z} \cdot \mathbf{x}}{x} \right)^2} - 1 \right\}, \frac{i}{2} \mathbf{z} \cdot \mathbf{r} \right] \]
\[-\alpha \mathbf{z} \left\{ 4\pi \delta(\mathbf{r}) + \frac{2}{i} \mathbf{r} \cdot \mathbf{r} \right\} \]
\[+ \frac{\kappa z}{i^3} \left[ \mathbf{z} \cdot \mathbf{r} (\mathbf{p} \cdot \mathbf{x}^2 + 1) \left\{ \sqrt{1 + \left( \frac{\mathbf{z} \cdot \mathbf{x}}{x} \right)^2} - 1 \right\}, \mathbf{z} \cdot \mathbf{r} \right] \]
\[= -4\pi \kappa z \delta(\mathbf{r}) - \frac{2\kappa z}{i^3} \mathbf{r} \cdot \mathbf{r} \]
\[+ \frac{2\kappa z}{i^3} (\mathbf{p} \cdot \mathbf{x}^2 + 1) \left\{ \sqrt{1 + \left( \frac{\mathbf{z} \cdot \mathbf{x}}{x} \right)^2} - 1 \right\} \]
Now expanding \( \{ \sqrt{1 + \left( \frac{k^2 z^2}{k^2} \right)^2} - 1 \} \), we have

\[ L_0, \ L_0, \ k z \]

\[-4 \pi k z \delta(k^2) - \frac{2 k^2 z^2}{k^2} \delta^2 k + \frac{2 k^2 z^2}{k^2} (\delta^2 k + 1) \frac{1}{2} \left( \frac{k^2 z^2}{k^2} \right)^2 \]

\[-4 \pi k z \delta(k^2) - \frac{2 k^2 z^2}{k^2} \delta^2 k \]

up to the accuracy of \( (k^2 z^2)^2 \)

Now we also see that

\[ Q^z = \bar{p}^z + \frac{i}{4} \{ \sqrt{1 + \left( \frac{k^2 z^2}{k^2} \right)^2} - 1 \} \left( k^2 z^2 \delta^2 k + 1 \left( \frac{k^2 z^2}{k^2} \right)^2 \right) \]

\[-\frac{1}{4} \left( \delta^2 k + 1 \right) \left\{ \sqrt{1 + \left( \frac{k^2 z^2}{k^2} \right)^2} - 1 \right\} + \frac{k^2}{4} \left\{ \sqrt{1 + \left( \frac{k^2 z^2}{k^2} \right)^2} - 1 \right\} \]

\[ = \bar{p}^z + 4 \pi k z \delta(k^2) \left( \delta^2 k + 1 \right) \left\{ \sqrt{1 + \left( \frac{k^2 z^2}{k^2} \right)^2} - 1 \right\} \]

\[ + \frac{2 k^2}{4} \left\{ \sqrt{1 + \left( \frac{k^2 z^2}{k^2} \right)^2} - 1 \right\} - \frac{1}{4} \left( \delta^2 k + 1 \right) \left\{ \sqrt{1 + \left( \frac{k^2 z^2}{k^2} \right)^2} - 1 \right\} \]

\[ + \frac{k^2}{4} \left[ 2 + \left( \frac{k^2 z^2}{k^2} \right)^2 - 2 \sqrt{1 + \left( \frac{k^2 z^2}{k^2} \right)^2} \right] \]

\[ = \bar{p}^z + 4 \pi k z \delta(k^2) \left( \delta^2 k + 1 \right) \left\{ \sqrt{1 + \left( \frac{k^2 z^2}{k^2} \right)^2} - 1 \right\} \]

\[-\frac{1}{4} \left( \delta^2 k + 1 \right) \left\{ \sqrt{1 + \left( \frac{k^2 z^2}{k^2} \right)^2} - 1 \right\} + \left( \frac{k^2 z^2}{k^2} \right)^2 \]
Expanding \( \{ \sqrt{1 + \left( \frac{\kappa z}{\kappa} \right)^2} - 1 \} \) we get collecting the terms up to the order \((\kappa z)^2\)

\[
Q^2 = \vec{p}^2 + 4 \pi \delta (z) (z^2 + 1) \left\{ \sqrt{1 + \left( \frac{\kappa z}{\kappa} \right)^2} - 1 \right\} - \left( \frac{\kappa z}{\kappa} \right)^2 \left[ \frac{1}{2 (z^2 + 1)} - 1 \right]
\]

Similarly one can show that to the required accuracy in our formulation

\[
Q^4 = \vec{p}^4
\]
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