# **RESURRECTION OF THE BOHR/SOMMERFELD**

### THEORY OF ATOMIC STRUCTURE

[3]

# MAGNETIC DIPOLE COUPLING.

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### ABSTRACT.

The Bohr/Sommerfeld theory of atomic structure as re-stated in [1], [2] and [3], is herein further developed to incorporate the effects of magnetic dipole coupling.

### 1 Introduction.

The splitting of the fine structure spectral emissions of single electron atoms and ions, is, in classical terms, attributed to a coupling between the magnetic flux density generated by the orbiting electron, and the magnetic moment produced by its spin. Even in the modern quantum mechanics theory, which considers the electron as a probabilistic wavefunction, this phenomenon is, in elementary treatises, initially described in such terms, [4],[5].

In the resurrected Bohr/Sommerfeld theory presented in this series of papers, in which the electron is treated as a real physical particle orbiting the nucleus, the above description is an exact one, and it is therefore necessary that its mathematical representation is developed accordingly. Consequently, its derivation in this paper is pursued along two lines. Firstly by a re-evaluation of the total electron orbital angular momentum via the principle quantum number criteria stated in [1]. This leads directly to a re-statement of the electron orbital energy equation with spin-orbit magnetic coupling fine structure splitting incorporated. From this relationship, the simple subtraction of the orbital energy without spin-orbit coupling, yields the spin-orbit energy term itself in isolation.

The second derivation is then completed in which this same energy term is obtained from first principles via consideration of the basic electrostatic, magnetic and mechanical concepts involved. Also, in this third Section, all other magnetic coupling terms, i.e. those involving the nucleus are also developed for inclusion into the extended electron orbital energy equation, and for use in future papers. In order to develop these last derivations from first principles, it is necessary to determine the manner in which the magnetic effects are generated. This is the subject of Section 2 of the paper, and also includes consideration of the effects due to the nucleus.

In the fourth Section the effects of electron spin reversal within an orbital are examined via presentation and discussion of a detailed example.

The development of this resurrected theory has, with the incorporation of the effects derived herein, now reached the point where it can, in detail, be compared with the equivalent theoretical relationships of the modern quantum mechanics theory of atomic structure. This comparison is effected in the fifth Section. In the third and final Appendix, calculated emission spectra for the first 7 to 3 orbital shells of hydrogen are presented, that can, in part, be compared with the listings in [6]. Calculated orbital energy levels are also included.

Finally, because specific magnetic attributes of the nucleus are included in this paper, all analyses will be restricted to the hydrogen atom, although all equations so derived will continue to incorporate the Atomic Number Z.

# 2 The Electric and Magnetic Characteristics of the Electron and the Nucleus, Pertinent to Magnetic Dipole Coupling.

# 2.1 <u>Preamble.</u>

Prior to attempting any mathematical derivation, it is necessary to discuss the contribution of the proton nucleus to this effect. In all treatises dealing with fine structure splitting, it has been attributed to the coupling between the magnetic dipoles generated by the electron's orbit and its spin. Much less mention has been made of the contributory effects of the proton nucleus. The fact that the proton orbits a common centre of rotation with the electron has, to some degree, been incorporated in previous papers in the series et al, by the use of the reduced electron mass m. However, the proton is also a charged particle and therefore due to its orbital rotation generates a magnetic field. In addition, it was stated in [3] that due to the nature of the proposed cause of electron spin, the proton would also be subject to spin induction. This spin of the proton would also induce the generation of a magnetic dipole. A fact which is generally accepted to be a constituent cause of the hyperfine structure. Consequently, both the orbital and spin magnetic dipoles of the proton could potentially couple with each other and with those of the orbiting electron. All of these potential reactions must be considered when analysing the magnetic contributions to atomic spectra and are therefore so included in this paper.

### 2.2 The Magnetic Coupling Characteristics of the Electron.

The orbital and spin magnetic dipoles of the electron are derived in Appendix B and are caused by the circular motion of its electrostatic charge. It is well known that the dipole due to the spin is purported to be "exactly" twice that due to its orbital motion. Because this is so for one and the same particle it infers that the effective charge in the spinning motion is twice that in the orbital. This can obviously not be so and therefore an alternative cause must be found. To address this point it is proposed that this effect is really a result of the way in which the two dipoles couple to produce a precessional force. To consider this, refer to Fig. 2.2 below. This figure shows the magnetic field lines generated by a spinning, orbiting electron.



### Fig. 2.1 - Electron Magnetic Field Coupling Geometry.

Assume the electron orbital motion is out of the page which represents a current flow into the page. The magnetic field so generated will then be as shown, (clockwise). If the electron is also spinning clockwise, (spin - up), the charge on its RHS is also moving out of the page so that the current flow this motion represents is also into the page. At point A the spin field and the orbit field add to cause a force  $F_R$  to be imparted to the electron. Because the spin rate of the electron is much greater than its orbit rate, at all points on the orbit the charge rotating past point A will be the full charge on the electron. The force  $F_R$  will therefore be proportional to this full charge. On the opposite LHS of the electron the charge spin motion is into the page so that the representative current is out of the page, resulting in the spin field line shown in Fig. 2.1. This field subtracts from the orbit field line thus causing force  $F_L$  on the electron. For the same reason as above  $F_L$  will also be proportional to the full charge. Consequently, the total force on the electron,  $F_R + F_L$  must be proportional to twice the electron charge. This can be mathematically represented in magnetic coupling equations by doubling the value of the spin magnetic dipole.

Thus (B.15) may be re-stated as

$$_{e}\Psi_{sp} = \frac{eh_{e}n_{sp}}{2\pi m_{e}c} \tag{2.1}$$

The orbit dipole remains at that derived in Appendix B, (B.7) as

$$_{e}\Psi_{or} = \frac{Zehn_{j}}{4\pi m_{e}c} \tag{2.2}$$

Where

 $_{e}\Psi_{sp}$  is the spin magnetic moment of the electron.

 $_{e}\Psi_{or}$  is the orbital magnetic moment of the electron.

 $\boldsymbol{e}$  is the electron charge.

h is Planck's constant.

 $_{e}n_{sp}$  is the spin quantum number of the electron.

 $m_e$  is electron mass, (rest).

c is the velocity of light

 $n_i$  is the orbital quantum number of the electron

Z is the atomic number

# 2.3 The Magnetic Coupling Characteristics of the Nucleus.

The magnetic dipoles of the proton nucleus are not currently theoretically derivable but the orbital dipole is known, as a result of experimental measurements, to be a function of the nuclear magneton thus

$${}_{p}\Psi_{or} = -\frac{Zehn_{j}\gamma_{p}}{4\pi m_{p}c}$$

$$\tag{2.3}$$

Where

 $_{p}\Psi_{or}$  is the orbital magnetic moment of the proton.

 $m_p$  is the rest mass of the proton.

 $\gamma_p$  is a constant of proportionality determined from experimental measurements to be 2.79275, [4].

The constant of proportionality in (2.3),  $\gamma_p$ , is thought to be due to the internal structure of the proton affecting the manner in which the motion of the charge generates a magnetic field, and consequently, for the same reason, the proton's spin magnetic dipole will be similarly affected. Also, for the same reason as above concerning the magnitude of the electron spin magnetic dipole, that of the proton nucleus would also be expected to be twice that of its orbit dipole. Consequently, it is proposed that this dipole can be represented by the following relationship

$$_{p}\Psi_{sp} = -\frac{Zeh_{p}n_{sp}\gamma_{p}}{2\pi m_{p}c}$$

$$\tag{2.4}$$

Where

 $_{p}\Psi_{sp}$  is the spin magnetic moment of the proton nucleus.

 $_{p}n_{sp}$  is the spin quantum number of the proton nucleus.

The proton dipoles are of opposite sign to those of the electron because of the opposite polarity of their respective electrostatic charge and because the proton is orbiting and spinning in the same direction as the electron which, as implicit in [3], is the norm.

Eqs.(2.1), (2.2), (2.3) and (2.4) can now be used to develop isolated magnetic dipole coupled energy terms. This is the subject of Section 3.3.

# 3 Derivation of the Total Electron Orbital Energy and the Isolated Spin-Orbit Magnetic Dipole Coupling Energies.

# 3.1 Derivation of Electron Orbital Energy Incorporating Spin-Orbit Coupling Via Re-Assessment of the Principle Quantum Number Criterion.

This is the simplest means of deriving the electron orbital energy incorporating spin-orbit magnetic coupling. However, it is to be noted that it only covers the magnetic coupling between the electron

spin and the electron orbit dipoles. This is because this couple is by far the largest contributor to fine structure splitting. Also, the results so obtained can thereby be compared directly with those of the comparable equations of the modern quantum theory of atomic structure. There are however, other smaller magnetic dipole coupling contributions which are derived in Section 3.3 and added to the extended electron orbital energy equation as appropriate.

The analysis is initiated from an expanded version of [1] Eq.(2.10). This approach is adopted here because it expresses more clearly the manner in which spin-orbit coupling is effected. Thus

$$nh = m_0 \oint v dl + \frac{m_0}{2c^2} \oint v^3 dl \tag{3.1}$$

Where now

 $\boldsymbol{n}$  is the primary quantum number

v is the total orbital velocity of the electron due to both the central coulomb force and the spin-orbit magnetic coupling force.

 $m_0$  is the reduced rest mass of the electron.

dl is an element of the orbit path length

The first integral in (3.1) is identical in form to that for a basic elliptic orbit and therefore has the solution

$$m_0 \oint v dl = \frac{2\pi \left( M_{\phi} + M_{so} \right)}{\left( 1 - \varepsilon^2 \right)^{1/2}}$$
(3.2)

Here

 $M_{\phi}$  is the angular momentum of the rest mass in the original elliptic orbit resulting from the central coulomb force

 $M_{so}$  is the angular momentum of the rest mass resulting from the spin-orbit magnetic coupling force.

 $\varepsilon$  is the eccentricity of the elliptic orbit.

The second integral in (3.1) is the rotation of the elliptic orbit due to the sum of the relativistic mass increase and spin-orbit precessions and is evaluated as follows

$$\frac{m_0}{2c^2} \oint v^3 dl = \frac{m_0}{2c^2} \oint \left({}_e \omega_\phi + {}_e \omega_{so}\right)^3 r_e^3 dl \tag{3.3}$$

Where

 $_e\omega_\phi$  is the angular rate due to the central coulomb force.

 $_e\omega_{so}$  is the angular rate due to spin-orbit coupling.

 $r_e$  is the radius vector magnitude from the electron to the focal point of rotation.

In (3.3),

$$dl = r_e d\phi \tag{3.4}$$

so that (3.3) becomes

$$\frac{m_0}{2c^2} \oint v^3 dl = \frac{m_0}{2c^2} \oint \left({}_e\omega_\phi + {}_e\omega_{so}\right)^3 r_e^4 d\phi \tag{3.5}$$

Where

 $\phi$  is the azimuth angle.

and (3.5) evaluates to

$$\frac{m_0}{2c^2} \oint v^3 dl = \frac{\pi \left(M_\phi + M_{so}\right)^3}{m_0^2 c^2 r_e^2}$$
(3.6)

So that from (3.2) and (3.6)

$$nh = \frac{2\pi \left(M_{\phi} + M_{so}\right)}{\left(1 - \varepsilon^2\right)^{1/2}} + \frac{\pi \left(M_{\phi} + M_{so}\right)^3}{m_0^2 c^2 r_e^2}$$
(3.7)

but in this case

$$r_e = \frac{\left(M_\phi + M_{so}\right)^2}{Ze^2 m_0}$$
(3.8)

which applies to the circular precession of the orbit in the second term in (3.7)This gives in (3.7)

$$\frac{nh}{2\pi} = \frac{(M_{\phi} + M_{so})}{(1 - \varepsilon^2)^{1/2}} + \frac{Z^2 e^4}{2c^2 (M_{\phi} + M_{so})}$$
(3.9)

Now

$$M_{\phi} = \frac{n_{\phi}h}{2\pi} \quad and \quad M_{so} = \frac{en_{sp}h}{2\pi} \tag{3.10}$$

Where

 $n_\phi$  is the azimuth quantum number associated with the rest mass of the electron.

The second term applies because the spin-orbit couple must be a direct function of electron spin and therefore directly dependent upon the spin quantum number. It is noted that this means that in this representation the spin-orbit angular momentum is identical to the spin angular momentum of the reduced electron mass as derived in [3].

Insertion of (3.10) into (3.9) gives

$$n = \frac{n_{\phi} + {}_{e}n_{sp}}{\left(1 - \varepsilon^{2}\right)^{1/2}} + \frac{Z^{2}e^{4}}{c^{2}h^{2}\left(n_{\phi} + {}_{e}n_{sp}\right)}$$
(3.11)

Inserting Sommerfeld's fine structure constant from [1], Eq.(3.34) gives

$$n = \frac{n_{\phi} + {}_{e}n_{sp}}{(1 - \varepsilon^2)^{1/2}} + \frac{\kappa^2 Z^2}{2(n_{\phi} + {}_{e}n_{sp})}$$
(3.12)

So that

$$(1 - \varepsilon^2)^{1/2} = \frac{n_{\phi} + {}_{e}n_{sp}}{n\left(1 - \frac{\kappa^2 Z^2}{2n\left(n_{\phi} + {}_{e}n_{sp}\right)}\right)}$$
(3.13)

Because  $\kappa^2 \ll 1$ , (3.13) can be approximated to

$$\left(1-\varepsilon^2\right)^{1/2} = \frac{n_\phi + {}_e n_{sp}}{n} \left(1 + \frac{\kappa^2 Z^2}{2n\left(n_\phi + {}_e n_{sp}\right)}\right)$$
(3.14)

So that

$$n(1-\varepsilon^{2})^{1/2} = n_{\phi} + {}_{e}n_{sp} + \frac{\kappa^{2}Z^{2}}{2n}$$
(3.15)

Which from [1], Eq.(3.43) becomes

$$n(1-\varepsilon^2)^{1/2} = n_{\phi}^* + {}_e n_{sp}$$
 (3.16)

Now, (3.7) can also be expressed as

$$nh = \frac{2\pi M_j^*}{\left(1 - \varepsilon^2\right)^{1/2}} \tag{3.17}$$

Where

 $M_j^\ast$  is the total orbital angular momentum of the electron due to the combined effects of the central coulomb field and spin-orbit coupling.

Accordingly, with

$$M_j^* = \frac{n_j h}{2\pi} \tag{3.18}$$

Where

 $n_j$  is the quantum number associated with  $M_j^\ast$  and is real, i.e. is integer and where adjacent values differ by unity.

Thus from (3.17) and (3.18)

$$n\left(1-\varepsilon^2\right)^{1/2} = n_j \tag{3.19}$$

Which gives in (3.16)

$$n_j = n_\phi^* + {}_e n_{sp} \tag{3.20}$$

Where

 $n_{\phi}^{*}$  is the azimuth quantum number associated with the relativistic energy mass of the electron.

The bound energy of the electron with spin-orbit magnetic coupling incorporated is then obtained by simply replacing  $n_{\phi}^*$  in [1], Eq.(3.46) by  $n_j$  thus

$${}_{e}E_{or} = -\frac{hR_{hy}Z^{2}}{n^{2}} \left[ 1 + \frac{\kappa^{2}Z^{2}}{n^{2}} \left( \frac{n}{n_{j}} - \frac{3}{4} \right) \right]$$
(3.21)

Where

 $_{e}E_{or}$  is the orbital energy of the electron

$$_e n_{sp} = \pm 1/_2$$
  
 $n = 1 \to \infty$ 

 $n_i$  is given by (3.20)

 $R_{hy}$  is Rydberg's constant for hydrogen

and the Selection Rules of [3] apply. It is a simple matter to prove that the above substitution of  $n_j$  for  $n_{\phi}^*$  is valid.

It is clear that (3.21) still takes the form of Sommerfeld's reduced equation as derived in [1], Eq. (3.46). A similar derivation exists for circular orbits.

It should be noted that the effective use of  $m_0$ , the reduced electron rest mass in the above derivation assumes that some of the energy in this expression is coupled into the proton orbit. This is incorrect, but the error so introduced is extremely small. This will be further discussed in Section 3.3.

To best demonstrate how (3.21) controls the emission spectra at this point in the development, it is recollected that n, the principle quantum number, must from the results of [1], be integer and its successive values differ by unity. Also, from the results of [3],  ${}_en_{sp}$  can only possess the values of  $\pm 1/2$ . Because  $n_j$  is the quantum number associated with the total angular momentum of the electron, it must also, in accordance with the results of [1], be an integer equal to or less than n, and successive values differ by unity. Accordingly,  $n_{\phi}^*$  the quantum number associated with the orbital angular momentum of the relativistically corrected electron mass, in order that the above criteria are met, must now take half integer values and successive values also differ by unity. These criteria can in turn best be demonstrated by rewriting [1] Table 3.1 as follows.

n	$oldsymbol{n}_{\phi}^{*}$	$_en_{sp}$	$n_j$	ε	Terms (Old)	Term (New)	Notes
1	$1/_{2}$	$+1/_{2}$	1	0	s	s(+)	
	$1/_{2}$	$+1/_{2}$	1	0.866	s	s(+)	2
2	$1^{1/2}$	+1/2	2	0	p(+)	p(+)	
	$1^{1/2}$	-1/2	1	0.866	p(-)	s(-)	1,2
	$^{1/2}$	$+1/_{2}$	1	0.943	s	s(+)	2
	$1^{1/2}$	$+1/_{2}$	2	0.745	p(+)	p(+)	2
3	$1^{1/2}$	-1/2	1	0.943	p(-)	s(-)	1,2
	$2^{1/2}$	$+1/_{2}$	3	0	d(+)	d(+)	
	$2^{1/2}$	-1/2	2	0.745	d(-)	p(-)	1,2
	$^{1/2}$	$+1/_{2}$	1	0.968	s	s(+)	2
	$1^{1/2}$	$+1/_{2}$	2	0.866	p(+)	p(+)	2
	$1^{1/2}$	-1/2	1	0.968	p(-)	s(-)	1,2
4	$2^{1/2}$	+1/2	3	0.661	d(+)	d(+)	2
	$2^{1/2}$	-1/2	2	0.866	d(-)	p(-)	1,2
	$3^{1/2}$	+1/2	4	0	f(+)	f(+)	
	$3^{1/2}$	-1/2	3	0.661	f(-)	d(-)	1,2

# Table 3.1 - Spin-Orbit Coupled Orbit Characteristics for the First Four Orbital Shells.

Table 3.1 shows how the four quantum numbers so far considered combine to produce the first four orbital shells and is largely self explanatory. There are however, two points worthy of comment and they are as follows.

<u>Note 1:</u> A second "Term" column has been added in Table 3.1, "Term (New)". In this column it is seen that the term for the  $_en_{sp} = -1/_2$  has been re-allocated. This is because it is clear from the values of  $n_j$  and  $\varepsilon$  that the orbitals in question are identical to the orbitals with  $_en_{sp} = +1/_2$  and  $n_{\phi}^*$  one quanta lower within the same orbital shell. This will be discussed in more detail in Section 4.0.

<u>Note 2:</u> Some orbitals for  $n \ge 2$  are elliptical and within them the electron is therefore subject to spin induction as described in [3]. The question therefore arises as to what happens when the electron traverses into the following quadrant and the direction of spin reverses, i.e. when in say 2s,  $_{e}n_{sp}$  is changed from +1/2 to -1/2. This reversal represents a net reduction of one quanta of orbital angular momentum. Consequently, by the law of conservation of angular momentum there must be a net increase of one quanta to balance this reduction. The only way this can be effected without violating other criteria associated with n or  $n_j$  is for  $n_{\phi}^*$  to increase by one quanta. This represents a zero energy change intra-shell orbital transition from say 2s, {or 2s(+) in the New Term column}, to 2p(-), {2s(-)}, and is clearly associated with the comments under Note 1 above. The process so described is the manner in which the potential anomalies discussed briefly in [3], Section 4.0, (iv) and (vi) are avoided. Further more detailed discussion of this feature is the subject of Section 4.0 where it is tracked around a complete orbit.

### 3.2 Isolation of the Electron Spin-Orbit Coupling Energy Term by Subtracting the Orbital Energy Without Spin-Orbit Coupling from that With.

If the effect of spin-orbit coupling is omitted from (3.21), the result is,

$${}_{e}E_{or} = -\frac{hR_{hy}Z^{2}}{n^{2}} \left[ 1 + \frac{\kappa^{2}Z^{2}}{n^{2}} \left( \frac{n}{n_{j} - {}_{e}n_{sp}} - \frac{3}{4} \right) \right]$$
(3.22)

It is important to note that (3.22) is not the same as [1], Eq.(3.46). The former is the orbital energy incorporating spin-orbit coupling but with the spin-orbit quantum term mathematically removed while [1], Eq.(3.46) is the orbital energy in a non spin-orbit coupled environment, i.e. there is a difference in the value of  $n_{\phi}^*$  in the two relationships as discussed at the end of sub-Section 3.1 above.

Subtracting (3.22) from (3.21) gives the isolated spin-orbit coupling energy term as

$${}_{e}E_{so} = \frac{hR_{hy}Z^2}{n^2} \frac{\kappa^2 Z^2}{n^2} \left\{ \frac{n_{e}n_{sp}}{n_j (n_j - {}_{e}n_{sp})} \right\}$$
(3.23)

This can be re-stated using (3.20) as

$${}_{e}E_{so} = \frac{hR_{hy}Z^2}{n^2} \frac{\kappa^2 Z^2}{n^2} \left\{ \frac{n_{e}n_{sp}}{n_{j} n_{\phi}^*} \right\}$$
(3.24)

Calculation of levels using (3.24) must take account of the Selection Rules as effectively embedded in Table 3.1. Of course in (3.24)  $n_{\phi}^*$  is the value in a spin-orbit coupled environment. Also the comment following (3.21) concerning the presence of  $m_0$  also applies here.

# 3.3 Derivation of All Isolated Magnetic Coupling Energy Terms from First Principles.

In any theory in which all events are to be described by real physical parameters, it is necessary that each event be separately derivable from first principles. In this resurrected Bohr/Sommerfeld theory of atomic structure it is therefore mandatory that each magnetic dipole coupling effect be so derivable. This must include those involving the proton nucleus. Such derivations are the subject of this sub-Section.

The coupling energy between any two magnetic dipoles is given by, [5]

$$E_m\left(\phi\right) = \frac{\mu_0}{4\pi} \left(\frac{\bar{\Psi}_{or}.\bar{\Psi}_{sp} - 3\bar{\Psi}_{or}.\bar{r}\;\bar{r}.\bar{\Psi}_{sp}}{r^3}\right)$$
(3.25)

Where

 $\bar{\Psi}_{or}$  is a magnetic dipole vector due to orbital motion.

 $\bar{\Psi}_{sp}$  is a magnetic dipole vector due to spin motion.

 $\bar{r}$  is the separation vector, magnitude r.

 $\mu_0$  is the permeability of free space.

In all cases considered here the dipole vectors are parallel so that (3.25) reduces to, ( $\mu_0 = 4\pi$  in cgs units),

$$E_m\left(\phi\right) = \frac{\Psi_{or}\Psi_{sp}}{r^3} \tag{3.26}$$

Eq.(3.26), together with the results of Section 2 can now be used to determine the various magnetic dipole coupling energies in hydrogen.

# 3.3.1 Relationship Between the Magnetic Dipoles of the Orbits of the Electron and the Proton Nucleus.

As shown by (2.2) and (2.3) these two dipoles are of opposite polarity. They are also coincident at the common focal point of both orbits and so no couple is generated between them. They simply subtract to produce the resultant magnetic field at that point. Thus

$$\Psi_{or} = {}_{e}\Psi_{or} + {}_{p}\Psi_{or} = \frac{Zehn_{j}}{4\pi m_{e}c} \left(1 - \frac{\gamma_{p}m_{e}}{m_{p}}\right)$$
(3.27)

3.3.2 Coupling Energy of the Electron Spin Dipole and the Net Orbit Dipole.

Insertion of (2.1) and (3.27) into (3.26) gives

$${}_{e}E_{so}\left(\phi\right) = \frac{Ze^{2}h^{2}\left(1 - \frac{\gamma_{p}m_{e}}{m_{p}}\right)n_{j\ e}n_{sp}}{8\pi^{2}m_{e}^{2}c^{2}r_{e}^{3}}$$
(3.28)

Eq.(3.28) is the electron spin-orbit coupling energy resulting from the orbital motions of the proton/electron pair due to the central coulomb force. However, the extra precessional motion of these orbits due to magnetic dipole coupling itself will also contribute to the coupling energy. This can be inserted into (3.28) by its product with the appropriate quantum number ratio thus

$${}_{e}E_{so}\left(or\right) = {}_{e}E_{so}\left(\phi\right)\frac{n_{j}}{n_{\phi}^{*}} = \frac{Ze^{2}h^{2}\left(1-\frac{\gamma_{p}m_{e}}{m_{p}}\right)n_{j}^{2} {}_{e}n_{sp}}{8\pi^{2}m_{e}^{2}c^{2}r_{e}^{3}n_{\phi}^{*}}$$
(3.29)

It is important to note that the  $n_{\phi}^*$  used here is the value in a spin-orbit coupled environment and is different from that in a non spin-orbit coupled environment. This was made clear in sub-Sections 3.1 and 3.2.

Eq.(3.29) shows that the electron spin-orbit coupling energy is a variable inversely proportional to the cube of the distance between the dipoles. To obtain a value that can represent the mean energy throughout the complete orbit means determining an appropriate average value for  $r_e$ . To maintain continuity here, that derivation is relegated to Appendix A. The result is

$$\langle r_e \rangle = \frac{L_e}{\left(1 - \varepsilon^2\right)^{1/2}} \tag{3.30}$$

Where

 $\langle r_e \rangle$  is the average value of  $r_e$  around the complete orbit.

 $L_e$  is the semi-latus rectum of the electron orbit.

With

$$L_e = \frac{M_j^{*2}}{Ze^2 m_e} = \frac{n_j^2 h^2}{4\pi^2 Ze^2 m_e}$$
(3.31)

Where

 $M_j^\ast$  is the total orbital angular momentum incorporating that component due to spin-orbit magnetic coupling.

From (3.19)

$$(1 - \varepsilon^2)^{3/2} = \frac{n_j^3}{n^3}$$
 (3.32)

So that (3.31) and (3.32) converts (3.29) to

$${}_{e}E_{so}\left(or\right) = \frac{8\pi^{4}Z^{4}e^{8}m_{e}\left(1 - \frac{\gamma_{p}m_{e}}{m_{p}}\right){}_{e}n_{sp}}{h^{4}c^{2}n_{j}n_{\phi}^{*}n^{3}}$$
(3.33)

Finally, insertion of [1], Eq.(3.8) and [1], Eq.(3.34), (the Rydberg constant and Sommerfeld's fine structure constant), gives

$${}_{e}E_{so}\left(or\right) = \frac{hR_{hy}Z^{2}}{n^{2}}\frac{\kappa^{2}Z^{2}}{n^{2}}\frac{m_{e}}{m_{0}}\left(1 - \frac{\gamma_{p}m_{e}}{m_{p}}\right)\frac{n_{e}n_{sp}}{n_{j}n_{\phi}^{*}}$$
(3.34)

With reference to the comment following (3.21) and (3.24), note here the appearance of the ratio  $m_e/m_0$ . Comparison of (3.34) with (3.24) is effected in sub-Section 3.4 below.

Eq.(3.34) is the main contributor to electron spin-orbit coupled precession but there are other magnetic coupling effects which contribute either directly or indirectly. These are derived below.

#### 3.3.3 Coupling Energy of the Spin Dipole of the Nucleus and the Net Orbit Dipole.

Although this couple does not affect the electron orbital energy in a direct sense, it does so in an indirect way. This will be demonstrated in the next paper. The coupling energy is derived as follows. Insertion of (2.4) and (3.27) into (3.26) gives

$${}_{p}E_{so}\left(\phi\right) = -\frac{Z^{2}e^{2}h^{2}\left(1 - \frac{\gamma_{p}m_{e}}{m_{p}}\right)\gamma_{p}\,n_{j\,p}n_{sp}}{8\pi^{2}c^{2}m_{e}m_{p}r_{p}^{3}}\tag{3.35}$$

Where

 $\boldsymbol{r}_p$  is the radius vector magnitude of the proton orbit.

Via an identical process to that in Section 3.3.2 above, the energy coupled into the proton orbit by the proton spin dipole becomes

$${}_{p}E_{so}\left(or\right) = -\frac{hR_{hy}Z^{2}}{n^{2}}\frac{\kappa^{2}Z^{2}}{n^{2}}\frac{m_{p}^{2}}{m_{0}m_{e}}Z\gamma_{p}\left(1-\frac{\gamma_{p}m_{e}}{m_{p}}\right)\frac{n_{p}n_{sp}}{n_{j}n_{\phi}^{*}}$$
(3.36)

The energy coupled into the proton orbit is therefore of opposite polarity to that coupled into the electron orbit from this source. It is also considerably greater in magnitude which, together with its orbit being so much smaller, results in the precession of the two particles being significantly different. This results in a small addition to the orbital energy of the electron which, in the next paper, will be shown to contribute to the Lamb Shift.

### 3.3.4 Coupling Energy of the Electron and Nucleus Spin Dipoles.

This is the final and smallest of the magnetic dipole coupling energies, and while it contributes to the orbital energy of the electron, (and the proton), its effect is minimal. It's main contribution to the emission spectra, as will be shown in a future paper, is to the hyperfine structure. Substitution of (2.1) and (2.4) into (3.26) gives

$$_{e,p}E_{ss}\left(\phi\right) = -\frac{Ze^{2}h^{2}\gamma_{p}\delta_{p\ e}n_{sp\ p}n_{sp}}{4\pi^{2}m_{e}m_{p}c^{2}r_{e}^{3}}$$
(3.37)

Where

 $_{e,p}E_{ss}(\phi)$  is the energy coupled into both the electron and proton orbits by the spin-spin magnetic dipole coupling of both particles.

Note that because this couple is of relativistic magnitude,  $r_e$  can be used instead of r to simplify the analysis. This substitution also ignores the fact that r is a dynamic function of  $\phi$  due to the different precession rate of the proton orbit, the effect of this variation on the magnetic couple also being of insignificant magnitude.

The parameter  $\delta_p$  is a constant of proportionality introduced to account for the effect of the rotation of the proton spin dipole about the common orbital point relative to the electron, also due to the different precession rate of the proton. This results in a field of magnetisation about the orbital focal point, the shape and therefore flux density of which, in a similar manner to  $\gamma_p$ , will depend upon the shape and internal structure of the proton. The value of  $\delta_p$  will, in a future paper, via a semi-empirical analysis associated with the hyperfine structure, be shown to be of the order of 3.3558912.

Via analysis similar to that above in Section 3.3.2, the energy coupled into both orbits by these spin dipoles is

$$_{e,p}E_{ss}\left(or\right) = -\frac{hR_{hy}Z^2}{n^2}\frac{\kappa^2 Z^2}{n^2}\frac{m_e^2}{m_0 m_p}2\gamma_p \delta_p \frac{n_e n_{sp} \ n_{sp}}{n_{\phi}^* n_j^2}$$
(3.38)

Clearly the energy contained in this expression is significantly smaller than that in (3.34). As stated earlier, (3.34) therefore represents the major source of fine structure splitting.

# 3.4 Total Electron Orbital Energy.

It is now possible to gather together all the terms, as so far developed, contributing to the orbital energy of the electron. These terms are (3.38), (3.34) and [1], Eq.(3.46). This group is preferred over one including (3.21) because of the minor discrepancies and omissions extant in that latter equation for reasons already partly explained and further summarised below. The overall electron orbital energy is therefore given by

$${}_{e}E_{or} = -\frac{hR_{hy}Z^{2}}{n^{2}} \left[ 1 + \frac{\kappa^{2}Z^{2}}{n^{2}} \left\{ \frac{n}{n_{\phi}^{*}} - \frac{m_{e}}{m_{0}} \left( 1 - \frac{\gamma_{p}m_{e}}{m_{p}} \right) \frac{n_{e}n_{sp}}{n_{j}n_{\phi}^{*}} + 2\frac{m_{e}^{2}}{m_{0}m_{p}} \gamma_{p}\delta_{p} \frac{n_{e}n_{sp}}{n_{\phi}^{*}n_{j}^{2}} - \frac{3}{4} \right\} \right]$$
(3.39)

Note that apart from the inclusion of the spin-spin term, (3.38), the difference between (3.21) and (3.39) is, in the electron spin-net orbit dipole couple term, the presence of the term  $\frac{m_e}{m_0} \left(1 - \frac{\gamma_p m_e}{m_p}\right)$ . This is the factor which (i) corrects (3.21) to represent only energy coupled into the electron orbit,  $\frac{m_e}{m_0}$ , and (ii) to include the energy effectively coupled into the electron orbit from the proton orbit dipole,  $\left(1 - \frac{\gamma_p m_e}{m_p}\right)$ . Eq.(3.39) is therefore considered a more accurate and complete representation of the total electron orbital energy. Consequently, it is this equation which is used to calculate emission spectra in Appendix C.

Finally, it is to be noted that (3.39) can quite easily be constructed via the analytical method of sub-Section 3.1, provided cognizance is taken of all contributory factors in the appropriate manner, i.e. by their orbital angular momentum contributions.

### 4 The Effect of Electron Spin Reversals Within an Elliptic Orbital.

Now that the effects of magnetic dipole coupling have been introduced into this resurrected theory, the question as to what happens when, due to spin induction, the electron spin reverses in an elliptic orbital, can, further to the brief dissertation in Section 3.1, Note 2 to Table 3.1, be discussed in more detail here.

If there were no dead zones in an elliptic orbit, the spin reversal would be "instantaneous" at the quadrant boundaries. This would result in a spin-orbit et al coupled energy change exemplified by the spin quantum number change  $\Delta_e n_{sp} = \pm 1$ , and therefore a  $\Delta n_j$  change of  $\pm 1$ . This could incur an inter-shell orbital transition of some kind. However, the dead zones impose a restriction on the magnitude of the spin change such there is no energy change, although there is an intra-shell transition. The manner in which these changes occur is best explained by means of an example, as follows. Consider Fig. 4.1.



Fig. 4.1 - Electron Orbital Spin Reversals, (Elliptic Orbital)

This shows electron spin directions, up, down or no spin, around the four quadrants and dead zones of an elliptic orbit. Consider the case of an electron in an ns orbital, n > 1. As the electron proceeds through the quadrants and dead zones, the quantum numbers change according to the spin reversals as depicted in Table 4.1 below.

Q/D	Quantum Number	Explanation
Q1	$e^{n_{sp}} = +1/2$ $n_{\phi}^{*} = 1/2$ $n_{j} = 1$	Orbital is $ns(+)$ , (See table 3.1)
D1	$e^{n_{sp}} = 0$ $n^*_{\phi} = 1$ $n_j = 1$	Change in $_{e}n_{sp}$ causes $^{1}/_{2}$ quanta reduction in spin-orbit coupled energy. $n_{j}$ is already at a minimum value and can only change by an integer. Therefore $n_{\phi}^{*}$ must increase by $^{1}/_{2}$ . The electron undergoes an intra-shell transition to $n_{s}$ as in [1], Table 3.1, (same $\varepsilon$ ).
Q2	$e^{n_{sp}} = -\frac{1}{2}$ $n_{\phi}^{*} = \frac{1}{2}$ $n_{j} = 1$	Spin induction causes ${}_{e}n_{sp}$ to change to ${}^{-1/2}$ causing a ${}^{1/2}$ quanta reduction in spin-orbit coupled energy. $n_{j}$ is already at a minimum value and can only change by an integer. Therefore $n_{\phi}^{*}$ must increase by ${}^{1/2}$ . The electron undergoes an intra-shell transition to $np(-)$ as in Table 3.1, (this paper).
D2	$e^{n_{sp}} = 0$ $n^*_{\phi} = 1$ $n_j = 1$	Change in $_{e}n_{sp}$ causes $1/_{2}$ quanta increase in spin-orbit coupled energy. $n_{j}$ is already at a minimum value and can only change by an integer. Therefore $n_{\phi}^{*}$ must reduce by $1/_{2}$ . The electron undergoes an intra-shell transition to $n_{s}$ as in [1], Table 3.1, (same $\varepsilon$ ).
Q3	$e^{n_{sp}} = +1/2$ $n_{\phi}^{*} = 1/2$ $n_{j} = 1$	Change in $_{e}n_{sp}$ causes $^{1}/_{2}$ quanta reduction in spin-orbit coupled energy. $n_{j}$ is already at a minimum value and can only change by an integer. Therefore $n_{\phi}^{*}$ must reduce by $^{1}/_{2}$ . The electron undergoes an intra-shell transition to $ns(+)$ as in Table 3.1, (this paper).
D3	Same as D1	As per Q1 to D1
Q4	Same as Q2	As per D1 to Q2
D4	Same as D2	As per Q2 to D2
Q1	Same as Q3	As per D2 to Q3

# <u>Table 4.1 - Intra-Shell Transition Characteristics for ns(+), (<u>n</u> > 1)</u>

Thus in the dead zones, D1 to D4, the orbital is that of ns in [1], Table 3.1. In quadrants Q1 and Q3, the orbital is that of ns(+) in Table 3.1, (this paper). In quadrants Q2 and Q4 the orbital is that of np(-),  $\{ns(-)\}$ , in Table 3.1, (this paper).

The same sequence of intra-shell transitions would occur for np, nd orbitals etc except where the orbital was circular within which there is no spin induction and therefore no reversals.

Note that in each change the non spin-orbit coupled orbital has the same geometrical characteristics as the spin-orbit coupled orbitals in the transition sequence and therefore there is no energy change in the transition. The angular momentum change that affects  $n_{\phi}^*$ , (the spin-orbit coupled environment value), will be shown in a future paper to be instrumental in the hyperfine structure of elliptic orbitals.

An important result of this feature is that for hydrogen, there is no pseudo ground state in which an electron exists in the 2s orbital. As a consequence, as no inter-shell transition path exists for a 2s orbital, an intra-shell transition of electrons that enter this orbital always takes place by which they move from the 2s orbital to the 2p(-),  $\{2s(-)\}$  orbital. This subsequently allows a normal inter-shell transition to the ground state 1s orbit. It must be noted that the above dissertation does not infer that electrons in the higher, (> 1s), orbitals can traverse the complete orbital before making an inter-shell transition. It is most likely that after insertion into any particular quadrant, due to spin induction, it will immediately make a further transition to a lower shell. Alternatively, it could traverse just one dead zone into the next quadrant before making such a transition with reversed spin. The one exception of course is an electron in the 2s orbital where, as described above, it must traverse one dead zone before making the transition to the ground state.

The above intra-shell transition sequences also lend significant credence to the renamed Term Scheme, (the "Term, (New)" column, in Table 3.1).

### 5 Comparison with the Atomic Structure Theory of Modern Quantum Mechanics.

The subject matter of this comparison is, in the quantum mechanics theory, the three relativistic terms that give rise to the fine structure and the splitting thereof into doublets, as presented in [4]. (The quantum mechanics quantum number l, referred to below, is the azimuth quantum number omitting spin-orbit coupling).

### 5.1 <u>The Relativistic Mass Increase Effects.</u>

### 5.1.1 In Quantum Mechanics theory for l = 0, the Darwin Term.

Adopting for this Section the energy designator of [4], this term is given in [4] as

$$\Delta E^{///} = \frac{hR_{hy}Z^2}{n^2} \frac{\kappa^2 Z^2}{n}$$
(5.1)

which in conjunction with the "relativistic mass increase effects" from [4] gives for the orbital energy in s orbitals

$$E = -\frac{hR_{hy}Z^2}{n^2} \left\{ 1 + \frac{\kappa^2 Z^2}{n^2} \left( n - \frac{3}{4} \right) \right\}$$
(5.2)

In the resurrected theory proposed here, the orbital energy is given by, (spin-orbit coupling omitted), [1], Eq.(3.46), repeated here for convenience

$$E = -\frac{hR_{hy}Z^2}{n^2} \left\{ 1 + \frac{\kappa^2 Z^2}{n^2} \left( \frac{n}{n_{\phi}^*} - \frac{3}{4} \right) \right\}$$
(5.3)

and for s orbitals  $n_{\phi}^* = 1$ , (the non-spin-orbit coupled value), so that (5.3) reduces to (5.2). Thus the resurrected Bohr/Sommerfeld theory is equivalent to the quantum mechanics theory at this stage.

### 5.1.2 In Quantum Mechanics theory for $l \neq 0$ .

Omitting spin-orbit coupling, the quantum mechanics theory gives for the mass increase effect, [4]

$$E = -\frac{hR_{hy}Z^2}{n^2} \left\{ 1 + \frac{\kappa^2 Z^2}{n^2} \left( \frac{n}{l + \frac{1}{2}} - \frac{3}{4} \right) \right\}$$
(5.4)

Reference to (5.3) shows that at this stage in the comparison

$$n_{\phi}^* = l + \frac{1}{2} \tag{5.5}$$

and consequently, in concert with Section 5.1.1 above, when

$$\begin{array}{ll} l = 0, & n_{\phi}^{*} = l + 1 \\ l \neq 0, & n_{\phi}^{*} = l + \frac{1}{2} \end{array}$$
 (5.6)

The difference of  $n_{\phi}^*$  to l for the two conditions of l in (5.6) is due solely to the fact that in the quantum mechanics theory the Darwin term is no longer present for  $l \neq 0$  and spin orbit coupling is not yet included.

# 5.2 Spin-Orbit Coupling.

The incorporation of spin-orbit coupling in quantum mechanics theory,  $(l \neq 0)$ , gives, [4]

$$E = -\frac{hR_{hy}Z^2}{n^2} \left\{ 1 + \frac{\kappa^2 Z^2}{n^2} \left( \frac{n}{j + \frac{1}{2}} - \frac{3}{4} \right) \right\}$$
(5.7)

where j is the inner quantum number given by  $j = l \pm 1/2$ , so that (5.7) becomes

$$E = -\frac{hR_{hy}Z^2}{n^2} \left\{ 1 + \frac{\kappa^2 Z^2}{n^2} \left( \frac{n}{l + \frac{1}{2} \pm \frac{1}{2}} - \frac{3}{4} \right) \right\}$$
(5.8)

In the resurrected Bohr/Sommerfeld theory under this condition the orbital energy is

$$E = -\frac{hR_{hy}Z^2}{n^2} \left\{ 1 + \frac{\kappa^2 Z^2}{n^2} \left( \frac{n}{n_j} - \frac{3}{4} \right) \right\}$$
(5.9)

Where

$$n_j = n_{\phi}^* + {}_e n_{sp} \tag{5.10}$$

Inserting (5.5) and [3], Eq.(3.4) gives

$$n_j = l + \frac{1}{2} \pm \frac{1}{2} \tag{5.11}$$

thus equating (5.9) with (5.8).

Also note that this means that for all values of l including zero

$$n_j = j + \frac{1}{2} \tag{5.12}$$

so that  $n_j$  is always integer as j is always half integer. As  $n_j$  is the quantum number associated with the total angular momentum of the electron, (as is j), this value of  $n_j$  is more in keeping with de Broglie's quantum hypothesis.

If desired this last comparison can be term specific wherein the isolated spin-orbit coupling term can be shown to be equivalent in both theories. However, this only applies when electron spin-orbit coupling is assumed to affect both the orbits of the electron and the proton nucleus, which has already been shown to be incorrect.

It is also clear that the above relationship comparison means that effectively,  $n_{\phi}^*$  is in part equivalent to the 1/2 quantum number zero point energy term in modern quantum mechanics theory.

# 5.3 Discussion.

In both theories, the primary quantum number, n, is a measure of the single valuedness of the electron matter wave around its orbit. In this respect the two theories are identical encompassing the same tenet. To some extent the same comment applies to the spin quantum numbers, s in quantum mechanics, (QM) theory;  $\#n_{sp}$  in the Bohr/Sommerfeld, (B/S) theory. Both have the same numerical value but, in view of the different treatment of the electron, there the similarity ends. In B/S theory  $en_{sp}$  results from the angular momentum of a real physical particle. This then leads directly to a properly defined quantised spin magnetic moment. In QM theory the spin quantum number, s, is still purported to be due to electron "spin", but because of the nature of

the electron in this theory, electron spin cannot be adequately defined. Accordingly, in QM theory the "spin" magnetic moment of the electron is subject to the same difficulties.

The main difference between the two theories however, concerns the azimuth quantum number,  $(l \text{ in } \text{QM}, n_{\phi}^* \text{ in } \text{B/S})$ . This comparison needs to be conducted in several parts because of the peculiarity in the interpretation of l.

(i) s Orbitals :- l = 0 :  $n_{\phi}^* = 1$ , (B/S Theory Spin-Orbit Coupling Omitted). In these orbitals in QM theory, azimuthal angular momentum is zero, so that accordingly spin-orbit coupling is also zero. Therefore, l = 0, and j = +1/2, and the orbital energy is given by, (i) the ubiquitous "zero point energy" of quantum mechanics, the "1/2" in the denominator of (5.4), and, (ii) the appearance of the Darwin term which only applies to s orbitals. The fact that there is no azimuthal angular momentum in QM theory is considered somewhat of an anomaly. Even with the electron treated as an orbiting probabilistic matter wave, this matter wave, as shown in [2], is a representation of kinetic energy, and accordingly will possess an equivalent mass in line with Einstein's renowned energy/mass relationship. The electron should still therefore generate an effective angular momentum. Consequently, spin-orbit magnetic coupling should also appear in QM theory in s orbitals.

In the resurrected B/S theory, in s orbitals, (with spin-orbit coupling omitted),  $n_{\phi}^*$  is effectively equivalent to the zero point energy plus the Darwin terms of QM theory. It cannot be actually so equated because it represents a different concept in that it is directly related to the angular momentum of a real physical electron particle. As a result spin-orbit coupling is present as is evident in Table 3.1. This leads directly to the next Sub-Section.

(ii) <u>s</u> Orbitals :- l = 0 :  $n_j = 1$ , (B/S Theory Spin-Orbit Coupling Incorporated). In this case the comments in (i) concerning the azimuth quantum number l of QM theory are still fully applicable. In discussing the resurrected B/S theory however, it is now  $n_j$  that is equivalent to the zero point energy and Darwin terms of QM theory, and as is clear from Table 3.1,  $n_j$  is composed of the azimuth quantum number  $n_{\phi}^*$ , (1/2 in s orbitals), plus the spin-orbit magnetic coupled quantum number,  $en_{sp}$ , (+1/2 in s orbitals).

(iii) All Other Orbitals :-  $l \neq 0$ ,  $j = l \pm 1/2$ :  $n_{\phi}^* > 1$ ,  $n_j = n_{\phi}^* +_e n_{sp}$ . In these orbitals both theories contain exactly the same components to make up the orbital energy and the differences are related to the meaning attributed to the azimuth quantum number l. Here l is the azimuth quantum number related to the angular momentum of the electron, (in wavefunction form), thus enabling spin-orbit coupling, so resulting in the inner quantum number j. The zero point energy term is still a separate addition. On the other hand  $n_{\phi}^*$  is now equivalent to l, this equivalence including the zero point energy term. The comparison between j and  $n_j$  is consequently identical to that between l and  $n_{\phi}^*$ .

(iv) <u>Other Differences.</u> Apart from the quantum number nomenclature and meanings, and the presence of spin-orbit coupling in s orbitals in the B/S theory, as discussed above, there are three other differences to the modern QM theory. Although at this juncture they have insignificant impact on the emission spectra, they will do so when the Lamb Shift and hyperfine structure are incorporated. These differences are exemplified in the derivations in Section 3.3 and discussed there. They are.

(a) The coupling energy between electron spin and electron orbit is only coupled into the electron orbit, not that of the proton nucleus. Hence the appearance of the term  $m_e/m_0$  in (3.34).

This correcting term is absent in the QM theory equivalent expression as represented by (5.7).

(b) The spin-orbit energy coupled into the electron orbit also, in the B/S theory, incorporates a term to reflect that effectively resulting from the proton dipole. Hence the appearance of the term  $\left(1 - \gamma_p m_{e/m_p}\right)$  in (3.34). This correcting term is absent in the QM equivalent expression as represented by (5.7).

(c) The magnetic dipole energy coupled into the electron orbit, in the B/S theory, also incorporates a term to reflect that resulting from the proton spin dipole, as represented by (3.38). No such term exists in the QM theory in the representative expression, (5.7), although this couple does receive detailed attention in the literature, [4], in discussion of the hyperfine structure for l > 0.

All of these other differences have very little impact on the orbital energy levels of the electron at this stage, but should be included because as the development continues to incorporate appropriate terms for the Lamb Shift and the hyperfine structure, they become to some extent the dominant features.

# 6 <u>Conclusions.</u>

The original intent of this series of papers was to resurrect the old quantum theory of Niels Bohr and Arnold Sommerfeld and, together with some input from modern quantum mechanics show that a theory of atomic structure could, for single electron atoms and ions, be developed in which the electron was interpreted as a real physical particle. With the incorporation of magnetic dipole coupling, it is proposed that this objective has been largely accomplished. This is considered to be a reasonable claim at this stage because the resurrected theory can now predict all that the modern quantum mechanics theory of atomic structure can predict. Further refinement in the latter theory, i.e. the Lamb Shift, has had to make recourse to additional techniques within quantum electrodynamics. Because of the philosophical intent of the resurrected Bohr/Sommerfeld theory, it will need to introduce this variation without recourse to quantum electrodynamics or similar disciplines. This will be the subject of the next paper.

Albeit the above statement on the maturity of the resurrected theory is considered justifiable at this stage, it must still be viewed as somewhat embryonic. This is because essentially, only the hydrogen atom has been considered in detail, and only to the point of fine structure splitting. To provide further substance to the theory, not only will it be necessary to incorporate an explanation for the Lamb Shift, but also a sound mathematical model for the hyperfine structure will need to be added. Both of these additions will require a physical interpretation in keeping with the original objective. Furthermore, it would also be very desirable to extend the theory to cover at the very least simple multi-electron atoms. However, this would be, as is well known, severely restricted by the difficulties inherent in solving three body, (and more), dynamic problems. Despite the fact that in the modern quantum mechanics theory of atomic structure, the electron is viewed as a probabilistic wavefunction, it is, strangely, subject to the same difficulties.

The comparison of the two theories, as so far developed, in Section 5.0, is from the mathematical point of view, favourable, minor differences aside. However, when the comparison is extended to include physical attributes, some anomalies result. Extending the comparison is justified despite the fact that the electron is viewed so differently in the quantum mechanics theory because that theory still makes extensive reference to such physical parameters as spin, angular momentum, magnetic moment and relativistic mass increase when discussing the electron. The extended comparison centres exclusively around the quantum numbers used to characterise the electron orbital energy

levels. The main consequence of this comparison is that in the quantum mechanics theory, the lack of s orbital angular momentum, results in the necessity for two separate equations to describe the orbital energy for all orbitals. One equation is required for s orbitals, in which the Darwin term is included but spin-orbit coupling excluded, and a second equation for all other orbitals with the Darwin term excluded and spin-orbit coupling included. The only terms common are those for the gross energy levels resulting from the basic central coulomb force and the "relativistic mass increase" of the electron.

In the resurrected Bohr/Sommerfeld theory only one equation is necessary incorporating the appropriate terms for the gross energy levels, the relativistic electron mass increase and all magnetic dipole coupling effects. All of these terms appearing in all orbitals. This is considered a superior aspect of the Bohr/Sommerfeld theory over the quantum mechanics.

Within the Bohr/Sommerfeld theory it has been possible to ascribe real physical meanings to all of the parameters involved and which appears free of apparent anomalies. Possible mechanisms have been identified for electron spin and photon emission, from which it has been possible to derive all except one of the so called Selection Rules. The one exception is for transitions in which  $\Delta n_j = \pm 2$ . These have been excluded in the resurrected theory for orbit transition path geometrical reasons. In the quantum mechanics theory, exclusion is for the inner quantum number change only. However, in this regard, it is noted that the orbital angular momentum Selection Rule governing transitions, is, even with spin-orbit coupling incorporated, still  $n_{\phi}^*$ , (or l), because only that quantum number is subject to a direct change when a photon emission occurs.

To complete the current phase of development, in addition to the incorporation of the Lamb Shift and the hyperfine structure, it will be useful to demonstrate the physical characteristics of all orbitals, the electron transition paths between them, and the strengths of the emitted spectra. These will be the subject of future papers.

Finally, as in previous papers in this series, the emission spectra as predicted by this theory are shown in Appendix C. If the Lamb Shift effect is removed from [6], the spectra of Appendix C are seen to compare very favourably provided allowance is made for the small differences in the values of the constants used.

### APPENDIX A.

# Derivation of the Median Value of the Radius Vector Magnitude from a Focal Point in an Elliptic Orbit.

In an elliptic orbit the radius vector magnitude is given by

$$r_e = \frac{L_e}{1 + \varepsilon \cos \phi} \tag{A.1}$$

The average value of  $r_e$  around the complete orbit is then

$$\langle r_e \rangle = \frac{L_e}{2\pi} \int_0^{2\pi} \frac{1}{1 + \varepsilon \cos \phi} d\phi \tag{A.2}$$

Because the orbit is symmetrical, (A.2) may be written

$$\langle r_e \rangle = \frac{L_e}{\pi} \int_0^\pi \frac{1}{1 + \varepsilon \cos \phi} d\phi \tag{A.3}$$

Using the substitution

$$b = \tan \frac{\phi}{2} \tag{A.4}$$

 $\operatorname{then}$ 

$$\cos \phi = \frac{1 - b^2}{1 + b^2}$$
 and  $d\phi = \frac{2db}{1 + b^2}$  (A.5)

The integration limits then become

when 
$$\phi = \pi$$
,  $b = \tan \pi/2 = \infty$  and when  $\phi = 0$ ,  $b = \tan 0 = 0$  (A.6)

These substitutions convert (A.3) to

$$\langle r_e \rangle = \frac{L_e}{\pi \left(1 - \varepsilon\right)} \int_0^\infty \frac{1}{\left(\frac{1 + \varepsilon}{1 - \varepsilon}\right) + b^2} db$$
 (A.7)

This is a standard integral that evaluates to

$$\langle r_e \rangle = \frac{L_e}{\left(1 - \varepsilon^2\right)^{1/2}} \tag{A.8}$$

It is interesting to note that the average value of the radius vector magnitude from a focal point around the complete orbit is equal to the semi-minor axis.

### APPENDIX B.

### Derivation of Electron Magnetic Dipole Strengths.

### B.1 The Orbital Magnetic Moment.

A magnetic moment elemental due to the radial normal component of the orbital motion of the electron is

$$\Delta \left( {}_{e}\bar{\Psi}_{\phi} \right) = \frac{i}{2c} \left( \bar{r} \, x \, d\bar{l} \right) \tag{B.1}$$

Where

 $d\bar{l}$  is a vector element of orbit path.

 $\bar{r}$  is the radius vector of the orbit.

i is the effective current due to the motion of the electron through the central coulomb field.

Thus

$$_{e}\bar{\Psi}_{\phi} = \frac{1}{2c} \oint i\bar{r} \, x \, d\bar{l} \tag{B.2}$$

and thus

$$_{e}\bar{\Psi}_{\phi} = \frac{Z}{2c} \int_{0}^{e} \bar{r} \, x \, \bar{v} \, de \tag{B.3}$$

So that, evaluating the vector cross product and taking the magnitude,

$$_{e}\Psi_{\phi} = \frac{ZM_{\varphi}^{*}}{2c} \int_{0}^{e} \frac{de}{m_{e}^{*}}$$
(B.4)

$$=\frac{ZM_{\varphi}^{*}}{2cm_{e}}\int_{0}^{e}\left(1-\frac{v^{2}}{c^{2}}\right)^{1/2}de$$
(B.5)

The relativistic term may be ignored because the spin-orbit coupling energy is already of relativistic magnitude. Eq.(B.5) therefore reduces to

$$_{e}\Psi_{\phi} = \frac{ZeM_{\varphi}^{*}}{2cm_{e}} = \frac{Zehn_{\phi}^{*}}{4\pi cm_{e}}$$
(B.6)

Eq.(B.6) is expressed in terms of a non-spin-orbit coupled environment. To express it in terms of a spin-orbit coupled environment  $n_j$  is substituted for  $n_{\phi}^*$  to give

$$_{e}\Psi_{or} = \frac{Zehn_{j}}{4\pi cm_{e}} \tag{B.7}$$

This substitution is valid because  $n_{\phi}^*$  has the same quantum value in a non-spin-orbit environment as  $n_i$  in a coupled environment.

Of course when  $Z = n_j = 1$ , (B.7) becomes the smallest unit of orbital magnetic dipole moment, the Bohr magneton.

### B.2 The Spin Magnetic Moment.

In order to complete this derivation it is necessary to consider the physical construction of the electron. For it to possess the appropriate spin angular momentum, it is proposed that it exhibits the mechanical attributes of a very thin wall spherical shell, with the electrostatic charge uniformly distributed on the outside surface. The derivation of spin magnetic dipole then proceeds as follows.



### Fig. B.1 - Electron Charge Configuration.

Referring to Fig. B1, if the charge on the elemental is

$$\Delta e = -\frac{e}{4\pi} \sin\theta d\theta d\phi \tag{B.8}$$

The effective current due to the spin motion of this elemental charge is then

$$i = \frac{velocity \ x \ charge}{path} = -\frac{e\omega_{sp}e\sin\theta d\theta d\phi}{8\pi^2} \tag{B.9}$$

Where

 $_{e}\omega_{sp}$  is the electron spin rate.

The dipole due to this elemental is then

$$_{e}\Psi_{sp} = \frac{\Delta\Lambda\,i}{c} = -\frac{_{e}\omega_{sp}\Gamma_{e}^{2}e\sin^{3}\theta d\theta d\phi}{8\pi c} \tag{B.10}$$

Where

 $\Delta\Lambda$  is the area bounded by the path of the elemental.

c is the velocity of light.

Integrating over the complete surface of the electron shell

$$_{e}\Psi_{sp} = -\frac{e\omega_{sp}\Gamma_{e}^{2}e}{8\pi c} \int_{0}^{\pi} \int_{0}^{2\pi} \sin^{3}\theta d\theta d\phi$$
(B.11)

These integrals are simple and evaluate to

$${}_{e}\Psi_{sp} = \frac{e\omega_{sp}\Gamma_{e}^{2}e}{3c} \tag{B.12}$$

From [3], Appendix A the non-relativistic angular momentum of the spinning electron shell may be stated as

$${}_eM_{sp} = \frac{2}{3}m_e {}_e\omega_{sp}\Gamma_e^2 \tag{B.13}$$

and because magnetic dipole coupling is of relativistic magnitude, (B.13) may be, for the purpose of this derivation, approximated by

$$_{e}M_{sp} = \frac{2}{3}m_{e\ e}\omega_{sp}\Gamma_{e}^{2} = \frac{en_{sp}h}{2\pi}$$
 (B.14)

Inserting (B.14) into (B.12) yields finally

$$_{e}\Psi_{sp} = \frac{eh_{e}n_{sp}}{4\pi m_{e}c} \tag{B.15}$$

This value is half that recognised in the literature, but is further addressed in the main text, sub-Section 2.2, to eliminate the difference.

### APPENDIX C.

### Calculated Emission Spectra for the First 7 to 3 Orbital Shells of Hydrogen, (as so far developed).

This Appendix presents calculated emission/absorption spectra for the first 7 to 3 orbit shells of hydrogen. They include the effects of relativistic mass correction and magnetic dipole coupling. The spectra are calculated using the formula

$$\lambda_{(n)(m)} = \frac{hc}{\left(E_{or(m)} - E_{or(n)}\right)} \tag{C.1}$$

together with the Selection Rules.

In (C.1)  $E_{or(\#)}$  is given by (3.39) within which  $R_{hy}$  is determined from the generalised relationship

$$R_{hy} = \frac{cR_{\infty} \{Zm_p + (J - Z)m_N\}}{\{Zm_p + (J - Z)m_N + m_e\}}$$
(C.2)

In this and the other relationships referred to, the values of the parameters used are as shown in the following Table.

Parameter	Name	Value	Units	Ref.
h	Planck's Constant	6.6260693E-27	erg secs	[7]
с	Velocity of Light in Vacuum	2.99792458E+10	cm/sec	[7]
R <sub>hy</sub>	Rydberg's Constant for Hy- drogen	See (C.2)	$sec^{-1}$	
$R_{\infty}$	Rydberg's Constant for Infi- nite Nuclear Mass	1.09737316E + 5	$\mathrm{cm}^{-1}$	[7]
Z	Atomic Number	1 for Hydrogen		
J	Mass Number	1 for Hydrogen		
$m_p$	Proton Mass	1.67262171E-24	$g sec^2/cm$	[7]
$m_N$	Neutron Mass	1.6749278E-24	$g sec^2/cm$	[7]
$m_e$	Electron Mass	9.10913826E-28	$g sec^2/cm$	[7]
e	Electron/Proton Charge	-/+ 4.8032044E-10	esu	See Note 1
$\gamma_p$	Proton magnetic moment constant of proportionality	2.79275	-	[4]
$\delta_p$	Proton spin dipole magnetisation constant of proportionality	3.3558912	-	-

# Table C1 - Parameter Values.

Note 1:- Calculated from e = 1.60217653E-20 abcoulombs x c.

Also the following factors have been used to convert energy from ergs to  $\rm cm^{-1}$ .

 $\begin{array}{l} {\rm Joules} = 1{\rm E}\text{-}7~{\rm ergs} \\ {\rm eV} = 6.24150948{\rm E}\text{+}18~{\rm Joules} \\ {\rm cm}^{-1} = 8.065541{\rm E}\text{+}3~{\rm eV} \end{array}$ 

The calculated spectra are shown below in Table C.2 expressed as wavelengths in Angstroms.

1.5         2.5         2.5           p(-)         d(+)         d(-)
1.5 1.5 p(+) p(-)
d (+)s (
p(+) p(-)
s(+)
s(+)
•*u
u
cm_

Orbital Ener	$_{BOB}$ - $E_{OR}$	From	↑ ₽	u	1		7				ñ		
		~		${}^{\phi}{}^{u*}$	0.5	0.5	1.5	1.5	0.5	1.5	1.5	2.5	2.5
ergs	$^{\mathrm{cm}-1}$	u	<sup>ф</sup> *и		s(+)	s(+)	p(+)	p(-)	s(+)	p(+)	p(-)	q(+)	(-)p
-6.051951E-13	106632.403	9	0.5	s(+)	N.P.	N.P.	4,102.9231	4,102.8623	N.P.	10941.123	10940.995	N.P.	N.P.
-6.051924E-13	106632.416	9	1.5	p(+)	937.8007	4,102.8595	N.P.	N.P.	10940.977	N.P.	N.P.	10941.149	10941.107
-6.051951E-13	106632.403	9	1.5	p(-)	937.8008	4,102.8617	N.P.	N.P.	10940.993	N.P.	N.P.	N.P.	10941.123
-6.051916E-13	106632.421	9	2.5	(+)p	N.P.	N.P.	4,102.9201	N.P.	N.P.	10941.101	N.P.	N.P.	N.P.
-6.051924E-13	106632.416	9	2.5	d(-)	N.P.	N.P.	4,102.9208	4,102.8601	N.P.	10941.107	10940.979	N.P.	N.P.
-6.051911E-13	106632.423	9	3.5	f(+)	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	10941.141	N.P.
-6.051915E-13	106632.421	9	3.5	f(-)	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	10941.144	10941.102
-6.051909E-13	106632.424	9	4.5	g(+)	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.
-6.051911E-13	106632.423	9	4.5	g(-)	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.
-6.051907E-13	106632.425	9	5.5	(+)ч	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.
-6.051908E-13	106632.424	9	5.5	h(-)	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.
-4.446327E-13	107440.693	7	0.5	s(+)	N.P.	N.P.	3,971.2234	3,971.1665	N.P.	10052.151	10052.043	N.P.	N.P.
-4.446310E-13	107440.701	7	1.5	p(+)	930.7456	3,971.1646	N.P.	N.P.	10052.033	N.P.	N.P.	10052.178	10052.143
-4.446327E-13	107440.693	7	1.5	p(-)	930.7456	3,971.1659	N.P.	N.P.	10052.042	N.P.	N.P.	N.P.	10052.151
-4.446305E-13	107440.704	7	2.5	d(+)	N.P.	N.P.	3,971.2216	N.P.	N.P.	10052.139	N.P.	N.P.	N.P.
-4.446310E-13	107440.701	7	2.5	q(-)	N.P.	N.P.	3,971.2220	3,971.1651	N.P.	10052.142	10052.034	N.P.	N.P.
-4.446302E-13	107440.705	7	3.5	f(+)	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	10052.174	N.P.
-4.446305E-13	107440.704	7	3.5	f(-)	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	10052.175	10052.140
-4.446300E-13	107440.706	7	4.5	g(+)	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.
-4.446302E-13	107440.705	7	4.5	g(-)	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.
-4.446299E-13	107440.707	7	5.5	(+)y	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.
-4.446300E-13	107440.706	7	5.5	h(-)	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.
-4.446299E-13	107440.707	7	6.5	i(+)	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.
-4.446299E-13	107440.707	7	6.5	i(-)	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.
N.P. = Not	Permitted by	the Sele	$ction R_{l}$	ıles.									

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