RESURRECTION OF THE BOHR/SOMMERFELD

THEORY OF ATOMIC STRUCTURE

[1]

BASIC ORBITS INCLUDING

RELATIVISTIC MASS INCREASE EFFECTS

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ABSTRACT.

This paper initiates the resurrection of the old Bohr/Sommerfeld quantum theory of atomic structure. The development stems from an investigation of the nature and characteristics of de Broglie matter waves, [1], in Pseudo-Euclidean Space-Time, as represented by the Relativistic Space-Time Domain D_0, [2].

Presented here is (i) a complete justification of the quantisation criteria related to the principle quantum number, leading to proof of validity of permitted orbits and non-validity of excluded orbits, (ii) derivation of the Bohr orbital momentum rules, (iii) derivation of generalised relativistic orbital energy levels, (at this stage excluding all spin effects), and (iv) quantisation of four sample permitted orbits.

This is the first in a series papers on this subject.

1   INTRODUCTION.

During the early part of the 20th century, investigations into the structure of the atom were primarily led by Niels Bohr and his collaborators. Niels Bohr was a Danish physicist working in Manchester. In the original Bohr theory for hydrogen like atoms with a single electron, (H, He$^+$, L^{++} etc), the atom was perceived with the electron as a real physical particle orbiting a central nucleus in a circular orbit. The energy levels of the orbits were specified by Niels Bohr based upon an empirical formula devised by Thomas Balmer, [3], [7], to portray the visible spectral lines of hydrogen. While such an arbitrary hypothesis is unsatisfactory as the basis for a theory of atomic structure, it was nevertheless developed to a point of considerable sophistication, e.g. to explain the fine structure of the hydrogen spectra, elliptic orbits together with relativistic mass correction effects were subsequently incorporated by the German physicist Arnold Sommerfeld. The energy levels of Niels Bohr were eventually shown to be theoretically derivable if the angular momentum of the electron in its orbit was quantised. However, there was in turn no theoretical basis for this stipulation and the entire theory, (the "old" quantum theory), was dropped. It was replaced by the newly emerging wave mechanics in which, subsequent to Planck's and de Broglie's hypotheses and Erwin Schrodinger's construction of his describing equation, the electron was represented as a wave function wherein, in a stable atomic "orbit", its orbital path length was stipulated to be an integral number of its wavelength. Despite the subsequent success that this approach has had

in describing atomic structure, it is considered that it suffers from similar deficiencies to those of the old quantum theory. For instance, it is acknowledged that Schrodinger's equation cannot be derived from first principles, or "proved", and is regarded as a fundamental hypothesis of the quantum mechanics theory of the atom, [4], [5]. It is believed that this is the only case in science where a second order differential equation is accepted as a basic hypothesis. Also there does not appear to be any theoretical justification for the criterion of quantisation, viz. the single valuedness of the electron matter wave wavelength in its "orbit" of the nucleus.

To avoid such difficulties, this paper presents a resurrection of the Bohr/Sommerfeld old quantum theory of atomic structure into which, based upon the results contained in [1], the primary quantisation criterion of the quantum mechanics theory, subsequent to its theoretical justification in this paper, can be re-interpreted and inserted. Justification for this is that in [1] it has been shown that in the Relativistic Space-Time D_0, the characteristics of de Broglie matter waves provide a sound theoretical basis by which the spatial part of the wavelength of such waves can be expressed as a function of the relativistic physical velocity of the matter particle they represent. viz. [1], Eq.(2.18). The resurrection of this theory will thereby provide an alternative to the unfortunate direction that quantum mechanics has taken in portraying the electron in probabilistic terms rather than physical. The former being completely foreign to the existence of real energy in a real space-time domain. Consequently, if in the resurrected Bohr/Sommerfeld theory, the electron is to be depicted as a real physical particle with finite extensions, albeit with a dual wave function existence, it will be necessary, wherever possible as the development proceeds, to provide a physical interpretation of the results.

Before the ideas in [1], as discussed above are linked into the resurrected theory, it is necessary to address some preliminary points. First, it will be useful to define the nomenclature for quantum numbers to be used in this paper for comparison with those in current practice. Next, in the derivation of the principle quantum number, the requirement that the orbit path length be an integral number of the electron's matter wave wavelength is itself an arbitrary stipulation without theoretical formalism. This must be provided. Next, this theoretical formalism should also provide a logical reasoning for which types of orbit are allowed and their basic characteristics. Also, a suitable expression for the bound energy of the electron is needed into which suitably quantised parameters can be inserted to produce a stable orbit energy level. This expression must allow for electron relativistic mass increase effects. All of the above points are addressed in the next Section.

It should be noted that this paper, particularly Section 2 should be read in conjunction with reference [1].

2   Resurrection of the Bohr/Sommerfeld Theory of Atomic Structure.

2.1   Quantum Number Nomenclature.

The current nomenclature for quantum numbers in atomic structure theory is not used in this paper. A new one, (similar to that of Sommerfeld), is used for two reasons. Firstly, it introduces a degree of rationalisation and secondly, the list differs slightly from those currently used. The table below provides a comparative list.

Name	Current Nomenclature	Value	New Nomenclature	Value
Principle	n	1 to ∞	n	1 to ∞
Azimuthal	k	1 to n	n_ϕ	1 to n
Orbital	l	0 to $(n-1)$	Not Used	-
Radial	$n^{/}$	$n - k$	n_r	$n - n_\phi$
Spin	s	$\sigma_1 = +1/2 \; \sigma_2 = -1/2$	n_{sp}	$\pm 1/2$
Inner	j	$1/2$ for $l = 0$ $l + s$ for $l \neq 0$	n_j	$n_\phi + n_{sp}$

Table 2.1 - Quantum Number Nomenclature.

Where relativistic effects are to be included, the azimuthal quantum number in the new nomenclature will be represented by n_ϕ^*. The reason for this will be discussed during the derivation.

In addition to the above, the current nomenclature lists a number of "term" letters for values of the orbital quantum number, l. The first five of these are:-

Quantum Number l	0	1	2	3	4
Term	s	p	d	f	g

This term scheme is adopted, but in relation to the azimuthal quantum number n_ϕ (and n_ϕ^*), in the new nomenclature. In this paper only the first three quantum numbers, n, n_ϕ, (and n_ϕ^*), and n_r will be involved. The other numbers resulting from the effects due to spin will appear in subsequent papers.

2.2   Justification of the Quantization Criteria & Determination of Permitted Orbits.

To begin this analysis, consider again the energy component of [1], Eq.(2.1). If this is to represent the orbital energy of a bound electron in an atom, for that electron orbit to be stable, it is necessary for the bound energy to be constant over an entire single orbit, e.g. there can be no net energy loss or gain. Thus for such a case, if the energy in [1], Eq.(2.1) is to be constant, then in [1], Eq.(2.15), f_v must also be constant over an entire orbit. In turn, this means that in a simple re-arrangement of [1], Eqs.(2.24) and (2.26),

$$v\lambda_{sv} = \frac{c^2}{f_v} \tag{2.1}$$

the product $v\lambda_{sv}$ must be similarly constant.
and where

      v is the electron's orbital velocity.

      λ_{sv} is the electron's orbital spatial matter wave wavelength.

c is the velocity of light.

f_v is the electrons spatial - temporal matter wave frequency.

It is noted that (2.1) appears to invoke the fictitious spatial "phase velocity" of the electron matter wave, viz [1], Eq.(2.19). However, although the quantity c^2/v appears in (2.1) it is only via a re-arrangement of the relationships between real parameters and is therefore acceptable as a mathematical descriptor.

In a stable elliptic orbit, the orbital velocity v cannot be constant because the distance of the orbiting electron from the central nucleus is continuously changing. Consequently for (2.1) to be constant for such an orbit, λ_{sv} while being single valued over an entire orbit , must however vary proportionately in precise inverse harmony to the variation in v within the orbit. This then ensures that the elliptical orbit is stable. In circular orbits, the distance of the electron from the central nucleus is constant and so the orbital velocity is constant. Thus in this case λ_{sv} is not only single valued over a complete orbit, but also exactly constant throughout it. The so called "pendulum orbits" are discussed at the end of this Section.

Now, to justify the criterion of quantisation, the single valuedness of λ_{sv} over a complete orbit, inserting the component parts of v for a basic elliptic orbit in (2.1) gives after minor re-arrangement

$$\lambda_{sv} = \frac{c^2}{f_v}\left(\dot{r} + \omega_\phi^2 r^2\right)^{-1/2} \tag{2.2}$$

where

r is the radial distance of the electron from the nucleus.

$\dot{r}$ is the radial velocity of the electron in its orbit.

ω_ϕ is the angular rate of the electron in its orbit.

Now, in any elliptic orbit it is well known that

$$r = \frac{L}{(1 + \varepsilon \cos \phi)}$$

$$so \quad that \tag{2.3}$$

$$\dot{r} = \frac{\omega_\phi L \varepsilon \sin \phi}{(1 + \varepsilon \cos \phi)^2}$$

Where

ϕ is the angular position of the radius vector from some axis origin.

L is the semi latus rectum of the elliptic orbit.

ε is the eccentricity of the orbit.

Substitution of (2.3) into (2.2) gives after minor reduction

$$\lambda_{sv} = \frac{c^2}{f_v}\frac{m_0 L}{M_\phi}\left(1 + \varepsilon^2 + 2\varepsilon \cos \phi\right)^{-1/2} \tag{2.4}$$

Where

M_ϕ is the angular momentum of the rest mass of the electron and is constant by the law of conservation.

m_0 is the rest mass of the electron.

On the RHS of (2.4) the only variable is the angular position so that it is clear that over a complete orbit

$$\lambda_{sv}|_{\phi=2\pi} = \lambda_{sv}|_{\phi=0} \tag{2.5}$$

Eq.(2.5) states that over the orbital path length of a stable orbit the orbiting electron's matter wave wavelength is an integer number. Therefore the criterion of quantisation is now linked to the requirement that, within a stable orbit, the bound energy of the orbiting electron must be constant. Accordingly, the criterion of quantisation is thus proved to be a necessary and sufficient condition for the stability of a basic electron orbit. The variability of λ_{sv} within the orbit is also clearly visible in (2.4).

If $\varepsilon = 0$ then (2.4) becomes

$$\lambda_{sv} = \frac{rm_0c^2}{f_v M_\phi} \tag{2.6}$$

and is constant throughout the complete orbit. This is the electron matter wave wavelength for circular orbits, $(r \equiv L)$.

In the case of the pendulum orbits, in (2.4) $L = 0$ and therefore $\lambda_{sv} = 0$. Accordingly from [1], Eq.(2.24) f_{sv} becomes infinite, which from [1], Eq.(2.26) requires that the orbital velocity v also becomes infinite. This contravenes the criterion of existence within the Relativistic Space-Time Domain D_0, and is a sufficient proof for the exclusion of the pendulum orbits. Note that for f_{sv} to be infinite would also necessitate infinite orbital energy.

In (2.4) if $\varepsilon = 1$, it becomes

$$\lambda_{sv} = \frac{m_0c^2L}{\sqrt{2}f_v M_\phi} (\sec\phi)^{1/2} \tag{2.7}$$

The orbit is parabolic and ϕ varies from $-(\pi - \delta)$ to $+(\pi - \delta)$. Quantisation does not apply because the orbit is not closed. The same comment applies to hyperbolic orbits, $(\varepsilon > 1)$.

2.3   Quantisation of the Bohr/Sommerfeld Atom.

In view of the results of the preceding Section, it is now permissible to apply the quantisation process to relativistically modified electron orbits to resurrect the Bohr/Sommerfeld theory of atomic structure.

Rewriting [1], Eq.(2.18) as

$$\frac{h}{\lambda_{sv}} = mv \tag{2.8}$$

where h is Planck's constant.

Because the wavelength is to be quantised for all orbit path lengths, both sides of (2.8) are integrated over the orbital path length to give

$$\frac{hl}{\lambda_{sv}} = \oint mvdl \tag{2.9}$$

where l is the length of the orbit path, and m the energy mass of the electron.

On the LHS if l is to be an integral number of wavelengths then (2.9) can be written

$$nh = \oint mvdl \tag{2.10}$$

Where n is an integer, the principle quantum number of the orbit. In (2.9) and (2.10) the circled integral sign indicates integration over the complete path of the orbit. It is (2.10) which will later be used as the source equation for the sample quantisation of a number of permitted orbits.

To show that the above derivation leads to the same quantisation results as in the original Bohr theory, it is sufficient to demonstrate that (2.10) leads to the original quantisation rules as propounded by Niels Bohr.

With

$$dl = vdt \tag{2.11}$$

insertion of this into (2.10) and expansion of the RHS gives

$$nh = \oint m \left(\dot{r}^2 + \omega_\phi^2 r^2 \right) dt \tag{2.12}$$

Splitting the RHS of (2.12) into two terms then gives

$$nh = \oint m\dot{r}dr + \oint m\omega_\phi r^2 d\phi \tag{2.13}$$

which can clearly be written

$$nh = \oint M_r^* dr + \oint M_\phi^* d\phi \tag{2.14}$$

where

M_r^* is the radial momentum of the relativistically mass corrected electron.

M_ϕ^* is the angular momentum of the relativistically mass corrected electron.

Eq.(2.14) is identical to the original quantisation rules of Niels Bohr with the minor exception that the momentum terms are corrected for the relativistic mass increase of the electron. Eq.(2.14) is perhaps the most elegant way of representing the quantisation process but simpler analysis results from the use of (2.10) as in Section 3 below.

2.4   Orbital Energy Levels.

In order to derive quantised orbital energy levels, an energy expression suitable for use in the process is required. To derive the form required here, use is made of the solution to the orbital equation of motion, which has been effected in [2]. The result however, requires considerable preliminary analysis before insertion into the orbital energy derivation process. For clarity, this preliminary analysis is relegated to Appendix A, Section A.1, the results of which are used in the following process.

Starting with Einstein's energy/momentum equation as stated at [1], Eq.(2.29), the bound energy of the electron is

$$E_{or} = m_0 c^2 \left(1 + \frac{M^2}{m_0^2 c^2} \right)^{1/2} - m_0 c^2 - \frac{Ze^2}{r} \tag{2.15}$$

where

E_{or} is the orbital or bound energy of the electron.

M is the spatial momentum of the electron in its orbit.

Z is the atomic number of the atom.

e is electronic charge.

It should be noted that although the atomic number has been included in this analysis, only hydrogen, ($Z = 1$), will be considered in detail when calculating spectra.

Via binomial expansion, retaining only second order relativistic terms, (2.15) reduces to

$$E_{or} = \frac{m_0 v^2}{2} + \frac{3}{8} \frac{m_0 v^4}{c^2} - \frac{Ze^2}{L} \left(1 + \varepsilon \cos \varphi \right) \tag{2.16}$$

where

L is the relativistically corrected orbit semi-latus rectum.

ε is the relativistically corrected orbit eccentricity.

and where (A.3) has been inserted for r. An expression for v is now required.
From (A.3)

$$\dot{r} = \frac{dr}{dt} = \frac{dr\,d\varphi}{d\varphi\,dt} = \frac{\omega_\varphi L\varepsilon\sin\varphi}{(1+\varepsilon\cos\varphi)^2} \tag{2.17}$$

The angular velocity of the electron is $\omega_\phi r$ which from (A.3) and (A.14) is

$$\omega_\phi r = \frac{\omega_\varphi L}{(1+\varepsilon\cos\varphi)}\left(1+\frac{Z^2 e^4}{c^2 M_\varphi^{*2}}\right)^{1/2} \tag{2.18}$$

So that from (2.17) and (2.18)

$$v^2 = \dot{r}^2 + \omega_\phi^2 r^2 = \frac{\omega_\varphi^2 L^2\varepsilon^2\sin^2\varphi}{(1+\varepsilon\cos\varphi)^4} + \frac{\omega_\varphi^2 L^2}{(1+\varepsilon\cos\varphi)^2}\left(1+\frac{Z^2 e^4}{c^2 M_\varphi^{*2}}\right) \tag{2.19}$$

which with (A.14) reduces to

$$v^2 = \frac{M_\varphi^{*2}}{m_0^2 L^2}\left\{1+2\varepsilon\cos\varphi+\varepsilon^2+\frac{Z^2 e^4}{c^2 M_\varphi^{*2}}(1+\varepsilon\cos\varphi)^2\right\}\left(1-\frac{v^2}{c^2}\right) \tag{2.20}$$

Solving (2.20) for v^2 gives

$$v^2 = \frac{\dfrac{M_\varphi^{*2}}{m_0^2 L^2}\left\{1+2\varepsilon\cos\varphi+\varepsilon^2+\dfrac{Z^2 e^4}{c^2 M_\varphi^{*2}}(1+\varepsilon\cos\varphi)^2\right\}}{\left[1+\dfrac{M_\varphi^{*2}}{m_0^2 c^2 L^2}\left\{1+2\varepsilon\cos\varphi+\varepsilon^2+\dfrac{Z^2 e^4}{c^2 M_\varphi^{*2}}(1+\varepsilon\cos\varphi)^2\right\}\right]} \tag{2.21}$$

Substitution of this into (2.16) gives for the orbital energy, after some reduction including binomial expansion to relativistic second order

$$E_{or} = \frac{M_\varphi^{*2}}{2m_0^2 L^2}\left\{1+2\varepsilon\cos\varphi+\varepsilon^2+\frac{Z^2 e^4}{c^2 M_\varphi^{*2}}(1+\varepsilon\cos\varphi)^2\right\}$$
$$-\frac{M_\varphi^{*4}}{8m_0^3 c^2 L^4}\left\{1+2\varepsilon\cos\varphi+\varepsilon^2\right\}^2-\frac{Ze^2}{L}(1+\varepsilon\cos\varphi) \tag{2.22}$$

Now, substituting for L from (A.14) gives, again after some reduction

$$E_{or} = \frac{Z^2 e^4}{2M_\varphi^{*2}}\left\{1+2\varepsilon\cos\varphi+\varepsilon^2\right\}-\frac{Z^2 e^4}{M_\varphi^{*2}}(1+\varepsilon\cos\varphi)$$
$$+\frac{Z^4 e^8}{c^2 M_\varphi^{*4}}\left\{\tfrac{1}{2}(1+\varepsilon\cos\varphi)^2-\tfrac{1}{2}(\varepsilon\cos\varphi+\varepsilon^2)(1-\varepsilon^2)-\tfrac{1}{8}(1+2\varepsilon\cos\varphi+\varepsilon^2)^2\right\} \tag{2.23}$$

which finally reduces to

$$E_{or} = -\frac{Z^2 e^4 m_0(1-\varepsilon^2)}{2M_\varphi^{*2}}\left(1-\frac{3}{4}\frac{Z^2 e^4}{c^2 M_\varphi^{*2}}(1-\varepsilon^2)\right) \tag{2.24}$$

This expression for the orbital energy can now be quantised for all permitted orbits by inserting the appropriate expression for $M_\varphi^{*2}/(1-\varepsilon^2)$. Non-relativistically corrected orbits can be treated by letting $c\to\infty$, and circular orbits by putting $\varepsilon=0$. Eq.(2.24) leads directly to the expanded version of Sommerfeld's equation for relativistically mass corrected elliptic orbits as will be shown in Section 3.5.

3   Quantisation of Permitted Orbits.

3.1   Preamble.

The orbital energy quantisations to be derived here will cover the following four cases.

(i) A simple circular orbit.

(ii) A simple elliptic orbit.

(iii) A relativistically mass corrected circular orbit

(iv) A relativistically mass corrected elliptic orbit.

All of these have been derived before and are therefore well documented in the literature, [3], [4] et al. However, they have been included here for a number of reasons as follows. First, they provide confirmation that the quantisation process presented in this paper, i.e. (2.10), is valid. Secondly, some of the derivation so produced is needed later in this and subsequent papers. Finally, it provides the means by which the values for the quantum numbers used here can be discussed, which realises several factors concerning orbit characteristics which may be new.

It should be noted that in the following derivations the mass referred to as electron mass is the effective mass of the electron as given in [3], i.e.

$$m_{\#} = \frac{m_e m_N}{m_e + m_N} \tag{3.1}$$

where

m_e is the mass of the electron.

m_N is the mass of the nucleus.

$m_{\#}$ is defined as rest mass, ($\# = 0$), or energy mass, ($\#$ absent)

This substitution accounts for the finite mass of the nucleus as it and the electron orbit around a common orbital focal point.

3.2   A Simple Circular Orbit.

In this case (2.10) becomes simply, (by letting $c \to \infty$)

$$nh = m_0 \oint \omega_\phi r dl \tag{3.2}$$

and with

$$dl = rd\phi \tag{3.3}$$

(3.2) becomes

$$nh = m_0 \int_0^{2\pi} \omega_\phi r^2 d\phi$$
$$= 2\pi M_\phi \tag{3.4}$$

so that

$$M_\phi = \frac{nh}{2\pi} \tag{3.5}$$

Thus from (2.24) the orbital energy, ($\varepsilon = 0$, and omitting the relativistic term)

$$E_{or} = -\frac{2\pi^2 Z^2 e^4 m_0}{n^2 h^2} \tag{3.6}$$

which finally becomes

$$E_{or} = -\frac{hR_{hy}Z^2}{n^2} \tag{3.7}$$

where

$$R_{hy} = \frac{2\pi^2 e^4 m_0}{h^3} \tag{3.8}$$

is Rydberg's constant (for hydrogen). Eq. (3.6) is well known as the Balmer energy term. Note that in this case

$$M_\phi = \frac{nh}{2\pi} = \frac{n_\phi h}{2\pi} \tag{3.9}$$

so that, in this case only

$$n_\phi = n \tag{3.10}$$

3.3   A Simple Elliptic Orbit.

In this case (2.10) reduces to

$$nh = m_0 \oint \left(\dot{r}^2 + \omega_\phi^2 r^2 \right)^{1/2} dl \tag{3.11}$$

and with

$$dl = \left(\dot{r}^2 + \omega_\phi^2 r^2 \right)^{1/2} dt \tag{3.12}$$

Eq.(3.11) becomes

$$nh = m_0 \oint \left(\dot{r}^2 + \omega_\phi^2 r^2 \right) dt \tag{3.13}$$

This reduces to

$$nh = M_\phi \int_0^{2\pi} \left\{ \frac{1}{r^2} \left(\frac{dr}{d\phi} \right)^2 + 1 \right\} d\phi \tag{3.14}$$

Introducing (2.3) yields

$$nh = M_\phi \int_0^{2\pi} \left\{ \frac{\varepsilon^2 \sin^2 \phi}{(1 + \varepsilon \cos \phi)^2} + 1 \right\} d\phi \tag{3.15}$$

Integrating the first term in (3.15) by parts gives

$$nh = M_\phi \int_0^{2\pi} \left\{ 1 - \frac{\varepsilon \cos \phi}{(1 + \varepsilon \cos \phi)} \right\} d\phi \tag{3.16}$$

Now multiplying (3.16) by 2 and (3.15) by -1 and adding gives

$$nh = -M_\phi \left[\int_0^{2\pi} \left\{ \frac{\varepsilon^2 \sin^2 \phi}{(1 + \varepsilon \cos \phi)^2} + 1 \right\} d\phi - 2 \int_0^{2\pi} \left\{ 1 - \frac{\varepsilon \cos \phi}{(1 + \varepsilon \cos \phi)} \right\} d\phi \right] \tag{3.17}$$

which reduces to

$$nh = M_\phi \int_0^{2\pi} \frac{1 - \varepsilon^2}{(1 + \varepsilon \cos \phi)^2} d\phi \tag{3.18}$$

From the first part of (2.3) this can be written

$$nh = M_\phi \frac{(1 - \varepsilon^2)}{L^2} \int_0^{2\pi} r^2 d\phi \tag{3.19}$$

This integral is well known as twice the area of an elliptic orbit so that it reduces to

$$nh = 2\pi M_\phi \frac{(1 - \varepsilon^2)}{L^2} pq \tag{3.20}$$

where p and q are the semi-major and semi-minor axes of the elliptic orbit. By virtue of the standard equations for an ellipse, (3.20) finally becomes

$$\frac{nh}{2\pi} = \frac{M_\phi}{\left(1 - \varepsilon^2\right)^{1/2}} \tag{3.21}$$

So that from (2.24) the orbital energy is, (omitting the relativistic term)

$$E_{or} = -\frac{hR_{hy}Z^2}{n^2} \tag{3.22}$$

identical to the circular case.

Note that the process here, from (3.14) onwards is essentially the same as presented in [3].

It should be noted that in the above derivation both the azimuthal, n_ϕ and the radial, n_r quantum numbers have been suppressed because the orbital energy is completely specified by the primary quantum number n. However, both n_ϕ and n_r are of extreme importance because they dictate the shape of the orbit.

The azimuthal quantum number n_ϕ is from (3.9) given by

$$n_\phi = \frac{2\pi M_\phi}{h} \tag{3.23}$$

So that from (3.21) and (3.23)

$$\left(1 - \varepsilon^2\right)^{1/2} = \frac{n_\phi}{n} \tag{3.24}$$

and with, by definition

$$n = n_\phi + n_r \tag{3.25}$$

the radial quantum number is determined.

The primary question is whether n_ϕ is an integer for this orbit. In the quantisation of the circular orbit just covered, n_ϕ and n are identical so n_ϕ is at all times an integer. In the case analysed here the only change to the orbit is that a radial component has been added. Consequently there is no change to the azimuthal component and with M_ϕ still being constant by the law of conservation, it is therefore determined that n_ϕ must still be integer. Note that this was effectively invoked in the use of (3.9) to obtain (3.23). Note also from (3.25) that with n and n_ϕ being integer, so must n_r be. As a result it is possible to determine exactly the characteristics of permitted simple orbits. The term schemes for the first four orbital shells are thus shown in the following table.

n	n_ϕ	n_r	ε	Current Term
1	1	0	0	s
2	1	1	0.87	s
	2	0	0	p
3	1	2	0.94	s
	2	1	0.75	p
	3	0	0	d
4	1	3	0.97	s
	2	2	0.87	p
	3	1	0.66	d
	4	0	0	f

Table 3.1 - Basic Orbit Characteristics for the First Four Shells.

From this table a number of orbit features are apparent. First, in the first shell, ($n =1$), only one orbit is permitted and this is clearly circular. This must be so in the atoms of all the elements. In the second shell, two orbits are allowed, one elliptical and one circular and this sequence of permitted orbits continues up through the orbit shells with an extra elliptical orbit being added per shell. The orbits correspond to the term letters shown in Section 2.1. Note that in each higher shell the eccentricity of the first orbit is higher than in the previous shell. Thus as $n \to \infty$, $\varepsilon \to$ 1 the orbit becomes parabolic and the atom is ionised. However, in a future paper, as additional relativistic correction terms are introduced it will be shown that ionisation takes place long before $n \to \infty$. Also, it can clearly be seen from the Table that if $n_\phi = 0$ then $n_r = n$, ($\varepsilon = 1$), and the so called pendulum orbits would result. However, these orbits were proved to be excluded in Section 2. Finally, it can also be seen from the Table that although all the orbitals have, via (3.7) and (3.22), exactly the same orbital energy, the shell/orbital configuration is exactly that which will result in the spectral fine structure when relativistic mass correction is introduced. This is shown in the next two Sections.

3.4 A Relativistically Mass Corrected Circular Orbit.

In this case (2.10) becomes

$$nh = \oint m\omega_\phi r dl \tag{3.26}$$

From (A.14) this becomes

$$nh = \left(1 + \frac{Z^2 e^4}{c^2 M_\varphi^{*2}}\right) \oint m\omega_\varphi r dl \tag{3.27}$$

Here

$$dl = r d\varphi \tag{3.28}$$

so that (3.27) becomes

$$nh = \left(1 + \frac{Z^2 e^4}{c^2 M_\varphi^{*2}}\right)^{1/2} \oint m\omega_\varphi r^2 d\varphi \tag{3.29}$$

which becomes

$$nh = \left(1 + \frac{Z^2 e^4}{c^2 M_\varphi^{*2}}\right)^{1/2} M_\varphi^* \int_0^{2\pi} d\varphi \tag{3.30}$$

which integrates to

$$nh = 2\pi M_\varphi^* \left(1 + \frac{Z^2 e^4}{2c^2 M_\varphi^{*2}}\right) \tag{3.31}$$

Re-arranging

$$M_\varphi^{*2} - \frac{nh}{2\pi} M_\varphi^* + \frac{Z^2 e^4}{2c^2} = 0 \tag{3.32}$$

Solving (3.32) for M_φ^* gives,

$$M_\varphi^* = \frac{nh}{2\pi} - \frac{\kappa^2 Z^2 h}{4\pi n} \qquad or \qquad \frac{\kappa^2 Z^2 h}{4\pi n} \tag{3.33}$$

where κ is Sommerfeld's Fine Structure Constant given by

$$\kappa = \frac{2\pi e^2}{hc} \tag{3.34}$$

Eq.(3.33) shows that theoretically, the electron can have two such circular orbits which satisfy the quantisation criteria. However, the second can be discounted for the purpose of determining atomic structure because it puts the electron "inside" the nucleus.

Insertion of the first root for M_φ^* in (3.31) into (2.24) then gives the orbital energy thus

$$E_{or} = -\frac{Z^2 e^4 m_0}{2\left(\frac{nh}{2\pi} - \frac{\kappa^2 Z^2 h}{4\pi n}\right)^2} \left\{ 1 - \frac{3}{4} \frac{Z^2 e^4}{c^2 \left(\frac{nh}{2\pi} - \frac{\kappa^2 Z^2 h}{4\pi n}\right)^2} \right\} \tag{3.35}$$

which with the insertion of (3.8) and (3.34), and because $\kappa^2 << 1$, (3.35) can be reduced to

$$E_{or} = -\frac{h R_{hy} Z^2}{n^2} \left(1 + \frac{\kappa^2 Z^2}{4n^2} \right) \tag{3.36}$$

Eq.(3.36) is the orbital energy for a relativistically corrected electron mass in a circular orbit and as expected is dependent only upon the principle quantum number. Nevertheless it is still of interest to discuss the quantisation value of the azimuthal quantum number n_ϕ. This number is still given by (3.9) but in the relativistically corrected case it is clear that it cannot be an integer. This is because M_ϕ is the angular momentum of the rest mass which in this case does not represent the total angular momentum of the orbiting electron. The relativistically added mass results in an increase in the angular momentum, and it is this plus the angular momentum of the rest mass which is quantised by an integer value, i.e. n_ϕ^*.

3.5   A Relativistically Mass Corrected Elliptic Orbit.

In this case (2.10) reduces to

$$nh = \oint m \left(\dot{r}^2 + \omega_\phi^2 r^2 \right)^{1/2} dl \tag{3.37}$$

which becomes with insertion of (3.12) for dl

$$nh = \oint m \left(\dot{r}^2 + \omega_\phi^2 r^2 \right) dt \tag{3.38}$$

In this integral the radial and angular terms must be treated separately. This is because the radial term must be integrated around the orbit as a function of the angle φ, whereas the angular term which includes the relativistic rotation of the orbit, must accordingly be integrated around the orbit as a function of the angle ϕ. Effecting this and, with insertion of (2.17) and (A.14), (3.38) becomes

$$nh = M_\varphi^* \left[\int_0^{2\pi} \left\{ \frac{1}{r^2} \left(\frac{dr}{d\varphi} \right)^2 \right\} d\varphi + \int_0^{2\pi} \left(1 + \frac{Z^2 e^4}{c^2 M_\varphi^{*2}} \right)^{1/2} d\phi \right] \tag{3.39}$$

Eq.(3.39) can most easily be solved by rewriting thus

$$nh = M_\varphi^* \left[\int_0^{2\pi} \left\{ \frac{1}{r^2} \left(\frac{dr}{d\varphi} \right)^2 + 1 \right\} d\varphi - \int_0^{2\pi} d\varphi + \int_0^{2\pi} \left(1 + \frac{Z^2 e^4}{c^2 M_\varphi^{*2}} \right)^{1/2} d\phi \right]$$

which, having inserted the standard equations for the semi major and minor axes of an ellipse, integrates to

$$\frac{nh}{2\pi} = \frac{M_\varphi^*}{(1 - \varepsilon^2)^{1/2}} + \frac{Z^2 e^4}{2c^2 M_\varphi^{*2}} \tag{3.40}$$

Re-arranging (3.40)

$$\frac{M_\varphi^{*2}}{(1 - \varepsilon^2)} - \frac{nh}{2\pi} \frac{M_\varphi^*}{(1 - \varepsilon^2)^{1/2}} + \frac{Z^2 e^4}{2c^2 (1 - \varepsilon^2)^{1/2}} = 0 \tag{3.41}$$

Solving (3.41) for $M_\varphi^* \big/ \left(1 - \varepsilon^2\right)^{1/2}$ then gives, taking the positive root

$$\frac{M_\varphi^*}{\left(1 - \varepsilon^2\right)^{1/2}} = \frac{nh}{2\pi} - \frac{\kappa^2 Z^2 h}{4\pi n \left(1 - \varepsilon^2\right)^{1/2}} \tag{3.42}$$

Where (3.34) has also been inserted. Now (3.24) also applies to this case except that the eccentricity is the relativistically modified value and so (3.24 becomes

$$\left(1 - \varepsilon^2\right)^{1/2} = \frac{n_\phi^*}{n} \tag{3.43}$$

Inserting this into the RHS of (3.42) finally gives

$$\frac{M_\varphi^*}{\left(1 - \varepsilon^2\right)^{1/2}} = \frac{nh}{2\pi} \left(1 - \frac{\kappa^2 Z^2}{2nn_\phi^*}\right) \tag{3.44}$$

insertion of (3.40) into (2.24) gives the orbital energy thus

$$E_{or} = -\frac{2\pi^2 Z^2 e^4 m_0}{n^2 h^2 \left(1 - \frac{\kappa^2 Z^2}{2nn_\varphi}\right)^2} \left\{ 1 - \frac{3}{4} \frac{4\pi^2 Z^2 e^4}{n^2 c^2 h^2 \left(1 - \frac{\kappa^2 Z^2}{2nn_\phi^*}\right)^2} \right\} \tag{3.45}$$

With the further introduction of (3.34) together with (3.8), and because $\kappa^2 \ll 1$ this finally reduces to

$$E_{or} = -\frac{h R_{hy} Z^2}{n^2} \left\{ 1 + \frac{\kappa^2 Z^2}{n^2} \left(\frac{n}{n_\phi^*} - \frac{3}{4}\right) \right\} \tag{3.46}$$

This is the expanded version of Sommerfeld's equation for the quantised energy levels of relativistically mass corrected elliptic orbits. For interest, the full version is derived in Appendix A.2.

In (3.46) it can be seen that the orbital energy is dependent upon the azimuthal quantum number as well as the principle.

Clearly the effect of the rotating orbit is to increase the orbital angular momentum by a very small amount according to the relativistic increase in mass of the orbiting electron. This rotating orbit is only treated as a unique additional factor in ensuring that the electron orbital path is an integral number of matter wave wavelengths, e.g. in (2.10). This ensures that the principle quantum number n and the relativistic azimuthal quantum number n_ϕ^* are both integers. The non-relativistic azimuthal quantum number, n_ϕ, being a descriptor of the rest mass angular momentum only, is therefore no longer an integer. The difference of n_ϕ from an integer value is however, relativistically small.

Thus from (3.46) it can be seen that each of the orbitals in Table 3.1, (with n_ϕ and n_r replaced by relativistic counterparts respectively), now possess a slightly different energy level by virtue of the presence of n_ϕ^* in (3.46). This results in the spectral fine structure as electrons make transitions from these orbitals to lower energy shells.

3.6   Selection Rules.

It is of course well known that in the spectral output of say hydrogen, only certain emission lines appear. For instance between shells 4 and 3 in Table 3.1 of the 12 apparently possible transitions, only 5 appear. This is due to the so called Selection Rules that govern which transitions are permitted. These rules are in turn governed by the manner in which the electron emits a photon

during the process of an orbital transition. The Selection Rule universally quoted at this point in development is

$$\Delta n_\phi^* = \pm 1 \qquad (3.47)$$

That is, that the electron in making the orbital transition will lose/gain exactly one quanta of orbital momentum, as well as one or more quanta of orbital energy. Because the mechanism resulting in (3.47) is closely related to the concept of electron spin, (3.47) is simply accepted for the purpose of this paper, and will be fully justified for a corpuscular theory of atomic structure in the next paper which will deal exclusively with the mechanical effects of electron spin.

4   Conclusions.

All of the results that have been derived here in Section 3 for the quantised energy levels of the bound electron, are well known and well documented throughout the literature. The significant difference with the derivations here is that they have all been achieved from first principles without the need for unsupported hypotheses or assumptions. This cannot be said for the original old quantum theory of Niels Bohr et al or the modern theory of atomic structure based upon quantum mechanics. Having said this it will of course be necessary to maintain this degree of rigour as the development of the resurrected Bohr/Sommerfeld theory is continued in order to maintain credibility.

The first principles referred to above are Planck's quantum hypothesis of energy and de Broglie's matter wave quantum hypothesis of momentum. Both of these have been verified experimentally. In [1] they were used as the starting point for the investigation of the characteristics of matter waves in the Relativistic Space-Time Domain D_0. The results of that investigation lead directly into the resurrection of the corpuscular theory of atomic structure pursued here. The primary results achieved, which have led to the derivation of the quantised orbital energy levels in Section 3 are reviewed as follows.

First and most important is the establishment of the link between the main quantisation criteria, the single valuedness of the orbital electron's matter wave wavelength, and the necessity that in a stable orbit, the bound energy of the electron must be constant over a complete orbit. This link provides the criteria with a necessary and sufficient formalism to fully justify its use within the overall development. Also the manner in which this link has been established has allowed visibility of the variability of the orbital electron's matter wave wavelength within a stable elliptic orbit, and how this becomes constant throughout a circular orbit. It has also provided a formal proof for the exclusion of the pendulum orbits as a result of their contravention of the primary criterion of existence within D_0.

The next most important aspect is the ease with which the development led to the relationship between the primary quantisation criteria and the physical orbital velocity of the electron. It is in fact a relativistic version of de Broglie's original quantum momentum hypothesis. It is this relationship which is then shown to be easily transformed into Bohr's quantised momentum rules although again it is the relativistically mass corrected versions that appear. This quantisation relationship is the one that is used to provide the input to the bound energy equation of the electron. It was subsequently used in this paper to provide such quantised inputs for the four orbital cases sampled in Section 3. The same relationship will be shown in the next paper to be just as applicable to further cases involving electron spin.

The orbital energy relationship into which the above quantised momentum relationships were inserted is really a partly developed Sommerfeld equation for relativistically mass corrected elliptic orbits. The version derived here does however permit the development of a complete mathematical model to be progressed in stages covering a variety of orbits as effectively demonstrated in Section

3.

It is important to note that in many of the derivations presented in this paper a number of simplifications in the form of relativistic approximations have been utilised. Most of these have been taken to the first, (v^2/c^2), relativistic term. While these approximations provide for a considerable degree of ease in the mathematical development, they will of course become the source of error, however small, in the calculation of line spectra wavelengths. The reason for the use of these approximations is essentially threefold thus, (i) mathematically necessary in that a fully rigorous solution was unattainable, (ii) ease of derivation as suggested above and, (iii) to ensure compatibility of results with those extant, i.e. Sommerfeld's energy equation. However, as further development proceeds and greater accuracy is needed, it may be necessary to refine some of the approximations used and such refinements will be introduced as needed.

Finally, everything that has been presented and discussed here has obviously ignored what is now accepted as an integral part of atomic structure, electron spin - howsoever viewed. This will be the subject of the next two papers, the first of which will deal with the mechanical aspects of electron spin, while the second deals with the magnetic. It is in the next paper that electron spin will be shown to be not just an integral part of atomic structure theory, but quite possibly the most important part.

APPENDIX A.

ORBITAL ENERGY.

A.1 Preliminary Analysis Involving the Solution to the Orbital Equation of Motion.

The relativistic orbit of the electron about the proton nucleus can be pictorially represented as in Fig. A.1
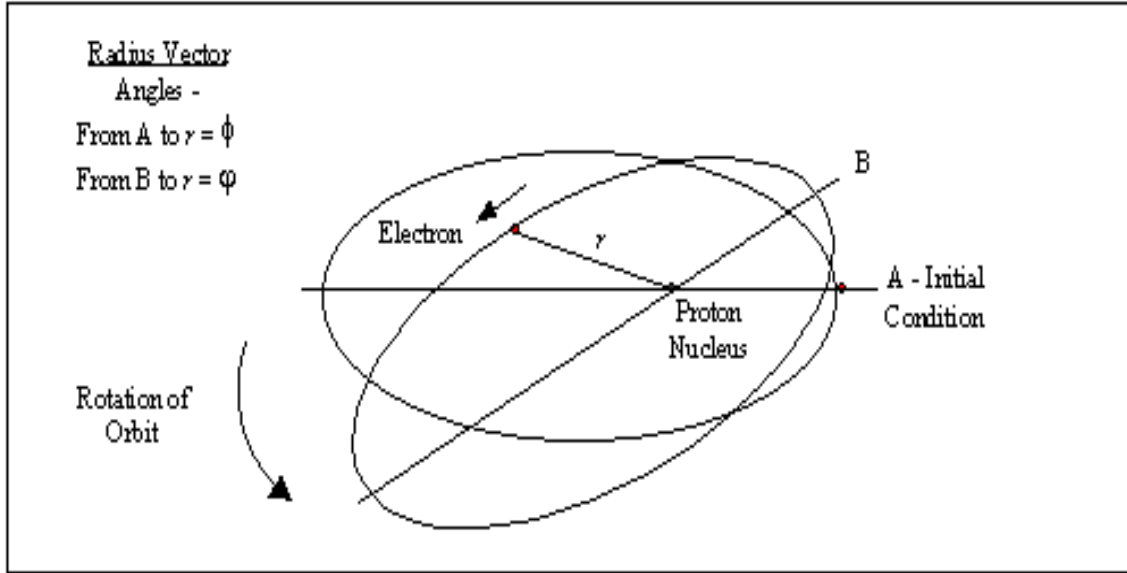

Fig. A.1 - Relativistic Electron Orbit.

The solution of the orbital equation of motion was, for a general case, effected in [2], Eq.(5.40) and is repeated here for convenience

$$\mu = \left[\frac{\left\{ \left(1 - h^2\mu_0^2/c^2\right)^{1/2} + F_0\mu_0/m_0c^2 \right\}}{\left(m_0h^2/F_0\right)\left(1 + F_0^2/m_0^2c^2h^2\right)} \right] \left[1 + \frac{\left\{ m_0h^2\mu_0/F_0 - \left(1 - h^2\mu_0^2/c^2\right)^{1/2} \right\}\cos\varphi}{\left\{ F_0\mu_0/m_0c^2 + \left(1 - h^2\mu_0^2/c^2\right)^{1/2} \right\}} \right] \quad (A.1)$$

where

$$\varphi = \phi \left(1 - \frac{F_0^2}{m_0^2c^2h^2} \right)^{1/2} \quad (A.2)$$

Here, for conformity with the nomenclature used in this paper, Φ in [2],Eq.(5.40) has been replaced with φ.

Eq.(A.1) is of the form

$$\mu = \frac{1 + \varepsilon\cos\varphi}{L} \quad (A.3)$$

Where

    L is the relativistically corrected orbit semi-latus rectum.

    ε is the relativistically corrected orbit eccentricity.

In order to obtain the required terms in the nomenclature of atomic structure as used in this series of papers, it is necessary to obtain suitable expressions for μ_0, h and L.Note that h in the above equation (A.1), is not Planck's constant but the swept area constant of the orbit as defined in [2].

Also note that in all of the ensuing analysis, all terms involving the velocity of light, c, will, where necessary, be binomially expanded to retain only those of relativistic second order.

First for μ_0, this can be determined from the eccentricity terms in (A.1) and (A.3), thus

$$\varepsilon = \frac{\left\{\dfrac{m_0 h^2 \mu_0}{F_0} - \left(1 + \dfrac{h^2 \mu_0^2}{c^2}\right)^{1/2}\right\}}{\left\{\left(1 + \dfrac{h^2 \mu_0^2}{c^2}\right)^{1/2} - \dfrac{F_0 \mu_0}{m_0 c^2}\right\}} \tag{A.4}$$

Solving this for μ_0 gives

$$\mu_0 = \frac{\dfrac{F_0}{m_0 h^2}\left(1 + \varepsilon\right)}{\left\{\left(1 - \dfrac{F_0^2}{m_0^2 c^2 h^2}\right)\left(1 - \dfrac{F_0^2 \varepsilon^2}{m_0^2 c^2 h^2}\right)\right\}^{1/2}} \tag{A.5}$$

Now, substitution of this into the semi-latus rectum half of (A.1), then gives after reduction

$$L = \frac{m_0 h^2}{F_0}\left\{1 - \frac{F_0^2}{2 m_0^2 c^2 h^2}\left(1 + \varepsilon^2\right)\right\} \tag{A.6}$$

To determine a suitable expression for h, from [2], Eq.(5.22)

$$h = \frac{\omega_\phi r^2}{\left(1 - \dfrac{v^2}{c^2}\right)^{1/2}} \tag{A.7}$$

and from (A.2) this becomes

$$h = \frac{\omega_\varphi r^2}{\left(1 - \dfrac{F_0^2}{m_0^2 c^2 h^2}\right)^{1/2}\left(1 - \dfrac{v^2}{c^2}\right)^{1/2}} \tag{A.8}$$

Which can be expressed as

$$h = \frac{M_\varphi^*}{m_0 \left(1 - \dfrac{F_0^2}{m_0^2 c^2 h^2}\right)^{1/2}} \tag{A.9}$$

Solving (A.9) for h gives

$$h = \frac{M_\varphi^*}{m_0}\left(1 + \frac{F_0^2}{c^2 M_\varphi^{*2}}\right)^{1/2} \tag{A.10}$$

Substitution of this into (A.6) then gives for L,

$$L = \frac{M_\varphi^{*2}}{m_0 F_0}\left\{1 + \frac{F_0^2}{2 c^2 M_\varphi^{*2}}\left(1 - \varepsilon^2\right)\right\} \tag{A.11}$$

Also from (A.8) and (A.10)

$$\omega_\varphi r^2 = \frac{M_\varphi^*}{m_0}\left(1 - \frac{v^2}{c^2}\right)^{1/2} \tag{A.12}$$

and also from (A.2) and (A.10)

$$\omega_\phi = \omega_\varphi \left(1 + \frac{F_0^2}{c^2 M_\varphi^{*2}}\right)^{1/2} \tag{A.13}$$

Eqs.(A.11), (A.12) and (A.13) are the required subsidiary equations to determine orbital energy and can be converted to atomic structure nomenclature by putting $F_0 = Ze^2$, thus

$$L = \frac{M_\varphi^{*2}}{Ze^2 m_0} \left\{1 + \frac{Z^2 e^4}{2c^2 M_\varphi^{*2}}\left(1 - \varepsilon^2\right)\right\}$$

$$\omega_\phi = \omega_\varphi \left(1 + \frac{Z^2 e^4}{c^2 M_\varphi^{*2}}\right)^{1/2} \tag{A.14}$$

$$\omega_\varphi r^2 = \frac{M_\varphi^*}{m_0}\left(1 - \frac{v^2}{c^2}\right)^{1/2}$$

These results are used in the derivation of electron orbital energy in the main text, Section 2.4, and in the quantisation of sample orbits thereafter.

A.2 Derivation of Sommerfeld's Full Relativistically Mass Corrected Elliptic Orbit Energy Equation.

In Section 3.5, the expanded version of Sommerfeld's equation for a relativistically mass corrected electron orbit energy level was derived. The full version is derived here for interest.

Multiplying out (2.24), adding the rest mass energy and binomially contracting gives

$$E_{or} = m_0 c^2 \left[1 + \frac{Z^2 e^4}{c^2 M_\varphi^2}\left(1 - \varepsilon^2\right)\right]^{-1/2} - m_0 c^2 \tag{A.15}$$

Inserting (3.34) and (3.44) then gives

$$E_{or} = m_0 c^2 \left[1 + \frac{\kappa^2 Z^2}{n^2 \left(1 - \frac{\kappa^2 Z^2}{2n n_\phi^*}\right)^2}\right]^{-1/2} - m_0 c^2 \tag{A.16}$$

This finally reduces to

$$E_{or} + E_0 = E_0 \left[1 + \frac{\kappa^2 Z^2}{\left\{n_r + \left(n_\phi^{*2} - \kappa^2 Z^2\right)^{1/2}\right\}^2}\right]^{-1/2} \tag{A.17}$$

which is Sommerfeld's equation, and where E_0 has been written for $m_0 c^2$.

APPENDIX B.

Calculated Emission Spectra for the First 7 to 4 Orbital Shells

of Hydrogen, (as so far developed).

This Appendix presents calculated emission/absorption spectra for all the relativistically mass corrected orbitals in the first 7 to 4 orbit shells of hydrogen. The spectra are calculated using the formula

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

together with the Selection Rule of (3.47).

In (B.1) $E_{or(\#)}$ is given by (3.46) within which R_{hy} is determined from the generalised relationship

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

In this and (B.1) 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	[6]
c	Velocity of Light in Vacuum	2.99792458E+10	cm/sec	[6]
R_{hy}	Rydberg's Constant for Hydrogen	See (B.2)	sec^{-1}	
R_{∞}	Rydberg's Constant for Infinite Nuclear Mass	1.09737316E+5	cm^{-1}	[6]
Z	Atomic Number	1 for Hydrogen		
J	Mass Number	1 for Hydrogen		
m_p	Proton Mass	1.67262171E-24	g sec^2/cm	[6]
m_N	Neutron Mass	1.6749278E-24	g sec^2/cm	[6]
m_e	Electron Mass	9.10913826E-28		[6]
e	Electron/Proton Charge	-/+ 4.8032044E-10	esu	See Note 1

Table B1 - 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 cm^{-1}.

Joules = 1E-7 ergs

eV = 6.24150948E+18 Joules

cm^{-1} = 8.065541E+3 eV

The calculated spectra are shown below in Table B2 expressed as wavelengths in Ångstroms.

Orbital Energy E_{OR} (ergs)	E_{OR} (cm^{-1})	From n	From n^*_ϕ	To n^*_ϕ	To n	1 — s	2 — s	2 — p	3 — s	3 — p	3 — d	4 — s	4 — p	4 — d	4 — f
-2.178715E-11	0	1	1	1	s	-									
-5.446804E-12	82259.1562	2	1	1	s	N.P.	-								
-5.446732E-12	82259.5213	2	1	2	p	1215.6642		-							
-2.420794E-12	97492.4415	3	1	1	s	N.P.	N.P.	6564.7267	-						
-2.420772E-12	97492.5496	3	1	2	p	1025.7190	6564.5227	N.P.		-					
-2.420765E-12	97492.5857	3	1	3	d	N.P.	N.P.	6564.6645			-				
-1.361693E-12	102824.0765	4	1	1	s	N.P.	N.P.	4862.7338	N.P.	18756.35	N.P.	-			
-1.361684E-12	102824.1221	4	1	2	p	972.5340	4862.6367	N.P.	18755.80	N.P.	18756.13		-		
-1.361681E-12	102824.1373	4	1	3	d	N.P.	N.P.	4862.7194	N.P.	18756.31	N.P.			-	
-1.361680E-12	102824.1449	4	1	4	f	N.P.	N.P.	N.P.	N.P.	N.P.	18756.23				-
-8.714821E-13	105291.8555	5	1	1	s	N.P.	N.P.	4341.7205	N.P.	12821.65	N.P.	N.P.	40523.00	N.P.	N.P.
-8.714775E-13	105291.8788	5	1	2	p	949.7405	4341.6473	N.P.	12821.43	N.P.	12821.67	40521.87	N.P.	40522.87	N.P.
-8.714759E-13	105291.8866	5	1	3	d	N.P.	N.P.	4341.7146	N.P.	12821.60	N.P.	N.P.	40522.49	N.P.	40522.86
-8.714751E-13	105291.8905	5	1	4	f	N.P.	N.P.	N.P.	N.P.	N.P.	12821.65	N.P.	N.P.	40522.67	N.P.
-8.714747E-13	105291.8928	5	1	5	g	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	40522.76
-6.051951E-13	106632.3747	6	1	1	s	N.P.	N.P.	4102.9237	N.P.	10941.12	N.P.	N.P.	26258.75	N.P.	N.P.
-6.051924E-13	106632.3883	6	1	2	p	937.8010	4102.8599	N.P.	10940.98	N.P.	10941.15	26258.34	N.P.	26258.76	N.P.
-6.051915E-13	106632.3928	6	1	3	d	N.P.	N.P.	4102.9206	N.P.	10941.10	N.P.	N.P.	26258.63	N.P.	26258.78
-6.051911E-13	106632.3950	6	1	4	f	N.P.	N.P.	N.P.	N.P.	N.P.	10941.14	N.P.	N.P.	26258.72	N.P.
-6.051908E-13	106632.3964	6	1	5	g	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	26258.76
-6.051906E-13	106632.3973	6	1	6	h	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.
-4.446327E-13	107440.6644	7	1	1	s	N.P.	N.P.	3971.2239	N.P.	10052.15	N.P.	N.P.	21661.22	N.P.	N.P.
-4.446310E-13	107440.6729	7	1	2	p	930.7458	3971.1650	N.P.	10052.03	N.P.	10052.18	21660.97	N.P.	21661.26	N.P.
-4.446305E-13	107440.6757	7	1	3	d	N.P.	N.P.	3971.2221	N.P.	10052.14	N.P.	N.P.	21661.17	N.P.	21661.28
-4.446302E-13	107440.6771	7	1	4	f	N.P.	N.P.	N.P.	N.P.	N.P.	10052.18	N.P.	N.P.	21661.24	N.P.
-4.446300E-13	107440.6780	7	1	5	g	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	21661.27
-4.446299E-13	107440.6785	7	1	6	h	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.
-4.446298E-13	107440.6789	7	1	7	i	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.	N.P.

N.P. = Not Permitted by the Selection Rule of Eq.(3.47)

Table B2 - Line Spectra for the First Seven to Four Orbital Shells of Hydrogen

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