Solutions of the Fermion Equation for atomic hydrogen and helium: derivation of the Pauli exclusion principle.

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Abstract.

The fermion equation is solved for the spectra of atomic hydrogen and helium. It is shown that the hydrogenic wavefunctions must be combinations of spin up and spin down wavefunctions, a result that is compatible with the fundamental Lorentz transforms of the right and left Pauli spinors. A summary of the relevant operator properties is given and key notation implemented for clarity. The fine structure of atomic H emerges straightforwardly from the angular part of the wavefunctions and the spin orbit coupling term. A summary of the solution for H is given for ease of reference and the Pauli Exclusion Principle derived from a straightforward use of parity inversion applied to the complete helium wavefunction.

Keywords: ECE theory, fermion equation, hydrogen and helium atoms, Pauli Exclusion Principle.

1. Introduction.

In the two preceding papers of this series [1–10] the first single particle fermion equation of physics has been derived and developed. It is given the appellation "fermion equation" to distinguish it from the Dirac equation. The fermion equation has multiple advantages which are being developed systematically [11]. Notably, the fermion equation removes the incorrect notion of "negative energy" from physics and therefore removes the need for a multi fermion interpretation [12] of the Dirac equation. It has been shown in UFT 172 and 173 (www.aias.us) that the fermion equation is an expression in one single first order differential equation of the two fundamentally important Lorentz transforms of the right and left Pauli spinors [12]. The fermion equation is preferred by Ockham´s Razor to the Dirac equation because it expresses the fermion field in terms of the two by two Pauli matrices and produces rigorously non negative energy. The origin of the fallacy of negative energy in physics has been shown to be Dirac´s incorrect choice of his four by four gamma matrices - the "standard representation". This error has been repeated dogmatically for eighty five years and has resulted in elaborate mathematical contrivances in quantum field theory and quantum electrodynamics. The fermion equation makes these complications unnecessary by Ockham´s Razor.

In Section 2 a summary is given for ease of reference of the operator properties used in this paper. In Section 3, details of the solution of the fermion equation are given for atomic H, and ket notation adopted for clarity. Some details are given of how the non relativistic quantum mechanics emerges as a limit of the relativistic theory. In Section 4 the fine spectral structure of the H atom is derived by straightforward consideration of the angular part of the wavefunction and the spin orbit term of the hamiltonian. Finally in Section 5 the Pauli Exclusion Principle is derived straightforwardly using the helium atom as an example. The fundamental origin of the principle is the fact that the hydrogenic wavefunctions must be combinations of spin up and spin down states, a conclusion that emerges from the fermion equation but not from the Dirac equation.

2. Summary of operator properties.

The basic operator in relativistic quantum mechanics [13, 14] is:

$$\hat{\kappa} = \begin{bmatrix} \hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}} + \hbar & 0 \\ 0 & -\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}} - \hbar \end{bmatrix} \tag{1}$$

where $\hat{\boldsymbol{\sigma}}$ is itself regarded as an operator [13]. Here $\hat{\boldsymbol{L}}$ is the orbital angular momentum operator and ħ is the reduced Planck constant with dimensions of angular momentum. Thus:

$$\hat{\kappa}\,\psi = -\kappa\,\hbar\,\psi \quad , \quad \kappa = \pm\left(j + \frac{1}{2}\right) \tag{2}$$

The square of this operator is defined by:

$$\hat{\kappa}^2 = (\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}} + \hbar)^2 = \hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}}\,\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}} + 2\,\hbar\,\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}} + \hbar^2 \quad . \tag{3}$$

From the algebra of Pauli matrices:

$$\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}}\,\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}} = \hat{\boldsymbol{L}}^2 + i\,\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}} \times \hat{\boldsymbol{L}} \quad . \tag{4}$$

The cross product of vector operators in the second term is non zero for the following reason. The basic commutator equations are:

$$\left[\hat{L}_X\,,\,\hat{L}_Y\right] = i\,\hbar\,\hat{L}_Z \tag{5}$$

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which in vector operator notation [14] are:

$$\hat{\boldsymbol{L}} \times \hat{\boldsymbol{L}} = i\,\hbar\,\hat{\boldsymbol{L}} \quad . \tag{6}$$

Therefore:

$$\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}}\,\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}} = \hat{L}^2 - \hbar\,\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}} \quad . \tag{7}$$

From Eq. (7) in Eq. (3):

$$\hat{\kappa}^2 = \hat{L}^2 + \hbar\,\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}} + \hbar^2 \quad . \tag{8}$$

As in UFT 173 and in reference [13]:

$$\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}}\;\varphi^R = \hbar\,(\,j - \frac{1}{2}\,)\;\varphi^R \tag{9}$$

$$\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}}\;\varphi^L = -\,\hbar\,(\,j + \frac{3}{2}\,)\;\varphi^L \quad . \tag{10}$$

where φ^R and φ^L are the right and left Pauli spinors:

$$\Phi^R = \begin{bmatrix} \psi_1^R \\ \psi_2^R \end{bmatrix} \quad , \quad \Phi^L = \begin{bmatrix} \psi_1^L \\ \psi_2^L \end{bmatrix} \quad . \tag{11}$$

The total angular momentum operator is:

$$\hat{\boldsymbol{J}} = \hat{\boldsymbol{L}} + \frac{1}{2}\hbar\hat{\boldsymbol{\sigma}} = \hat{\boldsymbol{L}} + \hat{\boldsymbol{S}} \quad . \tag{12}$$

This equation arose originally [13, 14] from an empirical suggestion that spin half explained many features of atomic spectra. The intrinsic spin angular momentum operator is defined as:

$$\hat{\boldsymbol{S}} = \frac{1}{2}\hbar\hat{\boldsymbol{\sigma}} \quad . \tag{13}$$

The square of the total angular momentum operator is therefore:

$$\begin{aligned}\hat{J}^2 &= \hat{L}^{\,2} + \hbar\,\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}} + \frac{\hbar^2}{4}\,\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{\sigma}} \\ &= \hat{L}^{\,2} + \hbar\,\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}} + \frac{3}{4}\,\hbar^2 \\ &= \hat{L}^{\,2} + 2\,\hat{\boldsymbol{S}}.\hat{\boldsymbol{L}} + \hat{\boldsymbol{S}}.\hat{\boldsymbol{S}} \quad ,\end{aligned} \tag{14}$$

in which has been used the result [12]:

$$\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{\sigma}} = 3\ . \tag{15}$$

Therefore:

$$\hat{\boldsymbol{\sigma}} = \begin{bmatrix} 1 & 1-i \\ 1+i & -1 \end{bmatrix}\ . \tag{16}$$

Therefore:

$$\hat{L}^{\,2}\,\Phi^R = \hbar^2\, l_-\,(l_- + 1\,)\,\Phi^R\ \ , \tag{17}$$

$$\hat{L}^{\,2}\,\Phi^L = \hbar^2\, l_+\,(l_+ + 1\,)\,\Phi^L \tag{18}$$

where:

$$l_\pm = \mathrm{j} \pm \frac{1}{2}\qquad . \tag{19}$$

Now consider the operator identity [13]:

$$\hat{\boldsymbol{\sigma}}.\,\hat{\boldsymbol{p}} = \hat{\boldsymbol{\sigma}}.\,\frac{\boldsymbol{r}}{r}\,\Big(\frac{\boldsymbol{r}}{r}\,.\,\hat{\boldsymbol{p}} + i\,\frac{\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}}}{r}\Big) \tag{20}$$

in radial coordinates, and construct the square:

$$\boldsymbol{\sigma}.\,\hat{\boldsymbol{p}}\ \boldsymbol{\sigma}.\,\hat{\boldsymbol{p}} = \frac{\boldsymbol{r}}{r}\,.\,\hat{\boldsymbol{p}}\,\frac{\boldsymbol{r}}{r}\,.\,\hat{\boldsymbol{p}} - \frac{\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}}\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}}}{r^2} + i\,\Big(\frac{\boldsymbol{r}}{r}\,.\,\hat{\boldsymbol{p}}\,\frac{\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}}}{r} + \frac{\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}}}{r}\,\frac{\boldsymbol{r}}{r}\,.\,\hat{\boldsymbol{p}}\,\Big) \tag{21}$$

The real part of this equation is:

$$\mathrm{Re}\,(\boldsymbol{\sigma}.\,\hat{\boldsymbol{p}}\ \boldsymbol{\sigma}.\,\hat{\boldsymbol{p}}\,) = \frac{\boldsymbol{r}}{r}\,.\,\hat{\boldsymbol{p}}\,\frac{\boldsymbol{r}}{r}\,.\,\hat{\boldsymbol{p}} - \frac{\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}}\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}}}{r^2} \tag{22}$$

where we have used:

$$\boldsymbol{\sigma}.\frac{\boldsymbol{r}}{r}\,\boldsymbol{\sigma}.\frac{\boldsymbol{r}}{r} = 1 \quad . \tag{23}$$

Now use:

$$\frac{\boldsymbol{r}}{r}\,.\,\hat{\boldsymbol{p}}\frac{\boldsymbol{r}}{r}\,.\,\hat{\boldsymbol{p}} = -\,\hbar^2\,\frac{\partial^2}{\partial x^2} \tag{24}$$

to find:

$$\boldsymbol{\sigma}.\hat{\boldsymbol{p}}\;\boldsymbol{\sigma}.\hat{\boldsymbol{p}} = -\,\hbar^2\,\frac{\partial^2}{\partial x^2} - \frac{\hat{L}^2}{r^2} + \frac{\hbar}{r^2}\,\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}} \tag{25}$$

However we know that:

$$\boldsymbol{\sigma}.\hat{\boldsymbol{p}}\;\boldsymbol{\sigma}.\hat{\boldsymbol{p}} = \hat{p}^2 = -\,\hbar^2\,\nabla^2 \tag{26}$$

so we obtain the operator identity:

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{\hat{L}^2}{\hbar^2 r^2} - \frac{\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}}}{\hbar\, r^2} \quad . \tag{27}$$

To make clear that these are all operator equations the symbol ^ has been placed over all operators.

The fine structure of atomic H can be deduced [14] straightforwardly using the operator equation:

$$\hat{J}^2 = \hat{L}^2 + \hat{S}^2 + 2\,\hat{\boldsymbol{L}}\,.\,\hat{\boldsymbol{S}}\,. \tag{28}$$

The energy levels of spin orbit coupling are given [14] by:

$$\hat{\boldsymbol{L}}\,.\,\hat{\boldsymbol{S}}\;\psi = \frac{1}{2}\,(\hat{J}^2 - \hat{L}^2 - \hat{S}^2)\,\psi \quad , \tag{29}$$

so the energy levels are:

$$E = \frac{\hbar^2}{2}\,(\mathrm{j}\,(\mathrm{j}+1) - l\,(l+1) - s\,(s+1)) < \psi^*|\,\xi\,(\mathrm{r})\,|\,\psi > \tag{30}$$

where ξ is defined in the next section.

3. Solution of the Fermion Equation for H.

The fermion equation produces the correct Lorentz transforms of the right and left

Pauli spinors, whereas the Dirac equation does not. The fermion equation is therefore the correct equation in physics. The fermion equation may be written as:

$$(\hat{E} - e\,\Phi + c\,\boldsymbol{\sigma}.\,\hat{\boldsymbol{p}}\,)\ \varphi^{L} = m\,c^{2}\boldsymbol{\Phi}^{R} \tag{31}$$

$$(\hat{E} - e\,\Phi - c\,\boldsymbol{\sigma}.\,\hat{\boldsymbol{p}}\,)\ \varphi^{R} = m\,c^{2}\boldsymbol{\Phi}^{L} \tag{32}$$

where the minimal prescription has been used to describe the effect of the Coulomb potential of the H atom:

$$E \longrightarrow E - e\,\varphi\ . \tag{33}$$

Here E is the total relativistic energy, - e is the charge on the electron, φ is the Coulomb potential, m is the mass of the electron and c the vacuum speed of light. Under the Lorentz transform [12]:

$$\boldsymbol{\Phi}^{R} \longrightarrow \exp\left(\frac{1}{2}\,\boldsymbol{\sigma}.\,\boldsymbol{\Phi}\right) \Phi^{R}\quad , \tag{34}$$

$$\boldsymbol{\Phi}^{L} \longrightarrow \exp\left(-\frac{1}{2}\,\boldsymbol{\sigma}.\,\boldsymbol{\Phi}\right) \Phi^{L}\ , \tag{35}$$

where $\boldsymbol{\Phi}$ denotes a vector angle. There are two fundamental Lorentz transforms [12] because the underlying group theory is one that is described by the Lorentz group extended by parity. The latter has the effect:

$$\hat{P}\ (\boldsymbol{\Phi}^{R}) = \boldsymbol{\Phi}^{L}\quad , \tag{36}$$

$$\hat{P}\ (\boldsymbol{\Phi}^{L}) = \boldsymbol{\Phi}^{R}\quad . \tag{37}$$

It is clear and simple to see that the rest energy:

$$E_{0} = mc^{2} \tag{38}$$

is always positive, and Eqs. (31) and (32) are interconverted by parity because:

$$\hat{P}\ (\hat{\boldsymbol{\sigma}}.\,\hat{\boldsymbol{p}}) = -\,\hat{\boldsymbol{\sigma}}.\,\hat{\boldsymbol{p}}\ . \tag{39}$$

The energy levels of the H atom are found by solving Eqs. (31) and (32) simultaneously. The basic problem [13] is to solve:

$$\left(\hat{L}^{2} + \hbar\,\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}} + \frac{3}{4}\,\hbar^{2}\right) \begin{bmatrix} \boldsymbol{\Phi}^{R} \\ \boldsymbol{\Phi}^{L} \end{bmatrix} = j\,(\,j+1\,)\,\hbar^{2} \begin{bmatrix} \boldsymbol{\Phi}^{R} \\ \boldsymbol{\Phi}^{L} \end{bmatrix} \tag{40}$$

and

$$(\hat{L}_Z + \frac{1}{2}\hbar\hat{\sigma}_Z) \begin{bmatrix} \Phi^R \\ \Phi^L \end{bmatrix} = m\hbar \begin{bmatrix} \Phi^R \\ \Phi^L \end{bmatrix} \quad . \tag{41}$$

There are two angular momenta present, the orbital and spin angular momentum of the electron. The permitted states [14] of the total angular momentum are given by the Clebsch Gordan series:

$$j = j_1 + j_2 , \ldots , | j_1 - j_2 | \ , \tag{42}$$

$$m_j = m_{j1} + m_{j2} \ . \tag{43}$$

When:

$$j_2 = \frac{1}{2} \tag{44}$$

then:

$$j = l + \frac{1}{2} \quad \text{or} \quad j = l - \frac{1}{2} \ . \tag{45}$$

The state of the system is defined by the key notation [14], which is related to the notation used by Merzbacher [13] as follows:

$$| \, j \, m_j \, l_+ > \ = \ Y^{jm}_{j+\frac{1}{2}} \quad , \tag{46}$$

$$| \, j \, m_j \, l_- > \ = \ Y^{jm}_{j-\frac{1}{2}} \quad . \tag{47}$$

Here:

$$l_\pm = j \pm \frac{1}{2} \ . \tag{48}$$

Using the operator equation (14) it follows that [14]:

$$\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}} \ | \, j \, m_j \, l > \ = \frac{1}{2} \hbar^2 \, (j (j + 1) - l (l + 1) - s (s + 1)) \, | \, j \, m_j \, l > \tag{49}$$

where j, l and s are quantum numbers. It follows from Eqs. (19) and (45) that:

$$\hat{\boldsymbol{\sigma}} . \hat{\boldsymbol{L}} \ | \, j \, m_j \, l_+ > \ = - (l_+ + 1) \, | \, j \, m_j \, l_+ > \ , \tag{50}$$

$$\hat{\boldsymbol{\sigma}} . \hat{\boldsymbol{L}} \ | \, j \, m_j \, l_- > \ = \ l_- \, | \, j \, m_j \, l_- > \ . \tag{51}$$

The following operator relation is given [13] by considerations of parity, because this operator is a pseudoscalar:

$$\hat{\boldsymbol{\sigma}}.\frac{\boldsymbol{r}}{r}\ |\, \mathrm{j}\ m_\mathrm{j}\, l_\pm > \ = \ -\,|\, \mathrm{j}\ m_\mathrm{j}\, l_\mp > \ . \tag{52}$$

Furthermore, this operator has the parity reversal effects:

$$\hat{\boldsymbol{\sigma}}.\frac{\boldsymbol{r}}{r}\,\frac{\partial}{\partial r} = -\frac{\partial}{\partial r} \quad , \quad \hat{\boldsymbol{\sigma}}.\frac{\boldsymbol{r}}{r}\,\frac{1}{r} = -\frac{1}{r} \quad . \tag{53}$$

It is clear that the spinors $\boldsymbol{\Phi}^R$ and $\boldsymbol{\Phi}^L$ are the physically meaningful wavefunctions because they obey the Lorentz transform and are given by fundamental considerations [12] of group theory, and, most importantly, because they give positive rest energy. In order to solve equations (31) and (32) the following mathematical transformations are used:

$$\boldsymbol{\Phi}^L \longrightarrow \boldsymbol{\Phi}_{\boldsymbol{S}}^R + \boldsymbol{\Phi}_{\boldsymbol{S}}^L \ , \tag{54}$$

$$\boldsymbol{\Phi}^R \longrightarrow \boldsymbol{\Phi}_{\boldsymbol{S}}^R - \boldsymbol{\Phi}_{\boldsymbol{S}}^L \ . \tag{55}$$

In ket notation, solutions must be of the format [13]:

$$\boldsymbol{\Phi}_{\boldsymbol{S}}^R = |\, \mathrm{j}\ m_\mathrm{j}\, l_- > \ , \quad \boldsymbol{\Phi}_{\boldsymbol{S}}^L = |\, \mathrm{j}\ m_\mathrm{j}\, l_+ > \tag{56}$$

so:

$$\boldsymbol{\Phi}^R = |\, \mathrm{j}\ m_\mathrm{j}\, l_- > - \ |\, \mathrm{j}\ m_\mathrm{j}\, l_+ > \tag{57}$$

$$\boldsymbol{\Phi}^L = |\, \mathrm{j}\ m_\mathrm{j}\, l_- > + \ |\, \mathrm{j}\ m_\mathrm{j}\, l_+ > \tag{58}$$

with the normalization:

$$\int \boldsymbol{\Phi}_{\boldsymbol{S}}^{+}\, \boldsymbol{\Phi}_{\boldsymbol{S}}\ d^3x = 1 \ . \tag{59}$$

In this notation:

$$\boldsymbol{\Phi}_{\boldsymbol{S}} = \begin{bmatrix} \boldsymbol{\Phi}_{\boldsymbol{S}}^R \\ \boldsymbol{\Phi}_{\boldsymbol{S}}^L \end{bmatrix} \ , \tag{60}$$

and:

$$\boldsymbol{\Phi}_{\boldsymbol{S}}^{+} = \begin{bmatrix} \boldsymbol{\Phi}_{\boldsymbol{S}}^{R*} \ , \ \boldsymbol{\Phi}_{\boldsymbol{S}}^{L*} \end{bmatrix} \tag{61}$$

so that:

$$\int (\psi_{\boldsymbol{S1}}^{R*}\, \psi_{\boldsymbol{S1}}^{R} + \ldots + \psi_{\boldsymbol{S1}}^{L*}\, \psi_{\boldsymbol{S1}}^{L}\,)\ d^3x = 1 \ . \tag{62}$$

From these considerations:

$$\psi_{\mathbf{1}}^{R} = \psi_{\mathbf{1}}^{R}\,(r)\,(|\,\mathrm{j}\; m_{\mathrm{j}}\, l_{-} > -\ |\,\mathrm{j}\; m_{\mathrm{j}}\, l_{+} >\ ) \quad , \tag{63}$$

$$\psi_{\mathbf{2}}^{R} = \psi_{\mathbf{2}}^{R}\,(r)\,(|\,\mathrm{j}\; m_{\mathrm{j}}\, l_{-} > -\ |\,\mathrm{j}\; m_{\mathrm{j}}\, l_{+} >\ ) \quad , \tag{64}$$

$$\psi_{\mathbf{1}}^{L} = \psi_{\mathbf{1}}^{L}\,(r)\,(|\,\mathrm{j}\; m_{\mathrm{j}}\, l_{-} > +\ |\,\mathrm{j}\; m_{\mathrm{j}}\, l_{+} >\ ) \quad , \tag{65}$$

$$\psi_{\mathbf{2}}^{L} = \psi_{\mathbf{2}}^{L}\,(r)\,(|\,\mathrm{j}\; m_{\mathrm{j}}\, l_{-} > +\ |\,\mathrm{j}\; m_{\mathrm{j}}\, l_{+} >\ ) \quad . \tag{66}$$

The fundamentally important result has been obtained that in order for the Lorentz transforms (34) and (35) to be obeyed correctly, the H wavefunctions must be the combinations (63) to (66). These are combinations of different spin states of the electron. The fact that energy is always positive in nature implies these combinations and vice versa. The eigenequation for $\hat{\boldsymbol{L}}\,.\,\hat{\boldsymbol{S}}$ is always the equation (49), giving the energy levels of the H atom as in Section 4.

The transformations (54) and (55) lead to:

$$(\,\hat{E} - e\,\varphi - m\,c^2)\boldsymbol{\Phi}_{\boldsymbol{S}}^{R} + c\,\boldsymbol{\sigma}.\,\hat{\boldsymbol{p}}\,\boldsymbol{\Phi}_{\boldsymbol{S}}^{L} = 0 \tag{67}$$

$$(\,\hat{E} - e\,\varphi + m\,c^2)\boldsymbol{\Phi}_{\boldsymbol{S}}^{L} + c\,\boldsymbol{\sigma}.\,\hat{\boldsymbol{p}}\,\boldsymbol{\Phi}_{\boldsymbol{S}}^{R} = 0 \quad . \tag{68}$$

Application of parity inversion leaves these equations unchanged because:

$$\hat{P}\;(\boldsymbol{\Phi}_{\boldsymbol{S}}^{R}) = \boldsymbol{\Phi}_{\boldsymbol{S}}^{R} \quad , \quad \hat{P}\;(\boldsymbol{\Phi}_{\boldsymbol{S}}^{L}) = -\,\boldsymbol{\Phi}_{\boldsymbol{S}}^{L} \quad . \tag{69}$$

In contrast, parity interconverts Eqs. (31) and (32). These considerations mean that Eqs. (67) and (68) are incomplete, they say nothing about parity. The Dirac equation is simply a combination of the incomplete equations (67) and (68), a combination using the four by four Dirac matrices in the standard representation [12]. The error made by Dirac, and repeated ever since, was to assert that the minus sign in Eq. (67) means “negative energy”, whereas it has no physical significance. The correct equations (31) and (32) keep the sign positive. The fermion equation is a combination of Eqs. (31) and (32), a combination constructed with Pauli matrices only. There is no need for the Dirac matrices in physics, and certainly no need for “negative energy”.

For the H atom, the transformed Eqs. (67) and (68) happen to have a semi analytical solution as follows. This solution must be regarded, however, as a solution of the correct equations (31) and (32). The significance of the transformations (54) and (55) is that the physical wavefunctions $\boldsymbol{\Phi}^{R}$ and $\boldsymbol{\Phi}^{L}$ must be combinations of different spin states. The Dirac equation does not give this fundamentally important result. By inspection [13] the solutions must take the format:

$$\boldsymbol{\Phi}_{\boldsymbol{S}}^{R} = \mathrm{F} \mid \mathrm{j}\ m_{\mathrm{j}}\, l_{-} > \quad , \qquad \boldsymbol{\Phi}_{\boldsymbol{S}}^{R} = -\, i f \mid \mathrm{j}\ m_{\mathrm{j}}\, l_{+} > \quad , \tag{70}$$

where the $- i$ has been introduced in order to give two real simultaneous equations at a later stage of the calculation. In these equations:

$$\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{p}} = \boldsymbol{\sigma}.\frac{\hat{\boldsymbol{r}}}{r}\left(-\, i\, \hbar \frac{\partial}{\partial r} + i\, \frac{\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}}}{r}\right) \tag{71}$$

with:

$$\boldsymbol{\sigma}.\frac{\hat{\boldsymbol{r}}}{r} \mid \mathrm{j}\ m_{\mathrm{j}}\, l_{\mp} > \, = - \mid \mathrm{j}\ m_{\mathrm{j}}\, l_{\pm} > \tag{72}$$

and:

$$\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}} \mid \mathrm{j}\ m_{\mathrm{j}}\, l > \, = \hbar\, (\, \mathrm{j}\, (\, \mathrm{j} + 1\,) - l\, (\, l + 1\,) - s\, (\, s + 1\,))\mid \mathrm{j}\ m_{\mathrm{j}}\, l > \tag{73}$$

where:

$$l_{\pm} = \mathrm{j} \pm \frac{1}{2}\ . \tag{74}$$

As shown in the following section the fine structure of the H atom is given completely by considerations of Eq. (73) alone [14], so it follows immediately that the fine structure is given by the fermion equation with the major advantage of keeping energy positive.

This result is emphasized by Eq. (71), which gives:

$$c\, \hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{p}}\ \boldsymbol{\Phi}_{\boldsymbol{S}}^{R} = -\, i\, \hbar\, c\, \left(\frac{\partial}{\partial r} - \frac{\mathrm{j} - \frac{1}{2}}{r}\right) \mathrm{F} \mid \mathrm{j}\ m\, l_{+} > \ , \tag{75}$$

$$c\, \hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{p}}\ \boldsymbol{\Phi}_{\boldsymbol{S}}^{L} = -\, \hbar\, c\, \left(\frac{\partial}{\partial r} + \frac{\mathrm{j} + \frac{3}{2}}{r}\right) f \mid \mathrm{j}\ m\, l_{-} > \ . \tag{76}$$

So Eqs. (67) and (68) become simultaneous differential equations in *f* and F:

$$(\, \hat{E} - e\, \varphi - m\, c^{2})\mathrm{F} \, - \hbar\, c\, \left(\frac{\partial}{\partial r} + \frac{\mathrm{j} + \frac{3}{2}}{r}\right) f \, = 0 \quad , \tag{77}$$

$$(\, \hat{E} - e\, \varphi + m\, c^{2}) f \, + \, \hbar\, c\, \left(\frac{\partial}{\partial r} - \frac{\mathrm{j} - \frac{1}{2}}{r}\right) \mathrm{F} \, = 0 \ . \tag{78}$$

which can be solved with some approximation [13] to give *E*, the energy levels of the H atom. The details of the result are given in the accompanying note 174(2) and are well known [13]. This solution is clearly a solution of the fermion equation, which gives all the fine structure of the H spectrum excluding the Lamb shift.

To derive Eqs. (77) and (78) use:

$$\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}} \mid \mathrm{j}\; m\, l_{-} > \; = \; (\mathrm{j} - \tfrac{1}{2}) \mid \mathrm{j}\; m\, l_{-} > \; , \tag{79}$$

$$\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}} \mid \mathrm{j}\; m\, l_{+} > \; = - \, (\mathrm{j} + \tfrac{3}{2}) \mid \mathrm{j}\; m\, l_{-} > \; . \tag{80}$$

and note that:

$$(\boldsymbol{\sigma}.\frac{\boldsymbol{r}}{r})\,\frac{\partial}{\partial r} = -\,\frac{\partial}{\partial r} \qquad , \qquad (\boldsymbol{\sigma}.\frac{\boldsymbol{r}}{r})\,\frac{1}{r} = -\,\frac{1}{r} \tag{81}$$

because of parity. Therefore:

$$\begin{aligned} \hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{p}}\; \Phi_{\boldsymbol{S}}^{R} &= \boldsymbol{\sigma}.\frac{\boldsymbol{r}}{r}\,(-\,i\,\hbar\,\frac{\partial}{\partial r} + i\,\frac{\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}}}{r}\,)\,\mathrm{F}\,\mathrm{j}\; m\, l_{-} > \\ &= -\,i\,\hbar\,\frac{\partial \mathrm{F}}{\partial r} \mid \mathrm{j}\; m\, l_{+} > + \; i\,\hbar\,\frac{(\mathrm{j} - \frac{1}{2})}{r}\,\mathrm{F} \mid \mathrm{j}\; m\, l_{+} > \\ &= -\,i\,\hbar\,(\frac{\partial}{\partial r} - (\frac{\mathrm{j} - \frac{1}{2}}{r}))\,\mathrm{F} \mid \mathrm{j}\; m\, l_{+} > \end{aligned} \tag{82}$$

which is Eq. (75). Similarly:

$$\begin{aligned} \hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{p}}\; \Phi_{\boldsymbol{S}}^{L} &= -\,i\;\boldsymbol{\sigma}.\frac{\boldsymbol{r}}{r}\,(-\,i\,\hbar\,\frac{\partial}{\partial r} + i\,\frac{\hat{\boldsymbol{\sigma}}.\hat{\boldsymbol{L}}}{r}\,)\,f \mid \mathrm{j}\; m\, l_{+} > \\ &= -\,\hbar\,\frac{\partial f}{\partial r} \mid \mathrm{j}\; m\, l_{-} > - \; \hbar\,\frac{(\mathrm{j} + \frac{3}{2})}{r}\,f \mid \mathrm{j}\; m\, l_{-} > \\ &= -\,\hbar\,(\frac{\partial}{\partial r} + \frac{(\mathrm{j} + \frac{3}{2})}{r}\,))\,f \mid \mathrm{j}\; m\, l_{-} > \end{aligned} \tag{83}$$

which is Eq. (76). The complete H wavefunctions are the combinations:

$$\boldsymbol{\Phi}^{L} = \; \boldsymbol{\Phi}_{\boldsymbol{S}}^{R} + \boldsymbol{\Phi}_{\boldsymbol{S}}^{L} = \mathrm{F} \mid \mathrm{j}\; m_{\mathrm{j}}\, l_{-} > \; -\,i\,f \mid \mathrm{j}\; m_{\mathrm{j}}\, l_{+} > \tag{84}$$

and

$$\boldsymbol{\Phi}^{R} = \; \boldsymbol{\Phi}_{\boldsymbol{S}}^{R} - \boldsymbol{\Phi}_{\boldsymbol{S}}^{L} = \mathrm{F} \mid \mathrm{j}\; m_{\mathrm{j}}\, l_{-} > \; +\,i\,f \mid \mathrm{j}\; m_{\mathrm{j}}\, l_{+} > \tag{85}$$

These combinations can be expressed in the simple format:

$$\Phi^L = e^{i\theta} \quad , \quad \Phi^R = e^{-i\theta} \tag{86}$$

where:

$$\cos\theta = \mathrm{F} \mid \mathrm{j}\ m_{\mathrm{j}}\ l_- > \quad , \quad \sin\theta = f \mid \mathrm{j}\ m_{\mathrm{j}}\ l_+ > \tag{87}$$

4. Non relativistic approximation and fine structure.

In the non relativistic approximation [12] used to derive the Landé and Thomas factors the total relativistic energy is expressed as:

$$E \longrightarrow m\,c^2 \tag{88}$$

where:

$$\mathrm{E} = \gamma\, m\, c^2 \quad , \quad \gamma = \left(1 - \frac{v^2}{c^2}\right)^{-½} \quad . \tag{89}$$

As described in UFT 172 and 173 (www.aias.us) this approximation leads to the hamiltonian:

$$\hat{H} = m\,c^2 + e\varphi + \frac{\hat{\boldsymbol{p}}^2}{2m} - \frac{e\hbar}{2m}\,\hat{\boldsymbol{\sigma}}.\boldsymbol{B} - \frac{e}{4m^2c^2}\,\hat{\boldsymbol{\sigma}}.(\hat{\boldsymbol{p}} - e\,\boldsymbol{A})\ \varphi\hat{\boldsymbol{\sigma}}.(\hat{\boldsymbol{p}} - e\,\boldsymbol{A}) + \ldots \tag{90}$$

where the vector potential $\boldsymbol{A}$ and magnetic flux density $\boldsymbol{B}$ have been introduced via the minimal prescription [1 – 14]:

$$\hat{\boldsymbol{p}} \longrightarrow \hat{\boldsymbol{p}} - e\,\boldsymbol{A} \tag{91}$$

Also:

$$\hat{H}\,\Phi^R = E\,\Phi^R \quad , \tag{92}$$

$$\hat{H}\,\Phi^L = E\,\Phi^L \quad , \tag{93}$$

and so:

$$\hat{H}\,\psi = E\,\psi \quad , \tag{94}$$

where the fermion spinor is defined as:

$$\psi = \begin{bmatrix} \psi_1^R & \psi_2^R \\ \psi_1^L & \psi_2^L \end{bmatrix} . \qquad (95)$$

The appellation "fermion spinor" is used to distinguish it from the Dirac spinor.

Rewrite Eq. (94) as:

$$\widehat{H}_1 \psi = (E - m c^2 + e\varphi) \psi \qquad (96)$$

where:

$$\widehat{H}_1 = \frac{\widehat{\boldsymbol{p}}^2}{2m} - \frac{e\hbar}{2m} \widehat{\boldsymbol{\sigma}}.\boldsymbol{B} - \frac{e}{4m^2c^2} \widehat{\boldsymbol{\sigma}}.(\widehat{\boldsymbol{p}} - e\boldsymbol{A}) \varphi \widehat{\boldsymbol{\sigma}}.(\widehat{\boldsymbol{p}} - e\boldsymbol{A}) + \ldots$$

$$:= \widehat{H}_2 + \widehat{H}_3 + \widehat{H}_4 \qquad (97)$$

In the absence of spin this equation becomes:

$$\frac{\hat{p}^2}{2m} \psi = (E - m c^2 + e\varphi) \psi \qquad (98)$$

and in the non relativistic limit:

$$E = m c^2 \longrightarrow \mathrm{T} = \frac{1}{2} m v^2 \quad . \qquad (99)$$

So Eq. (98) becomes the Schroedinger equation of the H atom:

$$\frac{\widehat{\boldsymbol{p}}^2}{2m} \psi = -\frac{\hbar^2}{2m} \nabla^2 \psi = E_{\mathrm{nr}} \psi \qquad (100)$$

where the total non-relativistic energy is the sum of the kinetic and potential energies:

$$E_{\mathrm{nr}} = T + V = T - \mathrm{e}\varphi \quad . \qquad (101)$$

It is well known [13, 14] that the Schroedinger equation gives the major features of the H spectrum but does not give the fine structure.

To obtain the fine structure consider Eq. (25):

$$\boldsymbol{\sigma}.\widehat{\boldsymbol{p}}\ \boldsymbol{\sigma}.\widehat{\boldsymbol{p}} = -\hbar^2 \frac{\partial^2}{\partial r^2} - \frac{\hat{L}^2}{r^2} + \frac{\hbar}{r^2} \widehat{\boldsymbol{\sigma}}.\widehat{\boldsymbol{L}} \qquad (102)$$

in which:

$$\hat{L}^2 \Phi^R = \hbar^2 l_- (l_- + 1) \Phi^R \qquad (103)$$

$$\hat{L}^2\,\Phi^L = \hbar^2\, l_+(\,l_+ + 1\,)\,\Phi^L \tag{104}$$

where:

$$l_\pm = \mathrm{j} \pm \frac{1}{2}\quad . \tag{105}$$

The first two terms on the right hand side of Eq. (102) are present in the Schroedinger equation of H [14] but the third term is absent from the Schroedinger equation. From the operator equation (14):

$$\hat{\boldsymbol{L}}.\hat{\boldsymbol{S}}\mid \mathrm{j}\; m_{\mathrm{j}}\, l> = \frac{1}{2}\;(\hat{J}^2 - \hat{L}^2 - \hat{S}^2\,)\mid \mathrm{j}\; m_{\mathrm{j}}\, l>$$

$$= \frac{1}{2}\,\hbar^2\,(\,\mathrm{j}\,(\,\mathrm{j}+1\,) - l\,(\,l+1\,) - s\,(\,s+1\,))\mid \mathrm{j}\; m_{\mathrm{j}}\, l>\quad . \tag{106}$$

The hamiltonian component $\hat{H}_3$ gives the g = 2 or Landé factor of the electron in the H atom (see UFT 172 and UFT 173). The hamiltonian component $\hat{H}_4$ gives the Thomas factor of 2 in the denominator of the spin orbit term as follows:

$$\hat{H}_4 = \frac{e^2}{8\pi m^2 c^2 r^3 \in_0}\;\hat{\boldsymbol{S}}.\hat{\boldsymbol{L}}\quad . \tag{107}$$

The evaluation of the radial integral in this approximation gives [14]:

$$<\frac{1}{r^3}> = \frac{a_0^3}{n^3 l\,(\,l + ½\,)(\,l+1\,)} \tag{108}$$

where the Bohr radius is:

$$a_0 = \frac{4\pi\in_0\hbar^2}{me^4} \tag{109}$$

Here n is the principal quantum number of H, and $\in_0$ is the vacuum permittivity. Denote:

$$\xi_{nl} = e^2\,(8\pi m^2 c^2 a_0^3 \in_0 n^3 l\,(\,l\,+\,½\,)(\,l\,+\,1\,)\,\hbar c)^{-1} \tag{110}$$

then the energy levels of the H atom are given in this approximation by:

$$E = \frac{1}{2}\,\hbar^2\,(\,\mathrm{j}\,(\,\mathrm{j}+1\,) - l\,(\,l+1\,) - s\,(\,s+1\,))<\mid \mathrm{j}\; m_{\mathrm{j}} l\mid\,\xi\mid \mathrm{j}\; mj\; l\mid>$$

$$= \frac{1}{2}\,\hbar c\;\xi_{nl}(\,\mathrm{j}\,(\,\mathrm{j}+1\,) - l\,(\,l+1\,) - s\,(\,s+1\,) \tag{111}$$

where:

$$\xi = \frac{e^2}{8\pi m^2 c^2 r^3 \epsilon_0} \quad . \tag{112}$$

5. Derivation of the Pauli exclusion principle.

By observation of atomic and molecular spectra, Pauli noticed in 1925 that no two electrons can have the same set of quantum numbers. He stated this observation as the principle that the complete wavefunction is antisymmetric under interchange of any two electrons, or more generally, fermions. This has become accepted [12–14] as a fundamental axiom of quantum mechanics. In H it has been shown in Section 2 that the wavefunctions of the single electron of H must be the combinations (63) to (66) in which the effect of parity is as follows:

$$\hat{P}\ (\Phi^R) = \Phi^L \quad , \quad \hat{P}\ (\Phi^L) = \Phi^R \quad . \tag{113}$$

Therefore parity has the following effect on F and *f*:

$$\hat{P}\ (\mathrm{F}) = \mathrm{F} \quad , \quad \hat{P}\ (f) = -f \quad . \tag{114}$$

These combinations of spin up and down states of the electron indicate that they are the fundamental origin of the Pauli exclusion principle, which therefore follows from the fermion equation.

Consider the mathematical structure of the Schroedinger Eq. (100), a structure of the type:

$$\hat{H}\ \psi = E\ \psi \tag{115}$$

This structure means [14] that in the helium atom, with two electrons, the total wavefunction must be the product:

$$\Psi\ (\boldsymbol{r}_1\ , \boldsymbol{r}_2) = \psi_{\boldsymbol{n}_1 \boldsymbol{l}_1 \boldsymbol{m}_1}(\boldsymbol{r}_1)\ \psi_{\boldsymbol{n}_2 \boldsymbol{l}_2 \boldsymbol{m}_2}(\boldsymbol{r}_2) \tag{116}$$

of the individual wavefunctions of each electron. If electron spin is now considered, there must be products such as:

$$\Psi_1^R\ (\mathrm{A})\ \Psi_1^R\ (\mathrm{B})\ , \ldots , \Psi_2^L\ (\mathrm{A})\ \Psi_2^L\ (\mathrm{B})\ , \tag{117}$$

where A and B denote electron A and electron B. Denote:

$$\mathrm{F}_1^-\ (\mathrm{A}) = \mathrm{F}_1 |\ \mathrm{j}\ m_\mathrm{j}\, l_- > \quad , \tag{118}$$

$$f_1^+\ (\mathrm{A}) = f_1 |\ \mathrm{j}\ m_\mathrm{j}\, l_+ > \quad , \tag{119}$$

and so on. A typical product of wavefunctions is:

$$\Psi_1^R\,(A)\,\Psi_1^R\,(B) = (F_1^-\,(A) + i\,f_1^+\,(A))\,(F_1^-\,(B) + i\,f_1^+\,(B)) \tag{120}$$

where the appearance of i is simply a consequence of the definitions (70) used for convenience. Now apply parity:

$$\hat{P}\;(\Psi_1^R\,(A)\,\Psi_1^R\,(B)) = (F_1^-\,(A) - i\,f_1^+\,(A))\,(F_1^-\,(B) - i\,f_1^+\,(B))\;. \tag{121}$$

Finally use the algebraic result:

$$(F_1^-\,(A) + i\,f_1^+\,(A))\,(F_1^-\,(B) + i\,f_1^+\,(B)) = (F_1^-\,(B) + i\,f_1^+\,(B))\,(F_1^-\,(A) + i\,f_1^+\,(A)) \tag{122}$$

and apply parity to the right hand side:

$$\hat{P}\,((F_1^-\,(A) + i\,f_1^+\,(A))\,(F_1^-\,(B) + i\,f_1^+\,(B)) = (F_1^-\,(A) - i\,f_1^+\,(A))\,(F_1^-\,(B) - i\,f_1^+\,(B)) \tag{123}$$

The Pauli exclusion principle is the result of the parity operation:

$$\hat{P}\,((F_1^-\,(A)\,f_1^+\,(B) + f_1^+(A)\,F_1^-\,(B)) = -\,(F_1^-\,(B)\,f_1^+\,(A) + f_1^+(B)\,F_1^-\,(A) \tag{124}$$

It is seen that the complete wavefunction is antisymmetric under interchange of A and B, meaning that if A is replaced by B, and B is replaced by A, the wavefunction changes sign. By observation of atomic and molecular spectra this is the observed wavefunction, one in which no two electrons have the same set of quantum numbers.

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