1) 173(7): Fine Structure of Hydrogen Atom from Fermion Equation.

Consider the fermion equation with positive energy eigenvalues:

$$\pi_\mu \phi \sigma^\mu = mc\sigma^1 \phi \quad -(1)$$

whose eigenfunction is the tetrad:

$$\phi = \begin{bmatrix} \phi_1^R & \phi_2^R \\ \phi_1^L & \phi_2^L \end{bmatrix}. \quad -(2)$$

As shown in detail in UFT 172 and notes for UFT 173 eq. (1) is equivalent to:

$$(\hat{E} + c\underline{\sigma} \cdot \hat{\underline{p}})\phi^L = mc^2\phi^R \quad -(3)$$

$$(\hat{E} - c\underline{\sigma} \cdot \hat{\underline{p}})\phi^R = mc^2\phi^L \quad -(4)$$

where the right and left Pauli spinors are:

$$\phi^R = \begin{bmatrix} \phi_1^R \\ \phi_2^R \end{bmatrix}, \quad \phi^L = \begin{bmatrix} \phi_1^L \\ \phi_2^L \end{bmatrix}. \quad -(5)$$

Note carefully that the eigenvalue mc^2 in eqs (3) and (4) is positive.

In order to solve eqs (3) and (4) for the H atom's fine structure, make the transform:

$$\phi^R \rightarrow \frac{1}{\sqrt{2}}(\phi^R + \phi^L) \quad -(6)$$

$$\phi^L \rightarrow \frac{1}{\sqrt{2}}(\phi^R - \phi^L) \quad -(7)$$

Using eqs (6) and (7) in (3) and (4):

$$(\hat{E} + c\underline{\sigma} \cdot \hat{\underline{p}})(\phi^R - \phi^L) = mc^2(\phi^R + \phi^L) \quad -(8)$$

$$(\hat{E} - c\underline{\sigma} \cdot \hat{\underline{p}})(\phi^R + \phi^L) = mc^2(\phi^R - \phi^L) \quad -(9)$$

Add (8) and (9):

$$(\hat{E} - mc^2)\phi^R = c\underline{\sigma}\cdot\hat{\underline{p}}\,\phi^L \quad -(10)$$

Subtract (9) from (8):

$$(\hat{E} + mc^2)\phi^L = c\underline{\sigma}\cdot\hat{\underline{p}}\,\phi^R \quad -(11)$$

Consider these equations in the presence of a potential so

$$\hat{E} \rightarrow \hat{E} - e\phi \quad -(12)$$

by the minimal prescription. Then:

$$c\underline{\sigma}\cdot\hat{\underline{p}}\begin{bmatrix}\phi^L \\ \phi^R\end{bmatrix} = \begin{bmatrix}\hat{E} - e\phi - mc^2 & 0 \\ 0 & \hat{E} - e\phi + mc^2\end{bmatrix}\begin{bmatrix}\phi^R \\ \phi^L\end{bmatrix} \quad -(13)$$

Now use:

$$\underline{\sigma}\cdot\hat{\underline{p}} = \left(\underline{\sigma}\cdot\frac{\underline{r}}{r}\right)\left(\frac{\underline{r}}{r}\cdot\hat{\underline{p}} + i\frac{\underline{\sigma}\cdot\hat{\underline{L}}}{r}\right) \quad -(14)$$

where $\hat{L}$ is the orbital angular momentum operator:

$$\underline{\sigma}\cdot\hat{\underline{L}}\,\phi^R = \pm\hbar\left(j + \tfrac{1}{2} \mp 1\right)\phi^R \quad -(15)$$

$$\underline{\sigma}\cdot\hat{\underline{L}}\,\phi^L = \mp\hbar\left(j + \tfrac{1}{2} \pm 1\right)\phi^L \quad -(16)$$

Denote:

$$\kappa := -\left(j + \tfrac{1}{2}\right). \quad -(17)$$

Assume:

$$\phi^L = i f(r)\, Y^{m_j}_{j l_L} \quad -(18)$$

$$\phi^R = g(r)\, Y^{m_j}_{j l_R} \quad -(19)$$

The operators $\hat{H}$, $\hat{J}_Z$, $\hat{J}^2$ and $\hat{\kappa}$ commute with the hamiltonian operator of the fermion equation to give the quantum numbers n_r, j, m_j and κ.

) with:
$$\hat{J}^2 = \hat{L}^2 + \hbar \underline{\sigma} \cdot \hat{\underline{L}} + \frac{3}{4}\hbar \quad -(20)$$
$$\hat{L}^2 \phi^R = \hbar^2 l_{\mp}(l_{\mp}+1)\phi^R \quad -(21)$$
$$\hat{L}^2 \phi^L = \hbar^2 l_{\pm}(l_{\pm}+1)\phi^L \quad -(22)$$
$$l_{\pm} = j \pm \frac{1}{2} \quad -(23)$$

With these definitions eq. (13) becomes:
$$\hbar c \begin{bmatrix} -\partial f/\partial r + (\kappa - 1) f/r \\ \partial g/\partial r + (\kappa+1) g/r \end{bmatrix} \begin{bmatrix} f \\ g \end{bmatrix} = \begin{bmatrix} E - e\phi - mc^2 \\ E - e\phi + mc^2 \end{bmatrix} \begin{bmatrix} g \\ f \end{bmatrix} \quad -(24)$$

Let
$$F = rf, \quad G = rg \quad -(25)$$

then:
$$\frac{\partial F}{\partial r} - \frac{\kappa F}{r} = \left(\frac{mc^2 - E + e\phi}{\hbar c} \right) G \quad -(26)$$
$$\frac{\partial G}{\partial r} + \frac{\kappa G}{r} = \left(\frac{mc^2 + E - e\phi}{\hbar c} \right) F \quad -(27)$$

For the H atom:
$$\frac{e\phi}{\hbar c} = -\frac{Z\alpha}{r} \quad -(28)$$

Let:
$$k_1 = \frac{mc^2 + E}{\hbar c}, \quad k_2 = \frac{mc^2 - E}{\hbar c}, \quad \rho = (k_1 k_2)^{1/2} \quad -(29)$$

then
$$\left(\frac{\partial}{\partial \rho} - \frac{\kappa}{\rho} \right) F - \left(\left(\frac{k_2}{k_1} \right)^{1/2} - \frac{Z\alpha}{\rho} \right) G = 0 \quad -(30)$$
$$\left(\frac{\partial}{\partial \rho} + \frac{\kappa}{\rho} \right) G - \left(\left(\frac{k_1}{k_2} \right)^{1/2} + \frac{Z\alpha}{\rho} \right) F = 0 \quad -(31)$$

4) Simultaneous solution of these equations give:

$$E = mc^2 \left(1 + \frac{Z^2 \alpha^2}{(n_r + ((j+1/2)^2 - Z^2\alpha^2)^{1/2})^2} \right) \quad -(32)$$

The Schroedinger equation gives:

$$E = \frac{Z^2 \alpha^2}{n_r^2} \quad -(33)$$

Eq. (32) gives the fine structure of the H atom from the fermion equation (1), Q. E. D.

For more complicated atoms and molecules, computational quantum chemistry has to be applied to eq. (1). The starting equations are (1), (3) and (4), the mathematical transform in eqs (6) and (7) has been used to transform eqn. (1) into the format (13), to which there is a well known solution given in this note.

Note carefully that the solution (32) has been obtained with positive mc^2 and positive:

$$E = (c^2 p^2 + m^2 c^4)^{1/2} \quad -(34)$$