174(1): Direct Solution of the Fermion Equation.

Consider the covariant format of the fermion equation:

$$\hat{\pi}_\mu \phi \sigma^\mu = mc\sigma^1\phi \quad -(1)$$

which is covariant notation for:

$$\hat{\pi}_\mu \phi \sigma^\mu = \sigma^0(\hat{p}_0 \phi \sigma^0) + \sigma^3(\hat{p}_i \phi \sigma^i) = mc\sigma^1\phi. \quad -(2)$$

Eq. (2) is an equation in the matrix eigenfunction:

$$\phi = \begin{bmatrix} \phi_1^R & \phi_2^R \\ \phi_1^L & \phi_2^L \end{bmatrix} \quad -(3)$$

so may be solved as a matrix equation.

Restrict development to the Z axis for clarity and simplicity. Then:

$$\hat{E}\phi\sigma^0 \quad c(\underline{\sigma}\cdot\hat{\underline{p}})(\phi\sigma^3) = mc^2\sigma^1\phi. \quad -(4)$$

If the energy levels of an atom or molecule are sought, then eq. (4) is an equation in which the operator $\underline{\sigma}\cdot\hat{\underline{p}}$ produces the energy levels E:

$$c(\underline{\sigma}\cdot\hat{\underline{p}})(\phi\sigma^3) = (E - e\phi - mc^2\sigma^1)\phi \quad -(5)$$

i.e.

$$c(\underline{\sigma}\cdot\hat{\underline{p}})(\phi\sigma^3) = ((E-\phi)\sigma^0 - mc^2\sigma^1)\phi \quad -(6)$$

in which:

$$\sigma^0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \sigma^1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma^3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad -(7)$$

and

2) $$\underline{\sigma} \cdot \hat{\underline{p}} = \left(\underline{\sigma} \cdot \frac{\underline{r}}{r}\right)\left(\frac{\underline{r}}{r} \cdot \hat{\underline{p}} + i\,\frac{\underline{\sigma} \cdot \hat{\underline{L}}}{r}\right) \quad -(8)$$

The numerical problem is to solve eq. (5) for the energy levels E. The operator $\hat{p}$ is the Schroedinger operator of quantum mechanics:

$$\hat{\underline{p}} = -i\hbar \underline{\nabla} \quad -(9)$$

while E in eq. (6) is regarded as the scalar energy. So:

$$-i\hbar c\, \underline{\sigma} \cdot \underline{\nabla}\left(\phi \sigma^3\right) = \left((E - e\phi)\sigma^0 - mc^2\sigma^1\right)\phi \quad -(10)$$

The potential ϕ is the Coulombic potential between electrons and protons in an atom or molecule. The simplest atom is H, atomic hydrogen, with one electron and one proton. In atomic H:

$$\phi = -\frac{e}{4\pi\epsilon_0 r} \quad -(11)$$

and the potential energy of interaction is:

$$V = e\phi = -\frac{e^2}{4\pi\epsilon_0 r} \quad -(12)$$

in S.I. units.

In order to solve eq. (10) by matrix methods multiply from the right by ϕ^{-1} on both sides:

$$c\left(\underline{\sigma} \cdot \hat{\underline{p}}\right)\left(\phi\sigma^3\right)\phi^{-1} = \left((E - e\phi)\sigma^0 - mc^2\sigma^1\right)\phi\phi^{-1} \quad -(13)$$

Here $$\phi\phi^{-1} = \sigma^0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad -(14)$$

and $$\sigma^0\sigma^0 = \sigma^0 \quad -(15)$$

$$\sigma^1\sigma^0 = \sigma^1. \quad -(16)$$

Therefore eq. (13) is:

$$\boxed{c(\underline{\sigma}\cdot\hat{\underline{p}})(\phi\sigma^3)\phi^{-1} = (E - e\phi)\sigma^0 - mc^2\sigma^1} \quad -(17)$$

This is a relatively simple equation for E, the energy levels of an atom or molecule. The inverse matrix is:

$$\phi^{-1} = \frac{\text{adj }\phi}{\det\phi} \quad -(18)$$

where $$\text{adj }\phi = \begin{bmatrix} \phi_2^L & -\phi_2^R \\ -\phi_1^L & \phi_1^R \end{bmatrix} \quad -(19)$$

$$\det\phi = \phi_1^R\phi_2^L - \phi_2^R\phi_1^L \quad -(20)$$

Therefore:

$$c(\underline{\sigma}\cdot\hat{\underline{p}})(\phi\sigma^3)\phi^{-1} = \frac{c\underline{\sigma}\cdot\underline{p}}{\det\phi}\left(\begin{bmatrix} \phi_1^R & \phi_2^R \\ \phi_1^L & \phi_2^L \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\right)\begin{bmatrix} \phi_2^L & -\phi_2^R \\ -\phi_1^L & \phi_1^R \end{bmatrix} \quad -(21)$$

$$= \frac{c\underline{\sigma}\cdot\hat{\underline{p}}}{\det\phi}\begin{bmatrix} \phi_1^R & -\phi_2^R \\ \phi_1^L & -\phi_2^L \end{bmatrix}\begin{bmatrix} \phi_2^L & -\phi_2^R \\ -\phi_1^L & \phi_1^R \end{bmatrix}$$

$$= \frac{c\underline{\sigma}\cdot\hat{\underline{p}}}{\det\phi}\begin{bmatrix} \phi_1^R\phi_2^L + \phi_2^R\phi_1^L & -(\phi_1^R\phi_2^R + \phi_2^R\phi_1^R) \\ \phi_1^L\phi_2^L + \phi_2^L\phi_1^L & \phi_1^L\phi_2^R + \phi_2^L\phi_1^R \end{bmatrix}$$

4) In eq. (21):

$$\underline{\sigma} \cdot \underline{\hat{p}} = \begin{bmatrix} \hat{p}_2 & 0 \\ 0 & -\hat{p}_2 \end{bmatrix} \quad -(21)$$

$$-(22)$$

Therefore eq. (17) is:

$$c \begin{bmatrix} \hat{p}_2 & 0 \\ 0 & -\hat{p}_2 \end{bmatrix} \begin{bmatrix} A & B \\ C & D \end{bmatrix} = \left(\begin{bmatrix} E - e\phi & 0 \\ 0 & E - e\phi \end{bmatrix} + \begin{bmatrix} 0 & mc^2 \\ mc^2 & 0 \end{bmatrix} \right) \det \phi \quad -(23)$$

where

$$A = \phi_1^R \phi_2^L + \phi_2^R \phi_1^L \quad -(24)$$

$$B = -\left(\phi_1^R \phi_2^R + \phi_2^R \phi_1^R \right) \quad -(25)$$

$$C = \phi_1^L \phi_2^L + \phi_2^L \phi_1^L \quad -(26)$$

$$D = \phi_1^L \phi_2^R + \phi_2^L \phi_1^R .$$

So:

$$c \begin{bmatrix} \hat{p}_2 A & \hat{p}_2 B \\ -\hat{p}_2 C & -\hat{p}_2 D \end{bmatrix} = \begin{bmatrix} E - e\phi & mc^2 \\ mc^2 & E - e\phi \end{bmatrix} \det \phi \quad -(27)$$

i.e.

$$c \hat{p}_2 A = (E - e\phi) \det \phi \quad -(28)$$

$$c \hat{p}_2 B = mc^2 \det \phi \quad -(29)$$

$$-c \hat{p}_2 C = mc^2 \det \phi \quad -(30)$$

$$-c \hat{p}_2 D = (E - e\phi) \det \phi \quad -(31)$$

and so:

$$c \hat{p}_2 (A - B) = (E - e\phi - mc^2) \det \phi \quad -(32)$$

$$-c \hat{p}_2 (D - C) = (E - e\phi - mc^2) \det \phi \quad -(33)$$

5) In eq. (32) for example:

$$c\hat{p}_Z\left(\phi_1^R\phi_2^L+\phi_2^R\phi_1^L+\phi_1^R\phi_2^R+\phi_2^R\phi_1^R\right) = \left(E-e\phi-mc^2\right)\left(\phi_1^R\phi_2^L-\phi_2^R\phi_1^L\right) \quad -(34)$$

i.e.

$$c\hat{p}_Z\left(\phi_1^R\left(\phi_2^L+\phi_2^R\right)+\phi_2^R\left(\phi_1^L+\phi_1^R\right)\right) = \left(E-e\phi-mc^2\right)\left(\phi_1^R\phi_2^L-\phi_2^R\phi_1^L\right) \quad -(35)$$

where

$$\hat{p}_Z = -i\hbar\frac{\partial}{\partial Z}. \quad -(36)$$

Eq. (33) is:

$$c\hat{p}_Z\left(C-D\right) = \left(E-e\phi-mc^2\right)\det\phi \quad -(37)$$

i.e.

$$c\hat{p}_Z\left(\phi_1^L\phi_2^L+\phi_2^L\phi_1^L-\left(\phi_1^L\phi_2^R+\phi_2^L\phi_1^R\right)\right) = \left(E-e\phi-mc^2\right)\left(\phi_1^R\phi_2^L-\phi_2^R\phi_1^L\right) \quad -(38)$$

or

$$c\hat{p}_Z\left(\phi_1^L\left(\phi_2^L-\phi_2^R\right)+\phi_2^L\left(\phi_1^L-\phi_1^R\right)\right) = \left(E-e\phi-mc^2\right)\left(\phi_1^R\phi_2^L-\phi_2^R\phi_1^L\right) \quad -(39)$$

Comparing eqns (35) and (39):

$$c\hat{p}_Z\left(\phi_1^R\left(\phi_2^L+\phi_2^R\right)+\phi_2^R\left(\phi_1^L+\phi_1^R\right)\right) = c\hat{p}_Z\left(\phi_1^L\left(\phi_2^L-\phi_2^R\right)+\phi_2^L\left(\phi_1^L-\phi_1^R\right)\right) \quad -(40)$$

6)

In addition to these equations it is known from eq. (1), via eqs. (5) of note 172(8) that:

$$c\hat{p}_Z \phi_1^R = (E - e\phi)\phi_1^R - mc^2\phi_1^L \quad -(41)$$

$$c\hat{p}_Z \phi_2^R = -(E - e\phi)\phi_2^R + mc^2\phi_2^L \quad -(42)$$

$$c\hat{p}_Z \phi_1^L = -(E - e\phi)\phi_1^L + mc^2\phi_1^R \quad -(43)$$

$$c\hat{p}_Z \phi_2^L = (E - e\phi)\phi_2^L - mc^2\phi_2^R \quad -(44)$$

so it is clear that eqs. (32) and (33) combine eqs. (41) to (44) in a hitherto unknown manner. This new information is given by the fermion equation.

Mathematically, eqs. (41) to (44) are four equations in five unknowns: E, ϕ_1^R, ϕ_2^R, ϕ_1^L and ϕ_2^L. With the new information given by eqs. (28) to (31) there are eight equations in the five unknowns. So the problem can be solved numerically.

Algorithm

Write an algorithm to solve, for example eqs. (41) to (44) with eq. (35). Use ϕ for any atom or molecule.