86(4): Simple Forms of the Dirac Equation for a Free Electron and Atomic H.

In previous notes to paper 86 it was shown that the Dirac equation for a free electron can be written as:

$$\boxed{\frac{1}{c}\frac{\partial\psi_1}{\partial t} + \frac{\partial\psi_3}{\partial Z} = -\frac{imc}{\hbar}\psi_1}, \quad -(1)$$

where:

$$\psi_1 = \psi_1^R + \psi_2^R + \psi_1^L + \psi_2^L, \quad -(2)$$

$$\psi_3 = \psi_1^R - \psi_2^R - \psi_1^L + \psi_2^L, \quad -(3)$$

and where the electron propagates in the Z axis. Here

$$\lambda = \frac{\hbar}{mc} \quad -(4)$$

is the Compton wavelength. Therefore eq. (1) is a simple linear equation in the combination of spinor components shown in eqs. (2) and (3).

For the sake of illustration consider the special case:

$$\psi_1 = \psi_3 \quad -(5)$$

i.e.

$$\psi_2^R = \psi_1^L = 0, \quad -(6)$$

and

$$\psi := \psi_1 = \psi_3 = \psi_1^R + \psi_2^L. \quad -(7)$$

Then eq. (1) simplifies further to:

2)

$$\left(\frac{1}{c} \frac{\partial}{\partial t} + \frac{\partial}{\partial Z} \right) \psi = - \frac{imc}{\hbar} \psi \quad - (8)$$

i.e

$$\boxed{\psi = \exp\left(- \frac{imc^2 t}{2\hbar} \right) \exp\left(- \frac{imc Z}{2\hbar} \right)} \quad - (9)$$

and

$$\psi \psi^* = 1 . \quad - (10)$$

If it is considered that:

$$\frac{Z}{t} = c \quad - (11)$$

then

$$2 \frac{\partial \psi}{\partial Z} = - \frac{imc}{\hbar} \psi$$

i.e

$$\boxed{\frac{\partial \psi}{\partial Z} = - \frac{imc}{2\hbar} \psi} \quad - (12)$$

or

$$\boxed{\frac{\partial \psi}{\partial t} = - \frac{imc^2}{2\hbar} \psi} \quad - (13)$$

Eq (13) is:

$$\boxed{i \frac{\partial \psi}{\partial t} = \frac{mc^2}{2\hbar} \psi = H \psi} \quad - (14)$$

where

$$H = \frac{mc^2}{2\hbar} .$$

3) which is the same form as the time-dependent Schrödinger equation. Therefore eq. (1) is the correctly relativistic form of the time dependent Schrödinger equation for a free electron moving in Z

H Atom Calculation

The Dirac equation for the H atom is:

$$\left(i\gamma^\mu \partial_\mu - \frac{mc}{\hbar} - \frac{\alpha}{r} \right) \psi_D = 0 \, ; \quad \psi_D = \begin{bmatrix} \psi_1^R \\ \psi_2^R \\ \psi_1^L \\ \psi_2^L \end{bmatrix} \quad -$$

which is:

$$\boxed{ i\gamma^\mu \partial_\mu \psi_D = \left(\frac{mc}{\hbar} + \frac{\alpha}{r} \right) \psi_D } \quad -(16)$$

where

$$r = \left(X^2 + Y^2 + Z^2 \right)^{1/2} \quad -(17)$$

and

$$\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c} \quad -(18)$$

is the fine structure constant. Eq (16) describes the relativistic interaction of a spin half electron with a spin half proton. This picture gives the atomic spectrum of H except for the Lamb shift. The latter is introduced by:

4)

$$\gamma^\mu \rightarrow \gamma^\mu\left(1+\frac{\alpha}{4\pi}\right) \quad -(19)$$

as in paper 85, when the Schrödinger equation was used. So this radiative correction gives:

$$\boxed{i\gamma^\mu\left(1+\frac{\alpha}{4\pi}\right)\partial_\mu \psi_{D1} = \left(\frac{mc}{\hbar}+\frac{\alpha}{r}\right)\psi_{D1}} \quad -(20)$$

It is known that the Lamb shift affects the 2s and 2p orbitals by only about two parts in ten million. Without a radiative correction, eq. (16) gives:

$$E_n(2s_{1/2}) = E_n(2p_{1/2}) \quad -(21)$$

and after the radiative correction:

$$E_n(2s_{1/2}) > E_n(2p_{1/2}) \quad -(22)$$

by about 0.03 cm^{-1}. So to a very good approximation:

$$\psi_{D1} = \psi_D. \quad -(23)$$

We now proceed as in paper 85 by realizing that the radiative correction is equivalent to a very tiny shift in r. This shift is denoted r(vac), defined by:

$$i\frac{\alpha}{4\pi}\gamma^\mu\partial_\mu\psi_D := -\frac{\alpha}{r(vac)}\psi_D \quad -(24)$$

because r(vac) has the effect:

5) $$-\frac{\alpha}{r} \rightarrow -\frac{\alpha}{r} + \frac{\alpha}{r(vac)} \qquad (25)$$

i.e. makes the Coulomb attraction energy less negative. This has the effect of increasing the total energy of $2S_{1/2}$ slightly more than increasing the total energy of $2P_{1/2}$, as observed.

So eq. (24) is:

$$\boxed{\gamma^\mu \partial_\mu \psi_D = -\frac{4\pi}{r(vac)} \psi_D} \qquad (26)$$

where ψ_D are the Dirac orbitals of the H atom without radiative corrections. These are very complicated (Metzbacher) but are known.

Computer Algebra Task.

Use the analytically known ψ_D in eq. (26) to find $r(vac)$ for $2S_{1/2}$ and $2P_{1/2}$. This is the relativistically correct Lamb shift.

Preliminary Hand Calculation

Eq. (16) can be simplified in a hand calculation as follows. This is helpful in revealing the structure of the Dirac equation of the H atom.

6)

Denote:

$$A := \frac{mc}{\hbar} + \frac{\alpha}{r} \quad -(27)$$

and use in eq. (16) the definitions of the Dirac matrices given in notes for paper 85. Thus

$$\frac{1}{c}\begin{bmatrix} 0&0&0&1\\ 0&0&1&0\\ 0&1&0&0\\ 1&0&0&0 \end{bmatrix}\frac{\partial\psi_D}{\partial t} + \begin{bmatrix} 0&0&0&-1\\ 0&0&-1&0\\ 0&1&0&0\\ 1&0&0&0 \end{bmatrix}\frac{\partial\psi_D}{\partial X} + \begin{bmatrix} 0&0&0&i\\ 0&0&-i&0\\ 0&-i&0&0\\ i&0&0&0 \end{bmatrix}\frac{\partial\psi_D}{\partial Y} + \begin{bmatrix} 0&0&-1&0\\ 0&0&0&1\\ 1&0&0&0\\ 0&-1&0&0 \end{bmatrix}\frac{\partial\psi_D}{\partial Z}$$

$$= -iA\begin{bmatrix} 1&0&0&0\\ 0&1&0&0\\ 0&0&1&0\\ 0&0&0&1 \end{bmatrix}\psi_D \quad -(28)$$

i.e.

$$\frac{1}{c}\frac{\partial\psi_2^L}{\partial t} - \frac{\partial\psi_2^L}{\partial X} + i\frac{\partial\psi_2^L}{\partial Y} - \frac{\partial\psi_1^L}{\partial Z} = -iA\psi_1^R \quad -(29)$$

$$\frac{1}{c}\frac{\partial\psi_1^L}{\partial t} - \frac{\partial\psi_1^L}{\partial X} - i\frac{\partial\psi_1^L}{\partial Y} + \frac{\partial\psi_2^L}{\partial Z} = -iA\psi_2^R \quad -(30)$$

$$\frac{1}{c}\frac{\partial\psi_2^R}{\partial t} + \frac{\partial\psi_2^R}{\partial X} - i\frac{\partial\psi_2^R}{\partial Y} + \frac{\partial\psi_1^R}{\partial Z} = -iA\psi_1^L \quad -(31)$$

$$\frac{1}{c}\frac{\partial\psi_1^R}{\partial t} + \frac{\partial\psi_1^R}{\partial X} + i\frac{\partial\psi_1^R}{\partial Y} - \frac{\partial\psi_2^R}{\partial Z} = -iA\psi_2^L \quad -(32)$$

Adding eqs (29) to (32):

$$\boxed{\frac{1}{c}\frac{\partial\psi_1}{\partial t} + \frac{\partial\psi_2}{\partial X} + \left(i\frac{\partial}{\partial Y} + \frac{\partial}{\partial Z}\right)\psi_3 = -iA\psi_1 \quad -(33)}$$

Where:

$$\psi_1 = \psi_1^R + \psi_2^R + \psi_1^L + \psi_2^L \quad -(34)$$

$$\psi_2 = \psi_1^R + \psi_2^R - \psi_1^L - \psi_2^L \quad -(35)$$

$$\psi_3 = \psi_1^R - \psi_2^R - \psi_1^L + \psi_2^L . \quad -(36)$$

In general:

$$A = \frac{mc}{\hbar} + \frac{\alpha}{(x^2+y^2+Z^2)^{1/2}} \quad -(37)$$

For the sake of illustration only consider:

$$A = \frac{mc}{\hbar} + \frac{\alpha}{Z} \quad -(38)$$

then:

$$\frac{1}{c}\frac{\partial\psi_1}{\partial t} + \frac{\partial\psi_3}{\partial Z} + i\frac{mc}{\hbar}\psi_1 = -i\frac{\alpha}{Z}\psi_1 . \quad -(39)$$

Assume:

$$\psi = \psi_1 = \psi_3 \quad -(40)$$

then:

$$\left(\frac{1}{c}\frac{\partial}{\partial t} + \frac{\partial}{\partial Z} + i\frac{mc}{\hbar}\right)\psi = -i\frac{\alpha}{Z}\psi . \quad -(41)$$

If

$$c = \frac{Z}{t} \quad -(42)$$

then:

$$\frac{\partial\psi}{\partial Z} + i\frac{mc}{2\hbar}\psi = -i\frac{\alpha}{2Z}\psi$$

or

$$\boxed{i\frac{\partial\psi}{\partial Z} = \frac{1}{2}\left(\frac{mc}{\hbar} + \frac{\alpha}{Z}\right)\psi} \quad -(42)$$

8) This is the relativistic form of a time-dependent Schrödinger equation:

$$\boxed{i\frac{\partial\psi}{\partial t} = \frac{1}{2}\left(\frac{mc^2}{\hbar} + \alpha\frac{c}{Z}\right)\psi = H\psi} \quad -(43)$$

Compare this with eq. (14) for the free electron:

$$i\frac{\partial\psi_0}{\partial t} = \frac{mc^2}{2\hbar}\psi_0 \quad -(44)$$

where

$$\psi_0 = \exp\left(-i\frac{mc^2}{2\hbar}t\right) \quad -(45)$$

The solution of eq. (43) will be:

$$\psi = \psi_0\psi_1 \quad -(46)$$

where ψ_1 is to be determined. If eq. (46) is used in eq. (43):

$$i\frac{\partial}{\partial t}(\psi_0\psi_1) = \frac{1}{2}\left(\frac{mc^2}{\hbar} + \frac{\alpha}{t_0}\right)(\psi_0\psi_1)$$

$$= i\left(\psi_1\frac{\partial\psi_0}{\partial t} + \psi_0\frac{\partial\psi_1}{\partial t}\right) \quad -(47)$$

Using eq. (44):

$$i\frac{\partial\psi_1}{\partial t} = \frac{\alpha}{2t}\psi_1 \quad -(48)$$

9)

i.e.

$$\frac{\partial \phi_1}{\partial t} = -\frac{ia}{t_o}\phi_1 \quad -(49)$$

where:

$$a = \frac{\alpha}{2} \quad -(50)$$

Therefore:

$$\boxed{\phi_1 = \log_e\left(-ia\frac{t}{t_o}\right)} \quad -(51)$$

and:

$$\phi = \exp\left(-\frac{imc^2}{\partial \hbar}t\right)\log_e\left(-i\frac{\alpha}{2}\frac{t}{t_o}\right) \quad -(52)$$

where t_o is a characteristic time:

$$t_o := \frac{Z_o}{c} \quad -(53)$$

If:

$$1+y := -i\frac{\alpha}{2}\frac{t}{t_o},$$

$$y = -\left(1 + i\frac{\alpha}{2}\frac{t}{t_o}\right)$$

then:

$$\log_e(1+y) = y - \frac{y^2}{2} + \frac{y^3}{3} - \frac{y^4}{4} + \dots$$

$$|y| < 1;$$

so:

$$\log_e\left(-i\frac{\alpha}{2}\frac{t}{t_o}\right) = \frac{1}{2}\left(1 + i\frac{\alpha}{2}\frac{t}{t_o}\right)^2$$

$$-\left(1 + i\frac{\alpha}{2}\frac{t}{t_o}\right) + \dots$$

10)

$$\text{Real}\left(\log_e\left(-\frac{i\alpha}{2}\frac{t}{t_0}\right)\right)$$

$$= -1 + \frac{1}{2} - \frac{\alpha}{4}\left(\frac{t}{t_0}\right)^2 + \cdots$$

$$= -\left(\frac{1}{2} + \frac{\alpha}{4}\left(\frac{t}{t_0}\right)^2\right) + \cdots \quad -(54)$$

and :

$$\phi = e^{-imc^2t/(2\hbar)}\left(-\left(1+i\frac{\alpha}{2}\frac{t}{t_0}\right) + \frac{1}{2}\left(1+i\frac{\alpha}{2}\frac{t}{t_0}\right)^2 + \cdots\right)$$

$$= \left(\cos\left(\frac{mc^2t}{2\hbar}\right) + i\sin\left(\frac{mc^2t}{2\hbar}\right)\right)\left(-\frac{1}{2} - \frac{\alpha^2}{4}\left(\frac{t}{t_0}\right)^2 + \cdots\right)$$

$$\boxed{\text{Real}\,\phi = -\frac{1}{2}\left(1+\frac{\alpha^2}{2}\left(\frac{t}{t_0}\right)^2 + \cdots\right)\cos\left(\frac{mc^2t}{2\hbar}\right)} \quad -(55)$$

i.e.

$$\boxed{\text{Real}\,\phi = -\frac{1}{2}\left(1+\frac{\alpha^2c^2}{2}\left(\frac{t}{\tau_0}\right)^2 + \cdots\right)\cos\left(\frac{mc^2t}{2\hbar}\right)} \quad -(56)$$

and as $\tau_0 \to \infty$ this becomes the real part of the free electron wave function.