

174(2) : Details of the Solution of the Dirac Equation for the Hydrogen Atom.

The Dirac equation produces the correct Lorentz transform of the right and left Pauli spinors, whereas the standard Dirac equation does not. The Dirac equation is therefore the correct equation in physics. The Dirac eqn. may be written as:

$$(\hat{E} - e\phi + c\vec{\sigma} \cdot \vec{p}) \phi^L = mc^2 \phi^R \quad (1)$$

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

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

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

Eqs (1) and (2) imply that under the Lorentz transform:

$$\phi^R \rightarrow \exp\left(\frac{1}{2} \vec{\sigma} \cdot \vec{\phi}\right) \phi^R \quad (4)$$

$$\phi^L \rightarrow \exp\left(-\frac{1}{2} \vec{\sigma} \cdot \vec{\phi}\right) \phi^L \quad (5)$$

(L. H. Ryder, "Quantum Field Theory" (C.U.P., 1996, 2nd. ed.) pp. 41 ff.)

It is clear that the eigenvalues mc^2 are always positive.

In the hydrogen atom, ϕ is the Coulomb potential between electron and proton. The energy levels E of the H atom are found by solving eqs. (1) and (2) simultaneously. It is instructive to give

2) the details of this calculation as follows. The basis are found in:

E. Merzbacher, "Quantum Mechanics" (Wiley, 2nd. ed., 1970), pp. 603 ff.

and we collected here for ease of reference.

First note that both $\underline{\sigma}$ and \underline{p} are operators.

First use:

$$\underline{\sigma} \cdot \underline{p} = \underline{\sigma} \cdot \frac{\underline{r}}{r} \left(\frac{r}{r} \cdot \underline{p} + i \frac{\underline{\sigma} \cdot \underline{L}}{r} \right) \quad - (6)$$

where $\frac{r}{r} \cdot \underline{p} = \frac{\hbar}{i} \frac{\partial}{\partial r} \quad - (7)$

Note that: $\underline{\sigma} \cdot \frac{\underline{r}}{r} Y_{j \pm \frac{1}{2}}^{jm} = - Y_{j \pm \frac{1}{2}}^{jm} \quad - (8)$

because $\underline{\sigma} \cdot \underline{r}$ is a pseudo-scalar. In the eigen-equation (8) the eigenfunctions are defined by Clebsch-Gordan coefficients. Next note that:

$$\underline{\sigma} \cdot \underline{L} Y_{j - \frac{1}{2}}^{jm} = (j - \frac{1}{2}) Y_{j - \frac{1}{2}}^{jm} \quad - (9)$$

$$\underline{\sigma} \cdot \underline{L} Y_{j + \frac{1}{2}}^{jm} = - (j + \frac{3}{2}) Y_{j + \frac{1}{2}}^{jm} \quad - (10)$$

and that:

$$\left(L^2 + \hbar \underline{L} \cdot \underline{\sigma} + \frac{3}{4} \hbar^2 \right) \begin{bmatrix} \phi^R \\ \phi^L \end{bmatrix} = j(j+1) \hbar^2 \begin{bmatrix} \phi^R \\ \phi^L \end{bmatrix} \quad - (11)$$

$$\left(L_z + \frac{1}{2} \hbar \sigma_z \right) \begin{bmatrix} \phi^R \\ \phi^L \end{bmatrix} = m \hbar \begin{bmatrix} \phi^R \\ \phi^L \end{bmatrix} \quad - (12)$$

Eqs. (1) and (2) may be solved by noting that

$$\phi^L = \phi_S^R + \phi_S^L \quad - (13)$$

$$\phi^R = \phi_S^R - \phi_S^L \quad - (14)$$

where:

$$\phi_S^R = F(r) Y_{j-1/2}^{jm} \quad - (15)$$

$$\phi_S^L = -i f(r) Y_{j+1/2}^{jm} \quad - (16)$$

The physically meaningful wave functions are:

$$\phi^L = F(r) Y_{j-1/2}^{jm} - i f(r) Y_{j+1/2}^{jm} \quad - (17)$$

and $\phi^R = F(r) Y_{j-1/2}^{jm} + i f(r) Y_{j+1/2}^{jm} \quad - (18)$

and are complex conjugates.

If the correct wave function (17) and (18) are used, the energy is always positive.

The operators are worked out as follows:

$$\underline{\sigma} \cdot \underline{\hat{p}} \phi_S^L = \underline{\sigma} \cdot \underline{\frac{r}{r}} \left(\underline{\frac{r}{r}} \cdot \underline{\hat{p}} + i \underline{\underline{\underline{\sigma} \cdot \underline{L}}}}{\underline{r}} \right) \phi_S^L \quad - (19)$$

and so on. \underline{L} eq. (19):

$$\underline{\sigma} \cdot \underline{\frac{r}{r}} \underline{\frac{r}{r}} \cdot \underline{\hat{p}} \phi_S^L = -i \hbar \frac{d}{dr} \left(\underline{\underline{\underline{\sigma} \cdot \underline{r}}}}{\underline{r}} \phi_S^L \right) \quad - (20)$$

where $\underline{\sigma} \cdot \underline{\frac{r}{r}} \phi_S^L = -i f(r) \underline{\underline{\underline{\sigma} \cdot \underline{r}}}}{\underline{r}} Y_{j+1/2}^{jm}$

$$= i f(r) Y_{j-1/2}^{jm} \quad - (21)$$

So: $\underline{\sigma} \cdot \underline{\frac{r}{r}} \underline{\frac{r}{r}} \cdot \underline{\hat{p}} \phi_S^L = \hbar \frac{df}{dr} Y_{j-1/2}^{jm} \quad - (22)$

Similarly:

$$\begin{aligned}
 & i \left(\underline{\sigma} \cdot \underline{\frac{r}{r}} \right) \left(\underline{\sigma} \cdot \underline{\hat{L}} \right) \left(-i f(r) Y_{j+\frac{1}{2}}^{jm} \right) \\
 &= -i \left(\underline{\sigma} \cdot \underline{\frac{r}{r}} \right) f(r) \left(j + \frac{3}{2} \right) Y_{j+\frac{1}{2}}^{jm} \\
 &= \hbar \left(j + \frac{3}{2} \right) f(r) Y_{j-\frac{1}{2}}^{jm} \quad - (23)
 \end{aligned}$$

Therefore:

$$c \underline{\sigma} \cdot \underline{\hat{p}} \phi_S^L = \hbar c \left(\frac{d}{dr} + \frac{j + 3/2}{r} \right) f(r) Y_{j-\frac{1}{2}}^{jm} \quad - (24)$$

and so on. With the transform (13) and (14), eqns (1)

and (2) become:

$$(E - mc^2 - e\phi) \phi_S^R = c \underline{\sigma} \cdot \underline{\hat{p}} \phi_S^L \quad - (25)$$

$$(E + mc^2 - e\phi) \phi_S^L = c \underline{\sigma} \cdot \underline{\hat{p}} \phi_S^R, \quad - (26)$$

with the physical wave functions (17) and (18). Note carefully that the Lorentz transform (4) and (5) give eqns. (1) and (2) and that eqns. (25) and (26) are the result of a mathematical transform made in order to solve eqns. (1) and (2). - (27)

(2). Eqs. (25) and (26) give:

$$(E + mc^2 - e\phi) f(r) + \hbar c \left(\frac{d}{dr} - \frac{j - \frac{1}{2}}{r} \right) F(r) = 0$$

$$(E - mc^2 - e\phi) F(r) - \hbar c \left(\frac{d}{dr} + \frac{j + 3/2}{r} \right) f(r) = 0 \quad - (28)$$

which may be solved for E in an approximation.

5) Using computers eqs. (27) and (28) may be solved to machine precision for E .

The result of the analytical solution is:

$$E = mc^2 \left(1 + \frac{(Zd)^2}{\left(\left(\left(j + \frac{1}{2} \right)^2 - (Zd)^2 \right)^{1/2} + n' \right)^2} \right)^{-1/2},$$

where $d = e^2 / (4\pi\epsilon_0 \hbar c)$, -(29)

where $n' = n - \left(j + \frac{1}{2} \right)$, -(30)

and $j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$ -(31)

$n' = 0, 1, 2, \dots$ -(32)

Here n is the principal quantum number in the non-relativistic theory of the H atom. Here:

$$\phi = -\frac{Ze}{r} \quad \text{--- (33)}$$

$$\text{--- (34)}$$

Eq. (29) is approximately:

$$E = mc^2 \left(1 - \frac{Z^2 e^4}{2n^2 d^2} - \frac{(Z^2 e^4)^2}{2n^4 d^4} \left(\frac{n}{j + \frac{1}{2}} - \frac{3}{4} \right) + \dots \right)$$

The non-relativistic result is:

$$E = -\frac{Z^2 e^4 mc^2}{2n^2 d^2} \quad \text{--- (35)}$$

$$= -\left(\frac{me^4}{32\pi^2 \epsilon_0^2 \hbar^2} \right) \frac{1}{n^2} \quad \text{--- (36)}$$

6) The $1S_{1/2}$ state is $n=1, l=0, j=1/2$,
 and $E(1S_{1/2}) = mc^2 \left(1 - \frac{Z^2 e^4}{d^2}\right) - (37)$
 The $2S_{1/2}$ state is $n=2, l=0, j=1/2$, and the
 $2P_{1/2}$ state is $n=2, l=1, j=1/2$, with the same
 energy: $E(2S_{1/2}) = E(2P_{1/2}) = \frac{mc^2}{\sqrt{2}} \left(1 + \left(1 - \frac{Z^2 e^4}{d^2}\right)^{1/2}\right)^{1/2} - (38)$

The radiative corrections cause the Lamb shift
 between $2S_{1/2}$ and $2P_{1/2}$.

Conclusion The well known results are given by
 the Dirac equation:
 $\nabla_\mu \psi = m c \sigma^\mu \psi - (39)$
 by expanding it into eqs (1) and (2). The
 wave function is:

$$\psi = \begin{bmatrix} \psi_1^R & \psi_2^R \\ \psi_1^L & \psi_2^L \end{bmatrix} - (40)$$

and the Pauli spinors are:

$$\phi^L = \begin{bmatrix} \psi_1^L \\ \psi_2^L \end{bmatrix} = F(r) Y_{j-\frac{1}{2}}^{jm} - i f(r) Y_{j+\frac{1}{2}}^{jm} - (41)$$

$$\phi^R = \begin{bmatrix} \psi_1^R \\ \psi_2^R \end{bmatrix} = F(r) Y_{j-\frac{1}{2}}^{jm} + i f(r) Y_{j+\frac{1}{2}}^{jm} - (42)$$