

174(6): Angular part of the wavefunction from the Fermi equation for Atomic H.

We use the ket notation, which is related to the spherical harmonic notation as follows:

$$|j m; l+\rangle = Y_{j+\frac{1}{2}}^{jm} \quad - (1)$$

$$|j m; l-\rangle = Y_{j-\frac{1}{2}}^{jm} \quad - (2)$$

where $l_{\pm} = j \pm \frac{1}{2} \quad - (3)$

The basic problem is to solve:

$$\left(\hat{L}_z + \frac{\hbar}{2} \hat{\sigma}_z \right) \begin{bmatrix} \phi_s^R \\ \phi_s^L \end{bmatrix} = m \hbar \begin{bmatrix} \phi_s^R \\ \phi_s^L \end{bmatrix} \quad - (4)$$

and $\left(\hat{L}^2 + \hbar \hat{L} \cdot \hat{\sigma} + \frac{3}{4} \hbar^2 \right) \begin{bmatrix} \phi_s^R \\ \phi_s^L \end{bmatrix} = j(j+1) \hbar^2 \begin{bmatrix} \phi_s^R \\ \phi_s^L \end{bmatrix} \quad - (5)$

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

$$j = j_1 + j_2, j_1 + j_2 - 1, \dots, |j_1 - j_2| \quad - (6)$$

$$m_j = m_{j1} + m_{j2} \quad - (7)$$

where $j_2 = \frac{1}{2} \quad - (8)$

then $j = l + \frac{1}{2} \text{ or } l - \frac{1}{2} \quad - (9)$

which is eq. (3).

2) We have:

$$\underline{\hat{\sigma}} \cdot \underline{\underline{r}} |j m; l_{\pm}\rangle = \dots - |j m; l_{\mp}\rangle$$

so the pseudoscalar operator $\underline{\hat{\sigma}} \cdot \underline{\underline{r}} / r$ (10) changes the spin of the electron from half to minus half.

Furthermore:

$$\underline{\hat{\sigma}} \cdot \underline{\underline{L}} |j m; l_{+}\rangle = -(l_{+} + 1) |j m; l_{+}\rangle \quad (11)$$

$$\text{and } \underline{\hat{\sigma}} \cdot \underline{\underline{L}} |j m; l_{-}\rangle = l_{-} |j m; l_{-}\rangle. \quad (12)$$

These results imply that:

$$\begin{aligned} \underline{\underline{L}} \cdot \underline{\underline{S}} |j m; l\rangle &= \underline{\underline{L}} \cdot \underline{\underline{S}} |n l s; j m\rangle \\ &= \frac{1}{2} \hbar^2 (j(j+1) - l(l+1) - s(s+1)) |j m; l\rangle \end{aligned} \quad (13)$$

$$\text{where: } \underline{\underline{S}} = \frac{1}{2} \hbar \underline{\hat{\sigma}} \quad (14)$$

Proof If $l_{-} = j - \frac{1}{2} \quad (15)$

then $s = -\frac{1}{2} \quad (16)$

so:

$$\begin{aligned} j(j+1) - l(l+1) - s(s-1) \\ = j(j+1) - (j - \frac{1}{2})(j + \frac{1}{2}) - \frac{3}{4} \end{aligned}$$

$$3) = j^2 + j - j^2 + \frac{1}{4} - \frac{3}{4} \\ = j - \frac{1}{2} = l - \quad - (17)$$

(Q.E.D.) Similarly, if

$$l = j + \frac{1}{2} \quad - (18)$$

then

$$s = \frac{1}{2} \quad - (19)$$

and

$$j(j+1) - l(l+1) - s(s+1) = j(j+1) - (j + \frac{1}{2})(j + \frac{3}{2}) - \frac{3}{4} \\ = j^2 + j - j^2 - 2j - \frac{3}{4} - \frac{3}{4} \\ = -j - \frac{3}{2} = -(j + \frac{1}{2} + 1) \\ = -(l + 1) \quad - (20)$$

(Q.E.D.) The following operator identity applies:

$$\underline{\hat{\sigma}} \cdot \underline{\hat{p}} = \underline{\hat{\sigma}} \cdot \frac{\underline{r}}{r} \left(\frac{\underline{r}}{r} \cdot \underline{\hat{p}} + i \frac{\underline{\hat{\sigma}} \cdot \underline{\hat{L}}}{r} \right) \quad - (21)$$

$$\text{i.e. } \underline{\hat{\sigma}} \cdot \underline{\hat{p}} = \underline{\hat{\sigma}} \cdot \frac{\underline{r}}{r} \left(-i\hbar \frac{\partial}{\partial r} + i \frac{\underline{\hat{\sigma}} \cdot \underline{\hat{L}}}{r} \right) \quad - (22)$$

Now consider the fermion equation in the

form:

$$\phi^R = \exp \left(\frac{1}{2} \underline{\hat{\sigma}} \cdot \underline{\phi} \right) \phi^R(0) \quad - (23)$$

$$\phi^L = \exp \left(-\frac{1}{2} \underline{\hat{\sigma}} \cdot \underline{\phi} \right) \phi^L(0) \quad - (24)$$

which are the Lorentz transforms of the right and left Pauli spinors. Eqs. (23) and (24) imply:

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

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

where:

$$\begin{aligned} \phi^R &= \phi_S^R - \phi_S^L \\ \phi^L &= \phi_S^R + \phi_S^L \end{aligned} \quad - (27)$$

Clearly, ϕ^R and ϕ^L are the physically meaningful wave functions because in eqs. (25) and (26) the rest energy is positive:

$$E_0 = mc^2 \quad - (28)$$

In ket notation:

$$\phi_S^R = |j m; l_- \rangle \quad - (29)$$

$$\phi_S^L = |j m; l_+ \rangle \quad - (30)$$

so:

$$\begin{aligned} \phi^R &= |j m; l_- \rangle - |j m; l_+ \rangle \\ \phi^L &= |j m; l_- \rangle + |j m; l_+ \rangle \end{aligned} \quad - (31)$$

with

$$\int \phi_S^\dagger \phi_S d^3x = 1 \quad - (32)$$

note that

$$\phi_S^R = \begin{bmatrix} \psi_{S1}^R \\ \psi_{S2}^R \end{bmatrix}, \quad \phi_S^L = \begin{bmatrix} \psi_{S1}^L \\ \psi_{S2}^L \end{bmatrix} \quad - (33)$$

5) and

$$\phi_s = \begin{bmatrix} \phi_s^R \\ \phi_s^L \end{bmatrix} \quad (34)$$

$$\phi_s^\dagger = \begin{bmatrix} \phi_s^{R*} & \phi_s^{L*} \end{bmatrix} \quad (35)$$

so

$$\int \left(\phi_{s1}^{R*} \phi_{s1}^R + \dots + \phi_{s2}^{L*} \phi_{s2}^L \right) d^3x = 1 \quad (36)$$

and

From eqs. (31) and (33):

$$\begin{aligned} \phi_1^R &= \phi_1^R(r) \left(|jm; l-\rangle - |jm; l+\rangle \right) \\ \phi_2^R &= \phi_2^R(r) \left(|jm; l-\rangle - |jm; l+\rangle \right) \\ \phi_1^L &= \phi_1^L(r) \left(|jm; l-\rangle + |jm; l+\rangle \right) \\ \phi_2^L &= \phi_2^L(r) \left(|jm; l-\rangle + |jm; l+\rangle \right) \end{aligned} \quad (37)$$

Physical Interpretation

In order for the fundamental Lorentz transforms (23) and (24) to be obeyed correctly, the wave functions in the H atom must be the combinations (37). These are combinations of spin up and spin down states of the electron. Keeping the energy the same implies these combinations. The eigen equation for $\vec{L} \cdot \vec{S}$ is always eq. (13), giving the energy levels E_n as in note 174(4). The combination in eq. (37) are always of different spin states of the electron.