1) 174(4): Non-Relativistic Approximations of the Fermion Equation for the H Atom.

Consider the non-relativistic approximation:

$$\hat{H}\phi^R = E\phi^R \quad -(1)$$

where E are atomic energy levels to be determined. Here

$$\hat{H} = mc^2 + e\phi + \frac{1}{2m}\underline{\hat{\sigma}}\cdot\underline{\hat{p}}\,\underline{\hat{\sigma}}\cdot\underline{\hat{p}} - \frac{e\hbar}{2m}\underline{\sigma}\cdot\underline{B}$$

$$- \frac{e}{4m^2c^2}\underline{\sigma}\cdot(\underline{\hat{p}} - e\underline{A})\,\phi\,\underline{\sigma}\cdot(\underline{\hat{p}} - e\underline{A})$$

$$+ \dots \quad -(2)$$

as in previous notes. We also have:

$$\hat{H}\phi^L = E\phi^L \quad -(3)$$

so

$$\hat{H}\phi = E\phi \quad -(4)$$

where

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

is the fermion spinor.

In this approximation:

$$E \longrightarrow mc^2 \quad -(6)$$

where

$$E = \gamma mc^2, \quad -(7)$$

$$\gamma = \left(1 - \frac{v^2}{c^2}\right)^{-1/2}. \quad -(8)$$

Rewrite eq. (1) as: $-(9)$

$$\hat{H}_1\phi = (E - mc^2 - e\phi)\phi$$

where:

$$\hat{H}_1 = \frac{1}{2m}\,\hat{\underline{\sigma}}\cdot\hat{\underline{p}}\;\hat{\underline{\sigma}}\cdot\hat{\underline{p}} - \frac{e\hbar}{2m}\,\underline{\sigma}\cdot\underline{B}$$

$$- \frac{e}{4m^2c^2}\,\hat{\underline{\sigma}}\cdot\left(\hat{\underline{p}} - e\underline{A}\right)\phi\;\hat{\underline{\sigma}}\cdot\left(\hat{\underline{p}} - e\underline{A}\right)$$

$$+ \cdots \qquad -(10)$$

$$:= \hat{H}_2 + \hat{H}_3 + \hat{H}_4 \qquad -(11)$$

Consider the eigenequation for $\hat{H}_2$:

$$\frac{1}{2m}\,\hat{\underline{\sigma}}\cdot\hat{\underline{p}}\;\underline{\sigma}\cdot\hat{\underline{p}}\;\phi = \left(E - mc^2 - e\phi\right)\phi \qquad -(12)$$

In the non-relativistic limit:

$$E - mc^2 = \gamma mc^2 - mc^2 \qquad -(13)$$

$$= \left(1 - \frac{v^2}{c^2}\right)^{-1/2} mc^2 - mc^2$$

goes to:

$$E - mc^2 \rightarrow T = \left(1 + \frac{1}{2}\frac{v^2}{c^2}\right)mc^2 - mc^2$$

$$= \frac{1}{2}mv^2 \qquad -(14)$$

where

$$T = \frac{1}{2}mv^2 \qquad -(15)$$

is the non-relativistic kinetic energy. So eq. (12) reduces to the Schroedinger equation:

$$\frac{\hat{p}^2}{2m}\phi = -\frac{\hbar^2}{2m}\nabla^2\phi = E_0\,\phi \qquad -(16)$$

where

$$E_0 = T - e\phi = T + V \qquad -(17)$$

3) The Schroedinger equation (16) produces the main features of the spectrum of H.

Now use in eq. (12):

$$\underline{\hat{\sigma}} \cdot \underline{\hat{p}}\, \underline{\hat{\sigma}} \cdot \underline{\hat{p}} = -\hbar^2 \frac{\partial^2}{\partial r^2} - \frac{\hat{L}^2}{r^2} + \frac{\hbar}{r^2}\, \underline{\hat{\sigma}} \cdot \underline{\hat{L}} \quad -(18)$$

in which:

$$\hat{L}^2 \phi^R = \hbar^2 \left(j - \frac{1}{2}\right)\left(j - \frac{1}{2} + 1\right) \phi^R \quad -(19)$$

$$\hat{L}^2 \phi^L = \hbar^2 \left(j + \frac{1}{2}\right)\left(j + \frac{1}{2} + 1\right) \phi^L \quad -(20)$$

where

$$l_- = j - \frac{1}{2} \quad -(21)$$

$$l_+ = j + \frac{1}{2} \quad -(22)$$

The first two terms on the right hand side of the Schroedinger equation, eq. (18) are present in the H but the third term gives the fine structure of the atom. If we denote:

$$\underline{\hat{S}} = \frac{1}{2}\hbar \underline{\hat{\sigma}} \quad -(23)$$

and the wave function in ket notation, $|nls; jm_j\rangle$, then:

$$\underline{\hat{L}} \cdot \underline{\hat{S}}\, |nls; jm_j\rangle = \frac{1}{2}\left(\hat{J}^2 - \hat{L}^2 - \hat{S}^2\right)|nls; jm_j\rangle \quad -(24)$$

$$= \frac{1}{2}\hbar^2 \left[j(j+1) - l(l+1) - s(s+1) \right] |nls; jm_j\rangle$$

and this gives all the details of the H atom's fine structure.

4) As in previous notes the hamiltonian $\hat{H}_3$ gives the $g = 2$ or Landé factor and $\hat{H}_4$ is the spin-orbit hamiltonian:

$$\hat{H}_4 = -\frac{e^2}{8\pi\epsilon_0 m^2 c^2 r^3} \underline{\hat{S}} \cdot \underline{\hat{L}} \quad -(25)$$

$$+ \ldots\ldots$$

The evaluation of the radial integral in the non-relativistic approximation for atomic H gives:

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{a_0^3}{n^3 l (l+\frac{1}{2})(l+1)} \quad -(26)$$

where the Bohr radius is:

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m e^4} \quad -(27)$$

Denote:

$$\zeta_{nl} := \frac{e^2}{8\pi\epsilon_0 m^2 c^2} \cdot \frac{1}{a_0^3} \cdot \frac{1}{n^3 l (l+\frac{1}{2})(l+1)\hbar c} \quad -(28)$$

then the energy levels of the H atom are:

$$E_{so} = \frac{1}{2}\hbar^2 \left[j(j+1) - l(l+1) - s(s+1) \right] . \quad -(29)$$

$$\langle nls; jm_j | \xi(r) | nls; jm_j \rangle$$

$$= \frac{1}{2}\hbar c\, \zeta_{nl} \left[j(j+1) - l(l+1) - s(s+1) \right]$$

where

$$\xi(r) := \frac{e^2}{8\pi\epsilon_0 m^2 c^2 r^3} \quad -(30)$$