250(7): Review of Calculations for UFT 250

The basis of UFT250 is a careful study of the various terms in the Dirac or fermion equation which lead to the conventional Zeeman effect hamiltonian:

$$\hat{H}\phi = \left(-\frac{e}{2m} \underline{L} \cdot \underline{B} - \frac{e\hbar}{2m} \underline{\sigma} \cdot \underline{B} - \xi \underline{S} \cdot \underline{L} \right) \phi \quad -(1)$$

where ξ is the conventional spin orbit coupling constant and

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

Eq. (1) is in fact a result which is obtained by a selective procedure as follows. In the appropriate approximation the fermion equation gives:

$$E\phi = \left(mc^2 + e\phi + \frac{1}{2m} \underline{\sigma} \cdot \underline{p} \, \underline{\sigma} \cdot \underline{p} - \frac{e}{2m} \left(\underline{\sigma} \cdot \underline{A} \, \underline{\sigma} \cdot \underline{p} + \underline{\sigma} \cdot \underline{p} \, \underline{\sigma} \cdot \underline{A} \right) + \frac{e^2}{2m} \underline{\sigma} \cdot \underline{A} \, \underline{\sigma} \cdot \underline{A} + \frac{e}{4m^2c^2} \underline{\sigma} \cdot (\underline{p} - e\underline{A}) \phi \, \underline{\sigma} \cdot (\underline{p} - e\underline{A}) \right) \phi \quad -(3)$$

$$= \left(mc^2 + e\phi + \frac{1}{2m} \underline{\sigma} \cdot (\underline{p} - e\underline{A}) \left(1 + \frac{e\phi}{2mc^2} \right) \underline{\sigma} \cdot (\underline{p} - e\underline{A}) \right) \phi \quad -(4)$$

The conventional hamiltonian (1) is obtained in

2) a carefully closer way by regarding $\underline{\sigma}$ either as a function or an operator. If $\underline{\sigma}$ is regarded as a function then:

$$\underline{\sigma} \cdot \underline{A}\, \underline{\sigma} \cdot \underline{p} = \underline{A} \cdot \underline{p} + i \underline{\sigma} \cdot \underline{A} \times \underline{p} \quad -(5)$$

and
$$\underline{\sigma} \cdot \underline{p}\, \underline{\sigma} \cdot \underline{A} = \underline{p} \cdot \underline{A} + i \underline{\sigma} \cdot \underline{p} \times \underline{A} \quad -(6)$$

Consider the term:

$$H_1 \psi = -\frac{e}{2m} \left(\underline{\sigma} \cdot \underline{A}\, \underline{\sigma} \cdot \underline{p} + \underline{\sigma} \cdot \underline{p}\, \underline{\sigma} \cdot \underline{A} \right) \psi \quad -(7)$$

<u>By regarding $\underline{\sigma}$ as a function</u>:

$$H_1 \psi = -\frac{e}{2m} \left(\underline{A} \cdot \underline{p} + \underline{p} \cdot \underline{A} + i \underline{\sigma} \cdot \underline{A} \times \underline{p} + i \underline{\sigma} \cdot \underline{p} \times \underline{A} \right) \psi \quad -(8)$$

For a uniform magnetic field:

$$\underline{A} = \frac{1}{2} \underline{B} \times \underline{r} \quad -(9)$$

so:

$$H_1 \psi = -\frac{e}{4m} \left(\underline{B} \times \underline{r} \cdot \underline{p} + \underline{p} \cdot \underline{B} \times \underline{r} + i \underline{\sigma} \cdot (\underline{B} \times \underline{r}) \times \underline{p} + i \underline{p} \times (\underline{B} \times \underline{r}) \right) \psi \quad -(10)$$

By regarding $\underline{p}$ as a function:

$$\underline{B} \times \underline{r} \cdot \underline{p} = \underline{p} \cdot \underline{B} \times \underline{r} = \underline{B} \cdot \underline{r} \times \underline{p} = \underline{B} \cdot \underline{L} \quad -(11)$$

so the hamiltonian (8) becomes:

$$H_1 \phi = -\frac{e}{2m} \underline{L} \cdot \underline{B} \phi + \left(i\underline{\sigma} \cdot \underline{A} \times \underline{p} + i\underline{\sigma} \cdot \underline{p} \times \underline{A} \right) \phi \quad -(12)$$

At this stage $\underline{p}$ is regarded as an operator

$$\underline{p} = -i\hbar \underline{\nabla} \quad -(13)$$

to obtain:

$$H_1 \phi = \left(-\frac{e}{2m} \underline{L} \cdot \underline{B} - \frac{e\hbar}{2m} \underline{\sigma} \cdot \underline{B} + \ldots \right) \phi \quad -(14)$$

$$= -\frac{e}{2m} \left(\underline{L} + 2\underline{S} \right) \cdot \underline{B} \phi$$

The total angular momentum $\underline{J}$ is conserved so eq. (14) is rewritten as:

$$H_1 \phi = -\frac{e}{2m} g_L \underline{J} \cdot \underline{B} \phi \quad -(15)$$

where $\underline{J}$ is defined by

$$\underline{J} = \underline{L} + \underline{S}, \ldots |\underline{L} - \underline{S}| \quad -(16)$$

and where g_L is the Landé factor, which is therefore given by the fermion or chiral Dirac equation.

The conventional spin orbit coupling term is given by the last term of eq. (3), in which the first $\underline{p}$ is an operator, but the

t) Second $\underline{p}$ is a function as in note 248(8), so the conventional spin-orbit hamiltonian is:

$$\hat{H}_{SO} = -\frac{ie\hbar}{4m^2c^2}\left(\underline{\sigma}\cdot\underline{\nabla}\phi\,\underline{\sigma}\cdot\underline{p}\right)\psi \quad -(17)$$

The standard physics assumption is now used:

$$\underline{E} = -\underline{\nabla}\phi \quad -(18)$$

so

$$\hat{H}_{SO} = -\frac{ie\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{E}\,\underline{\sigma}\cdot\underline{p} \quad -(19)$$

At this point $\underline{\sigma}$ is regarded as a function, so:

$$\underline{\sigma}\cdot\underline{E}\,\underline{\sigma}\cdot\underline{p} = \underline{E}\cdot\underline{p} + i\underline{\sigma}\cdot\underline{E}\times\underline{p} \quad -(20)$$

so the real valued part of the spin orbit hamiltonian is:

$$\hat{H}_{SO} = \frac{e\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{E}\times\underline{p} \quad -(21)$$

Finally the Coulomb law is used so:

$$\underline{E} = -\underline{\nabla}\phi = -\frac{e}{4\pi\epsilon_0 r^3}\,\underline{r} \quad -(22)$$

and

$$H_{22} = -\frac{e\hbar}{8\pi c^2\epsilon_0 m^2 r^3}\,\underline{\sigma}\cdot\underline{r}\times\underline{p} \quad -(23)$$

where

$$\underline{L} = \underline{r}\times\underline{p} \quad -(24)$$

5) The last term in eq. (1) is therefore:

$$-\xi \, \underline{S} \cdot \underline{L} = -\frac{e}{4\pi c^2 \epsilon_0 m^2 r^3} \, \underline{S} \cdot \underline{L} \quad - (25)$$

in which $\underline{\sigma}$ and $\underline{L}$ are now regarded as operators. It is seen that the use of $\underline{p}$ and $\underline{\sigma}$ as functions or operators is arbitrary. The results are accepted because they are correct experimentally.

However there are many other ways of using these operators or functions. In the derivation of the electron spin resonance (ESR) hamiltonian the following results of Pauli algebra are used, with $\underline{\sigma}$ and $\underline{p}$ used as functions:

$$\underline{\sigma} \cdot \underline{p} = \frac{1}{r^2} \underline{\sigma} \cdot \underline{r} \left(\underline{r} \cdot \underline{p} + i \underline{\sigma} \cdot \underline{L} \right) \quad - (26)$$

$$\underline{\sigma} \cdot \underline{A} = \frac{1}{r^2} \underline{\sigma} \cdot \underline{r} \left(\underline{r} \cdot \underline{A} + i \underline{\sigma} \cdot \underline{r} \times \underline{A} \right) \quad - (27)$$

so

$$\underline{\sigma} \cdot \underline{p} \, \underline{\sigma} \cdot \underline{A} = \frac{1}{r^2} \left(\underline{r} \cdot \underline{p} \, \underline{r} \cdot \underline{A} - \underline{\sigma} \cdot \underline{L} \, \underline{\sigma} \cdot \underline{r} \times \underline{A} \right) + \frac{i}{r^2} \left(\underline{r} \cdot \underline{p} \, \underline{\sigma} \cdot \underline{r} \times \underline{A} + \underline{\sigma} \cdot \underline{L} \, \underline{r} \cdot \underline{A} \right) \quad - (28)$$

For a uniform magnetic field defined by eq. (9):

$$\underline{r} \cdot \underline{A} = 0 \quad - (29)$$

so

$$\underline{\sigma} \cdot \underline{p} \, \underline{\sigma} \cdot \underline{A} = \frac{1}{r^2} \underline{\sigma} \cdot \underline{L} \, \underline{\sigma} \cdot \underline{A} \times \underline{r} + \frac{i}{r^2} \left(\underline{r} \cdot \underline{p} \, \underline{\sigma} \cdot \underline{r} \times \underline{A} \right) \quad - (30)$$

$$= \underline{p} \cdot \underline{A} + i \underline{\sigma} \cdot \underline{p} \times \underline{A}$$

6)

So:

$$\underline{p} \cdot \underline{A} = \frac{1}{r^2} \underline{\sigma} \cdot \underline{L}\, \underline{\sigma} \cdot \underline{A} \times \underline{r} \quad -(31)$$

and

$$\underline{\sigma} \cdot \underline{p} \times \underline{A} = \frac{1}{r^2} \underline{r} \cdot \underline{p}\, \underline{\sigma} \cdot \underline{r} \times \underline{A} \quad -(32)$$

If $\underline{\sigma}$ is regarded as a function eq. (31) reduces to:

$$\begin{aligned} \underline{p} \cdot \underline{A} &= \frac{1}{r^2} \underline{\sigma} \cdot \underline{L}\, \underline{\sigma} \cdot \underline{A} \times \underline{r} \\ &= \frac{1}{r^2} \underline{r} \times \underline{p} \cdot \underline{A} \times \underline{r} \end{aligned} \quad -(33)$$

$$= \frac{1}{r^2} (\underline{p} \cdot \underline{A})(\underline{r} \cdot \underline{r}) - (\underline{p} \cdot \underline{r})(\underline{r} \cdot \underline{A})$$

$$= \frac{1}{r^2} \underline{p} \cdot \underline{A}\, \underline{r} \cdot \underline{r} = \underline{p} \cdot \underline{A}$$

QED. This checks identity (31).

Identity (32) implies ~~that~~:

$$\underline{p} = \frac{\underline{r}}{|r^2|} \underline{r} \cdot \underline{p} = \hat{\underline{r}} (\hat{\underline{r}} \cdot \underline{p}) = \underline{p} \quad -(34)$$

QED.

Similarly,

$$\underline{\sigma} \cdot \underline{p} = \frac{1}{r^2} \underline{\sigma} \cdot \underline{r} (\underline{r} \cdot \underline{p} + i \underline{\sigma} \cdot \underline{L}) \quad -(35)$$

$$\underline{\sigma} \cdot \underline{A} = \frac{1}{r^2} \underline{\sigma} \cdot \underline{r} (\underline{r} \cdot \underline{A} + i \underline{\sigma} \cdot \underline{r} \times \underline{A}) \quad -(36)$$

So:

$$\underline{\sigma} \cdot \underline{A}\, \underline{\sigma} \cdot \underline{p} = \frac{1}{r^2} (\underline{r} \cdot \underline{A} + i \underline{\sigma} \cdot \underline{r} \times \underline{A})(\underline{r} \cdot \underline{p} + i \underline{\sigma} \cdot \underline{L})$$

(37)

) So

$$\underline{\sigma}\cdot\underline{A}\,\underline{\sigma}\cdot\underline{p} = \frac{1}{r^2}\left(\underline{A}\times\underline{r}\,\underline{\sigma}\cdot\underline{L} + i\,\underline{\sigma}\cdot\underline{r}\times\underline{A}\,\underline{r}\cdot\underline{p}\right) \quad -(38)$$

$$= \underline{A}\cdot\underline{p} + i\,\underline{\sigma}\cdot\underline{A}\times\underline{p}$$

Therefore:

$$\underline{A}\cdot\underline{p} = \frac{1}{r^2}\,\underline{\sigma}\cdot\underline{A}\times\underline{r}\,\underline{\sigma}\cdot\underline{L} \quad -(39)$$

$$\underline{\sigma}\cdot\underline{A}\times\underline{p} = \frac{1}{r^2}\,\underline{\sigma}\cdot\underline{r}\times\underline{A}\,\underline{r}\cdot\underline{p} \quad -(40)$$

Therefore the conventional Zeeman effect hamiltonian can be written as:

$$\hat{H}_2\phi = -\frac{e}{2m}\,\underline{L}\cdot\underline{B}\,\phi$$

$$= -\frac{e}{2m}\left(\underline{p}\cdot\underline{A} + \underline{A}\cdot\underline{p}\right)\phi \quad -(41)$$

$$= -\frac{e}{2mr^2}\left(\underline{\sigma}\cdot\underline{L}\,\underline{\sigma}\cdot\underline{A}\times\underline{r} + \underline{\sigma}\cdot\underline{A}\times\underline{r}\,\underline{\sigma}\cdot\underline{L}\right)\phi$$

where

$$\underline{A} = \frac{1}{2}\,\underline{B}\times\underline{r} \quad -(42)$$

The hamiltonian (41) can be written as:

$$\hat{H}_2\phi = -\frac{e}{mr^2}\,\underline{\sigma}\cdot\underline{A}\times\underline{r}\;\underline{\sigma}\cdot\underline{L}\,\phi \quad -(43)$$

If $\underline{\sigma}$ and $\underline{L}$ are regarded as functions then

$$H_2\phi = -\frac{e}{mr^2}\,\underline{A}\times\underline{r}\cdot\underline{L}\,\phi \quad -(44)$$

$\cdot$? A r and $\underline{L}$ are real valued.

8) so the magnetic field is defined by:

$$\underline{B} = \frac{2}{r^2} \underline{A} \times \underline{r} \quad - (45)$$

and

$$\hat{H}_2 \phi = -\frac{e}{2m} \underline{\sigma} \cdot \underline{B} \, \underline{\sigma} \cdot \underline{L} \phi \quad - (46)$$

At this point introduce the operators:

$$\underline{S} = \frac{\hbar}{2} \underline{\sigma} \quad - (47)$$

and

$$\underline{S} \cdot \underline{L} \phi = \frac{\hbar^2}{2} \left(j(j+1) - l(l+1) - s(s+1) \right) \phi \quad - (48)$$

so

$$H_2 \phi = E_2 \phi \quad - (49)$$

$$- (50)$$

where

$$H_2 = -\frac{e}{2m\hbar} \underline{\sigma} \cdot \underline{B} \, 2\underline{S} \cdot \hat{\underline{L}} \phi$$

and

$$E_2 = -\frac{e\hbar}{2m} \left(j(j+1) - l(l+1) - s(s+1) \right) \underline{\sigma} \cdot \underline{B} \quad - (51)$$

The complete hamiltonian (1) may now be expressed as:

$$H\phi = \left(-\frac{e}{2m} (\underline{L} + 2\underline{S}) \cdot \underline{B} - \xi \, \underline{S} \cdot \underline{L} \right) \phi$$

$$= \left(-\frac{e}{2m} g_L \underline{J} \cdot \underline{B} - \xi \, \underline{S} \cdot \underline{L} \right) \phi$$

$$= \underbrace{-\xi\, \underline{S}\cdot\underline{L}\,\phi}_{\text{conventional fine structure}} \underbrace{- \frac{e}{2m}\left(\frac{2\,\underline{S}\cdot\underline{L}}{\hbar} + \hbar\right)\underline{\sigma}\cdot\underline{B}\,\phi}_{\text{Electron spin orbit resonance (ESOR)}} \quad (52)$$

We obtain the very remarkable result that the original hamiltonian (4) can be expressed in entirely different ways, eqns. (1) and (52). The ESOR part of eq. (52) shifts and splits the ESR effect for one electron.