330(6): Development of the New Hamiltonian Term

From eq. (10) of Note 330(1) the new hamiltonian term is:

$$H_{01} = -\underline{\sigma} \cdot \underline{p} \frac{H_0}{4m^2c^2} \underline{\sigma} \cdot \underline{p} \quad -(1)$$

in the SU(2) basis. Here:

$$\underline{p} = \gamma p_0 \quad -(2)$$

is the relativistic momentum. Using the minimal prescription:

$$H_{01} = -\underline{\sigma} \cdot (\underline{p} - e\underline{A}) \frac{H_0}{4m^2c^2} \underline{\sigma} \cdot (\underline{p} - e\underline{A}) \quad -(3)$$

This is an entirely new type of spin orbit structure in spectroscopy.

For comparison, the conventional hamiltonian is:

$$H_{02} = \underline{\sigma} \cdot (\underline{p} - e\underline{A}) \frac{U}{4m^2c^2} \underline{\sigma} \cdot (\underline{p} - e\underline{A}) \quad -(4)$$

where

$$U = \frac{-e^2}{4\pi\epsilon_0 r} \quad -(5)$$

From the Schroedinger equation:

$$H_0 \phi = \left(-\frac{\hbar^2 \nabla^2}{2m} + U \right) \phi \quad -(6)$$

where ϕ are the hydrogenic wave functions.

Now use the following quantization scheme for eq. (1):

2) $$H_{01}\phi = \frac{i\hbar\, \underline{\sigma}\cdot\underline{\nabla}\, H_0}{4m^2c^2}\, \underline{\sigma}\cdot\underline{p}\,\phi \quad -(7)$$

In the first approximation assume that the relativistic ϕ are the ϕ from the Schroedinger equation. Therefore:

$$H_{01}\phi = \frac{i\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{\nabla}\left(H_0\,\underline{\sigma}\cdot\underline{p}\,\phi\right) \quad -(8)$$

$$= \frac{i\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{\nabla}\left(\underline{\sigma}\cdot\underline{p}\,H_0\phi\right).$$

Using the Leibnitz theorem:

$$H_{01}\phi = \frac{i\hbar}{4m^2c^2}\Big(H_0\phi\,\underline{\sigma}\cdot\underline{\nabla}\,\underline{\sigma}\cdot\underline{p} \quad -(9)$$
$$+\,\underline{\sigma}\cdot\underline{\nabla}\left(H_0\phi\right)\underline{\sigma}\cdot\underline{p}\Big)$$

There are two types of hamiltonian:

$$H_{011}\phi = \frac{i\hbar}{4m^2c^2}\,H_0\phi\,\underline{\sigma}\cdot\underline{\nabla}\,\underline{\sigma}\cdot\underline{p} \quad -(10)$$

and $$H_{012}\phi = \frac{i\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{\nabla}\left(H_0\phi\right) \quad -(11)$$

$$= \frac{i\hbar H_0}{4m^2c^2}\,\underline{\sigma}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{\nabla}\phi \quad -(11a)$$

because H_0 is a constant of motion.

3) Using Pauli algebra:

$$\underline{\sigma} \cdot \underline{\nabla}\, \underline{\sigma} \cdot \underline{p} = \underline{\nabla} \cdot \underline{p} + i \underline{\sigma} \cdot \underline{\nabla} \times \underline{p} \quad -(12)$$

and

$$\underline{\sigma} \cdot \underline{p}\, \underline{\sigma} \cdot \underline{\nabla} \phi = \underline{p} \cdot \underline{\nabla} \phi + i \underline{\sigma}\, \underline{p} \times \underline{\nabla} \phi \quad -(13)$$

Therefore:

$$\mathrm{Re}\, H_{011} \phi = -\frac{\hbar}{4m^2c^2} H_0 \phi\, \underline{\sigma} \cdot \underline{\nabla} \times \underline{p} \quad -(14)$$

and

$$\mathrm{Re}\, H_{012} \phi = -\frac{\hbar H_0}{4m^2c^2} \underline{\sigma} \cdot \underline{p} \times \underline{\nabla} \phi \quad -(15)$$

These are two new types of hamiltonian.
Using the minimal prescription:

$$\underline{p} \rightarrow \underline{p} - e\underline{A} \quad -(16)$$

in the presence of an electromagnetic field, a new type of ESR hamiltonian is obtained:

$$H_{ESR} \phi = \frac{e\hbar H_0 \phi}{4m^2c^2} \underline{\sigma} \cdot \underline{\nabla} \times \underline{A} \quad -(17)$$

$$= \frac{e\hbar H_0 \phi}{4m^2c^2} \underline{\sigma} \cdot \underline{B}$$

Its energy levels are given by:

4)

$$\langle H_{ESR} \rangle = \frac{e\hbar}{4m^2c^2} \underline{\sigma} \cdot \underline{B} \langle H_0 \rangle \quad -(18)$$

where:

$$\langle H_0 \rangle = -\frac{e^4}{32\pi^2 \epsilon_0^2 \hbar^2 c^2 n^2} \quad -(19)$$

This is the same result as eq. (8) of Note 329(6), providing a cross check.

Using the Bohr radius:

$$r_B = \frac{4\pi\epsilon_0 \hbar^2}{me^2} \quad -(20)$$

then

$$\langle H_0 \rangle = -\frac{e^2}{8\pi\epsilon_0 r_B n^2} \quad -(21)$$

$$= -\frac{\hbar c}{2} \left(\frac{\alpha}{r_B} \right) \frac{1}{n^2}$$

where the fine structure constant is:

$$\alpha = \frac{e^2}{4\pi\hbar c \epsilon_0} \quad -(22)$$

The conventional ESR hamiltonian is:

$$\langle H_{ESR0} \rangle = -\frac{e\hbar}{2m} \underline{\sigma} \cdot \underline{B} \quad -(23)$$

From eqs. (18) and (23):

5)

$$\langle H_{ESR} \rangle = -\frac{\langle H_0 \rangle}{2mc^2} \langle H_{ESRo} \rangle \quad -(24)$$

Fm eqs. (21) and (24):

$$\langle H_{ESR} \rangle = \frac{\hbar c}{4mc^2}\left(\frac{\alpha}{r_B}\right)\frac{1}{n^2}\langle H_{ESRo} \rangle \quad -(25)$$

$$= \frac{1}{4}\left(\frac{\hbar}{mc}\right)\left(\frac{\alpha}{r_B}\right)\frac{1}{n^2}\langle H_{ESRo} \rangle$$

where

$$\lambda_c = \frac{\hbar}{mc} \quad -(26)$$

is the Compton wavelength.

In S.I. Units:

$$\lambda_c = 3.861591 \times 10^{-13} m \quad -(27)$$

$$r_B = 5.29177 \times 10^{-11} m \quad -(28)$$

$$\alpha = 0.00729735 1 \quad -(29)$$

So

$$\boxed{\langle H_{ESR} \rangle = \frac{1.33128 \times 10^{-5}}{n^2} \langle H_{ESRo} \rangle} \quad -(30)$$

in the H atom. Therefore this new type of ESR appears in the MHz frequency range.

A new type of spectroscopy also appears from Eq. (11):

6) using:

$$H_0\phi = \left(-\frac{\hbar^2\nabla^2}{2m} + U\right)\phi \quad -(31)$$

$$= \left(-\frac{\hbar^2\nabla^2}{2m} - \frac{e^2}{4\pi\epsilon_0}\frac{\underline{r}}{r^2}\right)\phi$$

So:

$$H_{012}\phi = \frac{i\hbar}{4m^2c^2}\,\underline{\sigma}\cdot\underline{\nabla}(H_0\phi)\,\underline{\sigma}\cdot\underline{p}$$

$$= \frac{ie^2\hbar}{16\pi\epsilon_0 r^3}\,\underline{\sigma}\cdot\underline{r}\,\underline{\sigma}\cdot\underline{p}\,\phi - \frac{i\hbar^3}{8m^3c^2}\underline{\sigma}\cdot\underline{\nabla}(\nabla^2\phi)\,\underline{\sigma}\cdot\underline{p} \quad -(32)$$

The first part of this expression is the conventional spin orbit term

$$\mathrm{Re}\,H_{so}\phi = \frac{e^2\hbar}{16\pi\epsilon_0 m^2c^2r^3}\,\underline{\sigma}\cdot\underline{L}\,\phi \quad -(33)$$

where

$$\underline{L} = \underline{r}\times\underline{p} \quad -(34)$$

There is also a new term:

$$\mathrm{Re}\,H_2\phi = \frac{\hbar^3}{8m^3c^2}\,\underline{\sigma}\cdot\underline{\nabla}(\nabla^2\phi)\times\underline{p} \quad -(35)$$

In the presence of an electromagnetic field this gives the term:

7) $$\mathrm{Re}\, H_2 \psi = -\frac{e\hbar^3}{8m^3c^2} \underline{\sigma} \cdot \underline{\nabla}\left(\nabla^2 \psi\right) \times \underline{A} \quad -(36)$$

The energy levels of this term are:

$$\langle H_2 \rangle = -\frac{e\hbar^3}{8m^3c^2} \underline{\sigma} \cdot \int \psi^* \underline{\nabla}\left(\nabla^2 \psi\right) d\tau \times \underline{A} \quad -(37)$$

giving a completely new type of ESR