268(3): Spin Orbit Coupling from x Theory

In the non relativistic theory the hamiltonian is:

$$H\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{k}{r}\right)\psi \quad -(1)$$

where

$$r = \frac{\alpha}{1+\epsilon\cos\phi} \quad -(2)$$

For atomic H:

$$\langle E \rangle = \int \psi^* H \psi \, d\tau$$

$$= -\frac{\hbar^2}{2m}\int \psi^* \nabla^2 \psi \, d\tau - k\int \psi^* \frac{1}{r}\psi \, d\tau$$

$$= \frac{me^4}{32\pi^2\epsilon_0^2\hbar^2 n^2} - \frac{me^4}{16\pi^2\epsilon_0^2\hbar^2 n^2}$$

$$= -\frac{me^4}{32\pi^2\epsilon_0^2\hbar^2 n^2} \quad -(3)$$

For precessing orbits: $\quad -(4)$

$$H\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{x^2 k}{r} + (x^2-1)\frac{L^2}{2mr^2}\right)\psi,$$

and

$$r = \frac{\alpha}{1+\epsilon\cos(x\phi)} \quad -(5)$$

Therefore:

d)

$$\langle E \rangle = \left\langle \frac{p^2}{2m} \right\rangle - x^2 k \left\langle \frac{1}{r} \right\rangle + (x^2-1)\frac{L^2}{2m}\left\langle \frac{1}{r^2} \right\rangle \quad -(6)$$

The precession factor x is very small, so to an excellent approximation:

$$\alpha = r_B = \frac{L^2}{mk} \quad -(7)$$

where the Bohr radius is:

$$r_B = \frac{4\pi\epsilon_0 \hbar^2 n^2}{me^2} \quad -(8)$$

So:

$$\langle E \rangle = \left\langle \frac{p^2}{2m} \right\rangle - x^2 k \left\langle \frac{1}{r} \right\rangle + \frac{1}{2}(x^2-1) k r_B \left\langle \frac{1}{r^2} \right\rangle$$

$$= \frac{me^4}{32\pi^2\epsilon_0^2\hbar^2 n^2}(1-2x^2) + (x^2-1)\frac{\hbar^2 n^2}{2m}\left\langle \frac{1}{r^2} \right\rangle \quad -(9)$$

For the 1s orbital:

$$\left\langle \frac{1}{r^2} \right\rangle = \frac{1}{\pi r_B^3}\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta \, d\theta \int_0^{\infty} \exp\left(-\frac{2r}{r_B}\right) dr$$

$$= \frac{4}{r_B^3}\int_0^{\infty} \exp\left(-\frac{2r}{r_B}\right) dr \quad -(10)$$

3)

$$\left\langle \frac{1}{r^2} \right\rangle_{1s} = \frac{2}{r_B^2} \quad -(11)$$

Therefore:

$$\langle E \rangle_{1s} = \frac{me^4}{32\pi^2\epsilon_0^2\hbar^2}\left(1-2x^2\right) + \frac{\left(x^2-1\right)me^4}{16\pi^2\epsilon_0^2\hbar^2}$$

$$= -\frac{me^4}{32\pi^2\epsilon_0^2\hbar^2} \quad -(12)$$

There is no effect of x on the energy level of the 1s orbital if it is assumed that:

$$\alpha = r_B. \quad -(13)$$

The same result is true for the s orbitals from the fermion equation's spin orbit coupling term. The relevant hamiltonian to consider is:

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

$$= \left(\frac{p^2}{2m} + e\phi - \frac{e^2\hbar}{16\pi m^2c^2\epsilon_0 r^3}\,\underline{\sigma}\cdot\underline{L}\right)\phi \quad -(14)$$

The expectation value of the spin orbit hamiltonian is:

4) $$\langle E_{so} \rangle = -\frac{e^2 \hbar}{16\pi m^2 c^2 \epsilon_0} \int \psi^* \frac{\sigma \cdot L}{r^3} \psi \, d\tau \quad -(15)$$

$$= 0$$

for the s orbitals. $\quad -(16)$

From the fermion equation:

$$\langle E \rangle = \left\langle \frac{p^2}{2m} - \frac{k}{r} \right\rangle + \langle E_{so} \rangle$$

and from the precessing elliptical x theory:

$$\langle E \rangle = \left\langle \frac{p^2}{2m} \right\rangle + \left\langle -x^2 \frac{k}{r} + \frac{(x^2-1)L^2}{2mr^2} \right\rangle \quad -(17)$$

Therefore:

$$\langle E_{so} \rangle - \left\langle \frac{k}{r} \right\rangle = \left\langle \frac{(x^2-1)L^2}{2mr^2} \right\rangle - x^2 \left\langle \frac{k}{r} \right\rangle \quad -(18)$$

i.e.

$$\boxed{\langle E_{so} \rangle = (x^2-1)\left(\frac{L^2}{2m}\left\langle \frac{1}{r^2} \right\rangle - \left\langle \frac{k}{r} \right\rangle\right) = -\frac{e^2 \hbar}{16\pi m^2 c^2 \epsilon_0} \left\langle \frac{\sigma \cdot L}{r^3} \right\rangle \quad -(19)}$$

5) Comments

The result (19) has been obtained by assuming that the hamiltonians of the x theory and fermion equation are the same for the k orbital:

$$\left\langle \frac{(x^2-1)L^2}{2mr^2} \right\rangle - x^2 \left\langle \frac{k}{r} \right\rangle = -\left\langle \frac{k}{r} \right\rangle \quad -(20)$$

so from eq. (18):

$$\langle E_{so} \rangle = 0, \quad -(21)$$

and this is a self consistent result.

In general the computation of $\left\langle \frac{\underline{\sigma} \cdot \underline{L}}{r^3} \right\rangle$ is non trivial, but for a given x^2, Eq. (19) allows it to be calculated fairly simply. One method consists of using: $\quad -(22)$

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

$$= \frac{1}{2}\hbar^2\left(j(j+1) - l(l+1) - s(s+1)\right)\phi$$

so in this representation it is possible to obtain an expression for $\langle E_{so} \rangle$ as follows:

6)

$$\langle E_{so} \rangle = -\frac{e^2 \hbar^2 \left(\left(j(j+1) - \ell(\ell+1) - s(s+1) \right) \right)}{16\pi m^2 c^2 \epsilon_0} \left\langle \frac{1}{r^3} \right\rangle \quad -(20)$$

using:

$$\underline{S} = \frac{1}{2} \hbar \underline{\sigma}. \quad -(21)$$

From the Clebsch Gordan series:

$$j = \ell + s,\ \ell + s - 1, \ldots, |\ell - s| \quad -(22)$$

Eq. (18) can be written as:

$$\langle E_{so} \rangle = \left\langle \frac{k}{r} \right\rangle - (x^2 - 1) \frac{\hbar^2}{2m} \left\langle \frac{1}{r^2} \right\rangle - x^2 \left\langle \frac{k}{r} \right\rangle$$

$$= (x^2 - 1) \left(\frac{\hbar^2 n^2}{2m} \left\langle \frac{1}{r^2} \right\rangle - k \left\langle \frac{1}{r} \right\rangle \right) \quad -(23)$$

so from a combination of eqns. (20) and (23), x can be evaluated for a given n, j, ℓ and s.