

### 335(5): Expectation Value of the Corrected Spin-Orbit Hamiltonian.

This is calculated from:

$$H_{int} \psi = -\frac{g_N \mu_o e^2}{4\pi m_p m_e} \left( \frac{\gamma^2}{1+\gamma} \right)^{1/2} \frac{\underline{I} \cdot \underline{L}}{r^3} \psi \quad (1)$$

$$\text{and } E_{int} = \int \psi^* H_{int} \psi d\tau = -\frac{g_N \mu_o e^2}{4\pi m_p m_e} \left( \frac{\gamma^2}{1+\gamma} \right)^{1/2} \left\langle \frac{\underline{I} \cdot \underline{L}}{r^3} \right\rangle$$

This assumes that  $(\gamma^2/(1+\gamma))^{1/2}$  is a function but that  $\underline{I} \cdot \underline{L} / r^3$  is an operator. (2)

In direct analogy with the theory of electronic spin orbit splitting in H, the expectation value is:

$$\left\langle \frac{\underline{I} \cdot \underline{L}}{r^3} \right\rangle = \hbar^2 \left( \frac{J(J+1) - L(L+1) - I(I+1)}{2a_0^3 n^3 L(L+\frac{1}{2})(L+1)} \right) \quad (3)$$

where:  $J = L + I, L + I - 1, \dots, |L - I|$  (4)

For the proton in H:

$$\underline{I} = 1/2 \text{ or } -1/2 \quad (5)$$

2) As in previous work:

$$\frac{\gamma^2}{1+\gamma} = \left( \frac{1}{1 - \left(\frac{d}{n}\right)^2} + \left(1 - \left(\frac{d}{n}\right)^2\right)^{1/2} \right)^{-1} \quad (6)$$

where  $d$  is the fine structure constant.

In the presence of an external magnetic field  $\underline{B}$  the complete Hamiltonian is:

$$H = -\underline{m}_N \cdot \underline{B} - \underline{m}_N \cdot \underline{B}_{int}, \quad (7)$$

$$E = -g_N \frac{e\hbar}{2m_p} B_z m_I - E_{int} \quad (8)$$

where:

$$m_I = -I, \dots, I \quad (9)$$

and

$$E_{int} = -\frac{g_N \mu_N e^2}{4\pi m_p m_e} \left( \frac{\gamma^2}{1+\gamma} \right)^{1/2} \hbar^2 \left( \frac{J(J+1) - L(L+1) - I(I+1)}{2a_0^3 \hbar^3 L(L+1/2)(L+1)} \right) \quad (10)$$

The NMR resonance condition is:

$$\hbar\omega = E(m_I - 1) - E(m_I) \quad (11)$$


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