

35(2): Lande Factor for $S_{pi} - S_{pn}$ NMR

Consider the Hamiltonian made up of an electron and nucleus spin:

$$H = -\frac{e}{m_e} \underline{S} \cdot \underline{B} - g_N \frac{e}{2m_p} \underline{I} \cdot \underline{B} \quad (1)$$

where \underline{S} is the electron spin angular momentum and \underline{I} the nucleus spin angular momentum. Here m_e is the electron mass, m_p the nucleus mass and g_N the nucleus g factor. For a proton, the spin quantum number is $1/2$, $g_N = 5.5857$, for a neutron, $g_N = -3.82608$. In deuterium, $\underline{I} = 1$, $g_N = 0.85745$. Using the Zeeman series:

$$\underline{M} = \underline{I} + \underline{S}, \dots, |\underline{I} - \underline{S}| \quad (2)$$

Now develop the term in Eq. (1) as:

$$\underline{I} \cdot \underline{B} = \frac{1}{M^2} \underline{I} \cdot \underline{M} \underline{M} \cdot \underline{B} \quad (3)$$

$$\underline{S} \cdot \underline{B} = \frac{1}{M^2} \underline{S} \cdot \underline{M} \underline{M} \cdot \underline{B} \quad (4)$$

where:

$$2 \underline{I} \cdot \underline{M} = M^2 + \underline{I}^2 - \underline{S}^2 \quad (5)$$

$$2 \underline{M} \cdot \underline{S} = M^2 + \underline{S}^2 - \underline{I}^2 \quad (6)$$

It follows that:

$$H = -e g_m \underline{M} \cdot \underline{B} \quad (7)$$

where:

$$g_m = \frac{1}{2m} \left(\frac{1}{m_e} (m^2 + s^2 - I^2) + \frac{g_N}{m_p} (m^2 + I^2 - s^2) \right) \quad - (8)$$

Using expectation values:

$$g_m = \frac{1}{2} \left(\frac{1}{m_e} \left(\frac{1 + s(s+1) - I(I+1)}{m(m+1)} \right) + \frac{g_N}{m_p} \left(\frac{1 + I(I+1) - s(s+1)}{m(m+1)} \right) \right) \quad - (9)$$

Quantizing the Hamiltonian:

$$H\phi = -e g_m M_z B_z \phi \quad - (10)$$

where

$$M_z \phi = \hbar m_m \phi \quad - (11)$$

and

$$m_m = -m, \dots, m \quad - (12)$$

In Eq. (7):

$$\underline{m} = \underline{s} + \underline{I} \quad - (13)$$

So for electron spin resonance:

$$H_{\text{FSR}} = -e g_m \underline{s} \cdot \underline{B} + \dots \quad - (14)$$

and for nuclear magnetic resonance:

$$3) \quad H_{NMR} = -e g_m \frac{\underline{I} \cdot \underline{B}}{2m_p} + \dots \quad (15)$$

Upa quantization:

$$S_z \psi = \hbar m_s \psi \quad (16)$$

where

$$m_s = -S, \dots, S \quad (17)$$

and

$$I_z \psi = \hbar m_I \psi \quad (18)$$

where

$$m_I = -I, \dots, I \quad (19)$$

The correction due to the class are Hamiltonian can now be factored in to give:

$$H = -\frac{e}{m_e} \left(\frac{\gamma^2}{1+\gamma} \right) \underline{S} \cdot \underline{B} - g_N \frac{e}{2m_p} \underline{I} \cdot \underline{B} \quad (20)$$

So g_m is corrected to:

$$g_m = \frac{1}{2} \left(\frac{1}{m_e} \left(\frac{\gamma^2}{1+\gamma} \right) \left(\frac{1 + S(S+1) - I(I+1)}{m_I(m_I+1)} \right) + \frac{g_N}{m_p} \left(\frac{1 + I(I+1) - S(S+1)}{m_I(m_I+1)} \right) \right) \quad (21)$$

The ESR resonance frequency is:

$$\omega_{\text{ESR}} = g_m e B_z - (23)$$

and so it is split by the $s_{\uparrow\downarrow} s_{\uparrow\downarrow}$ interaction between the electron and the nucleus. The spectrum is also affected by the relativistic factor $\gamma^2/(1+\gamma)$.

Similarly, the NMR resonance frequency is obtained from:

$$H_{\text{NMR}} = -e g_m \underline{I} \cdot \underline{B} - (24)$$

so

$$H_{\text{NMR}} \phi = -e \hbar g_m m_I B_z - (25)$$

where

$$m_I = -I, \dots, I - (26)$$

and

$$\Delta m_I = 1. - (27)$$

Therefore the NMR spectrum is also split and also affected by $\gamma^2/(1+\gamma)$, QED.
