Lecture 22 Zeeman effect in Hyperfine structures

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In the last lecture, we understood the hyperfine structure that originates due to the interaction between the total angular momentum of electron and the nuclear angular momentum

In this lecture we will discuss the effect of static magnetic field on this hyperfine structure.

We will discuss this concept on the basis of the magnetic field strength.

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By now, we know that the nuclear magnetic moment is

$$\vec{\mu}_N = g_I\ \mu_B\ \vec{I}$$
$$= g_I^N\ \mu_B^N\ \vec{I} \qquad\qquad So,\ g_I = \frac{1}{1836} g_I^N$$

As discussed before, the total magnetic moment due to the electron is

$$\vec{\mu}_{electron} = \vec{\mu}_{orbital} + \vec{\mu}_{spin}$$
$$= \vec{\mu}_l + \vec{\mu}_s$$
$$= -\mu_B[\vec{L} + g_s \vec{S}]$$

So the total magnetic moment of the atom including the nuclear part is

$$\vec{\mu}_{total} = \vec{\mu}_{electron} + \vec{\mu}_{nucleus}$$
$$= -\mu_B \vec{L} - g_S \mu_B \vec{S} + g_I \mu_B \vec{I}$$

And the interaction energy with the applied magnetic field $\vec{B}_z$ is

$$E_{mag} = -\vec{\mu}_{total} . \vec{B}_z$$

We know that the Hamiltonian for the atom in the L-S coupling scheme including the interaction with nuclear magnetic moment is written as

$$H = \underbrace{H_{CF}}_{\substack{\left|l_1 m_{l_1}\right\rangle \left|s_1 m_{s_1}\right\rangle \\ \left|l_2 m_{l_2}\right\rangle \left|s_2 m_{s_2}\right\rangle}} + \underbrace{H_{ee}}_{\left|L m_l\right\rangle \left|S m_s\right\rangle} + \underbrace{H_{so}}_{\substack{\left|J m_J\right\rangle \\ \left|I\ \mathrm{m}_I\right\rangle}} + \underbrace{H_{hf}}_{\left|F m_F\right\rangle}$$

The total electronic quantum number *J* and *I* are not the good quantum number.

Here the hyperfine interaction is coupling the total angular momentum of the electron *J* and the nuclear angular momentum *I*. So the new angular momentum *F* which will be the good quantum number for the total Hamiltonian.

So we have

$\vec{F} = \vec{J} + \vec{I}$ and the eigenfunction is $\left|F\ m_F\right\rangle$ which will be the coupled state arising from the uncoupled states of $\left|J\ m_J\right\rangle \left|I\ m_I\right\rangle$

The hyperfine interaction energy

$$E_{HF} = A'_{HF}\ \vec{I} \cdot \vec{J}$$

When we apply the magnetic field, this will interact with the total magnetic moment of the atom.

There will be three situations of the interaction those depends on the magnitude of the magnetic field strength compared to the hyperfine interaction.

1. The weak field case
2. The intermediate field and
3. The strong field case.

Since the coupling strength between the nuclear spin and the total angular momentum of the electron is very small, the magnitude of the applied magnetic field should be very small.

On the other hand, the field considered to be strong compared to hyperfine interaction will be small compared to spin-orbit interaction.

Here we will discuss only two these cases.

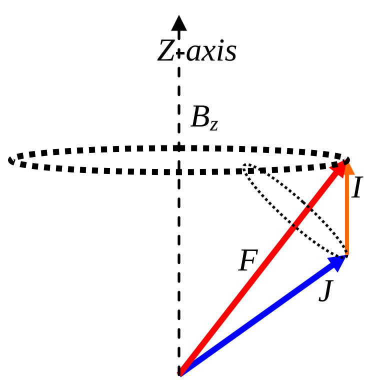
Case-I

Weak Field case

For this situation we can write the Hamiltonian as

$$H = \underbrace{H_{CF}}_{\substack{|l_1 m_{l_1}\rangle|s_1 m_{s_1}\rangle \\ |l_2 m_{l_2}\rangle|s_2 m_{s_2}\rangle}} + \underbrace{H_{ee}}_{|Lm_l\rangle|Sm_s\rangle} + \underbrace{H_{so}}_{\substack{|Jm_J\rangle \\ |I\,m_I\rangle}} + \underbrace{H_{hf}}_{|Fm_F\rangle} + H_{mag} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(22.1)$$

When this magnetic field is applied the total angular momentum F starts precessing around the magnetic field.



And the interaction energy with the applied magnetic field $\vec{B}_z$ is

$$\begin{aligned} E_{mag} &= \langle Fm_F | -\vec{\mu}_{total}.\vec{B}_z | Fm_F \rangle \\ &= \langle Fm_F | (\mu_B \vec{L} + g_S \mu_B \vec{S} - g_I \mu_B \vec{I}).\vec{B}_z | Fm_F \rangle \\ &= \mu_B B_z \langle Fm_F | (L_z + 2S_z - g_I I_z) | Fm_F \rangle \end{aligned}$$

Here we have substituted spin Lande g-factor $g_s = 2$.

So we have to calculate

$$\left\langle F\ m'_F \,|\, H_{mag} \,|\, F\ m_F \right\rangle = \mu_B B_z \left\langle F\ m_F \,|\, \left(L_z + 2S_z\right) - g_I\ I_z \,|\, F\ m_F \right\rangle \ \text{.......(22.2)}$$

Again using special case of Wigner-Eckart theorem, (Lande formula)

$$\left\langle J\, m' | \vec{A} | \, J\, m \right\rangle = \frac{\left\langle J\, m \,|\, \vec{A}\cdot\vec{J} \,|\, J\, m \right\rangle}{J\left(J+1\right)} \left\langle J\, m' \,|\, \vec{J} \,|\, J\, m \right\rangle$$

So,

$$\left\langle F\ m'_F \,|\, L_z + 2S_z \,|\, F\ m_F \right\rangle = \frac{\left\langle F\ m_F \,|\, \vec{J}\cdot\left(\vec{L}+2\vec{S}\right) | \, F\ m_F \right\rangle}{J\left(J+1\right)} \left\langle F\ m'_F \,|\, J_z \,|\, F\ m_F \right\rangle \text{....(22.3)}$$

Now,

$$\vec{J}\cdot\left(\vec{L}+2\vec{S}\right) = \vec{J}\cdot\left(\vec{L}+\vec{S}+\vec{S}\right) = \vec{J}\cdot\left(\vec{J}+\vec{S}\right)$$

$$= J^2 + \vec{J}\cdot\vec{S}$$

We have to find $\vec{J}\cdot\vec{S}$

So,

$$\vec{J} = \vec{L} + \vec{S}$$

$$J^2 + S^2 - 2\vec{J}.\vec{S} = L^2$$

$$\vec{J}.\vec{S} = \frac{J^2 + S^2 - L^2}{2}$$

Substituting, we get

$$\left\langle F\ m_F \,|\, \vec{J}\cdot\left(\vec{L}+2\vec{S}\right) | \, F\ m_F \right\rangle = \left\langle F\ m_F \,|\, J^2 + \vec{J}\cdot\vec{S} \,|\, F\ m_F \right\rangle$$

$$= \left\langle F\ m_F \,|\, J^2 + \frac{J^2 + S^2 - L^2}{2} \,|\, F\ m_F \right\rangle$$

$$= J\left(J+1\right) + \frac{J\left(J+1\right) + S\left(S+1\right) - L\left(L+1\right)}{2}$$

$$= \frac{3J\left(J+1\right) + S\left(S+1\right) - L\left(L+1\right)}{2}$$

From equation 22.3

$$\left\langle F\ m'_F \,|\, L_z + 2S_z \,|\, F\ m_F \right\rangle = \frac{3J(J+1)+S(S+1)-L(L+1)}{2J(J+1)} \left\langle F\ m'_F \,|\, J_z \,|\, F\ m_F \right\rangle$$

$$= \frac{3}{2} + \frac{S(S+1)-L(L+1)}{2J(J+1)} \left\langle F\ m'_F \,|\, J_z \,|\, F\ m_F \right\rangle$$

$$= g_J \left\langle F\ m'_F \,|\, J_z \,|\, F\ m_F \right\rangle$$

Where $g_J = \frac{3}{2} + \frac{S(S+1)-L(L+1)}{2J(J+1)}$ is known as Lande g-factor of electron

$$\left\langle F\ m'_F \,|\, J_z \,|\, F\ m_F \right\rangle = \frac{\left\langle F\ m_F \,|\, \vec{J}\cdot\vec{F} \,|\, F\ m_F \right\rangle}{F(F+1)} \left\langle F\ m'_F \,|\, F_z \,|\, F\ m_F \right\rangle$$

$$= \frac{F(F+1)+J(J+1)-I(I+1)}{F(F+1)} m_F$$

$$= a\, m_F$$

$$\left\langle F\ m'_F \,|\, I_z \,|\, F\ m_F \right\rangle = \frac{\left\langle F\ m_F \,|\, \vec{F}\cdot\vec{I} \,|\, F\ m_F \right\rangle}{F(F+1)} m_F$$

$$= \frac{F(F+1)+I(I+1)-J(J+1)}{F(F+1)} m_F$$

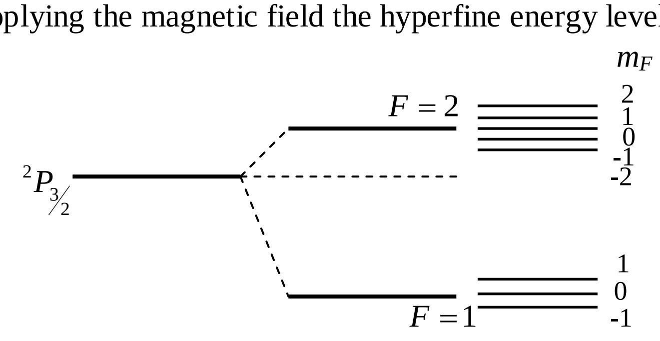
$$= b\, m_F$$

$$\left\langle F\ m'_F \,|\, H_{mag} \,|\, F\ m_F \right\rangle = \left(a\, g_J\, m_F - g_I\, b\, m_F\right) \mu_B B_z$$

$$= \left(a\, g_J - b\, g_I\right) m_F\ \mu_B B_z = g_{hf}\ m_F\ \mu_B B_z \quad \text{............(22.4)}$$

Where $g_{hf} = ag_J - bg_I$

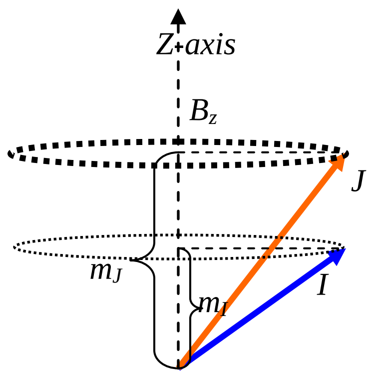
Thus applying the magnetic field the hyperfine energy levels will split as shown in the figure



Case –II :Strong field case:

For this situation we can write the Hamiltonian as

$$H = \underbrace{H_{CF}}_{\substack{\left|l_1 m_{l_1}\right\rangle\left|s_1 m_{s_1}\right\rangle \\ \left|l_2 m_{l_2}\right\rangle\left|s_2 m_{s_2}\right\rangle}} + \underbrace{H_{ee}}_{\left|L m_l\right\rangle\left|S m_s\right\rangle} + \underbrace{H_{so}}_{\substack{\left|J m_J\right\rangle \\ \left|I\, m_I\right\rangle}} + H_{mag} + A'\vec{I}.\vec{J} \quad \ldots\ldots\ldots\ldots\ldots..(22.5)$$



In *LS*-coupling, the spin-orbit interaction is stronger than the magnetic field interaction and hyperfine interaction is weaker so hyperfine interaction can not couple *J* and *I*.

If the magnetic field is applied in the *Z*-axis , *J* and *I* precess more rapidly about B_z .

This is known as Back-Goudsmit Effect which is strong field case.

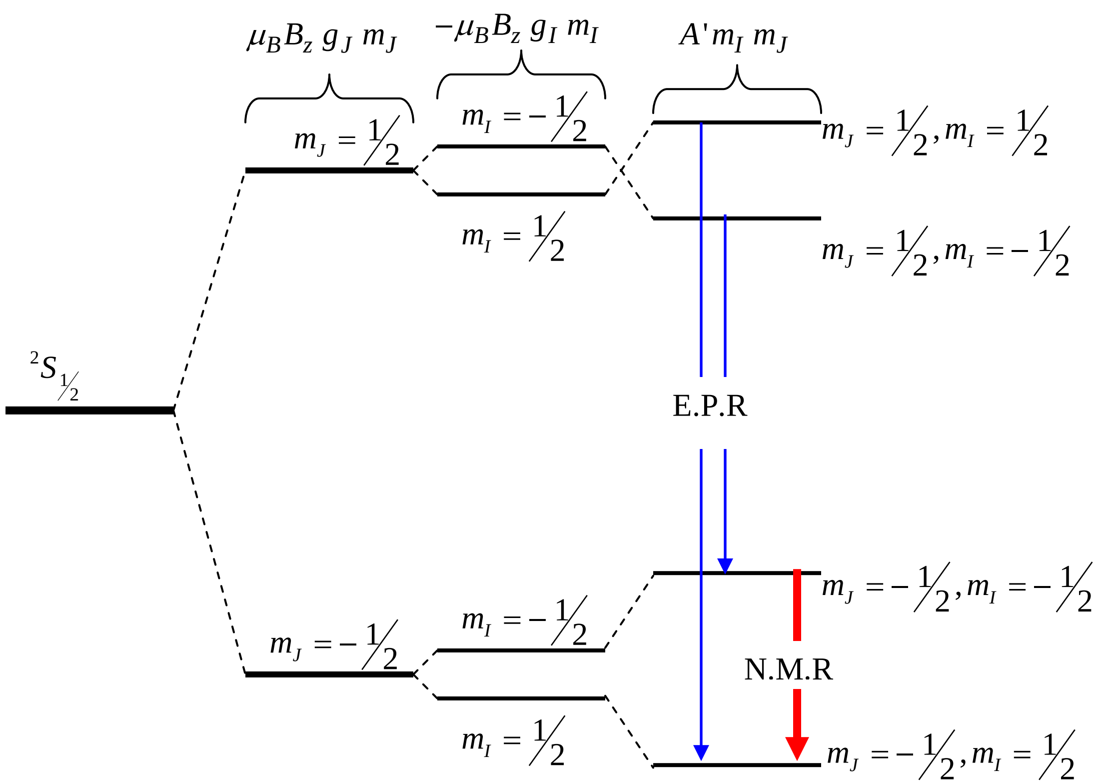
$$\begin{aligned} E_{mag} &= \mu_B B_z \left\langle J\ m_J \,|\left\langle I\ m_I \,|\left(L_z + 2S_z\right)|\, I\ m_I\right\rangle|\, J\ m_J\right\rangle \\ &= \mu_B B_z \left[\left\langle J\ m'_J \,|\, L_z + 2S_z \,|\, J\ m_J\right\rangle - \left\langle I\ m'_I \,|\, g_I\, I_z \,|\, I\ m_I\right\rangle\right] \\ &= \mu_B B_z\, g_J\, m_J - \mu_B B_z\, g_I\, m_I \end{aligned}$$

And the correction term = $\left\langle J\ m_J \,|\left\langle I\ m_I \,|\, A'\vec{I}.\vec{J} \,|\, I\ m_I\right\rangle|\, J\ m_J\right\rangle = A' m_I m_J$

So E_{mag}+ E_{hf} $= \left(m_J\, g_J - m_I\, g_I\right)\mu_B B_z + A' m_I\, m_J$ ………………….(22.6)

Here we take an example of the ground state of hydrogen $^2S_{1/2}$.

For this, $L = 0, S = 1/2, J = 1/2, \quad I = 1/2$. The energy level structure after applying the magnetic field is shown in the following diagram. It is to be noted that, each Zeeman level splits into (2I+1) level.



The transitions shown in blue lines corresponding to electron spin resonance (E.P.R) and the transitions in reds correspond to nuclear magnetic resonance.

Since these transitions are within the same electronic configuration, these are not electric dipole transitions. They are magnetic dipole transitions.

In the next two lectures, we will go through the details of E.P.R and N.M.R.

In this lecture we have gone through the interaction of the magnetic field and the total magnetic moment of the atom

In the weak field case each hyperfine level splits into $(2F+1)$ levels

In the strong magnetic field the hyperfine interaction does not couple I and J. Instead, I and J precess around the magnetic field.

This phenomenon is used to develop the electron spin resonance and nuclear spin resonance spectroscopy those are widely used for various fields of research.