

Lecture 21: Hyperfine Structure of Spectral Lines:

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In this lecture, we will go through the hyperfine structure of atoms.

Various origins of the hyperfine structure are discussed

The coupling of nuclear and electronic total angular momentum is explained.

When individual multiplet ($J \rightarrow J$ transitions) components are examined with spectral apparatus of the highest possible resolution, it is found that in many atomic spectra each of these components is still further split into a number of components lying extremely close together.

This splitting is called hyperfine structure.

The magnitude of the splitting is $\sim 2\text{ cm}^{-1}$.

Hyperfine structure is caused by properties of the atomic nucleus.

Isotopic effect:

Heavier isotopes present 1 in 5000 in ordinary hydrogen.

Therefore, different isotopes of same element have slightly different spectral lines.

Consider 1H (hydrogen) and 2H (deuterium):

$$R_H = R_\infty \frac{1}{1 + \frac{m}{M_H}} = 1.09677 \times 10^7 \text{ meter}^{-1}$$

$$R_D = R_\infty \frac{1}{1 + \frac{m}{M_D}} = 1.097074 \times 10^7 \text{ meter}^{-1}$$

The wavelength difference is therefore:

$$\begin{aligned} \Delta\lambda &= \lambda_H - \lambda_D = \lambda_H \left(1 - \frac{\lambda_D}{\lambda_H} \right) \\ &= \lambda_H \left(1 - \frac{R_H}{R_D} \right) \end{aligned}$$

This is known as isotope shift.

	<i>observed</i>	<i>calculated</i>
	(cm^{-1})	(cm^{-1})
H_α	1.79	1.787
H_β	1.33	1.323
H_γ	1.19	1.182
H_δ	1.12	1.117

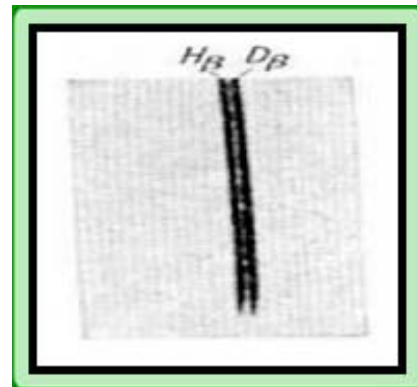


Figure shows the Balmer line of H & D

A quantitative explanation of the isotope effect is not simple, exception H atom. For the heavier elements the effect is traced back to the change of nucleus radius with mass.

$Sm^{150} - Sm^{152}$ is double that of $Sm^{152} - Sm^{154}$.

Usual increase is not from $Sm^{150} \rightarrow Sm^{152}$.

In many cases the isotope effect is not sufficient to explain the hyperfine structure.

The number of hyperfine structure components is often considerably greater than the number of isotopes.

In particular, elements which have only one isotope in appreciable amount also show hyperfine structure splitting.

Likewise, the number of components of different lines is frequently quite different for one and the same element.

These hyperfine structures can be quantitatively explained, when it is assumed that the “atomic nucleus possess an intrinsic angular momentum with which is associated a magnetic moment”.

This angular momentum can have different magnitudes for different nuclei and also of course, for different isotope of the same element.

This is known as Nuclear spin

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Magnetic moment & Angular momentum of the nucleus.

Nucleus consists of Proton & Neutron.

Proton:

- (i) Possesses angular momentum \vec{I}_P described by the spin quantum number $\frac{1}{2}$; this angular momentum obeys the general rules of quantization.

$$\text{Component along oz-axis } (I_P)_z = \pm \frac{1}{2} \hbar$$

$$\text{Magnitude } |I_P| = \sqrt{\left[\frac{1}{2} \left(\frac{1}{2} + 1 \right) \right]} \hbar$$

- (ii) Possesses a magnetic moment $\vec{\mu}_P$ parallel and in the same sense as its angular momentum I_P .

$$\text{Magnetic momentum of proton } \vec{\mu}_P = |(\mu_P)_z| = 2.79 \frac{e \hbar}{2MK} = 2.79 \mu_B^N$$

$$\mu_B^N = \text{nuclear magneton} = \frac{e \hbar}{2MK} \approx \mu_B \frac{m}{M} = \frac{1}{1836} \mu_B$$

$$\text{So, } \mu_B^N = \frac{\mu_B}{1836}$$

Neutron: also possesses magnetic moment

$$|\mu_{Neu}| = -1.913 \mu_B^N$$

But $\mu_{Neu} + \mu_P \neq$ total magnetic moment of the nucleus.

The structure of the nucleus is complex.

Inter nuclear forces are non-central forces involving angles between the magnetic moments and the radius vector joining the nucleus.

Further more, within the nucleus the nucleus possess an orbital angular momentum which can be zero for certain nuclei.

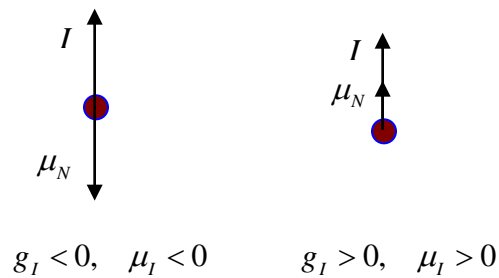
The nuclear magnetic moment μ_N is related to nuclear angular momentum I ,

$$\begin{aligned}\vec{\mu}_N &= g_I \mu_B \vec{I} \\ &= g_I^N \mu_B^N \vec{I} \quad \text{So, } g_I = \frac{1}{1836} g_I^N\end{aligned}$$

g_I or g_I^N is called nuclear Lande' factor.

The general adopted sign for g_I :

The Lande' factor is positive when the nuclear magnetic moment and angular momentum are in the same direction, and is considered negative when in the opposite direction.



Nuclear spin and Magnetic moment:

- (1) All isotopes having an even mass no. A and an even atomic number z , have zero nuclear spin and zero nuclear magnetic moment.

Example: ${}^4_2\text{He}$; ${}^{16}_8\text{O}$; ${}^{20}_{10}\text{Ne}$;

- (2) All isotopes having an even mass number A and an odd atomic number z , have an integral nuclear spin.

${}^2_1\text{D}, I=1$; ${}^6_3\text{Li}, I=1$; ${}^{10}_5\text{B}, I=3$;

- (3) All isotopes having an odd mass number A , have a half integral nuclear spin.

${}^1_1\text{H}, I = \frac{1}{2}$; ${}^3_2\text{He}, I = \frac{1}{2}$; ${}^{39}_{19}\text{K}, I = \frac{3}{2}$
 $1s$ $1s\ 2s$ $[-]4s$

Magnetic field due the orbital motion of electron:

A point charge is $q = -e$ is moving in a classical orbit with a velocity V . At a given instant, the field it creates at the nucleus, is

$$\begin{aligned}\vec{B} &= \frac{\mu_0}{4\pi} \frac{q \vec{r} \times \vec{V}}{r^3} = \frac{\mu_0}{4\pi} q V \times \frac{-\vec{r}}{r^3} = \frac{\mu_0}{4\pi m} \frac{q}{r^3} m \vec{r} \times \vec{V} \\ &= \frac{\mu_0 q}{4\pi m} \frac{\vec{L}}{r^3}\end{aligned}$$

r is directed from the nucleus towards the charge q .

Hence the magnetic field due to the orbital motion of the electron is

$$\vec{B}_l = \frac{\mu_0 q}{4\pi m} \frac{1}{r^3} \vec{L} = -\frac{\mu_0}{4\pi \hbar} 2\mu_B \frac{1}{r^3} \vec{L}$$

The interaction energy between the nuclear magnetic moment and the orbital motion of electron

$$E_l = -\vec{\mu}_N \cdot \vec{B}_l = \frac{\mu_0}{4\pi \hbar} 2g_I \mu_B^2 \frac{\vec{L} \cdot \vec{I}}{r^3}$$

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

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

$$\langle j m' | \vec{L} | j m \rangle = \frac{\langle j m | \vec{L} \cdot \vec{J} | j m \rangle}{j(j+1)} \langle j m' | \vec{J} | j m \rangle$$

So we can substitute, $\vec{L} = \frac{\vec{L} \cdot \vec{J}}{j(j+1)} \vec{J}$ and we get

$$E_l = \frac{\mu_0}{4\pi \hbar} 2g_I \mu_B^2 \frac{\vec{L} \cdot \vec{I}}{r^3} = \frac{\mu_0}{4\pi \hbar} 2g_I \mu_B^2 \frac{\vec{L} \cdot \vec{J}}{j(j+1)} \frac{1}{r^3} (\vec{I} \cdot \vec{J}) \dots\dots\dots(21.1)$$

The interaction energy between two magnetic dipole moments $\vec{\mu}_N$ and $\vec{\mu}_S$ separated by \vec{r} is given by

$$E_{Spin} = \frac{\mu_0}{4\pi} \left[\frac{\vec{\mu}_N \cdot \vec{\mu}_S}{r^3} + \frac{3(\vec{\mu}_N \cdot \vec{r})(\vec{\mu}_S \cdot \vec{r})}{r^5} \right] \dots\dots\dots(21.2)$$

Substituting the value of $\vec{\mu}_N$ and $\vec{\mu}_S$ in this equation, we get

$$E_{Spin} = \frac{\mu_0}{4\pi} \frac{g_I g_S \mu_B^2}{\hbar} \left[-\frac{\vec{I} \cdot \vec{S}}{r^3} + \frac{3(\vec{I} \cdot \vec{r})(\vec{S} \cdot \vec{r})}{r^5} \right] \dots\dots\dots(21.3)$$

Let us take the first term $\frac{\vec{I} \cdot \vec{S}}{r^3}$

Using the relation $\langle jm' | \vec{S} | jm \rangle = \frac{\langle jm | \vec{S} \cdot \vec{J} | jm \rangle}{j(j+1)} \langle jm' | \vec{J} | jm \rangle$

So we can substitute, $\vec{S} = \frac{\vec{S} \cdot \vec{J}}{j(j+1)} \vec{J}$ and we get

$$\frac{\vec{I} \cdot \vec{S}}{r^3} = (\vec{I} \cdot \vec{J}) \frac{\vec{J} \cdot \vec{S}}{j(j+1)} \frac{1}{r^3} = \frac{\vec{I} \cdot \vec{S} + S^2}{j(j+1)} \frac{1}{r^3} (\vec{I} \cdot \vec{J})$$

Now let us take the second term $\frac{3(\vec{I} \cdot \vec{r})(\vec{S} \cdot \vec{r})}{r^5}$

we can substitute, $\vec{r} = \frac{\vec{r} \cdot \vec{J}}{j(j+1)} \vec{J}$ and we get

$$\frac{3(\vec{I} \cdot \vec{r})(\vec{S} \cdot \vec{r})}{r^5} = \frac{3(\vec{I} \cdot \vec{J})(\vec{S} \cdot \vec{r})}{r^5} \frac{\vec{r} \cdot \vec{J}}{j(j+1)}$$

$$\begin{aligned}
 \vec{j} \cdot \vec{r} &= (\vec{l} + \vec{s}) \cdot \vec{r} \\
 \text{Now, } &= \vec{l} \cdot \vec{r} + \vec{s} \cdot \vec{r} \\
 &= 0 + \vec{s} \cdot \vec{r} \\
 &= \vec{s} \cdot \vec{r}
 \end{aligned}$$

$$\text{So, } \frac{3(\vec{l} \cdot \vec{r})(\vec{s} \cdot \vec{r})}{r^5} = \frac{3(\vec{l} \cdot \vec{j})(\vec{s} \cdot \vec{r})^2}{j(j+1)r^5}$$

Substituting the values in equation-21.3 of $\frac{\vec{l} \cdot \vec{s}}{r^3}$ and $\frac{3(\vec{l} \cdot \vec{r})(\vec{s} \cdot \vec{r})}{r^5}$, we get the interaction energy for spin

$$\begin{aligned}
 E_{Spin} &= \frac{\mu_0}{4\pi} \frac{g_l g_s \mu_B^2}{\hbar} \left[-\frac{\vec{l} \cdot \vec{s}}{r^3} + \frac{3(\vec{l} \cdot \vec{r})(\vec{s} \cdot \vec{r})}{r^5} \right] \\
 &= \frac{\mu_0}{4\pi} \frac{g_l g_s \mu_B^2}{\hbar} \left[\frac{3(\vec{l} \cdot \vec{j})(\vec{s} \cdot \vec{r})^2}{j(j+1)r^5} - \frac{\vec{l} \cdot \vec{s} + s^2}{j(j+1)} \frac{1}{r^3} (\vec{l} \cdot \vec{j}) \right] \dots\dots\dots(21.4) \\
 &= \frac{\mu_0}{4\pi} \frac{g_l g_s \mu_B^2}{\hbar} \frac{(\vec{l} \cdot \vec{j})}{j(j+1)} \left[\frac{3(\vec{s} \cdot \vec{r})^2}{r^5} - \frac{\vec{l} \cdot \vec{s} + s^2}{r^3} \right]
 \end{aligned}$$

Now we will calculate the total interaction energy due to electron orbital (equation 21.1) and spin (equation 21.4)

$$E_{HF} = E_l + E_{Spin}$$

$$= \frac{\mu_0}{4\pi\hbar} 2g_l \mu_B^2 \frac{\vec{l} \cdot \vec{j}}{j(j+1)} \frac{1}{r^3} (\vec{l} \cdot \vec{j}) + \frac{\mu_0}{4\pi} \frac{2g_l \mu_B^2}{\hbar} \frac{(\vec{l} \cdot \vec{j})}{j(j+1)} \left[\frac{3(\vec{s} \cdot \vec{r})^2}{r^5} - \frac{\vec{l} \cdot \vec{s} + s^2}{r^3} \right]$$

Here we have substitutes $g_s = 2$ for the electron.

So

$$E_{HF} = \frac{\mu_0}{4\pi} \frac{2g_l \mu_B^2}{\hbar} \frac{(\vec{l} \cdot \vec{j})}{j(j+1)} \left[\frac{\vec{l} \cdot \vec{j}}{r^3} + \frac{3(\vec{s} \cdot \vec{r})^2}{r^5} - \frac{\vec{l} \cdot \vec{s} + s^2}{r^3} \right]$$

$$= \frac{\mu_0}{4\pi} \frac{2g_l \mu_B^2}{\hbar} \frac{(\vec{l} \cdot \vec{j})}{j(j+1)} \left[\frac{\vec{l} \cdot \vec{s} + l^2}{r^3} + \frac{3(\vec{s} \cdot \vec{r})^2}{r^5} - \frac{\vec{l} \cdot \vec{s} + s^2}{r^3} \right]$$

$$= \frac{\mu_0}{4\pi} \frac{2g_l \mu_B^2}{\hbar} \frac{(\vec{l} \cdot \vec{j})}{j(j+1)} \left[\frac{l^2}{r^3} + \frac{3(\vec{s} \cdot \vec{r})^2}{r^5} - \frac{s^2}{r^3} \right]$$

Substituting $\vec{s} \cdot \vec{r} = \frac{1}{2}r$ and $s^2 = s(s+1) = \frac{1}{2}\left(\frac{1}{2}+1\right) = \frac{3}{4}$, we get

$$E_{HF} = \frac{\mu_0}{4\pi} \frac{2g_l \mu_B^2}{\hbar} \frac{(\vec{l} \cdot \vec{j})}{j(j+1)} \left[\frac{l(l+1)}{r^3} + \frac{3(r)^2}{4r^5} - \frac{3}{4r^3} \right]$$

$$= \frac{\mu_0}{4\pi} \frac{2g_l \mu_B^2}{\hbar} \frac{(\vec{l} \cdot \vec{j})}{j(j+1)} \left[\frac{l(l+1)}{r^3} \right] \dots\dots\dots(21.5)$$

$$= \frac{\mu_0}{4\pi} \frac{2g_l \mu_B^2}{\hbar} \frac{l(l+1)}{j(j+1)} \frac{1}{r^3} (\vec{l} \cdot \vec{j})$$

So the Hamiltonian including the hyperfine interaction for one electron system is

$$H = H_0 + H_{Spin-Orbit} + H_{Hyperfine}$$

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

So we define,

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

The interaction energy $E_{HF} = A'_{HF} \vec{I} \cdot \vec{j}$

$A'_{HF} \rightarrow$ constant, characteristic of the level j and l .

Note that the value of $A_{HF} = 0$ for $l = 0$, i.e. for the s -states.

However, experimentally splitting is observed for the $^2S_{1/2}$ state of hydrogen. This can not be explained by this classical explanation.

However, starting from the Dirac equation, if one evaluates the Hamiltonian for the hyperfine interaction including the vector potential (Reference: Atoms and Molecules by M. Weissbluth), it becomes

$$\begin{aligned} H_h &= \frac{\mu_0}{4\pi} \frac{2g_I\mu_B^2}{\hbar} \left[\frac{\ell(\ell+1)}{j(j+1)} \frac{1}{r^3} \vec{I} \cdot \vec{j} + \frac{8\pi}{3} \delta(r) (\vec{I} \cdot \vec{s}) \right] \\ &= A_{HF} \frac{\ell(\ell+1)}{j(j+1)} \vec{I} \cdot \vec{j} + A_F \vec{I} \cdot \vec{s} = A'_{HF} \vec{I} \cdot \vec{j} + A_F \vec{I} \cdot \vec{s} \dots\dots\dots(21.6) \end{aligned}$$

The first term is the dipole-dipole interaction with corresponding to classical expression as we derived earlier. The last term is known as Fermi Contact Interaction term, it has no classical analog and contributes only for s -states. Since $\psi(0)$ at $r = 0$ for non- s states is zero, Fermi contact term goes to zero for non- s states.

$$\delta(r) = |\psi(0)|^2 = \frac{1}{\pi a_0^3}$$

Where a_0 is the Bohr radius.

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For $\ell=0$; i.e. s states first term zero; second term is important. For penetrating orbit contact term is important.

$$\vec{F} = \vec{I} + \vec{s}$$

$$F^2 = I^2 + s^2 + 2\vec{I} \cdot \vec{s}$$

$$\Rightarrow \vec{I} \cdot \vec{s} = \frac{F^2 - I^2 - s^2}{2}$$

$$E_{HF} = \langle F m_F | A_F \vec{I} \cdot \vec{s} | F m_F \rangle = \frac{A_F}{2} [F(F+1) - I(I+1) - s(s+1)]$$

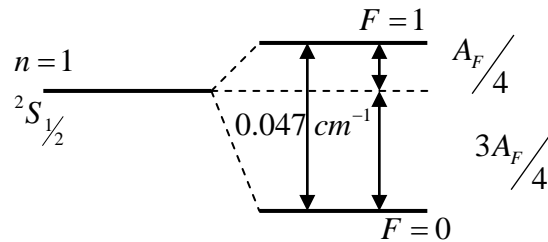
For hydrogen, $^2S_{1/2}$ state, $I = 1/2$, $s = 1/2$, $F = 0, 1$

$$\begin{aligned} E_{HF}(F=1) &= \frac{A_F}{2} \left[1(1+1) - \frac{1}{2} \left(\frac{1}{2} + 1 \right) - \frac{1}{2} \left(\frac{1}{2} + 1 \right) \right] \\ \text{So} \quad &= \frac{A_F}{2} \left[2 - \frac{3}{2} \right] = \frac{A_F}{4} \end{aligned}$$

$$\begin{aligned} E_{HF}(F=0) &= \frac{A_F}{2} \left[0(0+1) - \frac{1}{2} \left(\frac{1}{2} + 1 \right) - \frac{1}{2} \left(\frac{1}{2} + 1 \right) \right] \\ &= \frac{A_F}{2} \left[0 - \frac{3}{2} \right] = -\frac{3}{4} A_F \end{aligned}$$

The hyperfine splitting $= \Delta E_{HF} = E_{HF}(F=1) - E_{HF}(F=0) = A_F$

The calculated values of $A_F = 0.047 \text{ cm}^{-1}$.



For non s states, We have

$$E_{HF} = A_{HF} \frac{\ell(\ell+1)}{j(j+1)} \vec{I} \cdot \vec{j}$$

$$F^2 = I^2 + j^2 + 2 \vec{I} \cdot \vec{j}$$

$$\Rightarrow \vec{I} \cdot \vec{j} = \frac{F^2 - I^2 - j^2}{2}$$

$$E_{HF} = \frac{A_{HF}}{2} \frac{\ell(\ell+1)}{j(j+1)} [F(F+1) - I(I+1) - j(j+1)]$$

For hydrogen, $^2P_{3/2}$ state, $l=1$, $I = 1/2$, $j = 3/2$, $F = 2, 1$

So,

$$E_{HF}(F=2) = \frac{A_{HF}}{2} \frac{1(1+1)}{3/2(3/2+1)} \left[2(2+1) - \frac{1}{2} \left(\frac{1}{2} + 1 \right) - \frac{3}{2} \left(\frac{3}{2} + 1 \right) \right]$$

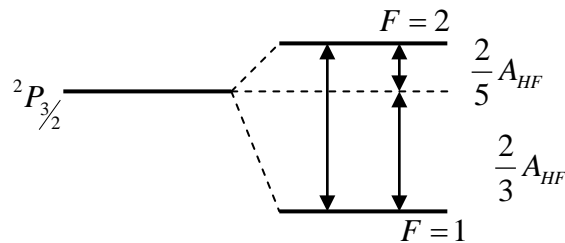
$$= \frac{A_F}{2} \frac{8}{15} \left[6 - \frac{18}{4} \right] = \frac{2}{5} A_{HF}$$

And

$$E_{HF}(F=1) = \frac{A_{HF}}{2} \frac{1(1+1)}{3/2(3/2+1)} \left[1(1+1) - \frac{1}{2} \left(\frac{1}{2} + 1 \right) - \frac{3}{2} \left(\frac{3}{2} + 1 \right) \right]$$

$$= \frac{A_F}{2} \frac{8}{15} \left[2 - \frac{18}{4} \right] = -\frac{2}{3} A_{HF}$$

The hyperfine splitting $= \Delta E_{HF} = E_{HF}(F=2) - E_{HF}(F=1) = \frac{16}{15} A_{HF}$



For hydrogen, $^2P_{1/2}$ state, $l=1$, $I = 1/2$, $j = 1/2$, $F = 0,1$

$$E_{HF}(F=1) = \frac{A_{HF}}{2} \frac{1(1+1)}{1/2(1/2+1)} \left[1(1+1) - \frac{1}{2} \left(\frac{1}{2} + 1 \right) - \frac{1}{2} \left(\frac{1}{2} + 1 \right) \right]$$

So,

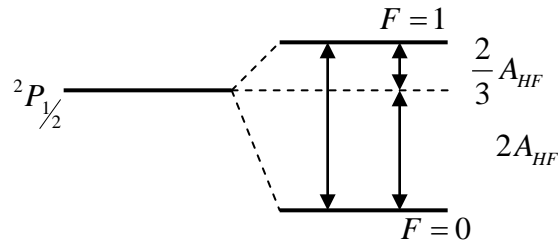
$$= \frac{A_F}{2} \frac{8}{3} \left[2 - \frac{3}{2} \right] = \frac{2}{3} A_{HF}$$

And

$$E_{HF}(F=0) = \frac{A_{HF}}{2} \frac{1(1+1)}{1/2(1/2+1)} \left[0(0+1) - \frac{1}{2} \left(\frac{1}{2} + 1 \right) - \frac{1}{2} \left(\frac{1}{2} + 1 \right) \right]$$

$$= \frac{A_F}{2} \frac{8}{3} \left[0 - \frac{3}{2} \right] = -2A_{HF}$$

The hyperfine splitting $= \Delta E_{HF} = E_{HF}(F=1) - E_{HF}(F=0) = \frac{8}{3} A_{HF}$



For multielectron atom

The interaction energy is $E_{HF} = A' \vec{I} \cdot \vec{J}$

$A' \rightarrow$ hyperfine constant, characteristic of the level J and L

$$F^2 = I^2 + J^2 + 2\vec{I} \cdot \vec{J}$$

$$\Rightarrow \vec{I} \cdot \vec{J} = \frac{F^2 - I^2 - J^2}{2}$$

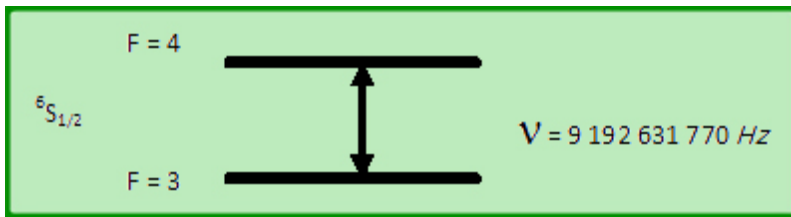
$$E_{HF}(F) = \frac{A'}{2} [F(F+1) - I(I+1) - J(J+1)]$$

$E_{HF}(F+1) - E_{HF}(F) =$ hyperfine splitting or hyperfine structure.

Hyperfine splitting is very small – measurements can be made to a high degree of precision.

The general conference of weights and measures (1964) defined “atomic second” from the transition between the hyperfine energy levels $F = 4, m_F = 0$ and $F = 3, m_F = 0$ of the $^6S_{1/2}$, Ground state of Cs atom $^{133}_{55}\text{Cs}$.

These two sublevels correspond to parallel and anti parallel orientations of the spins $S = 1/2$ of the valence electron and $I = 7/2$ of the nucleus of the Cs atom



Various Corrections:

Since the hyperfine splitting is very small, a lot of small corrections are needed.

- (1) Polarization of the inner shells: For atoms with many electrons, the resultant of the electron spins in the completed inner subshells cannot be regarded as zero, statistically each spin has a slight tendency to align parallel to the spins of the valence electrons. In evaluating the field B_0 , it is necessary to take account of this magnetization of the inner shells 30%.
- (2) Relativistic effect: As a result of high electrostatic charge of the nucleus with high atomic number z , the velocity of the electrons is high in the neighborhood of the nucleus and corrections are necessary. These corrections can modify the result with far heavy atoms for levels with small J , by a factor of the order of two.
- (3) Volume effects: With increasing t , the approximation of a point nucleus cannot be preserved.

Electric Quadrupole Effects

The distribution of the charge q_N within the nucleus is not spherically symmetric.

In classical theory, if the origin is taken as the center of gravity of the electric charges. Within the nucleus, the corresponding electric dipole moment is zero, there then remains the problem as to relative positions of the center of gravity of the electric charges and of the center of gravity of the masses within the nucleus.

In quantum theory, symmetry rules result in zero dipole moment for the nucleus. The first term in the multipole moment expansion corresponds to the interaction of electric quadrupole moment with electric field gradient create by the electrons in the region of the nucleus.

Let's assume that the nucleus has a cylindrical charge distribution around its own Oz axis, I is also Oz axis. The electron cloud has cylindrical symmetry around Oz axis (direction of J). The electric field gradient,

$$\phi_{zz} = -\frac{\partial E_z}{\partial z} = \frac{\partial^2 V}{\partial z^2}$$

$Q \rightarrow$ quadrupole moment of the nucleus

The additional energy ΔE_Q resulting from quadrupole coupling will be,

$$\Delta E_Q = \frac{eQ\phi_{zz}}{4} \left(\frac{3}{2} \cos^2 \theta - \frac{1}{2} \right)$$

Where θ is the angle between $Oz(I)$ and $Oz(J)$.

Define a quadrupole coupling constant $= D = eQ\phi_{zz}$

$$\Delta E_Q = \frac{D}{4} \left(\frac{3}{2} \cos^2 \theta - \frac{1}{2} \right)$$

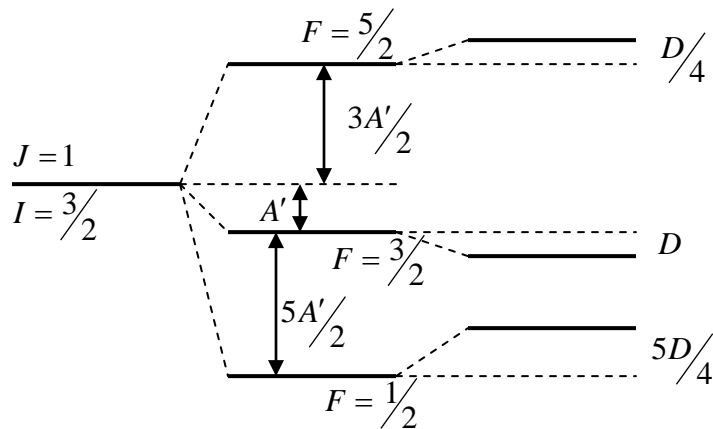
From vector model,

$$\cos \theta = \frac{F(F+1) - I(I+1) - J(J+1)}{2\sqrt{[I(I+1)J(J+1)]}}$$

Or, using quantum mechanics,

$$\Delta E_Q = \frac{D}{4} \frac{\frac{3}{2} C(C+1) - 2I(I+1)J(J+1)}{I(2I-1)J(2J-1)}$$

Where, $C = F(F+1) - I(I+1) - J(J+1)$



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Recap

In this lecture we came to know the origin of hyperfine structure such as isotope effect, hyperfine interaction etc.

The hyperfine structure is very small and can only be observed with a very high resolution.

We have understood the interaction of interaction of nuclear magnetic moment and the total electronic angular moment.

We now know that the ground state hyperfine splitting of hydrogen can not be described by classical concept.

The Fermi contact term is important to describe this splitting and quite accurately predict the experimental observation.

We have also understood the various corrections due to quadrupole effect, volume effect and relativistic effect.