# Lecture # 16



## The coupled basis: hyperfine interaction as an example

Recall: we solved the problem in the uncoupled basis.

$|m_s m_I\rangle$ ← eigen basis of $S_z, I_z$

energy correction & new states with $H'_{hf}$

$H'_{hf}$ is not diagonal in this basis ⇒ diagonalize

Is there a better way?

Before: $\{\vec{S}^2, \vec{I}^2, S_z, I_z\} \Rightarrow |S m_s ; I m_I\rangle$ shared basis

set of commuting observables

(or $|m_s m_I\rangle$ for short) uncoupled

Problem: $H'_{hf} \sim \vec{S}\cdot\vec{I}$ ← doesn't commute with $S_z$ & $I_z$

doesn't share the eigenbasis

Now: Introduce a new set of commuting observables which commute with $\vec{S}\cdot\vec{I}$!

$\{\vec{S}^2, \vec{I}^2, \vec{F}^2, F_z\} \Rightarrow |S I F m_F\rangle$ ← coupled basis

where $\vec{F} = \vec{S} + \vec{I}$ (so $F_z = S_z + I_z$)

($|S I F m_F\rangle \equiv |F m_F\rangle$ for short)

$\vec{F} \Rightarrow$ has the same properties as other ang. mom.! (2)

$\uparrow$ total ang. mom.

$\Rightarrow [F_x, F_y] = i\hbar F_z$

$$F_z |F m_F\rangle = \hbar m_F |F m_F\rangle$$

$$\vec{F}^2 |F m_F\rangle = \hbar^2 F(F+1) |F m_F\rangle$$

Importantly: $\vec{F}^2 = (\vec{S}+\vec{I})^2 = \vec{S}^2 + \vec{I}^2 + 2\vec{S}\cdot\vec{I}$

So $\vec{S}\cdot\vec{I} = \dfrac{\vec{F}^2 - \vec{S}^2 - \vec{I}^2}{2}$

Then, if $H'_{hf} = \underset{\uparrow \text{ recall!}}{\dfrac{A}{\hbar^2}} \vec{S}\cdot\vec{I} \Rightarrow H'_{hf} = \dfrac{A}{2\hbar^2}(\vec{F}^2 - \vec{S}^2 - \vec{I}^2)$

So $H'_{hf} \underbrace{|F m_F\rangle}_{\parallel\ |S I F m_F\rangle} = \dfrac{A}{2\hbar^2}\hbar^2 (F(F+1) - \overset{=1/2}{S}(S+1) - \overset{=1/2}{I}(I+1)) |F m_F\rangle$

$= \dfrac{A}{2}\left(F(F+1) - \dfrac{3}{2}\right) |F m_F\rangle$

$\rightarrow E^{(1)}_{hf} = \langle F m_F | H'_{hf} | F m_F\rangle = \dfrac{A}{2}\left(F(F+1) - \dfrac{3}{2}\right)$

So if we know $F \rightarrow$ we know the energy correction!

Need!
- given $S$ & $I \Rightarrow$ what are possible values of $F$?
- uncoupled vs coupled basis connection?
  $|++\rangle, |+-\rangle, |-+\rangle, |-+\rangle$ vs $|F m_F\rangle$

Consider $F_z|m_s m_I\rangle = (S_z + I_z)|m_s m_I\rangle =$ ③

$= \hbar(\underbrace{m_s}_{=\pm 1/2} + \underbrace{m_I}_{=\pm 1/2})|m_s m_I\rangle \Rightarrow$ $F_z$ matrix is diagonal in the $|m_s m_I\rangle$ basis

$\Uparrow$

it is also diagonal in $|F m_F\rangle$ basis

$$F_z \doteq \hbar \begin{array}{c} \begin{array}{cccc} |{+}{+}\rangle & |{+}{-}\rangle & |{-}{+}\rangle & |{-}{-}\rangle \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \end{array} \begin{array}{l} \langle{+}{+}| \\ \langle{+}{-}| \\ \langle{-}{+}| \\ \langle{-}{-}| \end{array}$$

$F_z|F m_F\rangle = \hbar m_F|F m_F\rangle$

$\underbrace{m_F}_{=1,0,0,-1} = m_s + m_I$

$|{+}{+}\rangle$ $|{+}{-}\rangle$ $|{-}{+}\rangle$ $|{-}{-}\rangle$

$\Downarrow$

$m_F$: $\underbrace{1, 0, -1}_{F=1}$ $\underbrace{0}_{F=0}$

Remember properties of ang. momenta!

$j \Rightarrow -j \le m_j \le j$

apply this to $F \Rightarrow$

if $m_F$ ranges from $-1$ to $1$ it hints that $F = 1$

Can we prove this?

$\vec{F}^2 = \vec{S}^2 + \vec{I}^2 + 2\vec{S}\cdot\vec{I} \rightarrow$ find a matrix representing this

Recall: $\vec{S}\cdot\vec{I} \doteq \begin{array}{c} \begin{array}{cccc} |{+}{+}\rangle & |{+}{-}\rangle & |{-}{+}\rangle & |{-}{-}\rangle \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \end{array} \frac{\hbar^2}{4}$

$\uparrow$

Lecture #15

$$\vec{S}^2 \doteq \hbar^2 \cdot \frac{3}{4}\begin{pmatrix} 1&0&0&0\\ 0&1&0&0\\ 0&0&1&0\\ 0&0&0&1 \end{pmatrix}; \quad \vec{I}^2 \doteq \hbar^2 \frac{3}{4}\begin{pmatrix} 1&0&0&0\\ 0&1&0&0\\ 0&0&1&0\\ 0&0&0&1 \end{pmatrix}$$

$$\underbrace{\hbar^2 S(S+1)\,|m_s m_I\rangle}_{\vec{S}^2 |m_s m_I\rangle} \qquad \underbrace{\hbar^2 I(I+1)\,|m_s m_I\rangle}_{\vec{I}^2 |m_s m_I\rangle}$$

Now add everything together $\Rightarrow$

$$\vec{F}^2 \doteq \hbar^2 \begin{array}{c} \begin{array}{cccc} |++\rangle & |+-\rangle & |-+\rangle & |--\rangle \end{array} \\ \begin{pmatrix} 2&0&0&0\\ 0&1&1&0\\ 0&1&1&0\\ 0&0&0&2 \end{pmatrix} \end{array} \Rightarrow \text{diagonalise!}$$

$$\Downarrow$$

$$\vec{F}^2 |F m_F\rangle = \underbrace{\hbar^2 F(F+1)}_{\text{find eigenvalues}} \underbrace{|F m_F\rangle}_{\text{eigenvectors}}$$

Eigenvalues:

$2\hbar^2$
$2\hbar^2$
$2\hbar^2$ $\Big\}\Rightarrow \boxed{F=1}$

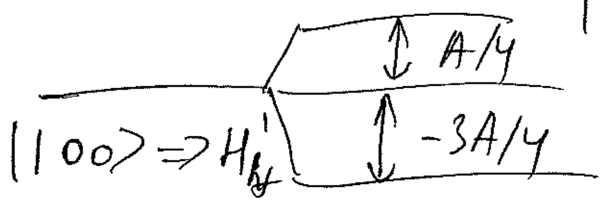
$0 \Rightarrow \boxed{F=0} \Rightarrow |F=0, m_F=0\rangle = \frac{1}{\sqrt{2}}\left(|+-\rangle - |-+\rangle\right)$ } singlet state

$$\underbrace{\begin{aligned} &|F=1, m_F=1\rangle\\ &|F=1, m_F=-1\rangle\\ &|F=1, m_F=0\rangle \end{aligned}}_{\text{coupled basis}} \begin{aligned} &= |++\rangle\\ &= |--\rangle\\ &= \underbrace{\tfrac{1}{\sqrt{2}}\left(|+-\rangle + |-+\rangle\right)}_{\text{uncoupled basis}} \end{aligned} \Bigg\} \text{ triplet state}$$

Putting everything together:

$$E^{(1)}_{hf} = \frac{A}{2}\left(F(F+1) - \frac{3}{2}\right) \Rightarrow \begin{cases} \frac{A}{4}, & F=1 \\ -\frac{3A}{4}, & F=0 \end{cases}$$

$|F\,m_F\rangle$: $|1 1\rangle, |1, 0\rangle, |1 -1\rangle$ ← triplet




$|00\rangle$ singlet

like before!

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Note: $H'_{hf}$ is diagonal in the $|F m_F\rangle$ basis!

$$\begin{array}{cc} & \begin{array}{cccc} |11\rangle & |10\rangle & |1-1\rangle & |00\rangle \end{array} \\ H'_{hf} \doteq \frac{A}{4} & \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix} \end{array}$$

Also note: $S = 1/2$; $I = 1/2 \Rightarrow F = 1, 0$

$\frac{1}{2} + \frac{1}{2}$ $\quad$ $\frac{1}{2} - \frac{1}{2}$

general rule:

If $\vec{J} = \vec{J}_1 + \vec{J}_2 \Rightarrow$

$j = j_1 + j_2, j_1 + j_2 - 1, \ldots, |j_1 - j_2|$

Finally: there is also a general rule on how to relate coupled & uncoupled bases!