Lecture #3

Now that we've discussed atomic structure, Look at transitions between atomic states.

For vector operators ($\hat{d}$ or $\hat{\mu}$) it is useful to use the spherical basis for the vector.
e.g. for electric field polarization $\vec{\epsilon}$

$\vec{\epsilon}_q = \sigma^+, \pi, \sigma^-$
$q=1 \quad q=0 \quad q=-1$

$\sigma^+ = \frac{\hat{x}+i\hat{y}}{\sqrt{2}}$

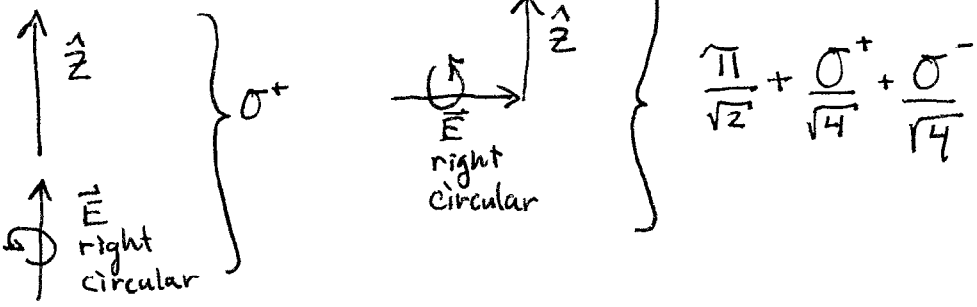
$\pi = \hat{z}$

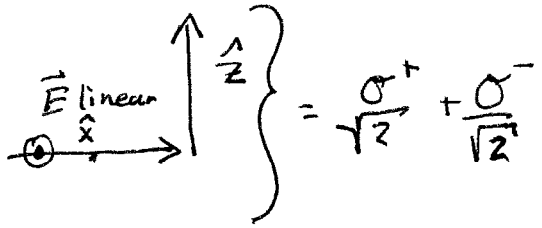
$\sigma^- = \frac{\hat{x}-i\hat{y}}{\sqrt{2}}$

$\sigma^+ \cdot \sigma^- = 0$
$\sigma^+ \cdot \sigma^+ = 1$
etc.

Note: σ^+ is not just right ~~circularly~~ circularly polarized light! It depends on the axis. ← quantization

e.g.





3-J symbols

Clebsch-Gordans are sometimes written in terms of the more symmetric 3-j symbols

$$\langle J' M'_j; Kq | J M_j \rangle = (-1)^{J'-K+M_j} \begin{pmatrix} J' & K & J \\ M'_j & q & -M_j \end{pmatrix} \sqrt{2J+1}$$

↓ a number depending on 6 parameters

not a matrix! it is a number depending on 6 parameters.

properties of Clebsch-Gordans, or equiv. 3-j's lead to selection rules!

e.g.

$$\begin{pmatrix} J_1 & J_2 & J_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = 0 \quad \text{unless } m_1 + m_2 + m_3 = 0$$

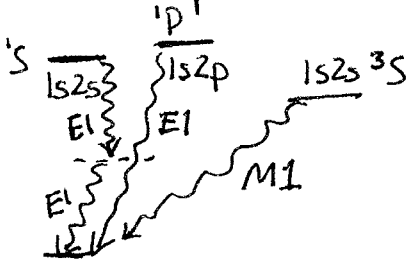
$$\begin{pmatrix} J_1 & J_2 & J_3 \\ 0 & 0 & 0 \end{pmatrix} = 0 \quad \text{unless } J_1 + J_2 + J_3 = \text{even}$$

etc.

Selection Rules

		Transition type: E1	M1	E2
Rigorous rules	1.	$\Delta J = 0, \pm 1$ ($0 \not\leftrightarrow 0$)	$\Delta J = 0, \pm 1$ ($0 \not\leftrightarrow 0$)	$\Delta J = 0, \pm 1, \pm 2$ ($0 \not\leftrightarrow 0$, $\frac{1}{2} \not\leftrightarrow \frac{1}{2}$, $0 \not\leftrightarrow 1$)
	2.	$\Delta m = 0, \pm 1$ ($J=0 \not\leftrightarrow J=0$)	$\Delta m = 0, \pm 1$ ($J=0 \not\leftrightarrow J=0$)	$\Delta m = 0, \pm 1, \pm 2$
	3.	Parity Change	No parity change	No parity Change
Rules for negligible configuration interaction	4.	one electron jumping config. $\Delta l = \pm 1$, Δn arbitrary	no change in electron config. $\Delta l = 0$, $\Delta n = 0$	no change in electron config. or one electron jumping with $\Delta l = 0, \pm 1, \pm 2$, Δn arb.
LS coupling is good	5.	$\Delta S = 0$	$\Delta S = 0$	$\Delta S = 0$
	6.	$\Delta L = 0, \pm 1$ ($L=0 \not\leftrightarrow L=0$)	$\Delta L = 0$, $\Delta J = \pm 1$ (change angle between $S \to L$)	$\Delta L = 0, \pm 1, \pm 2$ ($0 \not\leftrightarrow 0$, $0 \not\leftrightarrow 1$)

Example: (assume $I=0$)



Helium:

$1s2p\ ^1P \to 1s^2\ ^1S$ $\tau = 1.6\text{ns}$ dipole allowed. $\downarrow 10^{8}$

$1s2s\ ^1S \to 1s^2\ ^1S$ $\tau = 20\text{ms}$ E1, M1 E2 forbidden goes as a second order transition

$1s2s\ ^3S \to 1s^2\ ^1S$ $\tau = 8000\text{s}$

→ turns out to be M1, but highly suppressed by $\Delta S = 1$ requirement.

What about including nuclear moment $\vec{I}$?
This leads to coupling of yet more angular momenta, and Wigner 6-j symbols

$\vec{F} = \vec{J} + \vec{I}$
$\vec{F}' = \vec{J}' + \vec{I}$

Example: If $\hat{T}^k$ acts only on the electronic space:

$$\hat{T}^k = \hat{T}^k(J) \otimes \mathbb{1}(I)$$ → identity on nuclear space

then

$$\langle F M_F | \hat{T}^k_q | F' M_F' \rangle = \sum_{\substack{M_J M_I \\ M_J' M_I'}} \langle F M_F | J M_J I M_I \rangle \langle J M_J I M_I | \hat{T}^k_q | J' M_J' I M_I' \rangle \times \langle J' M_J' I M_I' | F' M_F' \rangle$$

Use Wig. Eckart on the JJ' matrix element:

$$= \frac{\langle J \| \hat{T}^k \| J' \rangle}{\sqrt{2J+1}} \sum_{\substack{M_J M_I \\ M_J' M_I'}} \langle F M_F | J M_J I M_I \rangle \langle J' M_J' ; kq | J M_J \rangle \langle J' M_J' I M_I' | F' M_F' \rangle$$

this is a sum over a product of 3 Clebsch Gordans

We can also apply Wig. Eckart to FF':

$$\langle F M_F | \hat{T}^k_q | F' M_F' \rangle = \frac{\langle F \| \hat{T}^k \| F' \rangle}{\sqrt{2F+1}} \langle F' M_F' ; kq | F M_F \rangle$$

equating these, we can solve for

$$\frac{\langle F \| \hat{T}^k \| F' \rangle}{\langle J \| \hat{T}^k \| J' \rangle} = \frac{\sqrt{2F+1}}{\sqrt{2J+1}} \frac{1}{\langle F' M_F', kq | F M_F \rangle_{M_J M_I'}} \sum_{M_J M_I} \langle F M_F | J M_J I M_I \rangle \langle J' M_J' kq | J M_J \rangle \times \langle J' M_J' I M_I' | F' M_F' \rangle$$

the above is independent of M_F', q, $M_F = M_F' + q$, so it can be evaluated at any convenient value, e.g.
$M_F' = q = M_F = 0$ (if allowed by selection rules)

Define the Wigner 6-j symbol as follows:

$$\frac{\langle F \| \hat{T}^k \| F' \rangle}{\langle J \| \hat{T}^k \| J' \rangle} = (-1)^{F'+J+K+I} \sqrt{(2F+1)(2F'+1)} \begin{Bmatrix} J & J' & K \\ F' & F & I \end{Bmatrix}$$

where $\begin{Bmatrix} J & J' & K \\ F' & F & I \end{Bmatrix}$ is the 6-j symbol, that gives a number for any six inputs.

6-j's have a lot of properties, such as they are invariant under permutation of columns or rows.

Given this definition, clearly $\frac{\langle F \| \hat{T}^k \| F' \rangle}{\langle J \| \hat{T}^k \| J' \rangle} = \frac{\langle F' \| \hat{T}^k \| F \rangle}{\langle J' \| \hat{T}^k \| J \rangle}$ up to a sign

⇒ Note: there is only one definition of the 6-j. The different definitions are in regard to the ~~Wigner~~ reduced Matrix elements.

Another $\langle F \| \hat{T}^k \| F \rangle$ definition is

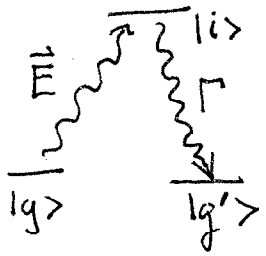
$$\frac{\langle F \| \hat{T}^k \| F' \rangle}{\langle J \| \hat{T}^k \| J' \rangle} = (-1)^{F'+J+K+I} \sqrt{(2F'+1)(2J+1)} \begin{Bmatrix} J & J' & K \\ F' & F & I \end{Bmatrix}$$

and $\frac{\langle F \| \hat{T}^k \| F' \rangle}{\langle J \| \hat{T}^k \| J' \rangle} = \frac{\sqrt{2F'+1}}{\sqrt{2F+1}} \frac{\sqrt{2J+1}}{\sqrt{2J'+1}} \frac{\langle F' \| \hat{T}^k \| F \rangle}{\langle J' \| \hat{T}^k \| J \rangle}$ up to a sign.

I don't know why there isn't a consistent definition.

Example: any second order process in a vector operator.

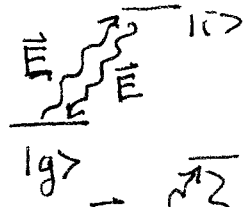
Scattering



$$\propto \left| \sum_i \frac{\langle g'|\hat{d}\cdot\epsilon E_0|i\rangle\langle i|\hat{d}\cdot\vec{E}|g\rangle}{\omega-\omega_i} \right|^2$$

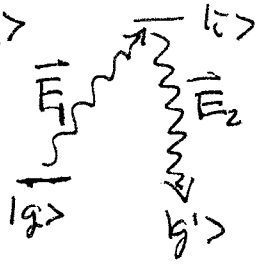
(single photon)

Light shift



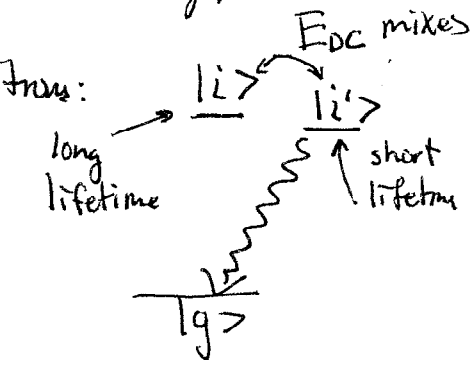
$$\Delta U \propto \sum_i \frac{\langle g|\hat{d}\cdot\vec{E}|i\rangle\langle i|\hat{d}\cdot\vec{E}|g\rangle}{\omega-\omega_i}$$

Raman Transitions



$$\Omega \propto \sum_i \frac{\langle g'|\hat{d}\cdot\vec{E}_2|i\rangle\langle i|\hat{d}\cdot E_1|g\rangle}{\omega-\omega_i}$$

Stark induce transitions:



$$\Gamma \propto \left| \sum_i \frac{\langle g|\hat{d}\cdot\epsilon E_0|i'\rangle\langle i'|E_{dc}|i\rangle}{\omega_i'-\omega_i} \right|^2$$

etc.

These all will have a form

$$A^0(E)\,\hat{T}^0(\hat{d}) + A^1_q(E)\cdot\hat{T}^1_q(\hat{d}) + A^2_q(E)\cdot\hat{T}^2_q(\hat{d})$$

e.g. $|E|^2|\hat{d}|^2 + (E\times E^*)\cdot(\hat{d}\times\hat{d}) + \sum_{\alpha\beta} E_\alpha E_\beta^* \frac{\hat{d}_\alpha\hat{d}_\beta + \hat{d}_\beta\hat{d}_\alpha}{2} - \frac{\delta_{\alpha\beta}}{3}\hat{d}^2$

So in principle they can make $\Delta F = 0, 1$ or 2 transitions.

this will be limited though by how the F states are coupled from $\vec{J}+\vec{I}$

Take the case for scattering light, and
⊕ Assume typical Hyperfine splittings.

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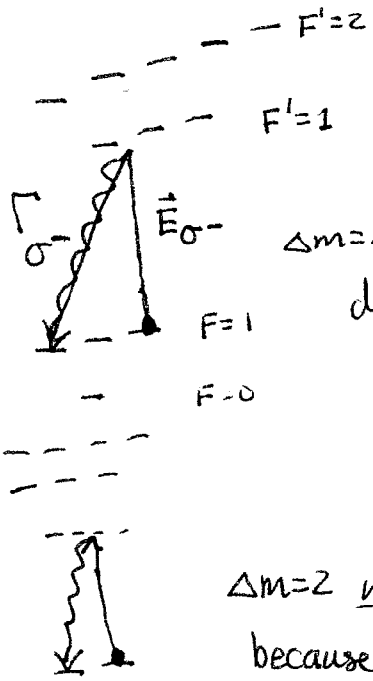
main result from the example:

$J'=3/2$ $I=1/2$ $F=2,1$ $\equiv$ } set of F'

$J=1/2$ $I=1/2$ $F=0,1$ = } set of F



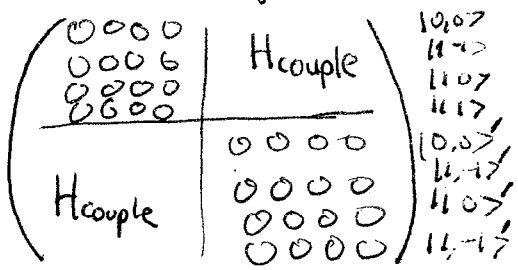
$\Delta m=2$ possible when detuned near hyperfine

$\Delta m=2$ not possible because hyperfine splitting is small compared to the detuning → so the nucleus is ignored.

Looks like a $J=1/2 \to J=3/2$ transition, ΔJ for ground state is at most $1/2 \to -1/2 = 1$.

$\Delta m=1$ only possible.

In the Mathematica notebook, the couplings are calculated as block off diagonal matrices, eg $F=0, F=1 \longleftrightarrow F'=0, F'=1$



8x8 total space, but only 4x4 off diagonal parts need to be calculated.

Transition strengths are often given in terms of the classical oscillator strength.

remember an electron on a spring decays at

$$\Gamma = \frac{e^2 \omega_0^2}{3mc^3} \frac{1}{4\pi\epsilon_0} = \frac{\pi e^2}{3mc\lambda^2\epsilon_0}$$

An oscillator strength is a unitless measure of a transition strength defined as

$$\Gamma_{ki} = \frac{2\pi e^2}{mc\lambda^2\epsilon_0} \frac{g_i}{g_k} f_{ki}$$

f_{ki} is the oscillator strength.

where g_i & g_k are the degeneracy factors for the states. (I don't know where/why the factor of 2/3 ~~3~~ 1/3 probably from average over all directions?)