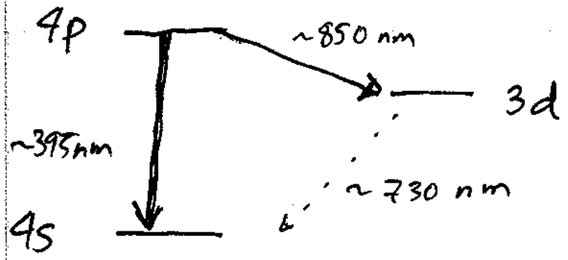
Lecture 10: Selection Rules, Multiplets, and decay

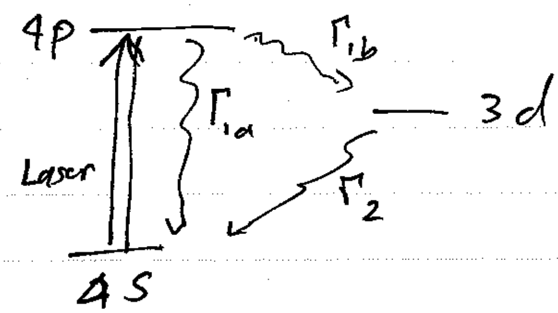
Given the selection rules for multiple transitions, we learn about the life times of excited states by spontaneous emission and branching ratios.

Consider, for example $^{40}Ca^+$ ions. This has one electron in the valence band (like an alkali). The first few energy levels:

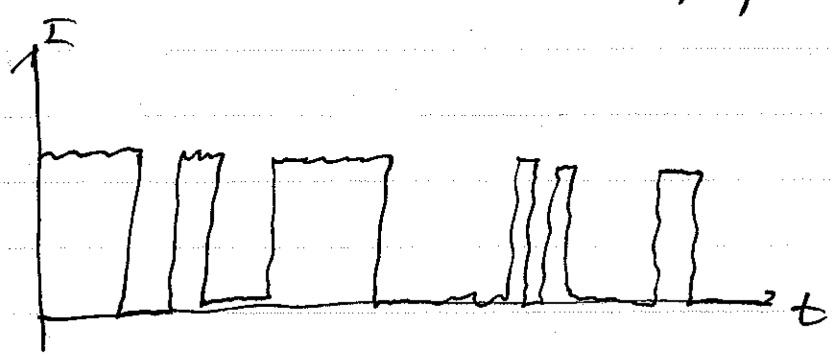


The $4p \to 4s$ and $4p \to 3d$ transitions are electric dipole alowed while 3d is forbidden (E2 transition only). The 3d state is thus meta-stable with a life time of approximately 1 second, whereas the 4p state decays very rapidly with a life time of approximately 15 nanoseconds. In addition, higher frequency and oscillator strength of $4p \to 4s$ vs. $4p \to 4d$ transition leads to a "branching ratio" of 16:1 for decay, i.e. it is 16 times more likely for the ion to decay on the $4p \to 4s$ transition than the $4p \to 4d$ transition. This fact was use in an ingenious method by Hans Dehmelt (1975)

To determine the lifetime of the meta-stable state. Termed "electron shelving", the strong transition "amplifies" the weak transition.

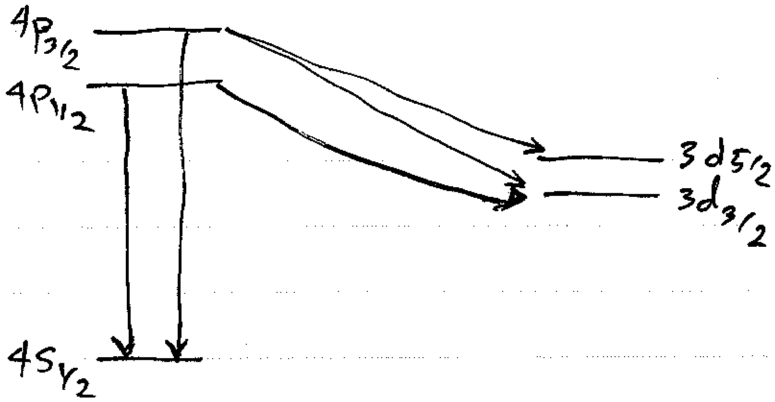


A laser is tuned to the $4s \to 4p$ transition. Most of the time the atom ~~fluoresce~~ fluoresces, decaying back to 4s. Every one in a while (approx 1 in 16 times) the atom decays to 3d. It is long lived, eventually decays back to 4s and the cycle repeats. Thus, every decay of 3d is heralded by the scattering of lots of laser photons, (for reasonable intensity say 10^9 photons). For a single trapped ion, we thus see a random telegraph signal



The dark periods determine times we the atom is "shelved" in 3d. By examining statistics $\Rightarrow$ lifetime of 3d.
Experiment: D.J. Wineland, 1986 (with Hg^+)

If we include the ~~[illegible]~~ fine structure



The $4p_{3/2} \to 3d$ has two channels for decay, whereas the $4p_{1/2} \to 3d$ has one channel. What are the "branching ratios"?

If we ignore the frequency difference of the fine-structure spiliting the decay rate from any initial state $|nL'S'J'M_J'\rangle$ to $|nLSJM_J\rangle$ for all possible J M_J

$$\Gamma^{(J')}_{n'S'L' \to nSL} = \sum_{J} \Gamma_{n'L'S'J' \to nLSJ}$$

$$\Gamma_{n'L'S'J' \to nLSJ} = \sum_{M_J} \frac{4}{3}\frac{k^3}{\hbar} |\langle n'L'S'J'M_J'|\hat{\vec{d}}| nLSJM_J\rangle|^2$$

$$= \frac{4}{3}\frac{k^3}{\hbar} |\langle n'L'S'J'\|d\|nLSJ\rangle|^2$$

Expressing in uncoupled basis

$$\cancel{\Gamma^{(J')}_{n'S'L' \to nSL} = \sum_{JM_J}' \sum_{\substack{M_LM_L' \\ M_SM_S'}}' |\langle n'L'M_L'|\hat{\vec{d}}|nLM_L\rangle|^2 |\langle J'M_J'|L'M_L' S'M_S'\rangle|^2 |\langle JM_J|LM_L SM_S\rangle|^2 \delta_{SS'} \delta_{M_SM_S'}}$$

Only one M_J fullfills selection rule for each M_L M_S

$$\Gamma^{(J')}_{n'S'L' \to nSL} = \frac{4k^3}{3\hbar} \sum_{JM_J}' \left| \sum_{\substack{M_L M_S \\ M_L' M_S'}} \langle J'M_J' | L'M_L' S'M_S' \rangle \langle JM_J | LM_L S M_S \rangle \langle nL'M_L' | \vec{d} | nLM_L \rangle \underbrace{\langle S'M_S' | SM_S \rangle}_{\delta_{SS'}\,\delta_{M_S M_S'}} \right|^2$$

$$= \frac{4k^3}{3\hbar} \sum_{\substack{M_L M_L' \\ M_{L_1} M_{L_1}' \\ M_S M_{S_1}}} \sum_{JM_J}' \langle L'M_{L_1}' S'M_{S_1} | J M_J' \rangle \langle J M_J' | L M_L' S' M_S \rangle \langle LM_{L_1} S M_{S_1} | J M_J \rangle \langle J M_J | LM_L S M_S \rangle \delta_{SS'} \langle nL'M_L' | \vec{d} | nLM_L \rangle \langle nL'M_{L_1}' | \vec{d} | nLM_{L_1} \rangle$$

Sum over $JM_J \Rightarrow \delta_{M_{L_1} M_L} \; \delta_{M_S M_{S_1}}$

$$\Rightarrow M_J' = M_{L_1} + M_S \quad \text{and} \quad M_J' = M_{L_1}' + M_S$$

$$\Rightarrow \delta_{M_{L_1} M_{L_1}'}$$

$$\Gamma^{(J')}_{n'S'L' \to nSL} = \delta_{SS'} \frac{4k^3}{3\hbar} \sum_{M_L, M_L', M_S} |\langle nL'M_L' | \vec{d} | nLM_L \rangle|^2 \, |\langle J'M_J' | LM_L' S M_S \rangle|^2$$

$$= \delta_{SS'} \sum_{M_L} |\langle nL'M_L' | \vec{d} | nLM_L \rangle|^2 \frac{4k^3}{3\hbar}$$

$$= \delta_{SS'} \; \Gamma_{n'S'L' \to nSL}$$

Independent of initial <u>~~hyperfine~~ multiplet state J</u> within a fine structure manifold.

To find the branching ratio, note:

$$\Gamma^{(J')}_{n'S'L \to nSL} = \delta_{SS'} \frac{4}{3}\frac{k^3}{\hbar} |\langle n L' \| d \| n L \rangle|^2$$

Whereas

$$\Gamma^{(J \to J')}_{n'S'L' \to nSL} = \delta_{SS'} \frac{4}{3}\frac{k^3}{\hbar} |\langle n L' S' J' \| d \| n L S J \rangle|^2$$

How are these reduced matrix elements related?

6J Symbols

To deal with the problem we've set out for ourselves, we need to develop the formalism to treat the addition of <u>three</u> <u>angular momenta</u> (here, the electron spin, orbital ang moment, and photon angular momentum).

Let $\vec{J} = \vec{j}_1 + \vec{j}_2 + \vec{j}_3$ $\qquad \vec{j}_{12} = \vec{j}_1 + \vec{j}_2$, $\quad \vec{j}_{23} = \vec{j}_2 + \vec{j}_3$

$$= \vec{j}_{12} + \vec{j}_3 = \vec{j}_1 + \vec{j}_{23}$$

Because in quantum mechanics the ~~~~ states of coupled angular momenta for two j's is different from the uncoupled representation, there are different ways of writing the coupling of 3 j's

e.g.

$$|j m\, j_1 j_2 (j_{12})\, j_3\rangle = \sum_{m_{12} m_3} \langle j m | j_{12} m_{12}\, j_3 m_3\rangle\, |j_{12} m_{12}\rangle |j_3 m_3\rangle$$

$$\Rightarrow |jm\, j_1 j_2 (j_{12}) j_3\rangle = \sum_{m_{12}\, m_1 m_2 m_3} \langle jm | j_{12} m_{12}\, j_3\, m_3\rangle \langle j_{12}\, m_{12} | j_1 m_1\, j_2 m_2\rangle\, |j_1 m_1\rangle \otimes |j_2 m_2\rangle \otimes |j_3 m_3\rangle$$

Similarly

$$|jm\, j_1 j_2 j_3 (j_{23})\rangle = \sum_{m_{23},\, m_1 m_2 m_3} \langle jm | j_1 m_1\, j_{23}\, m_{23}\rangle \langle j_{23} m_{23} | j_2 m_2\, j_3 m_3\rangle\, |j_1 m_1\rangle \otimes |j_2 m_2\rangle \otimes |j_3 m_3\rangle$$

Define:

$$\langle jm\, j_1 j_2 j_3 (j_{23}) | jm\, j_1 j_2 (j_{12}) j_3\rangle \equiv (-1)^{j_1+j_2+j_3+j} \sqrt{(2j_1+1)(2j_{23}+1)} \boxed{\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{Bmatrix}}$$

Wigner 6-J symbols

The funny signs and normalization are chosen so that the 6J symbols have maximum symmetry

$\Rightarrow$ • Exchangable by any two ~~cols~~ columns

• Exchangable w.r.t. upper and lower arguments of any two columns.

$$\Rightarrow \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{Bmatrix} = \frac{(-1)^{j_1+j_2+j_3+j}}{\sqrt{(2j_1+1)(2j_{23}+1)}} \sum_{\substack{m_1 m_2 m_3 \\ m_{12}, m_{23}}} \langle jm | j_{12} m_{12}\, j_3\, m_3\rangle \langle jm | j_1 m_1\, j_{23}\, m_{23}\rangle \cdot \langle j_{12} m_{12} | j_1 m_1\, j_2 m_2\rangle \langle j_{23}\, m_{23} | j_2 m_2\, j_3\, m_3\rangle$$

To find the relationship between the reduced matrix elements consider

$$\langle J'M' j_1' j_2' | \hat{T}_Q^{(K)} \otimes \mathbb{1} | J M j_1 j_2 \rangle$$

where $\hat{T}_Q^{(K)}$ acts only on subsystem 1

$$= \langle J'M' | KQ\, JM \rangle \langle J' j_1' j_2' \| \hat{T}^{(K)} \| J j_1 j_2 \rangle$$

$$= \sum_{\substack{m_1 m_2 \\ m_1' m_2'}} \langle J'M' | j_1' m_1' j_2' m_2' \rangle \langle j_1' m_1' | \hat{T}_Q^{(K)} | j_1 m_1 \rangle \underbrace{\langle j_2' m_2' | j_2 m_2 \rangle}_{\delta_{j_2 j_2'} \delta_{m_2 m_2'}} \langle JM | j_1 m_1 j_2 m_2 \rangle$$

$$= \sum_{m_1 m_1' m_2} \langle J'M' | j_1' m_1' j_2' m_2' \rangle \langle JM | j_1 m_1 j_2 m_2 \rangle \langle j_1' m_1' | KQ\, j_1 m_1 \rangle \langle j_1' \| T^{(K)} \| j_1 \rangle$$

Now use

$$\langle J' j_1 j_2' \| \hat{T}^{(K)} \| J j_1 j_2 \rangle = \sum_{M, M'} (-1)^{J+M} \sqrt{\frac{2K+1}{2J'+1}} \langle J'M' | KQ\, J{-M} \rangle \langle J'M' | \hat{T}^{(K)} | JM \rangle$$

Since $\langle J'M' | K Q\, J{-M} \rangle = (-1)^{J-M} \langle KQ | J'M' JM \rangle \sqrt{\frac{2J'+1}{2K+1}}$

$$\Rightarrow \langle J' j_1' j_2' \| \hat{T}^{(k)} \| J j_1 j_2 \rangle$$

$$= \underbrace{\sum_{\substack{m_1 m_1' m_2 \\ M' M'}}' \left(4\ \text{C-J coeffs} \right)}_{\Downarrow} \times \langle \cancel{j}_1 \| \hat{T}^{(k)} \| j_2 \rangle \, \delta_{j_2 j_2'}$$

$$(-1)^{j_1' + j_2 + J + K} \sqrt{(2J+1)(2J'+1)} \begin{Bmatrix} j_1' & J' & j_2 \\ J & j_1 & K \end{Bmatrix}$$

Example

$$\boxed{\langle J' L' S \| d \| J L S \rangle = (-1)^{L' + S + J + 1} \sqrt{(2J+1)(2J'+1)} \begin{Bmatrix} L' & J' & S \\ J & L & 1 \end{Bmatrix} \langle L' \| d \| L \rangle}$$

Relative decay rate $f_{J'L' \to JL} = (2J+1)(2J'+1) \left| \begin{Bmatrix} L' & J' & S \\ J & L & 1 \end{Bmatrix} \right|^2$

$$\sum_J' f_{J'L' \to JL} = 1$$