

Problem 1

Spontaneous decay rate on a dipole transition $|\psi_e\rangle \rightarrow |\psi_g\rangle$
 summed over all possible final states

$$\Gamma = \frac{4}{3\hbar} k^3 \sum_f |\langle \psi_f | \hat{\mathbf{d}} | \psi_e \rangle|^2$$

Hydrogen, including fine-structure $(nLJM_J) \rightarrow \sum_{M'_J} (n'L'J'M'_J)$

$$\Gamma = \frac{4}{3\hbar} k^3 \sum_{M'_J} |\langle n'L'J'M'_J | \hat{\mathbf{d}} | nLJM_J \rangle|^2$$

(4) Expand in spherical basis $\hat{\mathbf{d}} = \sum_f \hat{\mathbf{e}}_f^* \hat{d}_f$ and
 use W.E.T

$$\Gamma = \frac{4}{3\hbar} k^3 |\langle n'L'J' || \hat{d} || nLJ \rangle|^2 \underbrace{\sum_{M'_J} |\langle J'M'_J | 1_q | J M_J \rangle|^2}_{= 1 \text{ by normalization}}$$

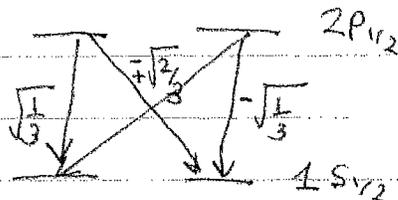
$$\Rightarrow \boxed{\Gamma = \frac{4}{3\hbar} k^3 |\langle n'L'J' || \hat{d} || nLJ \rangle|^2 \text{ independent of } M_J}$$

This makes sense physically. The vacuum is isotropic and will not care what direction the angular momentum of the atom is pointing in.

Aside: Note that $\Gamma \propto \omega^3$. Thus high frequency transitions decay much more rapidly than low frequency transitions. This makes sense from classical electromagnetic theory: The Larmor power (rate of energy radiated from an oscillating dipole) goes as ω^3 .

(b) Life of of $2p_{1/2}$ in Hydrogen

Allowed transitions



Note branching ratios

for decay:

$$\frac{1}{3} + \frac{2}{3} = 1 \quad \checkmark$$

(Note Lamb shift puts $2s_{1/2}$ above $2p_{1/2}$)

From part (a), we need only consider one initial M_J since Γ is the same for all

$$\Rightarrow \Gamma(2p_{1/2}) = \frac{4k^3}{3\hbar} |\langle 1s_{1/2} || d || 2p_{1/2} \rangle|^2$$

To calculate the reduced matrix element, pick some allowed transition and use the W.E.T.

$$\langle 1s_{1/2}, M_J = \frac{1}{2} | d_z | 2p_{1/2}, M_J = \frac{1}{2} \rangle = \langle 1s_{1/2} || d || 2p_{1/2} \rangle \underbrace{\langle \frac{1}{2} \frac{1}{2} | 1 0 \frac{1}{2} \frac{1}{2} \rangle}_{= -\frac{1}{\sqrt{3}}}$$

Must uncouple spin & orbit ang. mom.

$$|2p_{1/2}, \frac{1}{2}\rangle = \sqrt{\frac{1}{3}} |2p, 0\rangle |\frac{1}{2}\rangle - \sqrt{\frac{2}{3}} |2p, 1\rangle |-\frac{1}{2}\rangle \quad (\text{From p.s. \#1 part 3})$$

$$|1s_{1/2}, \frac{1}{2}\rangle = |1s, 0\rangle |\frac{1}{2}\rangle$$

$$\Rightarrow \langle 1s_{1/2}, \frac{1}{2} | d_z | 2p_{1/2}, \frac{1}{2} \rangle = \frac{1}{\sqrt{3}} \langle 1s, 0 | d_z | 2p, 0 \rangle = -\frac{e}{\sqrt{3}} \langle 1s, 0 | z | 2p, 0 \rangle$$

Aside = $\langle 1s, 0 | z | 2p, 0 \rangle = \int d^3x \psi_{2p,0}^*(\vec{x}) z \psi_{1s,0}(\vec{x})$

$$z = \sqrt{\frac{4\pi}{3}} r Y_1^0(\theta, \phi)$$

$$\Rightarrow \langle 1s, 0 | z | 2p, 0 \rangle = \sqrt{\frac{4\pi}{3}} \int_0^\infty dr u_{1s}(r) r u_{2p}(r) \int d\Omega Y_0^0 Y_1^0 Y_0^0$$

Aside continued:

$$\int_0^{\infty} dr r u_{10}(r) u_{21}(r) = \frac{a_0}{\sqrt{6}} \int_0^{\infty} \bar{r}^4 e^{-\frac{3}{2}\bar{r}} d\bar{r} = 1.29 a_0$$

$$\int d\Omega Y_0^0 Y_0^1 Y_0^1 = \frac{1}{\sqrt{4\pi}} \underbrace{\int d\Omega Y_0^1 Y_0^1}_{=1} = \frac{1}{\sqrt{4\pi}}$$

$$\Rightarrow \langle 1s_{v_2} \frac{1}{2} | \hat{d}_z | 2p_{v_2} \frac{1}{2} \rangle = \left(-\frac{e}{\sqrt{3}}\right) \left(\sqrt{\frac{4\pi}{3}}\right) (1.29 a_0) \left(\frac{1}{\sqrt{4\pi}}\right)$$

$$= -0.43 e a_0$$

$$\Rightarrow \langle 1s_{v_2} || d || 2p_{v_2} \rangle = \sqrt{3} 0.43 e a_0 = 0.74 e a_0$$

Thus, $\Gamma(2p_{v_2}) = (0.74)^2 \frac{4}{3\hbar} k^3 (e a_0)^2$

Aside: In atomic units: $\frac{\hbar\Gamma}{e^2/a_0} = \frac{4}{3} (ka_0)^3 \left(\frac{\langle d \rangle}{e a_0}\right)^2$

$$k = \frac{\omega}{c} = \frac{\hbar\omega}{\hbar c} = \epsilon \frac{E_0}{\hbar c} = \epsilon \frac{e^2}{\hbar^2 c a_0} = \alpha \epsilon \frac{1}{a_0}$$

$$\Rightarrow \hbar\Gamma (e^2/a_0) = \epsilon^3 \frac{4}{3} \alpha^3 \left(\frac{\langle d \rangle}{e a_0}\right)^2$$

Here $\frac{\langle d \rangle}{e a_0} = 0.74$

$\alpha = \frac{1}{137}$

$\epsilon = \frac{\hbar\omega}{E_0} = \frac{3}{8} \frac{E_0}{E_0} = \frac{3}{8}$

(Photon for $n=2 \rightarrow n=1$)

$$\Rightarrow \hbar\Gamma / (e^2/a_0) = 1.5 \times 10^{-8}$$

$$\frac{e^2}{a_0} = 27.2 \text{ eV} = 4.1 \times 10^{16} \text{ s}^{-1}$$

$$\Rightarrow \Gamma = 6.2 \times 10^8 \text{ s}^{-1}$$

$$\Rightarrow \text{Life time } \tau = \frac{1}{\Gamma} = 1.6 \text{ ns}$$

Problem Light-Shift (multi-level atoms)

Arbitrary, vector monochromatic field $\vec{E}(\vec{x}, t) = \text{Re}(\vec{E}(\vec{x}) e^{-i\omega t})$

driving ground \leftrightarrow excited manifolds

$$\{ |g; J_g\rangle \leftrightarrow |e; J_e\rangle \}$$

Light-shift operator on ground manifold

$$\hat{V}_{LS}(\vec{x}) = -\frac{1}{4} \vec{E}(\vec{x})^* \cdot \hat{\alpha} \cdot \vec{E}(\vec{x})$$

where $\hat{\alpha} = -\frac{\hat{d}_{ge}}{\hbar \Delta}$

\uparrow
polarizability tensor

$$\hat{d}_{eg} = \hat{P}_e \hat{d} \hat{P}_g$$

\uparrow projectors

$$\hat{d}_{ge} = \hat{d}_{eg}^\dagger$$

(a) Explicit representation in basis of mag-sublevels:

$$\hat{d}_{eg} = \hat{P}_e \hat{d} \hat{P}_g = \sum_{M_e = -J_e}^{J_e} \sum_{M_g = -J_g}^{J_g} |e; J_e M_e\rangle \langle e; J_e M_e| \hat{d} |g; J_g M_g\rangle \langle g; J_g M_g|$$

Spherical basis expansion: $\hat{d} = \sum_q (1)^q \vec{e}_{-q} \hat{d}_q = \sum_q \vec{e}_q^* \hat{d}_q$

$$\Rightarrow \hat{d}_{eg} = \sum_{M_e, M_g} \vec{e}_q^* \langle e; J_e M_e | \hat{d}_q | g; J_g M_g \rangle |e; J_e M_e\rangle \langle g; J_g M_g|$$

Aside: W. E.T.

$$\langle e; J_e M_e | \hat{d}_q | g; J_g M_g \rangle = \langle e; J_e || d || g; J_g \rangle \langle J_e M_e | 1 q J_g M_g \rangle$$

Selection rule $M_e = M_g + q$

$$\Rightarrow \hat{d}_{eg} = \sum_{M_g, q} \vec{e}_q^* C_{M_g}^{M_g+q} |e; J_e M_g+q\rangle \langle g; J_g M_g| \langle e || d || g \rangle$$

where I have used a short hand

for the dipole C-G coef: $C_{M_g}^{M_g+q} = \langle J_e M_g+q | 1 q J_g M_g \rangle$

Similarly $\hat{d}_{ge} = \hat{d}_{eg}^\dagger = \sum_{M_g, q} \vec{e}_q C_{M_g}^{M_g+q} |g; J_g M_g\rangle \langle e; J_e M_g+q| \langle e || d || g \rangle^*$

$$\Rightarrow \hat{d}_{ge} \hat{d}_{eg} = \sum_{M_g, M_g'} \sum_{q, q'} \vec{e}_q \vec{e}_{q'}^* C_{M_g'}^{M_g'+q'} C_{M_g}^{M_g+q} |e; J_e M_g'+q'\rangle \langle g; J_g M_g\rangle \langle g; J_g M_g' | e; J_e M_g+q \rangle \langle g; J_g M_g' | 1 q' J_e M_g'+q' \rangle \langle e || d || g \rangle^* \langle e || d || g \rangle$$

Note:

Two sums must have two sets of indices

$$|g; J_g M_g'\rangle \langle e; J_e M_g'+q' | e; J_e M_g+q \rangle \langle g; J_g M_g' | 1 q' J_e M_g'+q' \rangle \langle e || d || g \rangle^* \langle e || d || g \rangle$$

$$\delta_{M_g'+q', M_g+q}$$

\Rightarrow Selection rule: $M_g' - M_g = q - q'$
(conservation of angular momentum)

$$\delta_{M_g'} = M_g + q - q'$$

(Next Page)

Thus,

$$\hat{d}_{ge} \hat{d}_{eg} = |k_{el} d_{llg}|^2 \sum_{M_g} \sum_{q, q'} \vec{e}_{q'} \vec{e}_q^* C_{M_g+q, q'}^{M_g+q} C_{M_g}^{M_g+q}$$

$|g; J_g, M_g+q\rangle \langle J_g, M_g|$

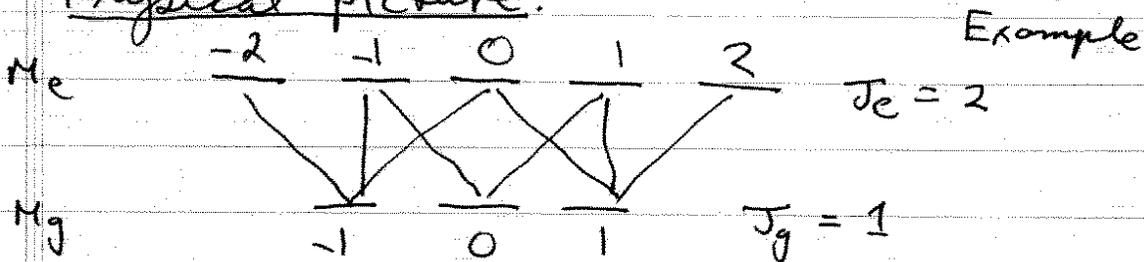
Putting this together, the polarizability tensor in a spherical basis representation:

$$\hat{\alpha} = \tilde{\alpha} \left(\sum_{M_g, q} |C_{M_g}^{M_g+q}|^2 \vec{e}_q |g; J_g, M_g\rangle \langle g; J_g, M_g| \vec{e}_q^* \right) + \sum_{M_g, q \neq q'} C_{M_g+q, q'}^{M_g+q} C_{M_g}^{M_g+q} \vec{e}_{q'} |g; J_g, M_g+q\rangle \langle J_g, M_g| \vec{e}_q^*$$

Here I explicitly write diagonal + off-diag terms

where $\tilde{\alpha} = - \frac{|\langle e; J_e, l_{llg} \rangle|^2}{\hbar \Delta}$ (reduced matrix element)

Physical picture:

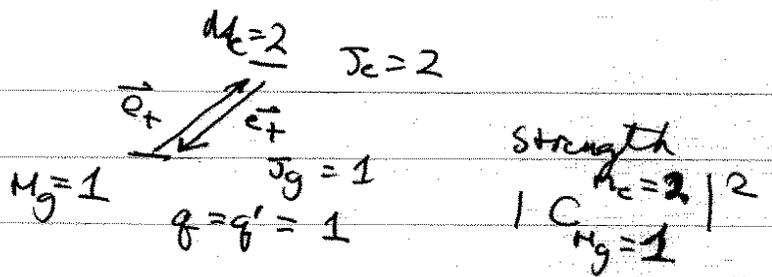


The shift can be thought of as resulting from virtual absorption and emission of photons.

If the atom absorbs and re-emits a photon of helicity $q \Rightarrow$ comes back to the same state \Rightarrow Oscillator strength $M_g \leftrightarrow M_e$.

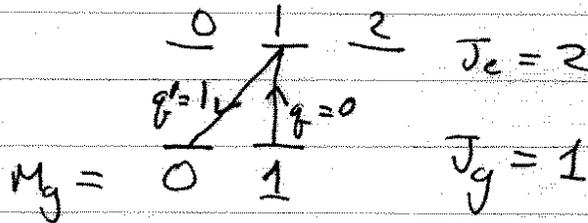
If the atom absorbs photon helicity q and emits q' , the deficit goes into atomic ang. mo. $M \Rightarrow M = M_e + q \rightarrow M_a = M_e - q'$

ex: Diagonal term



example: Off-diagonal term

Strength
 $\begin{pmatrix} C_0 & C_1 \\ C_0 & C_1 \end{pmatrix}$



(b) Plane polarized case: $\vec{E}(\vec{r}) = E_1 \vec{e}_L e^{i\vec{k} \cdot \vec{r}}$

$$\Rightarrow \hat{V}_{LS} = -\frac{1}{4} |E_1|^2 \vec{e}_L^* \cdot \hat{\alpha} \cdot \vec{e}_L$$

Case (i): Linear polarization along z $\vec{e}_L = \vec{e}_0$

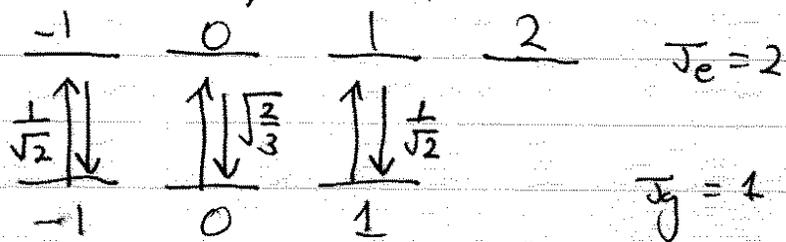
$$\Rightarrow \hat{V}_{LS} = -\frac{1}{4} |E_1|^2 \vec{e}_0 \cdot \hat{\alpha} \cdot \vec{e}_0$$

$$= \underbrace{-\frac{\alpha^2}{4} |E_1|^2}_{V_1} \sum_{M_g} |C_{M_g}^{M_g}|^2 |g; J_g M_g\rangle \langle g; J_g M_g|$$

\Rightarrow Only diagonal terms (see picture above)

Case $|g; J_g = 1\rangle \rightarrow |e; J_c = 2\rangle$

Only π -polarization



Clebsch-Gordan coeff $C_{M_g}^{M_c} = \langle 2 M_g | 1 0 1 M_g \rangle$

→ For $\vec{E}_L = \vec{e}_z$ $|J_g=1\rangle \rightarrow |J_e=2\rangle$

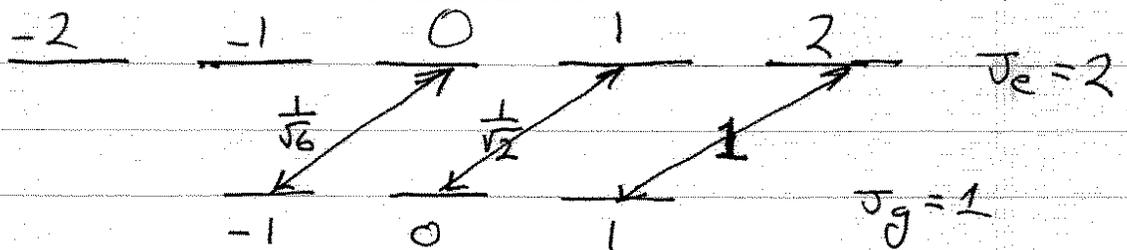
Eigenvectors: Magnetic sublevels $|J_g, J_g\rangle$

Eigenvalues: $\frac{1}{2}V_1$, $\frac{2}{3}V_1$

Sketch: $\Delta < 0 \Rightarrow V_1 < 0$

M_g -1 0 1 Shifted levels

Case $\vec{E}_L = \vec{e}_+$ $|J_g=1\rangle \rightarrow |J_e=2\rangle$



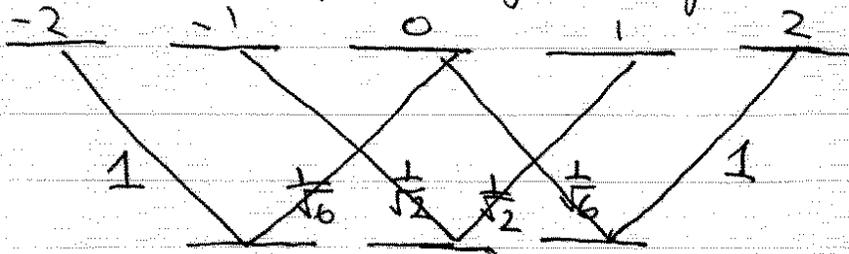
Eigenvectors: $|J_g, M_g\rangle$

Eigenvalues: $M_g = -1 : \frac{1}{6}V_1$, $M_g = 0 : \frac{V_1}{2}$, $M_g = +1 : V_1$

M_g -1 0 1 ($V_1 < 0$ here)

Case $\vec{E}_L = \vec{e}_x$ $|J_g=1\rangle \rightarrow |J_e=2\rangle$

$\vec{e}_x = \frac{-\vec{e}_+ + \vec{e}_-}{\sqrt{2}}$; Not one of spherical basis
 \Rightarrow Not just diagonal elements



Light Shift operator for $\vec{\epsilon}_L = \vec{\epsilon}_x = \frac{1}{\sqrt{2}}(-\vec{\epsilon}_+ + \vec{\epsilon}_-)$

$$\hat{V}_L(\vec{x}) = V_1 \left[\sum_{M_g, \delta} |C_{M_g}^{M_g+\delta}|^2 (\vec{\epsilon}_x \cdot \vec{\epsilon}_\delta) |J_g M_g\rangle \langle J_g M_g| (\vec{\epsilon}_\delta^* \cdot \vec{\epsilon}_x) \right. \\ \left. + \sum_{M_g, \delta, \delta'} C_{M_g+\delta}^{M_g+\delta'} C_{M_g}^{M_g+\delta} (\vec{\epsilon}_x \cdot \vec{\epsilon}_\delta) |J_g, M_g+\delta-\delta'\rangle \langle J_g M_g| \vec{\epsilon}_\delta \right]$$

$$= \frac{V_1}{2} \left[\sum_{M_g} (|C_{M_g}^{M_g+1}|^2 + |C_{M_g}^{M_g-1}|^2) |J_g M_g\rangle \langle J_g M_g| \right. \\ \left. - \sum_{M_g} (C_{M_g+2}^{M_g+1} C_{M_g}^{M_g+1} |J_g, M_g+2\rangle \langle J_g M_g| + h.c.) \right]$$

$$= \frac{V_1}{2} (|0\rangle\langle 0| + \frac{1}{12} (|1\rangle\langle 1| + |1\rangle\langle -1| + |1\rangle\langle -1| - |1\rangle\langle 1| - |1\rangle\langle 1|))$$

here I have simplified notation $|M_g\rangle \equiv |J_g, M_g\rangle$

Eigenvalues are eigenvectors

In the basis $\{|0\rangle, |1\rangle, |-1\rangle\}$

$$\hat{V}_L \doteq \frac{V_1}{2} \begin{bmatrix} 1 & 0 & 0 \\ 0 & \frac{7}{12} & -\frac{1}{12} \\ 0 & -\frac{1}{12} & \frac{7}{12} \end{bmatrix}$$

Block diagonal.
We must diagonalize the 2x2 matrix

$$\begin{bmatrix} \frac{7}{12} & -\frac{1}{12} \\ -\frac{1}{12} & \frac{7}{12} \end{bmatrix} = \frac{7}{12} \mathbb{1} - \frac{1}{12} \sigma_x \Rightarrow \text{eigenvalues } \frac{7}{12} \pm \frac{1}{12} = \frac{6}{12}, \frac{8}{12}$$

eigenvectors $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$

$\vec{\epsilon}_L = \vec{\epsilon}_x \Rightarrow$

$J_g = 1 \Rightarrow J_e = 2$	Eigenvector / eigenvalue
	$ 0\rangle : \frac{V_1}{2}$
	$\frac{ 1\rangle + -1\rangle}{\sqrt{2}} : \frac{V_1}{2}$
	$\frac{ 1\rangle - -1\rangle}{\sqrt{2}} : \frac{2}{3} V_1$

Thus we see that the eigenvalues for $\vec{E}_L = \vec{e}_z$ and $\vec{E}_L = \vec{e}_x$ are equal. This is as it must be. What direction we call "x" or "y" or "z" is irrelevant. The choice of "quantization axis" is arbitrary.

What about the eigenvectors for these two cases?

For $\vec{E}_L = \vec{e}_z$ with z-quantization we found eigenvectors $|M_z = 0\rangle$, $|M_z = \pm 1\rangle$ with eigenvalues $\hat{V}_L = \frac{2}{3}V_1$, $\frac{1}{2}V_1$ (doubly degenerate)

Thus for $\vec{E}_L = \vec{e}_x$ with x-quantization we must have eigenvectors $|M_x = 0\rangle$, $|M_x = \pm 1\rangle$ with eigenvalues $\hat{V}_L = \frac{2}{3}V_1$, $\frac{1}{2}V_1$ (doubly degenerate)

Now $|M_x\rangle = \hat{D} |M_z\rangle$ where \hat{D} is a rotation matrix

For $J_y = 1$ we can explicitly calculate the rotation matrix, or use symmetry arguments via the spherical basis (see Phys 521, P.S. #6)

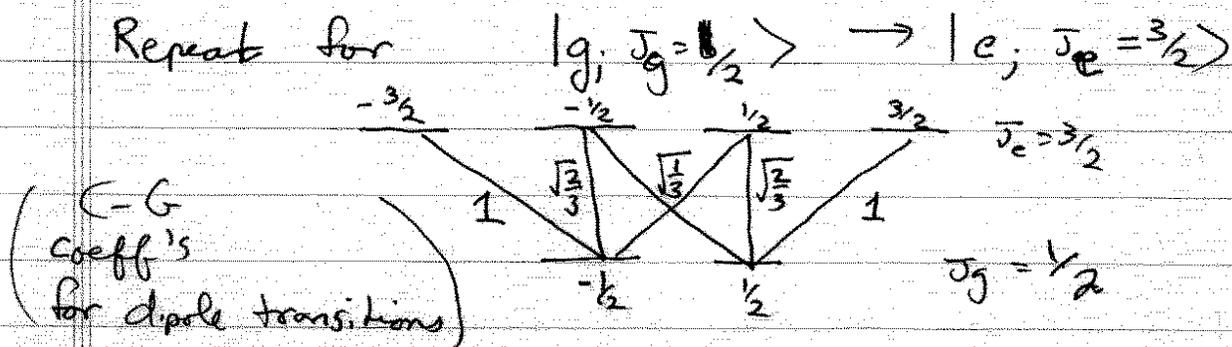
$$|1, M_x = 0\rangle = \frac{-1}{\sqrt{2}} (|1, M_z = +1\rangle - |1, M_z = -1\rangle)$$

$$|1, M_x = \pm 1\rangle = \frac{-i}{\sqrt{2}} \left[\pm |1, M_z = 0\rangle + \frac{1}{\sqrt{2}} (|1, M_z = 1\rangle + |1, M_z = -1\rangle) \right]$$

$$\text{thus } \hat{V}_L |M_x = 0\rangle = \frac{2}{3}V_1 |M_x = 0\rangle$$

$$\hat{V}_L |M_x = \pm 1\rangle = \frac{1}{2}V_1 |M_x = \pm 1\rangle$$

So it all makes sense! ∇



Case (i) $\vec{E}_L = \vec{e}_z$

Eigenvectors $|J_g, M_g = \pm 1/2\rangle$
 Eigenvalues $\frac{2}{3} V_1$ (doubly degenerate)

Case (ii) $\vec{E}_L = \vec{e}_+$

Eigenvectors $|J_g, M_g = \pm 1/2\rangle$
 Eigenvalues $|M_g = 1/2\rangle: V_1, |M_g = -1/2\rangle: \frac{1}{3} V_1$

Case (iii) $\vec{E}_L = \vec{e}_x = \frac{1}{\sqrt{2}}(\vec{e}_+ + \vec{e}_-)$

Unlike the $J_g = 1$ case, the light-shift operator is diagonal here since there are no $\Delta M_g = \pm 2$ coherences possible in the ground state

$$\begin{aligned} \hat{V}_{LS} &= \frac{V_1}{2} \sum_{M_g} (|C_{M_g}^{J_g+1}|^2 + |C_{M_g}^{J_g-1}|^2) |J_g, M_g\rangle \langle J_g, M_g| \\ &= \frac{V_1}{2} \left[\left(1 + \frac{1}{3}\right) |1/2\rangle \langle 1/2| + \left(\frac{1}{3} + 1\right) |-1/2\rangle \langle -1/2| \right] \\ &= \frac{2}{3} V_1 \left(|1/2\rangle \langle 1/2| + |-1/2\rangle \langle -1/2| \right) \end{aligned}$$

\Rightarrow Eigenvectors $|J_g, M_g = \pm 1/2\rangle$
 Eigenvalues $\frac{2}{3} V_1$ (doubly degenerate)

Same as $\vec{E}_L = \vec{e}_z$ as it must be

(c) The polarizability tensor can be written in terms of irreducible tensors

Let $\hat{T}_{ij} = d_{ge}^i d_{eg}^j$ outer product of two vectors

As discussed in class, any such Cartesian tensor can be expanded in terms of irreducible tensors

$$\hat{T}_{ij} = \hat{T}_{ij}^{(0)} + \hat{T}_{ij}^{(1)} + \hat{T}_{ij}^{(2)}$$

where $\hat{T}_{ij}^{(0)} = \text{Trace}(\hat{T}_{ij}) \frac{\delta_{ij}}{3} = \frac{1}{3} \hat{d}_{ge} \cdot \hat{d}_{eg}$

Antisymmetric: $\hat{T}_{ij}^{(1)} = \frac{d_{ge}^i d_{eg}^j - d_{ge}^j d_{eg}^i}{2} = \frac{1}{2} \epsilon_{ijk} (\hat{d}_{ge} \times \hat{d}_{eg})_k$

Symmetric, Traceless: $\hat{T}_{ij}^{(2)} = \frac{d_{ge}^i d_{eg}^j + d_{ge}^j d_{eg}^i}{2} - \frac{1}{3} \hat{d}_{ge} \cdot \hat{d}_{eg}$

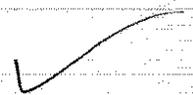
Thus with $\hat{\alpha}_{ij} = -\frac{1}{k\Delta} \hat{T}_{ij}$

we arrive at the desired expansion

$$\hat{V}_{Ls} = -\frac{1}{4} \vec{E}^*(\vec{x}) \cdot \hat{\alpha} \vec{E}(\vec{x}) = -\frac{1}{4} E_i^* E_j \hat{\alpha}_{ij}$$

$$= -\frac{1}{4} (\alpha^{(0)} |\vec{E}(\vec{x})|^2 + \alpha^{(1)} \cdot (\vec{E}^* \times \vec{E}) + \vec{E}^* \cdot \hat{\alpha}^{(2)} \cdot \vec{E})$$

$$\hat{\alpha}_{ij}^{(k)} = -\frac{1}{k\Delta} \hat{T}_{ij}^{(k)}$$



(d) For the particular case $|g; J_g = 1/2\rangle \rightarrow |e; J_e = 3/2\rangle$

\hat{V}_{LS} acts on the ground manifold $\{|J_g, 1/2\rangle, |J_g, -1/2\rangle\}$

The rank-2 part $\hat{V}_{LS}^{(2)} = -\frac{1}{4} E_c^* E_j \hat{\alpha}_{ij}^{(2)}$

has matrix elements $\langle J_g = 1/2, M_g | \hat{V}_{LS}^{(2)} | J_g = 1/2, M_g \rangle$

$$= \langle \frac{1}{2} || \hat{V}_{LS}^{(2)} || \frac{1}{2} \rangle \underbrace{\langle \frac{1}{2} M_g | 2q - \frac{1}{2} M_g \rangle}$$

this C-G coeff vanishes
by the triangle inequality

Thus,

$$\hat{V}_{LS} = -\frac{1}{4} |\vec{E}|^2 \hat{\alpha}^{(0)} - \frac{1}{4} (\vec{E}^* \times \vec{E}) \cdot \hat{\alpha}^{(1)}$$

↓

Scalar

↓

vector

Acting on spin- $1/2$ the scalar part must be proportional to the identity and the vector part to $\hat{\sigma}$ since any operator acting on the 2D Hilbert space is of this form

Thus,
$$\hat{V}_{LS} = V_0(\vec{x}) \hat{1} + \vec{B}_{\text{eff}}(\vec{x}) \cdot \hat{\sigma}$$

Where
$$V_0(\vec{x}) = \frac{1}{2} \text{Tr}(\hat{V}_{LS})$$

$$\vec{B}_{\text{eff}} = \frac{1}{2} \text{Tr}(\hat{V}_{LS} \hat{\sigma})$$