Lecture 22: Further Applications of the Wigner-Eckart Thrm

Higher order multipole transitions

We derived last lecture the selection rules for electric dipole driven transitions. More generally, given a slowly varying E/M field such that the characteristic time of change $T << \frac{R}{c}$ = (time for light to propagate across distribution of size R) or equivalently

$$R << cT \sim \frac{c}{\omega} \sim \lambdabar \quad (\text{i.e. charge in near field})$$

size of atom

we have the multipole expansion for interaction energy:

(position of atom)

$$\hat{H}_{int} = -\hat{\vec{d}} \cdot \vec{E}(\vec{x}_0, t) - \hat{\vec{\mu}} \cdot \vec{B}(\vec{x}_0, t) + \frac{1}{2} \sum_{ij} \hat{Q}_{ij} \, \partial_i E_j(\vec{x}_0, t) + \cdots$$

where $\hat{\vec{d}}$ = electric dipole operator

$\hat{\vec{\mu}}$ = magnetic dipole operator

$\hat{Q}_{ij} = \sum_\alpha q_\alpha \left(x_i^\alpha x_j^\alpha - \frac{1}{3} r_\alpha^2 \delta_{ij} \right)$: electric quadrapole tensor

Note: this expression is for a special choice of Gauge ("The Poincaré Gauge", obtained from the usual Hamiltonian via the "Power-Wooley" transf.)

The multipole moments driven by the incident field are dominated by the lowest nonvanishing term. However, if for example, the transition does not satisfy the E1 selection rules, transition is still possible via a higher order multipole.

Magnetic dipole transitions (M1)

As with E1 transition, the absorption rate is proportional to the square of the matrix element

$$W_{f\leftarrow i} \sim |\langle \psi_f | \hat{\vec{\mu}} \cdot \vec{B}(\vec{x}_0) | \psi_i \rangle|^2$$

$$= |\langle \psi_f | \underbrace{\hat{\mu}_q^{(1)}}_{\text{Rank 1 tensor operator}} | \psi_i \rangle|^2 \; |\vec{e}_q^{\,*} \cdot \vec{B}(\vec{x}_0)|^2$$

For Fine structure states $|n L S J M_J\rangle$:

$$\langle n'L'S'J'M_J' | \hat{\mu}_q^{(1)} | n L S J M_J \rangle = \langle n'L'S'J' \| \hat{\mu}^{(1)} \| n L S J \rangle \langle J' M_J' | 1 q \, J M_J \rangle$$

$\Rightarrow$ As in E1: $\Delta J = 0, \pm 1$ (no $J=0 \rightarrow J'=0$)

$\Delta M_J = 0, \pm 1$

What about S and L?

Electron $\vec{\mu} = -\mu_B(\vec{L} + 2\vec{S}) \Rightarrow [\vec{\mu}, \vec{L}^2] = [\vec{\mu}, \vec{S}^2] = 0$

$\Rightarrow \Delta S = 0$

$\Delta L = 0, \pm 1$ by rotation. What about parity

Recall $\vec{\mu} = \gamma \vec{J}$ and $\vec{J}$ is <u>even</u> under parity

(e.g. $\vec{J} = \vec{x} \times \vec{p}$ <u>even</u>)

$\Rightarrow \vec{\mu}$ is even under parity

$\Rightarrow \Delta L = 0$:

<u>Summary:</u> (M1)

$\Delta J = 0, \pm 1$ $\quad \Delta M_J = 0, \pm 1 \longrightarrow$ Depends on polarization of $\vec{B}$

$\Delta S = 0$

$\Delta L = 0$

Example in Hydrogen $2P_{3/2} \to 2P_{1/2}$ transition (10 GHz):

$$\Delta J = 1, \quad \Delta L = 0, \quad \Delta S = 0 \qquad \Delta M_J = 0, \pm 1$$

How does transition rate for M1 compare to E1?

Atomic units: $d_A = e a_0$

$$\mu_A = \frac{e\hbar}{mc} = e \underset{\substack{\uparrow \\ \text{Compton}}}{\lambda_c} = e(\alpha a_0) \qquad \alpha = \frac{e^2}{\hbar c}$$

$$\Rightarrow \frac{|\mu_A|^2}{|d_A|^2} = \alpha^2 = \left(\frac{1}{137}\right)^2 \cong 5 \times 10^{-5}$$

Recall $\alpha = \frac{v}{c}$ in Hydrogen $\Rightarrow$ $\alpha = \frac{R}{Tc} = \frac{R}{\lambda}$ small parameter

<u>Electric Quadrupole</u> (E2)

Must consider matrix elements $\langle \psi_f | \hat{Q}_{ij} | \psi_i \rangle \; \partial_j E_i$

$\hat{Q}_{ij}$ is a symmetric traceless cartesian tensor: irreducible

Five independent components related to the five spherical components $\hat{Q}^{(2)}_q$ (see Jackson)

thus
$$\langle n'L'S'J'M_J' | \hat{Q}^{(2)}_q | nLSJM_J \rangle = \langle n'L'S'J' \| \hat{Q}^{(2)} \| nLSJ \rangle \langle J'M_J' | 2\, q\, J M_J \rangle$$

$\Rightarrow$

$\Delta J = 0, \pm 1, \pm 2$

$\Delta M_J = 0, \pm 1, \pm 2$

$\Delta S = 0$

$\Delta L = 0, \cancel{\pm 1}, \pm 2$

forbidden by parity (Q is <u>even</u>)

Note: For $\Delta L = 0$ $\Delta M_J = 0, \pm 1$ both M1 and E2 are allowed. They can interfer.

Size of E2 compared to E1 and M1

Transition rate $\sim \frac{Q^2}{D^2}$ where D is the scale over which $\vec{E}$ has gradient

For plane wave: $D = \frac{1}{ƛ} \Rightarrow \frac{1}{D} = k$

$$\Rightarrow \frac{Q}{D} \sim \frac{e a_0^2}{ƛ} = e a_0^2 k = e a_0^2 \frac{\omega}{c}$$

$\omega \hat{=}$ frequency of resonance $\Rightarrow \hbar\omega = \frac{e^2}{a_0}$

$$\Rightarrow \frac{Q}{D} \sim e a_0^2 \frac{e^2}{\hbar c a_0} = \alpha e a_0 = \mu_A$$

So for a plane wave with $|E| = |\vec{B}|$, the strength of M1 and E2 are equal. Of course, in other situations this may not be true. For example, in a microwave cavity, or Rf coil $\vec{B}$ can be large, but the gradient of $|\vec{E}|$ small $\Rightarrow$ M1 transition

Question: How can E2 transitions generate $\Delta J = 2$ transitions. Doesn't the photon only carry one unit of angular momentum? No, this is the spin of the photon. It can also have orbital ang. mom.

Partial wave expansion: $e^{i\vec{k}\cdot\vec{x}} = 4\pi \sum_{l=0}^{\infty} i^l j_l(kr) \sum_{m=-l}^{l} Y_m^{l*}(\hat{k}) Y_m^l(\hat{r})$

Spher. Bessel fnct.

Contraction and reduction of spherical tensors

We have seen for cartesian tensors we can "contract" indicies to obtain tensors of lower rank.

Eg. $\sum_{j=1}^{3} \hat{T}_{ij} \hat{U}_j = \hat{W}_i$ Contraction of a rank-2 tensor with a vector

Eg: $\sum_{ij} Q_{ij} (\partial_i E_j) = \hat{H}^{(2)}$ Contraction of two rank-2 tensors $\Rightarrow$ scalar

We would like to contract two irreducible spherical tensors to obtain another irred. sph. ten.

Rule:
$$\hat{T}_Q^{(K)} = \sum_{q_1 q_2} \langle K Q | k_1 q_1 \, k_2 q_2 \rangle \hat{T}_{q_1}^{(k_1)} \hat{T}_{q_2}^{(k_2)}$$

is a rank(K) irreducible tensor

Check: $\hat{D} \hat{T}_Q^{(K)} \hat{D}^{\dagger} = \sum_{Q'} \hat{T}_{Q'}^{(K)} D_{Q'Q}^{(K)}$

Use direct sum: $D_{QQ'}^{(K)} = \bigoplus \left(D_{q_1}^{(k_1)} \otimes D_{q_2}^{(k_2)} \right)$

So, contracting tensors is like the addition of angular momentum.

We can also go in the other direction to express the direct product of two irreps as a sum of irreps

$$\hat{T}_{q_1}^{(k_1)} \hat{T}_{q_2}^{(k_2)} = \sum_{K=|k_1-k_2|}^{k_1+k_2}{}' \sum_{Q=-K}^{K}{}' \langle K Q | k_1 q_1 \, k_2 q_2 \rangle \hat{T}_Q^{(K)}$$

Example: Making a vector from two other vectors

Consider
$$\hat{W}_Q^{(1)} = \sum_{q_1 q_2} \langle 1Q | 1q_1 1q_2 \rangle \hat{U}_{q_1}^{(1)} \hat{V}_{q_2}^{(1)}$$

$$\Rightarrow \hat{W}_0^{(1)} = \frac{1}{\sqrt{2}}\left(-\hat{U}_{-1}^{(1)} \hat{V}_{+1}^{(1)} + \hat{U}_{+1}^{(1)} \hat{V}_{-1}^{(1)}\right)$$

$$\hat{W}_{\pm 1}^{(1)} = \frac{1}{\sqrt{2}}\left(\pm \hat{U}_{\pm 1}^{(1)} \hat{V}_0^{(1)} \mp \hat{U}_0^{(1)} \hat{V}_{\pm 1}^{(1)}\right)$$

Expressing in Cartesian component
$$\hat{W}_q^{(1)} = \frac{1}{i\sqrt{2}} (\hat{\vec{U}} \times \hat{\vec{V}})_q$$ as we saw in Lecture 11

Example: Making a scalar from two tensors
$$\hat{S} = \sum_Q \langle 00 | KQ\, K{-Q} \rangle \hat{T}_Q^{(K)} \hat{U}_{-Q}^{(K)}$$

Aside: $\langle 00 | KQ\, K{-Q} \rangle = \frac{(-1)^K}{\sqrt{2K+1}} (-1)^Q$

$$\Rightarrow \hat{S} = \frac{(-1)^K}{\sqrt{2K+1}} (\hat{T} \cdot \hat{U})$$

$$\boxed{\hat{T}^{(K)} \cdot \hat{U}^{(K)} = \sum_Q (-1)^Q \hat{T}_Q^{(K)} \hat{U}_{-Q}^{(K)}}$$

Example: Magnetic dipole-dipole interaction
$$\hat{H} = H_0 \left(\frac{\hat{r}^2 \hat{\sigma}_1 \cdot \hat{\sigma}_2 - 3(\hat{\vec{x}} \cdot \hat{\sigma}_1)(\hat{\vec{x}} \cdot \hat{\sigma}_2)}{r^3} \right)$$
r^3 ← relative coor

$$= H_0 (\hat{T}^{(2)} \cdot \hat{U}^{(2)})$$

$$\hat{T}_{ij}^{(2)} = \frac{\hat{r}^2 \delta_{ij} - 3\hat{x}_i \hat{x}_j}{r^3} \qquad \hat{U}_{ij}^{(2)} = \hat{\sigma}_1 \cdot \hat{\sigma}_2 \delta_{ij} - 3(\hat{\sigma}_1)_i (\hat{\sigma}_2)_j$$

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The dipole-dipole Hamiltonian is a <u>non central force</u> (force depends on direction of $\vec{r}$, not just its magnitude)

Thus, angular momentum of the motion of the spins is not conserved.

Given states $|L\, M_L\rangle \otimes |S\, M_S\rangle$

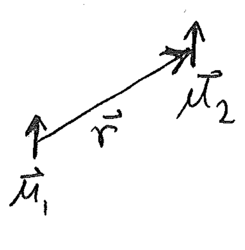
$$\langle L' M_L'\, S' M_S' | \hat{H} | L M_L\, S M_S\rangle = H_0 \langle L' M_L'\, S' M_S' | \hat{T}^{(2)} \cdot \hat{U}^{(2)} | L M_L\, S M_S\rangle$$

$$= H_0 \sum_Q (-1)^Q \langle L' M_L' | \hat{T}^{(2)}_Q | L M_L\rangle \langle S' M_S' | \hat{U}^{(2)}_{-Q} | S\, M_S\rangle$$

W.E.T. $\Rightarrow$ $M_L' = M_L + Q \qquad M_S' = M_S - Q$

$$\Rightarrow \boxed{M_L' + M_S' = M_L + M_S}$$

Total angular momentum is conserved. A change in orbital angular moment ΔM_L must be compensated by a change in internal angular momentum $\Delta M_S = -\Delta M_L$



Physical picture: rotating dipoles