# Lecture #18



## Properties of spherical tensors

Example of spherical tensor $\Rightarrow$ spherical harmonic

$$Y_{\ell}^{m \leftarrow \text{component}} \Longleftrightarrow T_q^{(k)\leftarrow \text{rank}}$$

$\ell$ ↑ rank, $q$ ↑ component

$|m| \le \ell \qquad |q| \le k$

$\ell = 0$, $m = 0$ $\Rightarrow Y_0^0 = \frac{1}{\sqrt{4\pi}} \leftarrow$ const

↑ 0th order spherical tensor $\rightarrow$ scalar

$$\ell = 1 \Rightarrow Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta, \quad Y_1^{\pm 1} = \mp \sin\theta e^{\pm i\varphi}\sqrt{\frac{3}{8\pi}}$$

$$\left.\begin{aligned} x &= r\sin\theta\cos\varphi \\ y &= r\sin\theta\sin\varphi \\ z &= r\cos\theta \end{aligned}\right\} \Rightarrow Y_1^0 = \sqrt{\frac{3}{4\pi}}\frac{z}{r}; \quad Y_1^{\pm 1} = \sqrt{\frac{3}{4\pi}}\frac{1}{r}\left(\mp\frac{x \pm iy}{\sqrt{2}}\right)$$

$$\sin\theta e^{\pm i\varphi} = \sin\theta(\cos\varphi \pm i\sin\varphi) = \frac{1}{r}(x \pm iy)$$

$\Downarrow$

Instead of $\vec{r} = (x, y, z)$

Introduce new vector components

$\Downarrow$

$$r_1^1 = -\frac{x+iy}{\sqrt{2}}; \quad r_1^{-1} = \frac{x-iy}{\sqrt{2}}; \quad r_1^0 = z$$

$$\vec{r} = x\vec{i} + y\vec{j} + z\vec{k} = -r_1^1\vec{e}_1^{\,-1} - r_1^{-1}\vec{e}_1^{\,1} + r_1^0\vec{e}_1^{\,0}$$

↑ in Cartesian coordinates ↖ in spherical basis

$$\vec{\epsilon}_1^{\,1} = -\frac{\vec{i}+i\vec{j}}{\sqrt{2}}\;; \quad \vec{\epsilon}_1^{\,0} = \vec{k}\,, \quad \vec{\epsilon}_1^{\,-1} = \frac{\vec{i}-i\vec{j}}{\sqrt{2}}$$

$$\underset{\uparrow \atop k}{\phantom{\epsilon}} \qquad (\vec{\epsilon}_1^{\,1}\cdot\vec{\epsilon}_1^{\,-1*} = 0)$$

<u>Morning coffee exercise</u>: check that the expansion is

So, $\tilde{r}_1^{\pm 1} = \sqrt{\frac{4\pi}{3}}\, r\, Y_1^{\pm 1}$ ; $\tilde{r}_1^{0} = \sqrt{\frac{4\pi}{3}}\, r\, Y_1^{0} \Rightarrow$

$$\underset{\uparrow \text{ rank}}{\tilde{r}_1^{q}} = \sqrt{\frac{4\pi}{3}}\, r\, Y_1^{q} \Rightarrow \vec{r} = \sqrt{\frac{4\pi}{3}}\, r \sum_{q=-1}^{1} (-1)^q Y_1^q \underset{\nwarrow \text{rank}}{\vec{\epsilon}_1^{\,-q}}$$

$\uparrow$ expansion in terms of spherical harmonics

<u>Note</u>: In general, any vector $\vec{V}$ can be decomposed in the spherical basis:

$$\vec{V} = V_x\vec{i} + V_y\vec{j} + V_k\vec{k} = \sum_{q=-1}^{1} (-1)^q V_q^{(1)} \vec{\epsilon}_1^{\,-q}\,, \quad (\text{rank})$$

$$\underbrace{V_{\pm 1}^{(1)}}_{q} = \mp\frac{V_x \pm iV_y}{\sqrt{2}}\;; \quad V_0^{(1)} = V_z$$

<u>Also note</u>: Beyond the rank 1, it is no longer possible to express Cartesian and spherical tensors of the <u>same</u> rank in terms of each other.

Recall last lecture: $\underbrace{T_{ij}}_{N=2} \Rightarrow \underset{\uparrow \atop k=0}{T^{(0)}} + \underset{\parallel \atop T^{(1)} \leftarrow k}{\underline{T_{ij(a)}}} + \underset{\parallel \atop T^{(2)} \leftarrow k}{\underline{T_{ij(s)}}}$

Cartesian tensor of rank $N \Rightarrow 3^N$ components

Spherical tensor of rank $K \Rightarrow (2K+1)$-components

$\begin{matrix} N=0 \\ K=0 \end{matrix} \Rightarrow 3^0 = 1 = 2\cdot 0+1$ ; $N=1,\ K=1 \Rightarrow 3^1 = 2\cdot 1+1$

For any other $\underset{(k)}{N} \Rightarrow 3^N \neq 2k+1$

Selection rules $\quad \langle j', m' | T_q^{(k)} | j, m \rangle = 0$

unless $k + j \geq j' \geq |k - j|$

$m' = m + q$

Example

Consider the (H)-atom and its energy levels. In the electric dipole approximation, what are the allowed radiative transitions?

Hint: The probability per unit time for an electric dipole transition from the initial state $|i\rangle$ to the final state $|f\rangle$ is $\sim |M_{fi}|^2$, where $M_{fi} = \langle f | \vec{\epsilon} \cdot \underbrace{(e\vec{r})}_{\text{dipole moment}} | i \rangle$ is the electric dipole matrix element for this transition. $\vec{\epsilon}$ is the polarization of light.

Solution: Since $\vec{\epsilon} \cdot (-e\vec{r})$ acts on the orbital angular momentum space and can't change the spin state $\Rightarrow$ use only orbital degrees of freedom.

$$|i\rangle = |n_i, l_i, m_i\rangle, \quad |f\rangle = |n_f, l_f, m_f\rangle$$

$$M_{fi} = -e \langle n_f, l_f, m_f | \vec{\epsilon} \cdot \vec{r} | n_i, l_i, m_i \rangle$$

selection rules depend on the polarization of light

Linear polarization: $\vec{\epsilon} = (0,0,1)$ (along $Oz$)

$$\vec{\epsilon}\cdot\vec{r} = z = r\cos\theta = \sqrt{\frac{4\pi}{3}}\, r\, Y_1^0(\theta,\varphi)$$

Circular polarization: $\vec{\epsilon}\cdot\vec{r} = \frac{1}{\mp\sqrt{2}}(x \pm iy) = \mp\sqrt{\frac{4\pi}{3}}\, r\, Y_1^{\pm 1}(\theta$

$\Downarrow$

$$M_{fi} \underset{\substack{\uparrow \\ \text{for any } q}}{\sim} \int R^*_{n_f l_f}(r)\, r\, R_{n_i l_i}(r)\, r^2 dr.$$

$q = \underset{\substack{\uparrow \\ \parallel z}}{0}, \underbrace{\pm 1}_{\substack{\uparrow \\ \text{circular}}}$

$$\cdot \int Y_{l_f}^{m_f *}(\theta,\varphi)\, Y_1^q(\theta,\varphi)\, Y_{l_i}^{m_i}(\theta,\varphi)\, \sin\theta\, d\theta\, d\varphi$$

Use: $Y_l^{\pm m} \sim e^{\pm i m\varphi} \Rightarrow$

$$\int_0^{2\pi} e^{-im_f\varphi}\, e^{iq\varphi}\, e^{im_i\varphi}\, d\varphi = \int_0^{2\pi} e^{i(m_i+q-m_f)\varphi}\, d\varphi =$$

$$= \frac{e^{i(m_i+q-m_f)2\pi} - 1}{i(m_i+q-m_f)} = 0 \ \underline{\underline{\text{unless}}}\ \boxed{m_i + q = m_f}$$

$\Downarrow$

$$\Delta m = m_f - m_i = \underset{\substack{\uparrow \\ \text{linear} \\ \parallel Oz}}{0}, \underbrace{\pm 1}_{\substack{\uparrow \\ \text{circular}}}$$

Are there any selection rules for $\ell$? $\Rightarrow$

$$\int Y_{\ell_f}^{m_f *} Y_1^{q} Y_{\ell_i}^{m_i} \sin\theta \, d\theta = a \int Y_{\ell_f}^{m_f *} Y_{\ell_i+1}^{m_i+q} \sin\theta \, d\theta \; +$$

$$+ \, b \int Y_{\ell_f}^{\overbrace{m_f}^{=m_i+q} *} Y_{\ell_i-1}^{m_i+q} \sin\theta \, d\theta =$$

Properties of $Y_\ell^m$

$\Downarrow$

$$Y_1^q Y_\ell^m = a Y_{\ell+1}^{m+q} + b Y_{\ell-1}^{m+q}$$

also, see lecture #17

$$= a \cdot \tilde{C}_1 \delta_{\ell_f, \ell_i+1} \delta_{m_f, m_i+q} + b \tilde{C}_2 \delta_{\ell_f, \ell_i-1} \delta_{m_f, m_i+q}$$

$\Downarrow$

$$\ell_f - \ell_i = \boxed{\Delta \ell = \pm 1}$$

Note: $\Delta \ell = 0$ is rejected due to parity

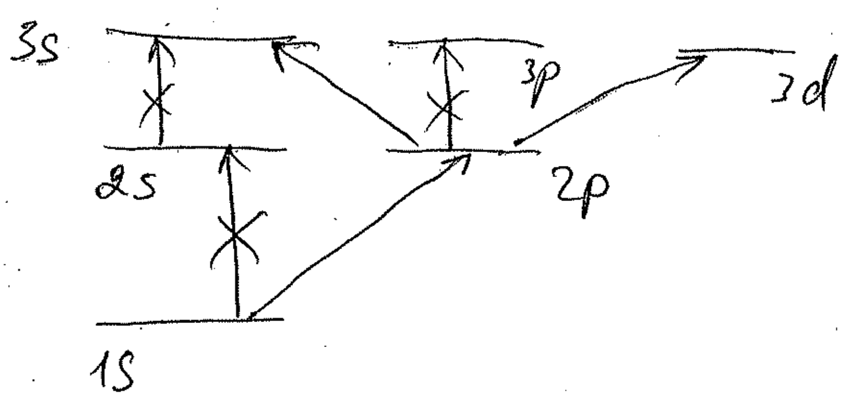
$\mathcal{J}_i Y_\ell^m \sim (-1)^\ell Y_\ell$

parity

Energy levels of $H$-atom:

$$E_n = -\frac{E_I}{n^2}$$

doesn't depend on $\ell, m$




(in reality $\Rightarrow$

$$H = H_{Coulomb} + H_{SO} + H_{hf} + \ldots$$

removes degeneracy)

spin-orbital coupling

spin-spin coupl.