Lecture 7: Tensor operators and the Wigner-Eckart theorem

Motivation: We have seen the relationship between symmetries and conservation laws in physics. In quantum theory, this tells us what are "good quantum numbers", i.e., which quantities are associated with stationary states. In addition this leads to selection rules for absorption/emission.

Example: In lecture 4 we saw the "parity" selection rule

Recall $\langle \psi_f | \hat{\vec{d}} | \psi_i \rangle = \langle \psi_f | \hat{\Pi}^\dagger \underbrace{\hat{\Pi} \hat{\vec{d}} \hat{\Pi}^\dagger}_{} \hat{\Pi} | \psi_i \rangle$

eigenstates of parity $\langle \psi_f | (-1)^{\Pi_f} \; -\hat{\vec{d}} \; (-1)^{\Pi_i} | \psi_i \rangle$

$$\Rightarrow (-1)^{\Pi_f + \Pi_f} = 1 \qquad \Rightarrow \boxed{\Pi_i = -\Pi_f}$$

$\hat{\vec{d}}$ is odd parity, so a dipole transition must change parity of the initial $\rightarrow$ final state

This is an example of "conservation of parity". We associate with the photon, one unit of parity.

We ~~~~ now seek selection rules arising from rotational symmetry, i.e., conservation of angular mom.

Recall, under a rotation, the three components of a vector operator transform as

$$\hat{\mathcal{D}}^\dagger(\vec{e}_n, \theta) \; \hat{V}_i \; \hat{\mathcal{D}}(\vec{e}_n, \theta) = \sum_{j=1}^{3} \mathbb{R}_{ij}(\vec{e}_n, \theta) \; \hat{V}_j = \hat{V}_i'$$

where $\hat{\mathcal{D}}(\vec{e}_n, \theta) = e^{-i/\hbar \, \theta \, \hat{\vec{J}} \cdot \vec{e}_n}$ (unitary operator)

$$\mathbb{R}_{ij}(\vec{e}_n, \theta) = 3\times 3 \text{ rotation matrix}$$

Generally, we define rank-K tensor with components such that

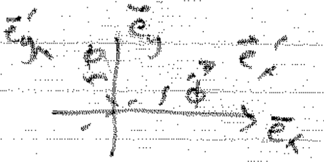
$$\hat{T}'_{i_1 i_2 \cdots i_K} = \sum_{j_1 j_2 \cdots j_K} \mathbb{R}_{i_1 j_1} \mathbb{R}_{i_2 j_2} \cdots \mathbb{R}_{i_K j_K} T_{j_1 j_2 \cdots j_K}$$

$$= \hat{\mathcal{D}}^{\dagger}(\mathbb{R}) \, \hat{T}_{i_1 i_2 i_3 \cdots i_K} \, \hat{\mathcal{D}}(\mathbb{R})$$

These are known as the "Cartesian" components of the tensor. They are not the natural objects as we will see.

Consider a rotation by angle ϕ about z-axis

$$\mathbb{R}(\vec{e}_z, \phi) = \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}$$



One can easily diagonalize this matrix to find its eigenvectors/values

Eigenvalues: $\{e^{-i\phi}, e^{i\phi}, 1\} = \{e^{-iq\phi}, q = -1, 0, +1\}$

Eigenvectors: $\left\{ -\left(\frac{\vec{e}_x + i\vec{e}_y}{\sqrt{2}}\right), \frac{\vec{e}_x - i\vec{e}_y}{\sqrt{2}}, \vec{e}_z \right\} = \{\vec{e}_q\}$

These vectors lie in a complex space. They are normalized according to $\vec{e}_q^{\,*} \cdot \vec{e}_q = 1$.
The phase is convention, to be discussed.

The set $\{\vec{e}_q\}$ is known as the "spherical basis". They are the natural objects, being eigenvectors of rotation about the polar axis, z.

Note: $\vec{e}_q^{\,*} = (-1)^q \vec{e}_{-q}$

The components of a vector in this basis are

$$V_q = \vec{e}_q \cdot \vec{V}$$

$$\Rightarrow \quad \vec{V} = \sum_q \vec{e}_q^{\,*} V_q = \sum_q (-1)^q \vec{e}_{-q} V_q$$

Thus $V_{+1} = -\frac{V_x + iV_y}{\sqrt{2}}$, $V_{-1} = \frac{V_x - iV_y}{\sqrt{2}}$, $V_0 = V_z$

Consider position $\vec{x} = (x, y, z)$

$$\Rightarrow \quad x_{\pm 1} = \mp \frac{x \pm iy}{\sqrt{2}} = \mp \frac{r}{\sqrt{2}} \sin\theta\, e^{\pm i\phi} = \sqrt{\frac{4\pi}{3}}\, r\, Y_{1\pm1}(\theta,\phi)$$

$$x_0 = z = r\cos\theta = \sqrt{\frac{4\pi}{3}}\, r\, Y_{1,0}(\theta,\phi)$$

Thus $\quad x_q = \sqrt{\frac{4\pi}{3}}\, r\, Y_{1,q}(\theta,\phi)$

The components in the spherical basis have the same angular dependence as the $Y_{\ell,m}(\theta,\phi)$.
This is no surprise, since the $Y_{\ell m}$'s are eigenfunctions of rotation about the z-axis. It does allow us to generalize "irreducible" (i.e. eigenfunction) tensor components beyond vector (rank 1)

Define "<u>Solid harmonic</u>"

$$\mathcal{Y}_{\ell,m}(\vec{x}) = r^\ell\, Y_{\ell,m}(\theta,\phi), \quad \text{where } r,\theta,\phi$$

$r = |\vec{x}| \quad \theta = \cos^{-1}\left(\frac{z}{r}\right)$

$\phi = \tan^{-1}\left(\frac{y}{x}\right)$

$$= \mathcal{Y}_{\ell,m}(x,y,z)$$

For a given ℓ, there are $2\ell+1$ $\mathcal{Y}_{\ell,m}$

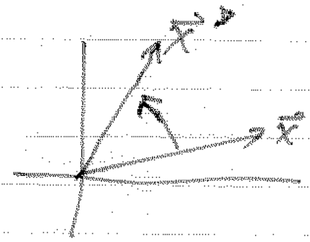
The functions $\mathcal{Y}_{\ell,m}(x,y,z)$ are known as components "irreducible spherical tensors". They transform differently under rotations than cartesian components:

Using Dirac notion: Rember $Y_{\ell,m}(\theta,\phi) = \langle \vec{e}_r | \ell m \rangle$

$$\Rightarrow \mathcal{Y}_{\ell,m}(\vec{x}) = \langle \vec{x} | \ell m \rangle$$

$|\vec{x}\rangle$ = position eigenket

Rotated position



$$|\vec{x}'\rangle = \underset{\substack{\uparrow \\ \text{rotation operator} \\ \text{(unitary)}}}{\hat{\mathcal{D}}} |\vec{x}\rangle$$

Consider $\mathcal{Y}_{\ell,m}(\vec{x}') = \langle \vec{x}' | \ell m \rangle = \langle \vec{x} | \underset{\uparrow}{\,}\hat{\mathcal{D}}^{\dagger} | \ell m \rangle$

$$\sum_{m'=-\ell}^{\ell} |\ell m'\rangle\langle \ell m'|$$

$$\Rightarrow \mathcal{Y}_{\ell,m}(\vec{x}') = \sum_{m'} \underbrace{\langle \vec{x} | \ell m' \rangle}_{\mathcal{Y}_{\ell m'}(\vec{x})} \underbrace{\langle \ell m' | \hat{\mathcal{D}}^{\dagger} | \ell m \rangle}_{\langle \ell m | \hat{\mathcal{D}} | \ell m' \rangle^{*} = \mathcal{D}^{(\ell)*}_{mm'}}$$

$\mathcal{D}^{(\ell)*}_{mm'}$: unitary rotation matrix for subspace (ℓ)

$$\Rightarrow \boxed{\mathcal{Y}_{\ell m}(\vec{x}') = \sum_{m'=-\ell}^{\ell} \mathcal{D}^{(\ell)*}_{mm'} \, \mathcal{Y}_{\ell m'}(\vec{x})}$$

Transformation of irreducible spherical tensor components under rotation.

Now consider operator $\mathcal{Y}_{\ell,m}(\hat{x})$

$$\Rightarrow \boxed{\hat{\mathcal{D}}^\dagger \mathcal{Y}_{\ell,m}(\hat{x}) \hat{\mathcal{D}} = \sum_{m'=-\ell}^{\ell} \mathcal{D}^{(\ell)*}_{mm'} \mathcal{Y}_{\ell m'}(\hat{x})}$$

An object with transforms this way is known as an irreducible (spherical) tensor operator

Generally rank $K \Rightarrow 2K+1$ components

$$\boxed{\hat{\mathcal{D}}^\dagger \hat{T}^{(K)}_q \hat{\mathcal{D}} = \sum_{q'=-K}^{K} \mathcal{D}^{(K)*}_{qq'} \hat{T}^{(K)}_{q'}}$$

Using $\hat{\mathcal{D}} = e^{-\frac{i}{\hbar}\theta \vec{e}_n \cdot \hat{\vec{J}}}$

This relationship can also be expressed as

$$[\hat{J}_z, \hat{T}^{(K)}_q] = q\, \hat{T}^{(K)}_q$$

$$[\hat{J}_\pm, \hat{T}^{(K)}_q] = \sqrt{K(K+1) \mp q(q\pm 1)}\; \hat{T}^{(K)}_{q\pm 1}$$

The most important use of spherical tensors is to calculate matrix elements between states with well defined angular momentum. The Wigner-Eckart Theorem (W.E.T.) will allow us to express these matrix elements in terms of a factor that depends <u>solely on geometry</u>. This leads to "selection rules" in, for example, absorption and emission of photons by atoms. Such selection rules are statements of conservation of angular momentum.

<u>Motivation</u>

Consider the dipole matrix elements of the spherical tensor operator $\hat{d}_q = -e\,\hat{x}_q$ between two Hydrogen eigenfunctions (no spin)

$$M_{(n'\ell'm')\leftarrow(n\ell m)} = \langle n'\ell'm'|\hat{d}_q|n\ell m\rangle = -e\int d^3x\ \psi^*_{n'\ell'm'}(\vec{x})\ x_q\ \psi_{n\ell m}(\vec{x})$$

$$\text{Now}\quad x_q = r\,Y^1_q(\theta,\phi)\sqrt{\tfrac{4\pi}{3}}$$

$$\Rightarrow M_{(n'\ell'm')\leftarrow(n\ell m)} = \underbrace{e\int r^2dr\ R_{n'\ell'}(r)\ r\ R_{n\ell}(r)}_{C(n'\ell'|n\ell)}\ \underbrace{\int d\Omega\ Y^{\ell'*}_{m'}(\theta,\phi)\ Y^1_q(\theta,\phi)\ Y^{\ell}_m(\theta,\phi)}_{\substack{=0 \text{ unless} \\ m'=m+q \\ |\ell-1|\le\ell'\le|\ell+1|}}$$

independent of angular geometry

Thus we see that the matrix element <u>factorizes</u> into a part independent of angular geometry and a factor that looks like addition of angular momenta

The Wigner–Eckart theorem : Statement

Given a tensor operator $\hat{T}^{(k)}_q$

$$\boxed{\langle \alpha'; j'm' | \hat{T}^{(k)}_q | \alpha; jm \rangle = \langle \alpha'; j' \| \hat{T}^{(k)} \| \alpha, j \rangle \langle j'm' | kq\, jm \rangle}$$

- Here α' and α are all other eigenvalues other than $j\,M$.
- $\langle j'm' | kq\, jm \rangle$ is the C.G coeff for addition
$$\vec{J}' = \vec{J} + \vec{K}$$
- $\langle \alpha'; j' \| \hat{T}^{(k)} \| \alpha, j \rangle$ is the "reduced matrix element" independent of m, m' and q

Notes: • We have chosen a particular convention for the reduced matrix element. Sakurai chooses a different normalization

• In our convention, the r.m.e. is not a true "matrix element" $\langle \alpha' j' \| \hat{T}^{(k)} \| \alpha j \rangle^* \neq \langle \alpha j \| \hat{T}^{(k)} \| \alpha' j' \rangle$

In words, the W.E.T. states that all matrix elements of $\hat{T}^{(k)}_q$ are proportional, ~~with~~ factorizing into a component independent of angular geometry, and a C.G. coeff. the C.G. coeff determines the <u>selection rules</u> according to conservation of angular momentum $\vec{J}' = \vec{J} + \vec{K}$. The tensor operator thus acts an object that carries to angular momentum K with z-projection q

The Wigner-Eckart theorem: Proof

Lemma: $\langle j'm' | kq\, jm \rangle$

$$= \sum_{q' m_1' m_1} D^{(j')*}_{m_1' m'}(R)\, D^{(k)}_{q'q}(R)\, D^{(j)}_{m_1 m}(R)\, \langle j' m_1' | k q' j m_1 \rangle$$

Proof: $\langle j'm' | kq\, jm \rangle = \langle j'm' | D^{\dagger}(R)\, D(R) |kq\rangle \otimes |jm\rangle$

Aside $D(R) |j' m'\rangle = \sum_{m_1'} |j' m_1'\rangle D^{(j')}_{m_1' m_1}$

$$D(R) |kq\rangle \otimes |jm\rangle = \sum_{q' m_1} |kq', j m_1\rangle D^{(k)}_{q'q}\, D^{(j)}_{m_1 m}$$

$$\Rightarrow \langle j'm' | kq\, jm \rangle = \sum_{q' m_1 m_1'} \langle j' m_1' | k q' j m_1 \rangle D^{(j')*}_{m_1' m'}\, D^{(k)}_{q'q}\, D^{(j)}_{m_1 m}$$

Now consider: $\langle \alpha'; j'm' | \hat{T}^{(k)}_{q} | \alpha, jm \rangle$

$\qquad\qquad D^{\dagger}D \quad D^{\dagger}D$

$$= \sum_{q' m_1' m_1} \langle \alpha'; j' m_1' | \hat{T}^{(k)}_{q'} | \alpha j\, m_1 \rangle D^{(j')*}_{m_1' m'}\, D^{(k)}_{q'q}\, D^{(j)}_{m_1 m}$$

Since those of linearly independent equation

$$\Rightarrow \langle \alpha' j' m_1' | \hat{T}^{(k)}_{q'} | \alpha j m \rangle = C(\alpha' j', k, \alpha j)\, \langle j'm' | kq\, jm \rangle$$

C is the reduced matrix element

Q.e.d.

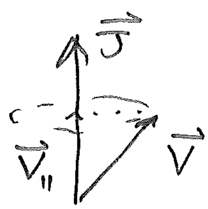
An important application of Wigner–Eckart is the <u>Landé–Projection theorem</u>:

- Consider a vector, $\hat{\vec{V}}$, w.r.t. rotations generated by $\hat{\vec{J}}$
- Consider matrix element in a manifold with definate j

$\Rightarrow$ As shown in homework

$$\langle j m' | \hat{\vec{V}} | j m \rangle = \left(\frac{\langle j m | \hat{\vec{V}} \cdot \hat{\vec{J}} | j m \rangle}{j(j+1)} \right) \langle j m' | \hat{\vec{J}} | j m \rangle$$

$\hat{\vec{V}} \propto \hat{\vec{J}}$, depending on its projection



$$\vec{V}_{\parallel} = \left(\frac{\vec{V} \cdot \vec{J}}{J^2} \right) \vec{J}$$

But since $\vec{V} \cdot \vec{J}$ is a scaller, independent of m

$\Rightarrow$ When calculated in a fixed manifold j

$$\hat{\vec{V}} = C(j)\, \hat{\vec{J}}$$

$$C(j) = \frac{\langle j m | \hat{\vec{V}} \cdot \hat{\vec{J}} | j m \rangle}{j(j+1)}$$ pick any m

Example: Hyperfine splitting for $l \neq 0$ states

For $l \neq 0$ the contact term vanishes, and the hyperfine interaction is

$$\hat{H}_{HF} = 2 g_N \mu_B \mu_N \left(\frac{(\hat{\vec{L}} - \hat{\vec{S}}) \cdot \hat{\vec{I}} + 3(\hat{\vec{S}} \cdot \vec{e}_r)(\hat{\vec{I}} \cdot \vec{e}_r)}{r^3} \right)$$

$$= -\hat{\vec{\mu}}_N \cdot \hat{\vec{B}}_e(\vec{r}) = -g_N \mu_N \hat{\vec{I}} \cdot \hat{\vec{B}}_e(\vec{r})$$

where $\vec{\mu}_N = g_N \vec{I}$, $\quad \hat{\vec{B}}_e = -2 \frac{\mu_B \hat{\vec{L}}}{r^3} + 2\mu_B \frac{(\hat{\vec{S}} - 3(\hat{\vec{S}} \cdot \vec{e}_r)\vec{e}_r)}{r^3}$

$$\Rightarrow \hat{H}_{HF} = \frac{\beta}{r^3} \hat{\vec{I}} \cdot \hat{\vec{b}} \qquad \text{where } \vec{b} = \vec{L} - \vec{S} + 3(\vec{S} \cdot \vec{e}_r)\vec{e}_r$$

Now, there are three angular momenta $\vec{I}, \vec{S}, \vec{L}$

$\Rightarrow$ $\hat{H}_{HF}$ scalar under rotation by $\vec{F} = \vec{I} + \vec{J}$
$\vec{J} = \vec{L} + \vec{S}$

The Hyperfine interaction is small w.r.t. fine-structure. Thus, to first order, the hyperfine perturbs the $(2i+1)(2j+1)$ manifold $|n j l s m_j\rangle |i m_i\rangle$

Consider, thus, the coupled representation

$$|n(j l s i) F m_F\rangle$$

$$|i - j| \leq F \leq |i + j|$$

Landé: $\hat{\vec{b}}$ is a vector w.r.t. $\vec{J} = \vec{L} + \vec{S}$

$\Rightarrow$ In a manifold with fixed j

$$\hat{\vec{b}} = \frac{\langle j\ell s \| \vec{b}\cdot\vec{J} \| j\ell s\rangle}{j(j+1)} \vec{J}$$

$$\Rightarrow \boxed{\hat{H}_{HF} = \frac{\beta}{r^3} \frac{\langle j\ell s| \vec{b}\cdot\vec{J} | j\ell s\rangle}{j(j+1)} \vec{I}\cdot\vec{J} \qquad (\ell \neq 0)}$$

Aside: $\vec{b}\cdot\vec{J} = \vec{b}\cdot(\vec{L}+\vec{S}) = (\vec{L}-\vec{S})\cdot(\vec{L}+\vec{S}) + 3(\vec{S}\cdot\vec{e}_r)(\vec{e}_r\cdot(\vec{L}+\vec{S}))$

$$= \hat{\vec{L}}^2 - \hat{\vec{S}}^2 + 3(\vec{S}\cdot\vec{e}_r)(\vec{S}\cdot\vec{e}_r)$$

(Double aside: $(\vec{S}\cdot\vec{e}_r)(\vec{S}\cdot\vec{e}_r) = \frac{1}{4}(\hat{\vec{\sigma}}\cdot\vec{e}_r)(\hat{\vec{\sigma}}\cdot\vec{e}_r)$

$$= \frac{1}{4}(\hat{\vec{\sigma}}^2)(\vec{e}_r\cdot\vec{e}_r) = \frac{1}{4}$$

and $\hat{\vec{S}}^2 = \frac{3}{4}\mathbb{1}$ (spin $\frac{1}{2}$ always for electron)

$$\Rightarrow \vec{b}\cdot\vec{J} = \vec{L}^2$$

$$\therefore \boxed{\hat{H}_{HF} = \frac{\beta}{r^3} \frac{\ell(\ell+1)}{j(j+1)} \hat{\vec{I}}\cdot\hat{\vec{J}}}$$ in fine-structure manifold with fixed j, ℓ

Once again, we can diagonalyzed by going to the coupled representation

$$\vec{I}\cdot\vec{J} = \frac{1}{2}\left(F^2 - I^2 - J^2\right)$$

$\Rightarrow$ Shifts in eigenvalues:

$$\boxed{\Delta E_{HF}(n\,l\,j\,i\,f) = \frac{\beta}{2}\left\langle \frac{1}{r^3}\right\rangle_{nl} \frac{l(l+1)}{j(j+1)}\left(f(f+1) - i(i+1) - j(j+1)\right)}$$

For hydrogen $\left\langle \frac{1}{r^3}\right\rangle_{nl} = \dfrac{1}{a_0^3 n^3 l(l+1)(l+\frac{1}{2})}$, $i = \frac{1}{2}$)

$$\Rightarrow \boxed{\Delta E_{HF}(n\,l\,\cancel{j}\,i\,f) = \frac{1}{2}\left(\frac{m_e}{m_p}\right)\frac{\alpha^2}{n^3}\,\frac{f(f+1) - j(j+1) - \frac{3}{4}}{j(j+1)(2l+1)}}$$

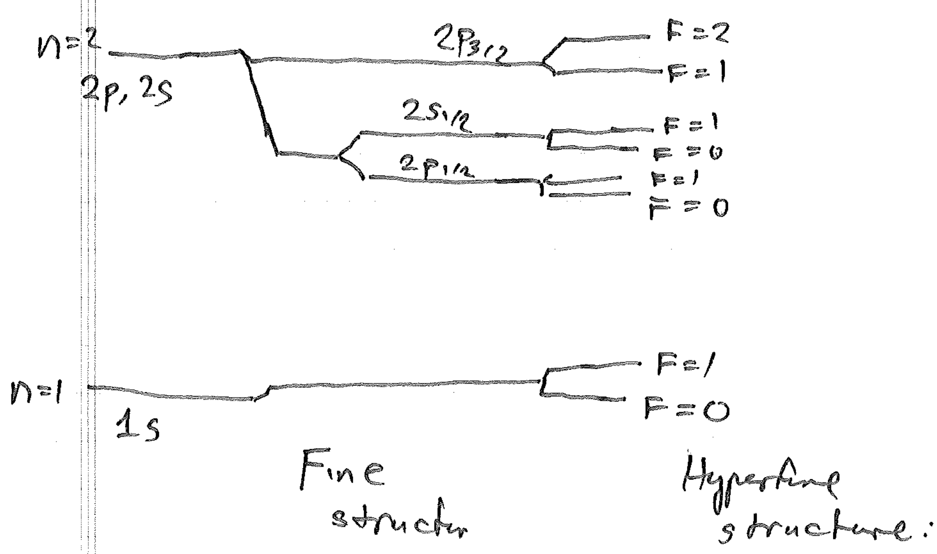
in atomic units

Note, the difference in the shifts for ~~adjacent~~ adjacent f:

$$\boxed{\Delta E_{HF}(f) - \Delta E_{HF}(f-1) = Cf}$$

Landé interval rule

Hydrogen energy level diagram



Note: the addition of small quadrapole effects breaks the Lande interval rule.