Lecture 20: Tensor Operators and the Spherical Basis

Motivation: We have seen many times now the relationship between symmetries and conservation laws in physics. In quantum theory this tells us what are the "good quantum numbers", i.e. which physical quantities are associated with stationary states. In addition this leads to selection rules when a quantum system is perturbed.

Example: In lecture 4 we saw the "parity selection rule" for electric dipole transitions. Recall derivation

$$\langle \underset{\uparrow}{\psi_f} | \hat{\vec{d}} | \underset{\uparrow}{\psi_i} \rangle = \langle \underbrace{\psi_f | \hat{\Pi}^\dagger}_{\langle \psi_f | \Pi_f} \underbrace{\hat{\Pi}\, \hat{\vec{d}}\, \hat{\Pi}^\dagger}_{-\hat{\vec{d}}} \underbrace{\hat{\Pi} | \psi_i}_{\Pi_i | \psi_i\rangle} \rangle = -\Pi_i \Pi_f \langle \psi_f | \hat{\vec{d}} | \psi_i \rangle$$

eigenstates of parity

$$\Rightarrow -\Pi_i \Pi_f = 1 \quad \Rightarrow \quad \boxed{\Pi_i = -\Pi_f}$$

$\hat{\vec{d}}$ is odd under parity, so the initial and final states must have opposite parity

This is an example of conservation of parity. The photon carries one unit of intrinsic parity so the atomic transition must change parity.

We want to find selection rules arising from rotational symmetry, i.e. conservation of angular momentum

Transformations under rotation and conservation

The fundamental object to study under rotations is the vector. A vector operator is defined as a three component object $\hat{V}_i$ $i=1,2,3$ which transforms as:

$$\boxed{\hat{D}^\dagger(\mathbb{R})\ \hat{V}_i\ \hat{D}(\mathbb{R}) = \sum_{j=1}^{3} \mathbb{R}_{ij}\ \hat{V}_j}\qquad \mathbb{R} = \text{rotation} \in SO(3)$$

$$\hat{\vec{V}} = \sum \hat{V}_i\ \vec{e}_i \qquad \vec{e}_i : \text{Cartesian unit vectors}$$

Infinitesimal form: $\hat{D}(\mathbb{R}) = \hat{\mathbb{1}} - i\,\vec{e}_n\cdot\hat{\vec{J}}\,\theta$

$$\Rightarrow [\vec{e}_n\cdot\hat{\vec{J}}, \hat{\vec{V}}] = -i(\vec{e}_n \times \vec{V})$$

$$\boxed{[\hat{J}_i, \hat{V}_j] = i\,\epsilon_{ijk}\,\hat{V}_k}\qquad \text{"}\vec{V}\text{ is a vector wrt. }\vec{J}\text{"}$$

Application to selection rule: Consider dipole operator $\hat{d}_z$: Invariant under rotation about z

$$\hat{D}_z^\dagger\ \hat{d}_z\ \hat{D}_z = d_z \quad \text{or} \quad \hat{D}_z\ \hat{d}_z\ \hat{D}_z^\dagger = d_z$$

Given eigenstate $|J, M_J\rangle$: $\hat{D}_z |J M_J\rangle = |J M_J\rangle e^{-i\theta M_J}$

$$\Rightarrow \langle J M_J' | \hat{d}_z | J M_J\rangle = \langle J M_J' | \hat{D}_z^\dagger \hat{D}_z\ \hat{d}_z\ \hat{D}_z^\dagger \hat{D}_z | J M_J\rangle$$

$$= e^{-i\theta(M_J - M_J')}\ \langle J M_J' | \hat{d}_z | J M_J\rangle$$

$\Rightarrow$ $\boxed{\text{Require } M_J = M_J' \quad \text{for dipole along quantization axis}}$

Photon intrinsic angular momentum

Tensors

Beyond vectors, we have more generally tensors

E.g. Multipole expansion of charge density $\rho(\vec{x})$

$$q = \int d^3x\, \rho(\vec{x}) \qquad \vec{d} = \int d^3x\, \vec{x}\, \rho(\vec{x}) \qquad \overleftrightarrow{Q} = \int d^3x \left(\frac{3\vec{x}\vec{x}}{2} - \overleftrightarrow{1}\right)\rho(\vec{x})$$

monopole (scalar) dipole (vector) Quadrapole (rank 2 tensor)

Define rank-K tensor operator $\hat{T}_{i_1 i_2 i_3 \cdots i_K}$ K components

$$\mathcal{D}^\dagger(\mathbb{R})\, \hat{T}_{i_1 \cdots i_K}\, \mathcal{D}(\mathbb{R}) = \sum_{\{j\}} \mathbb{R}_{i_1 j_1} \mathbb{R}_{i_2 j_2} \cdots \mathbb{R}_{i_K j_K}\, \hat{T}_{j_1 j_2 \cdots j_K}$$

Example: Outer product

Consider two vector operators $\hat{\vec{V}}$ and $\hat{\vec{W}}$

Define $\hat{\overleftrightarrow{T}} = \hat{\vec{V}}\, \hat{\vec{W}}$ (dyadic) $\hat{T}_{ij} = \hat{V}_i \hat{W}_j$

$\Rightarrow$ $\hat{T}_{ij}$ is a rank-2 tensor

$\hat{T}_{ij}$ is reducible into pieces that transform differently under rotation

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

Scalar	$\hat{T}_{ij}^{(0)} = \frac{1}{3}\delta_{ij}\, \mathrm{Trace}(\hat{T}) = \frac{1}{3}\delta_{ij} (\hat{\vec{V}} \cdot \vec{W})$	One component $(\vec{V}\cdot\vec{W})$
Vector	$\hat{T}_{ij}^{(1)} = \frac{1}{2}(\hat{T}_{ij} - \hat{T}_{ji}) = \frac{1}{2}\epsilon_{ijk}(\vec{V}\times\vec{W})_k$	Three components $\vec{V}\times\vec{W}$
Tensor	$\hat{T}_{ij}^{(2)} = \frac{1}{2}(\hat{T}_{ij} + \hat{T}_{ji}) - \hat{T}_{ij}^{(0)}$ symmetric traceless	5 components

Generally we have rank-l "irreducible" Cartesian tensors: $l = 0$ trace over all indicies

$l = 1$ antisymmetrize

$l > 1$ symmetric / traceless

Note: For the case we studied, the number of independent components for $\hat{T}^{(l)}_q$ was $2l+1$ $\Rightarrow$ Intimate relation with angular mom

Spherical Basis and Spherical Harmonics

To find the irreducible tensor components it is usually (though not always) more convenient to work in the "spherical bases" rather than Cartesian

Recall spherical basis $\{\vec{e}_q,\ q = -1, 0, 1\}$

$$\vec{e}_0 \equiv \vec{e}_z, \quad \vec{e}_{\pm} \equiv \mp\left(\frac{\vec{e}_x \pm i\,\vec{e}_y}{\sqrt{2}}\right) \qquad \text{Note } \vec{e}_q^{\,*} = (-1)^q \vec{e}_{-q}$$

Eigenvectors of rotation about z-axis by ϕ

$$\mathbb{R}\,\vec{e}_q = e^{-i\phi q}\,\vec{e}_q$$

$\vec{e}_q \cdot \vec{e}_{q'}^{\,*} = \delta_{qq'}$: Complex vector space: Components $V_q = \vec{e}_q \cdot \vec{V}$

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

Spherical Harmonics $Y^l_m(\theta,\phi)$: eigenfunctions of rotation about z-axis

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Solid Harmonics $\mathcal{Y}^{\ell}_{m}(\vec{x}) = r^{\ell} Y^{\ell}_{m}(\theta, \phi)$

(also eigenfunctions of rotation about z)

$z = r\cos\theta \qquad x = r\sin\theta\cos\phi \qquad y = r\sin\theta\sin\phi$

$\mathcal{Y}^{\ell}_{m}$ are polynomials of order ℓ in spherical basis components x_q

e.g. $\ell = 1 \qquad \mathcal{Y}^{\ell=1}_{q}(\vec{x}) = N_1 \, x_q$ normalization

$\mathcal{Y}^{1}_{0} = N_1 z = r(N_1 \cos\theta) \qquad \mathcal{Y}^{1}_{\pm 1} = \mp N_1 \left(\frac{x \pm iy}{\sqrt{2}}\right) = r\left(\mp \frac{N_1}{\sqrt{2}} \sin\theta \, e^{\pm i\phi}\right)$

Suppose we replace $\vec{x}$ by the vector operator $\hat{\vec{x}}$

Let $\hat{T}^{(1)}_{q} = \mathcal{Y}^{\ell=1}_{q}(\hat{\vec{x}}) = N_1 \hat{x}_q$

$\Rightarrow \hat{D}^{\dagger}_{z} \hat{T}^{(1)}_{q} \hat{D}_{z} = e^{\mp iq\phi} \, \hat{T}^{(1)}_{q}$

More generally $|\ell m\rangle' = \hat{D}(\mathbb{R}) \, |\ell m\rangle$

and: recall $\langle \ell m' | \hat{D}(\mathbb{R}) | \ell m\rangle \equiv D^{(\ell)}_{m'm}$

$\langle \vec{x} | \ell m\rangle' = \langle \vec{x} | \mathcal{D}^{\dagger}(\mathbb{R}) | \ell m\rangle = \langle \vec{x}' | \ell m\rangle$

rotated vector

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

$\vec{x} \Rightarrow$ operator

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

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or equivalently

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

$Y^{\ell}_{m}(\hat{\vec{x}})$ is an example of a <u>irreducible spherical tensor operator</u>

More generally, given a vector operator $\hat{\vec{V}}$ define

$$\hat{V}^{(k)}_{q} = Y^{(k)}_{q}(\hat{\vec{V}})$$ Spherical tensor of rank (k)

$$\boxed{\hat{\mathcal{D}}\, \hat{V}^{(k)}_{q}\, \hat{\mathcal{D}}^{+} = \sum_{q'=-k}^{k} \mathcal{D}^{(k)}_{q'q}\, \hat{V}^{(k)}_{q'}}$$

↑ Definition of irreducible spherical tensor $\hat{T}^{(k)}_{q}$

Here
$$\hat{V}^{(1)}_{0} = N_1\, V_z$$
$$\hat{V}^{(1)}_{\pm 1} = N_1 \left[\mp\left(\frac{\hat{V}_x \pm i\hat{V}_y}{\sqrt{2}}\right)\right]$$
$$\hat{V}^{(2)}_{\pm 2} = N_2 \left(\frac{\hat{V}_x \pm i\hat{V}_y}{\sqrt{2}}\right)^2 \quad \text{etc.}$$

Infinitesimal version: $\hat{\mathcal{D}} = \hat{1} - i\,\theta\, \vec{e}_n \cdot \hat{\vec{J}}$

$$\Rightarrow \boxed{\begin{aligned} \left[\hat{J}_z, \hat{T}^{(k)}_{q}\right] &= q\, \hat{T}^{(k)}_{q} \\ \left[\hat{J}_\pm, \hat{T}^{(k)}_{q}\right] &= \sqrt{k(k+1) - q(q\pm 1)}\; \hat{T}^{(k)}_{q\pm 1} \end{aligned}}$$