Lecture #16

Scalar, vector, and tensor operators

Depending on how an object changes upon rotation
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(a) Consider an operator A

$$\underset{\substack{\uparrow \\ \text{after rotation}}}{A'} = \mathcal{D}(R)\, A\, \mathcal{D}^{\dagger}(R) \leftarrow \text{see Lecture \#10}$$

see Lecture #10

$\mathcal{D}(R) = 1 - \frac{i}{\hbar}(\vec{J}\cdot\vec{n})\,d\varphi$

If $A' = A$ ← scalar operator
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$$[\vec{J}\cdot\vec{n}, A] = 0$$

<u>Recall</u>: for an arbitrary operator A ⇒

$$A' = A - \frac{i}{\hbar}\,d\varphi\,[\vec{J}\cdot\vec{n}, A]$$

↑ infinitesimal rotation by $d\varphi$ around $\vec{n}$

In classical physics or math : scalar is a number, doesn't change upon rotation

(b) Vector or vector operator in QM ⇒ $V_i' = \sum_j R_{ij} V_j$

↑ rotation operator (or rotation matrix) in CM

$N \times N$ ← dimension of space

$$V_i' = \mathcal{D}(R)\, V_i\, \mathcal{D}^\dagger(R) \underset{\uparrow}{=} V_i - \frac{i}{\hbar} d\varphi\, [\vec{J}\cdot\vec{n}, V_i] =$$

Lecture #9

$$= \sum_j R_{ij} V_j =$$

$$\underset{\substack{\uparrow \\ \text{HW \#}}}{=} V_i + d\varphi\, \underbrace{[\vec{n} \times \vec{V}]_i}_{\sum_{jk} \varepsilon_{ijk} n_j V_k} \quad \Rightarrow \quad [\vec{J}\cdot\vec{n}, V_i] = i\hbar\, [\vec{n}\times\vec{V}]_i$$

$$\vec{n} \parallel \vec{i} \Rightarrow [J_i, V_i] = i\hbar\, [\vec{i} \times \vec{V}]_i = 0$$

$$\vec{n} \parallel \vec{j} \Rightarrow [J_j, V_i] = i\hbar\, [\vec{j} \times \vec{V}]_i \underset{\uparrow}{=} -i\hbar V_k$$

$$\begin{vmatrix} i & j & k \\ 0 & 1 & 0 \\ V_i & V_j & V_k \end{vmatrix} = \vec{i}\,(-V_k)$$

Generally:

$$[V_i, J_j] = i\hbar\, \varepsilon_{ijk} V_k$$

assume summation

Valid for any vector operator or, in other words, a definition of a vector operator

Examples $\vec{V} = \vec{J} \Rightarrow [J_i, J_j] = i\hbar\, \varepsilon_{ijk} J_k$ ← as we know

$$\underset{(\vec{J} = \vec{L})}{\vec{V} = \vec{P}} \Rightarrow [P_i, L_j] = [P_i, r_k P_i - r_i P_k] =$$

$$(\vec{r} \times \vec{P})_j = r_k P_i - r_i P_k$$

$$= [P_i, -r_i P_k] = -[P_i, r_i] P_k = i\hbar P_k$$

(c) Tensor

$$\underbrace{T_{ijk\ldots}}_{N \text{ indices}}' = \sum \underbrace{R_{ii'} R_{jj'} R_{kk'} \ldots}_{N \text{ rotation matrices}} T_{i'j'k'\ldots}$$

N of indices = rank of tensor

Cartesian tensor

Examples of tensors:

$N=2$ ⇒ • I_{ij} ← tensor of inertia of a rigid body $L_i = I_{ij} w_j$ ← angular momentum

• ε_{ij} ← dielectric tensor

$$D_i = \varepsilon_{ij} E_j$$

D_i ← displacement; E_j ← electric field

$$\varepsilon_{ij} = 1 + 4\pi \chi_{ij}^{(1)}$$ ← linear susceptibility

$\vec{P} = \chi^{(1)} \vec{E} \Rightarrow P_i = \chi_{ij}^{(1)} E_j$

$\vec{P}$ ← polarization

⇑ linear optics

$N = \cancel{2}\,3, 4$ ⇒ $$\vec{P} = \chi^{(1)} E + \underbrace{\chi^{(2)} E^2 + \chi^{(3)} E^3 + \ldots}_{\text{Nonlinear optics}}$$

SHG: $P_i = \chi_{ijk}^{(2)} E_j E_k$

SHG ← second harmonic generation; $\chi_{ijk}^{(2)}$ ← $N=3$

THG: $P_i = \chi_{ijkl}^{(3)} E_j E_k E_l$

THG ← third harmonic generation; $\chi_{ijkl}^{(3)}$ ← $N=4$

Cartesian tensor $\Rightarrow \underset{\substack{\uparrow \\ \text{3D-space}}}{3}{}^{N}$ components

Note: vector is a tensor of rank 1, scalar – of rank 0.

The problem with Cartesian tensor: reducible under rotation
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i.e. can be decomposed into objects that transform differently under rotations

<u>Example</u>

$N=2 \Rightarrow T_{ij}$ ← tensor of 2nd rank

$\vec{u}, \vec{v}$ – vectors

$$\hat{T} = \vec{u} \otimes \vec{v} \Rightarrow T_{ij} = u_i v_j \Rightarrow \hat{T} = \begin{bmatrix} u_1 v_1 & u_1 v_2 & u_1 v_3 \\ u_2 v_1 & u_2 v_2 & u_2 v_3 \\ u_3 v_1 & u_3 v_2 & u_3 v_3 \end{bmatrix}$$

↑ dyadic $\qquad i,j = 1,2,3 \qquad$ ↑ 9 indep. comp.

Now rotate $\hat{T} \Rightarrow \hat{T}'$ ← in a general case all 9 new components

Can we introduce some other 9 components defining the tensor, which preserve their properties upon rotation;

Find the origin of the problem (why is the Cartesian tensor reducible)?
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$$u_i v_j = \frac{\vec{u}\cdot\vec{v}}{3}\delta_{ij} - \frac{\vec{u}\cdot\vec{v}}{3}\delta_{ij} + \frac{u_i v_j}{2} + \frac{u_i v_j}{2} + \frac{u_j v_i}{2} - \frac{u_j v_i}{2}$$

$$= \underbrace{\frac{\vec{u}\cdot\vec{v}}{3}\delta_{ij}}_{\substack{\text{scalar part} \\ T^{(0)}\delta_{ij}}} + \underbrace{\frac{u_i v_j - u_j v_i}{2}}_{\substack{\text{anti-symmetric} \\ \text{tensor } T_{ij(a)} \text{ (vector)}}} + \underbrace{\left(\frac{u_i v_j + u_j v_i}{2} - \frac{\vec{u}\cdot\vec{v}}{3}\delta_{ij}\right)}_{\text{symmetric tensor } T_{ij(s)}}$$

↑ re-group

Independent components:

Scalar: 1 ; antisymmetric tensor $\Rightarrow u_i v_j - u_j v_i = \varepsilon_{ijk}(\vec{u}\times\vec{v})_k$

$\uparrow$ independent components

$$\underset{\substack{\uparrow \\ i=j=1,2,3 \\ \text{cases } 3 \text{ times}}}{9 - 3} - \underset{\substack{\uparrow \\ ij \leftrightarrow ji \\ 3 \text{ times}}}{3} = 3 \text{ independent components}$$

symmetric tensor

$$T_{ij(s)} = \frac{u_i v_j + u_j v_i}{2} - \frac{\vec{u}\cdot\vec{v}}{3}\delta_{ij} \Rightarrow 9 - \underset{\substack{\uparrow \\ ij \to ji \\ 3 \text{ times}}}{3} - \underset{\substack{\uparrow \\ \text{traceless}}}{1} = 5$$

$i = j \Rightarrow$

$$\mathrm{Tr}\,(T_{\underbrace{ij}_{i}(s)}) = -\frac{u_1 v_1 + u_2 v_2 + u_3 v_3}{3}\underbrace{\delta_{ij}}_{1\cdot 3} + \sum_{i=1}^{3} u_i \underbrace{v_j}_{i}$$

$$\mathrm{Tr}\, T_{ij}(s) = -\vec{u}\cdot\vec{v} + \overset{(i=j)}{\vec{u}\cdot\vec{v}} = 0 \leftarrow \text{traceless} \leftarrow T_{11} = -T_{22} - T_{33}$$

Check: $5 + 3 + 1 = 9$ independent components

So, instead of 9-component T_{ij} (cartesian tensor) introduce a one-component scalar $T^{(0)} = \sum_i T_{ii} = \mathrm{Tr}\,\hat{T}$, 3-component antisymmetric tensor $T_{ij(a)} = \frac{1}{2}(T_{ij} - T_{ji})$ and 5-component traceless symmetric tensor

$$T_{ij(s)} = \frac{1}{2}(T_{ij} + T_{ji}) - \frac{1}{3}T^{(0)}\delta_{ij}.$$

Why are $T^{(0)}$, $T_{ij(a)}$, $T_{ij(s)}$ better than T_{ij}? $\Rightarrow$ they transform within the same set under rotation:

scalar remains scalar (doesn't change),

$T_{ij\,(a)} \xrightarrow[\text{rotation}]{R} T_{i'j'\,(a)}$, $T_{ij\,(s)} \xrightarrow{R} T_{i'j'\,(s)}$ $\Rightarrow$ $T^{(0)}$, $T_{ij\,(a)}$, $T_{ij\,(s)}$, form an irreducible representation

So, in terms of the components of Cartesian tensor $\hat{T}$, the new components are; (for the simplest case of $N=2$-rank tensor)

$$T^{(0)} = T_{11} + T_{22} + T_{33} \quad \Leftarrow 1 \text{ component}$$

$$\hat{T}_{(a)} = \begin{pmatrix} 0 & \frac{1}{2}(T_{12}-T_{21}) & \frac{1}{2}(T_{13}-T_{31}) \\ -\frac{1}{2}(T_{12}-T_{21}) & 0 & \frac{1}{2}(T_{23}-T_{32}) \\ -\frac{1}{2}(T_{13}-T_{31}) & -\frac{1}{2}(T_{23}-T_{32}) & 0 \end{pmatrix} \Leftarrow 3 \text{ indep. components} \Uparrow \text{vector}$$

$$\hat{T}_{(s)} = \begin{pmatrix} T_{11} - \frac{1}{3}T^{(0)} & \frac{T_{12}+T_{21}}{2} & \frac{T_{13}+T_{31}}{2} \\ \frac{T_{12}+T_{21}}{2} & T_{22} - \frac{1}{3}T^{(0)} & \frac{T_{23}+T_{32}}{2} \\ \frac{T_{13}+T_{31}}{2} & \frac{T_{23}+T_{32}}{2} & T_{33} - \frac{1}{3}T^{(0)} \end{pmatrix} \Leftarrow 5 \text{ Indep. comp.}$$

$$T_{33} - \frac{1}{3}T^{(0)} = -(T_{11}+T_{22}) + \frac{2}{3}T^{(0)}$$

$T^{(0)}$, $\hat{T}_{(a)}$, $\hat{T}_{(s)}$ $\leftrightarrow$ irreducible spherical tensors

Definition of a spherical tensor

The $(2K+1)$ - component operator $\underbrace{\{T_q^{(K)}\}}_{\hat{T}^{(K)}}$ $(q=-K,-K+1,\dots,+K)$ is an irreducible K-th-order spherical tensor operator, if the components $T_q^{(K)}$ transform under rotation as:

$$\mathcal{D}(R)\,T_q^{(K)}\,\mathcal{D}^{+}(R)=\sum_{q'=-K}^{K}\underbrace{\mathcal{D}_{q'q}^{(K)}(R)}_{\text{rotation matrix}}\,T_{q'}^{(K)}$$

Recall Lecture # 13

$$\mathcal{D}_{m'm}(R)=\langle j,m'|\mathcal{D}(R)|j,m\rangle$$

rotation matrix $= \langle K', q'|\mathcal{D}(R)|K,q\rangle = \mathcal{D}_{q'q}^{(K)}\,\delta_{K'K}$

$\Longleftrightarrow$ $K=j$, $q=m$

$\delta_{K'K}$ reflects the fact that the angular momentum does not change under rotation $\Leftarrow$ angular momentum conservation

$$\mathcal{D}_{q'q}^{(K)}=\langle K,q'|e^{-\frac{i}{\hbar}\varphi\vec{J}\cdot\vec{n}}|K,q\rangle$$

$(2K+1)\times(2K+1)$ - matrix

From the previous example, $T^{(0)}\to K=0$ $\leftarrow$ rank of spherical tensor

components $\to$ $2K+1=3\Rightarrow \hat{T}_{(a)}\to K=1$

$2K+1=5\Rightarrow \hat{T}_{(s)}\to K=2$

Properties of the components of spherical tensors ⑧

$$[J_\pm, T_q^{(k)}] = \hbar\sqrt{k(k+1)-q(q\pm1)}\; T_{q\pm1}^{(k)}$$
$$[J_z, T_q^{(k)}] = \hbar q\, T_q^{(k)}$$
HW!

Other properties: let's act on $|j,m\rangle$ with $T_q^{(k)}$ and rotate the obtained state;

$$\mathcal{D}(R)\left[T_q^{(k)}|j,m\rangle\right] = \mathcal{D}(R)\left[T_q^{(k)}\underbrace{\mathcal{D}^\dagger(R)\mathcal{D}(R)}_{I \text{ identity}}|j,m\rangle\right]$$

$$= \underbrace{\left[\mathcal{D}(R)T_q^{(k)}\mathcal{D}^\dagger(R)\right]}_{\sum_{q'}\mathcal{D}_{q'q}^{(k)} T_{q'}^{(k)}} \underbrace{\sum_{m'}\mathcal{D}_{m'm}^{(j)}|j,m'\rangle}_{\mathcal{D}(R)|j,m\rangle} =$$

Lecture #13

$$= \sum_{q',m'}\mathcal{D}_{q'q}^{(k)}\mathcal{D}_{m'm}^{(j)}\underbrace{\left[T_{q'}^{(k)}|j,m'\rangle\right]}_{|k,q'\rangle\otimes|j,m'\rangle} = \sum_{m'}\mathcal{D}_{m'm}^{(j)}\sum_{q'}\mathcal{D}_{q'q}^{(k)}T_{q'}^{(k)}|j,m'\rangle$$

⇓

Acting on a state with $T_q^{(k)}$ is equivalent to adding the angular momentum (k,q) to a state (j,m).

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

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

$m' = m+q$