Lect 16 Irreducible spherical tensor operators

● §1. We have studied the transformation of state vectors $|jm\rangle$ under rotation operator $D(g) = e^{-i\vec{J}\cdot\hat{n}\theta}$. We have

$$\boxed{D(g)\,|jm\rangle = \sum_{m'} |jm'\rangle\, D^j_{m'm}(g)} \leftarrow D^j_{m'm}(g) = \langle jm'|\, e^{-i\vec{J}\cdot\hat{n}\theta}\, |jm\rangle$$

we can further extend this idea to the transformation of a set of operators denoted as T_{jm} $(m=-j,\cdots j)$. Under rotation, if they transformation satisfy

$$\boxed{D(g)\, T_{jm}\, D^{\dagger}(g) = \sum_{m'} T_{jm'}\, D^j_{m'm}(g)}$$

● we say T_{jm} $(m=-j,\cdots j)$ form the rank-j irreducible tensor operators, and T_{jm} is the m-th component.

Example: Consider spherical harmonics $r^l Y_{lm}(\hat{r})$ as operators, they form l-th rank tensor. (They are useful for studying electron transition in atoms)

$$D(g)\,\vec{r}\,D^{\dagger}(g) = g^{-1}\vec{r},$$

$$D(g)\, r^l\, Y_{lm}(\hat{r})\, D^{\dagger}(g) = r^l\, Y_{lm}(g^{-1}\hat{r}),$$

$$Y_{lm}(g^{-1}\hat{r}) = \langle g^{-1}\hat{r}\,|\,lm\rangle = \langle \hat{r}|\quad D(g)\,|lm\rangle = \sum_{m'} \langle \hat{r}|lm'\rangle\, D_{m'm}(\hat{g})$$

● $\Rightarrow$ $$\boxed{D(g)\, r^l\, Y_{lm}(\hat{r})\, D^{\dagger}(g) = \sum_{m'} r^l\, Y_{lm'}(\hat{r})\, D^j_{m'm}(g)}$$

if $l=1$, we have

$$\boxed{\begin{aligned} rY_{11} &= -\frac{1}{\sqrt{2}}(x+iy) \\ rY_{10} &= z \\ rY_{1-1} &= \frac{1}{\sqrt{2}}(x-iy) \end{aligned}}$$

generally speaking, if operators A_x, A_y, A_z are Cartisian vecter we can form the rank-1 irreducible (spherical) tensors

$$A_{11} = -\frac{1}{\sqrt{2}}(A_x + iA_y), \quad A_{10} = A_z; \quad A_{1-1} = \frac{1}{\sqrt{2}}(A_x - iA_y)$$

§2. Hower, the above definition on page 1 is not convenient to use, let us take derivatives with respective to ~~rotation~~ angles, we arrive at

$$\boxed{[\vec{J}\cdot\hat{n},\ T_{jm}] = \sum_{m'} T_{jm'}\ \langle jm'|\ \vec{J}\cdot\hat{n}\ |jm\rangle}$$

Ex: Prove this.

and, we have

$$\boxed{\begin{aligned} [J_\pm,\ T_{jm}] &= \sqrt{(j\mp m)(j\mp m+1)}\ T_{j\,m\pm1} \\ [J_z,\ T_{jm}] &= m\,T_{jm} \end{aligned}}$$

We can also prove that we can ~~start~~ from $[\vec{J}\cdot\hat{n},\ T_{jm}] = \sum_{m'} T_{jm'} \langle jm'|\vec{J}\cdot\hat{n}|jm\rangle$ to derive

$$D^{+}(g)\ T_{jm}\, D(g) = \sum_{m'} T_{jm'}\ \langle jm'|\ D(g)\ |jm\rangle.$$

In other words, these two defenations are equivalent. One is the infinitsimal form, and the other is the finite angle form.

Proof: from $[\vec{J}\cdot\hat{n}, T_{jm}] = \sum_{m'} T_{jm'} \langle jm'|\vec{J}\cdot\hat{n}|jm\rangle$

$$\rightarrow (1 - i\vec{J}\cdot\hat{n}\,\delta\theta)\, T_{jm} (1 + i\vec{J}\cdot\hat{n}\,\delta\theta) = \sum_{m'} T_{jm'} \langle jm'|(1 - i\vec{J}\cdot\hat{n}\,\theta)|jm\rangle$$

For infinitismall angle $\delta\theta$, we have $\boxed{e^{-i\hat{n}\cdot\vec{J}\delta\theta}\, T_{jm}\, e^{i\hat{n}\cdot\vec{J}\delta\theta} = \sum_{m'} T_{jm'} \langle jm'| e^{-i\hat{n}\cdot\vec{J}\delta\theta} |jm\rangle}$.

For finite angle θ, we can decompose it as $\theta = N\cdot\delta\theta$, $\Rightarrow$

$$e^{-i\hat{n}\cdot\vec{J}\delta\theta} (e^{-i\hat{n}\cdot\vec{J}\delta\theta} \cdots T_{jm}\, e^{i\hat{n}\cdot\vec{J}\delta\theta} \cdots e^{i\hat{n}\cdot\vec{J}\delta\theta}$$

$$= \sum_{m_1, \cdots m_N} T_{jm_N} \langle jm_N'| e^{-i\hat{n}\cdot\vec{J}\delta\theta} |jm_{N-1}\rangle \langle jm_{N-1}| e^{-i\hat{n}\cdot\vec{J}\delta\theta} |jm_{N-2}\rangle \cdots$$
$$\langle jm_1| e^{-i\hat{n}\cdot\vec{J}\delta\theta} |jm\rangle$$

$$= \boxed{\sum_{m} T_{jm'} \langle jm'| e^{-i\hat{n}\cdot\vec{J}\theta} |jm\rangle = e^{-i\hat{n}\cdot\vec{J}\theta}\, T_{jm}\, e^{i\hat{n}\cdot\vec{J}\theta}}$$

§ The action of irreducible tensors on $|jm\rangle$.

Let us first prove the decomposition relation of the D-matrix.

$$\boxed{\begin{gathered} D^{j}_{qm}(g)\, D^{j'}_{q'm'}(g) = \sum_{J}\sum_{QM} \langle JQ|jqj'q'\rangle\, D^{J}_{QM}(g) \langle JM|jmj'm'\rangle \\ \text{with } (J = |j-j'|, \cdots j+j') \end{gathered}}$$

$$|jm\rangle \otimes |j'm'\rangle = \sum_{JM} |JM\rangle \langle JM|jmj'm'\rangle$$

$$\langle jq| \otimes \langle j'q'| = \sum_{JQ} \langle JQ|jqj'q'\rangle \langle JQ|$$

Then $D(g)\,|jm\rangle \otimes |j'm'\rangle = e^{-iJ.n\theta}|jm\rangle \otimes e^{-iJ'.n\theta}|j'm'\rangle$

$$= \sum_{qq'} |jq\rangle|j'q'\rangle \quad \langle jq|e^{-iJ.n\theta}|jm\rangle\langle j'q'|e^{-iJ'n\theta}|j'm'\rangle$$

$$= \sum_{qq'} |jq\rangle \otimes |j'q'\rangle\, D^j_{qm}(g)\, D^{j'}_{q'm'}(g)$$

on the other hand

$$D(g)\;|jm\rangle \otimes |j'm'\rangle = D(g) \sum_{JM} |JM\rangle \langle JM|jmj'm'\rangle$$

$$\Rightarrow \qquad = \sum_{JQM} |JQ\rangle\, {}_{JQ}\langle\, |D(g)|JM\rangle \langle JM|jmj'm'\rangle$$

$$= \sum_{JQM} |JQ\rangle\, D^J_{QM}(g)\, \langle JM|jmj'm'\rangle$$

$$\Rightarrow \langle jq| \otimes \langle j'q'|\, D(g)\,|jm\rangle \otimes |j'm'\rangle = \sum_{JQM} \langle JQ|jqj'q'\rangle \langle JM|jmj'm'\rangle\, D^J_{QM}(g).$$

Now we will use it for tensors. Consider the combination $T_{jm}|j'm'\rangle$.

$$D(g)\;T_{jm}|j'm'\rangle = D(g)\,T_{jm}\,D^\dagger(g)\;D(g)\,|j'm'\rangle$$

$$= \sum_{qq'} D^j_{qm}(g)\; T_{jq} \quad D^{j'}_{q'm'}(g)\; |j'q'\rangle$$

$$= \sum_{qq'} \sum_{JQM} D^J_{QM}(g)\, \langle JQ|jqj'q'\rangle \langle JM|jmj'm'\rangle \;\; T_{jq}\, |j'q'\rangle$$

$$\Rightarrow D(g) \sum_{mm'} \langle JM | jm j'm' \rangle \left(T_{jm} | j'm' \rangle \right)$$

$$= \sum_{qq'} \sum_{J'QM'} T_{jq} | j'q' \rangle \langle J'Q | jq j'q' \rangle \sum_{mm'} \langle J'M' | jm j'm' \rangle \langle JM | jm j'm' \rangle \, D^{J'}_{QM'}(g)$$

$$\sum_{mm'} \langle J'M' | jm j'm' \rangle \langle JM | jm j'm' \rangle = \delta_{JJ'} \delta_{MM'}$$

$$\Rightarrow D(g) \sum_{mm'} \langle JM | jm j'm' \rangle \left(T_{jm} | j'm' \rangle \right) = \sum_{Q} \left(\sum_{qq'} \langle JQ | jq j'q' \rangle \, T_{jq} | j'q' \rangle \right) D^{J}_{QM}(g)$$

define $|(T) JM\rangle = \sum_{mm'} \langle JM | jm j'm' \rangle \, T_{jm} | j'm' \rangle \Rightarrow$

$$\boxed{D(g) |(T) JM\rangle = \sum_{Q} |(T) JQ\rangle \, D^{J}_{QM}(g)}$$

Thus $|(T) JM\rangle$ forms the $2J+1$ multiplet of angular momentum, and the decomposition follows the same C-G coefficients.

§ Wigner-Eckart theorem:

Now we consider the matrix elements $\langle \eta_1 j_1 m_1 | T_{jm} | \eta_2 j_2 m_2 \rangle$. $\eta_{1,2}$ are another set quantum numbers compatible with angular momentum. Wigner-Eckart theorem says it can be decompsed into two parts: one part does not depend on $m_{1,2}$, m, and the dependence on m and $m_{1,2}$ is through CG coefficient!

Proof: consider $T_{jm}|\eta_2 j_2 m_2\rangle$, we can decompose it as

$$T_{jm}|\eta_2 j_2 m_2\rangle = \sum_{JM} |(T\eta_2)\, JM\rangle \langle JM | jm\, j_2 m_2\rangle$$

a symbol to denote its dependance of T, η_2

$$\Rightarrow \langle \eta_1 j_1 m_1 | T_{jm} | \eta_2 j_2 m_2\rangle = \langle \eta j_1 m_1 | (T\eta_2) j_1 m_1\rangle \langle j_1 m_1 | jm\, j_2 m_2\rangle$$

matrix-elements. CG

As we proved in Lect 13, since $|\eta j_1 m_1\rangle$ and $|(T\eta_2) j_1 m_1\rangle$ are angular momentum eigenstates with quantum number $j_1 m_1$, then ~~its ind~~

$\langle \eta j_1 m_1 | (T\eta_2) j_1 m_1\rangle$ is independent on m_1, but it can depend on j_1. We denote it as the standard form

$$\langle \eta j_1 m_1 | (T\eta') j_1 m_1\rangle = \frac{1}{\sqrt{2j_1+1}} \underbrace{(\eta j_1 \| T(j) \| \eta' j_2)}_{\text{reduced matrix elements.}}$$

These matrix elements do not depend on $m, m_{1,2}$, only depend on representations but NOT on which basis of representation.

$$\boxed{\langle \eta_1 j_1 m_1 | T_{jm} | \eta' j_2 m_2\rangle = \frac{1}{\sqrt{2j_1+1}} (\eta j_1 \| T(j) \| \eta' j_2) \langle j_1 m_1 | jm\, j_2 m_2\rangle}$$

Example: Solution to HW 2 ①

1. From lecture notes, we learn that we can follow $Y_{lm}(r)$ $(m=\pm1,0$

$$Y_{11} \propto -\frac{1}{\sqrt{2}}(x+iy)$$
$$Y_{10} \propto z$$
$$Y_{1-1} \propto \frac{1}{\sqrt{2}}(x-iy).$$

For a cartisian vecter, such as J_x, J_y, J_z, we form rank-1 tensor

$$\boxed{\begin{aligned} J_{11} &= -\frac{1}{\sqrt{2}}(J_x+iJ_y) = \frac{-1}{\sqrt{2}}J_+ \\ J_{10} &= J_z \\ J_{1-1} &= \frac{1}{\sqrt{2}}(J_x-iJ_y) = \frac{1}{\sqrt{2}}J_- \end{aligned}}$$

we have

$$\langle j'm'|\,J_{11}\,|jm\rangle = \frac{-1}{\sqrt{2}}\langle j'm'|J_+|jm\rangle = \frac{-\delta_{jj'}}{\sqrt{2}}\delta_{m',m+1}\sqrt{(j-m)(j+m+1)}$$

$$\langle j'm'|\,J_{10}\,|jm\rangle = \delta_{jj'}\; m\,\delta_{m'm}$$

$$\langle j'm'|\,J_{1-1}\,|jm\rangle = \frac{1}{\sqrt{2}}\langle j'm'|J_-|jm\rangle = \frac{\delta_{jj'}}{\sqrt{2}}\delta_{m',m-1}\sqrt{(j+m)(j-m+1)}$$

Next, let us quote the C-G coefficients $\langle jm'|1q\,jm\rangle$

$$\langle jm\,|10\,jm\rangle = \frac{m}{\sqrt{j(j+1)}}$$

$$\langle jm+1\,|11\,jm\rangle = -\sqrt{\frac{(j+m+1)(j-m)}{2j(j+1)}}$$

$$\langle j\,m-1\,|1\text{-}1\,jm\rangle = \sqrt{\frac{(j+m)(j-m+1)}{2j(j+1)}}$$

$-2 \quad \sqrt{j+1}$

we can express

$$\langle j'm' | J_{1q} | j m \rangle = \delta_{jj'} \sqrt{j(j+1)} \quad \langle j'm' | 1 q j m \rangle$$

according to the definition of reduced matrix elements,

we have $\frac{1}{\sqrt{2j+1}} (j' || J || j) = \delta_{jj'} \sqrt{j(j+1}$

$$\Rightarrow (j' || J || j) = \delta_{jj'} \sqrt{j(j+1)(2j+1)}$$