Wigner-Eckart theorem
Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton
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1. Vector operators

The operators corresponding to various physical quantities will be characterized by their behavior under rotation as scalars, vectors, and tensors.

$$V_i \to \sum_j \Re_{ij} V_j$$

We assume that the state vector changes from the old state $|\psi\rangle$ to the new state $|\psi'\rangle$.

$$|\psi'\rangle = \hat{R}|\psi\rangle$$

or

$$\langle\psi'| = \langle\psi|\hat{R}^+$$

A vector operator $\hat{\mathbf{V}}$ for the system is defined as an operator whose expectation is a vector that rotates together with the physical system.

$$\langle\psi'|\hat{V}_i|\psi'\rangle = \sum_j \Re_{ij} \langle\psi|\hat{V}_j|\psi\rangle$$

or

$$\hat{R}^+\hat{V}_i\hat{R} = \sum_j \Re_{ij}\hat{V}_j$$

or

$$\hat{V}_i = \hat{R}\sum_j \Re_{ij}\hat{V}_j\hat{R}^+$$

We now consider a special case, infinitesimal rotation.

$$\hat{R} = \hat{1} - \frac{i}{\hbar}\varepsilon\hat{\mathbf{J}}\cdot\mathbf{n}$$

$$\hat{R}^{+} = \hat{1} + \frac{i}{\hbar}\varepsilon\hat{\mathbf{J}}\cdot\mathbf{n}$$

$$(\hat{1} + \frac{i}{\hbar}\varepsilon\hat{\mathbf{J}}\cdot\mathbf{n})\hat{V}_i(\hat{1} - \frac{i}{\hbar}\varepsilon\hat{\mathbf{J}}\cdot\mathbf{n}) = \sum_j \Re_{ij}\hat{V}_j$$

$$\hat{V}_i - \frac{i\varepsilon}{\hbar}[\hat{V}_i, \hat{\mathbf{J}}\cdot\mathbf{n}] = \sum_j \Re_{ij}\hat{V}_j$$

For $\boldsymbol{n} = \boldsymbol{e}_z$,

$$\Re_z(\varepsilon) = \begin{pmatrix} 1 & -\varepsilon & 0 \\ \varepsilon & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\hat{V}_1 - \frac{i\varepsilon}{\hbar}[\hat{V}_1, \hat{J}_z] = \Re_{11}\hat{V}_1 + \Re_{12}\hat{V}_2 + \Re_{13}\hat{V}_3 = \hat{V}_1 - \varepsilon\hat{V}_2$$

$$\hat{V}_2 - \frac{i\varepsilon}{\hbar}[\hat{V}_2, \hat{J}_z] = \Re_{21}\hat{V}_1 + \Re_{22}\hat{V}_2 + \Re_{23}\hat{V}_3 = \varepsilon\hat{V}_1 + \hat{V}_2$$

$$\hat{V}_3 - \frac{i\varepsilon}{\hbar}[\hat{V}_3, \hat{J}_z] = \Re_{31}\hat{V}_1 + \Re_{32}\hat{V}_2 + \Re_{33}\hat{V}_3 = \hat{V}_3$$

or

$$[\hat{V}_1, \hat{J}_z] = -i\hbar\hat{V}_2, \qquad [\hat{V}_2, \hat{J}_z] = i\hbar\hat{V}_1, \qquad [\hat{V}_3, \hat{J}_z] = 0$$

For $\boldsymbol{n} = \boldsymbol{e}_x$,

$$\Re_x(\varepsilon) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & -\varepsilon \\ 0 & \varepsilon & 1 \end{pmatrix}$$

$$\hat{V}_1 - \frac{i\varepsilon}{\hbar}[\hat{V}_1, \hat{J}_x] = \Re_{11}\hat{V}_1 + \Re_{12}\hat{V}_2 + \Re_{13}\hat{V}_3 = \hat{V}_1$$

$$\hat{V}_2 - \frac{i\varepsilon}{\hbar}[\hat{V}_2, \hat{J}_x] = \Re_{21}\hat{V}_1 + \Re_{22}\hat{V}_2 + \Re_{23}\hat{V}_3 = \hat{V}_2 - \varepsilon\hat{V}_3$$

$$\hat{V}_3 - \frac{i\varepsilon}{\hbar}[\hat{V}_3, \hat{J}_x] = \Re_{31}\hat{V}_1 + \Re_{32}\hat{V}_2 + \Re_{33}\hat{V}_3 = \varepsilon\hat{V}_2 + \hat{V}_3$$

or

$$[\hat{V}_1, \hat{J}_x] = 0, \quad [\hat{V}_2, \hat{J}_x] = -i\hbar\hat{V}_3, \quad [\hat{V}_3, \hat{J}_x] = i\hbar\hat{V}_2$$

For For $\boldsymbol{n} = \boldsymbol{e}_y$,

$$\Re_y(\varepsilon) = \begin{pmatrix} 1 & 0 & \varepsilon \\ 0 & 1 & 0 \\ -\varepsilon & 0 & 1 \end{pmatrix}$$

$$\hat{V}_1 - \frac{i\varepsilon}{\hbar}[\hat{V}_1, \hat{J}_y] = \Re_{11}\hat{V}_1 + \Re_{12}\hat{V}_2 + \Re_{13}\hat{V}_3 = \hat{V}_1 + \varepsilon\hat{V}_3$$

$$\hat{V}_2 - \frac{i\varepsilon}{\hbar}[\hat{V}_2, \hat{J}_y] = \Re_{21}\hat{V}_1 + \Re_{22}\hat{V}_2 + \Re_{23}\hat{V}_3 = \hat{V}_2$$

$$\hat{V}_3 - \frac{i\varepsilon}{\hbar}[\hat{V}_3, \hat{J}y_x] = \Re_{31}\hat{V}_1 + \Re_{32}\hat{V}_2 + \Re_{33}\hat{V}_3 = -\varepsilon\hat{V}_1 + \hat{V}_3$$

or

$$[\hat{V}_1, \hat{J}_y] = i\hbar\hat{V}_3, \quad [\hat{V}_2, \hat{J}_y] = 0, \quad [\hat{V}_3, \hat{J}_y] = -i\hbar\hat{V}_1$$

Using the Levi-Civita symbol, we have

$$[\hat{V}_i, \hat{J}_j] = i\hbar\varepsilon_{ijk}\hat{V}_k$$

We can use this expression as the defining property of a vector operator.

Levi-Civita symbol: ε_{ijk}

$\varepsilon_{123}=\varepsilon_{231}=\varepsilon_{312}=1$

$\varepsilon_{132}=\varepsilon_{213}=\varepsilon_{321}=-1$

all other $\varepsilon_{ijk.}$ =0.

((**Example**))

When $\hat{V} = \hat{\mathbf{J}}$,

$$[\hat{J}_i, \hat{J}_j] = i\hbar\varepsilon_{ijk}\hat{J}_k$$

When $\hat{\boldsymbol{V}} = \hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{A}} = \hat{\boldsymbol{r}}$,

$$[\hat{x}_i, \hat{L}_j] = i\hbar\varepsilon_{ijk}\hat{x}_k$$

When $\hat{\boldsymbol{A}} = \hat{\boldsymbol{p}}$, and $\hat{\boldsymbol{A}} = \hat{\boldsymbol{r}}$,

$$[\hat{p}_i, \hat{L}_j] = i\hbar\varepsilon_{ijk}\hat{p}_k$$

2. Cartesian tensor operators

The standard definition of a Cartesian tensor is that each of its suffix transforms under the rotation as do the components of an ordinary 3D vector,
The Cartesian tensor operator is defined by

$$\langle\psi'|\hat{T}_{ij}|\psi'\rangle = \sum_{k,l}\Re_{ik}\Re_{jl}\langle\psi|T_{kl}|\psi\rangle$$

under the rotation specified by the 3x3 orthogonal matrix $\Re$.

$$\hat{T}_{ij} = \hat{R}\sum_{k,l}\Re_{ik}\Re_{jl}\hat{T}_{kl}\hat{R}^{+}$$

The simplest example of a Cartesian tensor of rank 2 is a dyadic formed out of two vectors $\hat{\mathbf{U}}$ and $\hat{\mathbf{V}}$.

$$\hat{T}_{ij} = \hat{U}_i\hat{V}_j$$

where $\hat{U}_i$ and $\hat{V}_i$ are the components of ordinary 3D vector operators. There are nine components: 1+3+5 = 9. This Cartesian tensor is reducible. It can be decomposed into the three parts.

$$\hat{U}_i\hat{V}_j = \frac{\hat{\mathbf{U}}\cdot\hat{\mathbf{V}}}{3}\delta_{ij} + \frac{\hat{U}_i\hat{V}_j - \hat{U}_j\hat{V}_i}{2} + (\frac{\hat{U}_i\hat{V}_j + \hat{U}_j\hat{V}_i}{2} - \frac{\hat{\mathbf{U}}\cdot\hat{\mathbf{V}}}{3}\delta_{ij})$$

The first term on the right-hand side, $\hat{\mathbf{U}}\cdot\hat{\mathbf{V}}$ is a scalar product invariant under the rotation. The second is an anti-symmetric tensor which can be written as

$$\varepsilon_{ijk}(\hat{\mathbf{U}}\times\hat{\mathbf{V}})_k$$

There are 3 independent components.

$$\begin{pmatrix} 0 & a_{12} & a_{13} \\ -a_{12} & 0 & a_{23} \\ -a_{13} & -a_{23} & 0 \end{pmatrix}$$

The third term is a 3x3 symmetric traceless tensor with 5 independent components (=6-1, where 1 comes from the traceless condition.

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{pmatrix}$$

with $a_{11}+a_{22}+a_{33}=0$

In conculsion, the tensor $\hat{T}_{ij}=\hat{U}_i\hat{V}_j$ can be decomposed into spherical tensors of rank 0, 1, and 2.

3. Spherical tensor

Notice the numbers of elements of these irreducible subgroups: 1, 3, and 5. These are exactly the numbers of elements of angular momentum representations for j = 0, 1, and 2!

The first term is trivial: the scalar by definition is not affected by rotation, and neither is an j = 0 state.

To deal with the second and third terms, we introduce tensor operators having three and five components, such that under rotation these sets of components transform among themselves just as do the sets of eigenkets of angular momentum in the j = 1 and j = 2 representation, respectively.

Suppose we take a spherical harmonics $Y_l^m(\theta,\phi)=Y_l^m(\mathbf{n})$, where the orientation of the unit vector ***n*** is characterized by θ and ϕ. We now replace ***n*** by some vector $\hat{\mathbf{V}}$. Then we have a spherical tensor of rank *k* (in place of *l*) with magnetic quantum number (in place of *m*).

$$T_q^{(k)}=Y_{l=k}^{m=q}(\hat{\mathbf{V}})$$

The quantity

$$P_{l,m}(x,y,z) = r^l Y_l^m(\theta,\phi)$$

is a homogeneous polynomial of order *l*.

The quantity $P_{1,q}(x,y,z) = \sqrt{\frac{4\pi}{3}} r Y_1^q(\theta,\phi)$ is a first order homogeneous polynomial in *x*, *y*, and *z*.

(i)

$$P_{1,1}(x,y,z) = \sqrt{\frac{4\pi}{3}} r Y_1^1(\theta,\phi) = -\frac{x+iy}{\sqrt{2}}$$

$$T_1^{(1)} = -\frac{\hat{V}_x + i\hat{V}_y}{\sqrt{2}}$$

(ii)

$$P_{1,0}(x,y,z) = \sqrt{\frac{4\pi}{3}} r Y_1^0(\theta,\phi) = z$$

$$T_0^{(1)} = \hat{V}_z$$

(iii)

$$P_{1,-1}(x,y,z) = \sqrt{\frac{4\pi}{3}} r Y_1^{-1}(\theta,\phi) = \frac{x-iy}{\sqrt{2}}$$

$$T_{-1}^{(1)} = \frac{\hat{V}_x - i\hat{V}_y}{\sqrt{2}}$$

The above example is the simplest nontrivial example to illustrate the reduction of a Cartesian tensor into irreducible spherical tensors.

$$T_q^{(k)} = Y_{l=k}^{m=q}(\hat{\mathbf{V}})$$

$$|\mathbf{n}'\rangle = \hat{R}|\mathbf{n}\rangle$$

$$\langle\mathbf{n}'| = \langle\mathbf{n}|\hat{R}^+$$

$$\hat{R}^{+}|l,m\rangle = \sum_{m'} |l,m'\rangle\langle l,m'|\hat{R}^{+}|l,m\rangle$$

$$\langle \mathbf{n}'|l,m\rangle = \langle \mathbf{n}|\hat{R}^{+}|l,m\rangle = \sum_{m'} \langle \mathbf{n}|l,m'\rangle\langle l,m'|\hat{R}^{+}|l,m\rangle$$

or

$$Y_l^m(\mathbf{n}') = \sum_{m'} Y_l^{m'}(\mathbf{n})\langle l,m|\hat{R}|l,m'\rangle^*$$

$$D_{m,m'}^{(l)}(\hat{R}) = \langle l,m|\hat{R}|l,m'\rangle$$

If there is an operator that acts like $Y_l^m(\hat{\mathbf{V}})$, it is then reasonable to expect

$$\hat{R}^{+}Y_l^m(\hat{\mathbf{V}})\hat{R} = \sum_{m'} Y_l^{m'}(\hat{\mathbf{V}})\langle l,m|\hat{R}|l,m'\rangle^* = \sum_{m'} Y_l^{m'}(\hat{\mathbf{V}}){D_{mm'}^{(l)}}^*(\hat{R})^*$$

We define a spherical tensor operator of rank k as a set of $2k$+1, $\hat{T}_q^{(k)}$, $q = k$, k-1,…, -k such that under rotation they transform like a set of angular momentum eigenkets,

$$\hat{R}^{+}\hat{T}_q^{(k)}\hat{R} = \sum_{q'=-k}^{k} {D_{qq'}^{(k)}}^*(\hat{R})\hat{T}_{q'}^{(k)}\ , \qquad (1)$$

where

$$\hat{T}_q^{(k)} = Y_{l=k}^{m=q}(\hat{\mathbf{V}})$$

$$D_{qq'}^{(k)}(\hat{R}) = \langle k,q|\hat{R}|k,q'\rangle$$

or

$${D_{qq'}^{(k)}}^*(\hat{R}) = \langle k,q|\hat{R}|k,q'\rangle^* = \langle k,q'|\hat{R}^{+}|k,q\rangle$$

with $q = k$, k-1,…, -k. This can be rewritten as

$$\hat{R}^{+}\hat{T}_q^{(k)}\hat{R} = \sum_{q'=-k}^{k} D_{q'q}^{(k)}(\hat{R}^{+})\hat{T}_{q'}^{(k)}$$

The switching of $\hat{R} \to \hat{R}^{+}$ leads to another expression

$$\hat{R}\hat{T}_q^{(k)}\hat{R}^+ = \sum_{q'=-k}^{k} D_{q'q}^{(k)}(\hat{R})\hat{T}_{q'}^{(k)} \tag{2}$$

Considering the infinitesimal form of the expression (1), we have

$$(\hat{1}+\frac{i\varepsilon\hat{\mathbf{J}}\cdot\mathbf{n}}{\hbar})\hat{T}_q^{(k)}(\hat{1}-\frac{i\varepsilon\hat{\mathbf{J}}\cdot\mathbf{n}}{\hbar}) = \sum_{q'=-k}^{k} \hat{T}_{q'}^{(k)}\langle k,q'|\hat{1}+\frac{i\varepsilon\hat{\mathbf{J}}\cdot\mathbf{n}}{\hbar}|k,q\rangle$$

or

$$\hat{T}_q^{(k)}+\frac{i\varepsilon}{\hbar}[\hat{\mathbf{J}}\cdot\mathbf{n},\hat{T}_q^{(k)}] = \hat{T}_q^{(k)}+\frac{i\varepsilon}{\hbar}\sum_{q'=-k}^{k}\hat{T}_{q'}^{(k)}\langle k,q'|\hat{\mathbf{J}}\cdot\mathbf{n}|k,q\rangle$$

or

$$[\hat{\mathbf{J}}\cdot\mathbf{n},T_q^{(k)}] = \sum_{q'=-k}^{k}\hat{T}_{q'}^{(k)}\langle k,q'|\hat{\mathbf{J}}\cdot\mathbf{n}|k,q\rangle$$

In general, we have

$$[\hat{\boldsymbol{J}},T_q^{(k)}] = \sum_{q'=-k}^{k}\hat{T}_{q'}^{(k)}\langle k,q'|\hat{\boldsymbol{J}}|k,q\rangle$$

Using the Wigner-Eckart theorem, this can be rewritten as

$$\begin{aligned}
[\hat{J}_\mu,T_q^{(k)}] &= \sum_{q'=-k}^{k}\hat{T}_{q'}^{(k)}\langle k,q'|\hat{J}_\mu|k,q\rangle \\
&= \sum_{q'=-k}^{k}\hat{T}_{q'}^{(k)}\langle k,1;q,\mu|k,1;k,q'\rangle < k\,||\,\hat{\boldsymbol{J}}\,||\,k > \\
&= \langle k,1;q,\mu|k,1;k,q+\mu\rangle < k\,||\,\hat{\boldsymbol{J}}\,||\,k > \hat{T}_{q+\mu}^{(k)} \\
&= \sqrt{k(k+1)}\langle k,1;q,\mu|k,1;k,q+\mu\rangle\hat{T}_{q+\mu}^{(k)}
\end{aligned}$$

This can be also described as

$$[\hat{J}_\mu,T_q^{(k)}] = (-1)^{k-1+q+\mu}\sqrt{k(k+1)(2k+1)}\begin{pmatrix} k & 1 & k \\ q & \mu & -(q+\mu)\end{pmatrix}\hat{T}_{q+\mu}^{(k)}$$

using the Wigner 3j symbol.

For $\boldsymbol{n} = \boldsymbol{e}_x, \boldsymbol{e}_y, \boldsymbol{e}_z$

$$[\hat{J}_z, T_q^{(k)}] = \sum_{q'=-k}^{k} \hat{T}_{q'}^{(k)} \langle k, q' | \hat{J}_z | k, q \rangle = \hbar q \hat{T}_q^{(k)} \tag{3}$$

$$[\hat{J}_x, T_q^{(k)}] = \sum_{q'=-k}^{k} \hat{T}_{q'}^{(k)} \langle k, q' | \hat{J}_x | k, q \rangle$$

$$[\hat{J}_y, T_q^{(k)}] = \sum_{q'=-k}^{k} \hat{T}_{q'}^{(k)} \langle k, q' | \hat{J}_y | k, q \rangle$$

$$[\hat{J}_\pm, T_q^{(k)}] = \sum_{q'=-k}^{k} \hat{T}_{q'}^{(k)} \langle k, q' | \hat{J}_\pm | k, q \rangle = \hbar \sqrt{(k \mp q)(k \pm q + 1)} \hat{T}_{q\pm 1}^{(k)} \tag{4}$$

These two commutation relations can also be taken as a definition of a spherical tensor of rank *k*.

We now consider

$$\hat{R} \hat{T}_q^{(k)} \hat{R}^+ = \sum_{q'=-k}^{k} D_{q'q}^{(k)}(\hat{R}) \hat{T}_{q'}^{(k)}$$

This equation is rewritten as

$$\hat{R} \hat{T}_q^{(k)} = \sum_{q'=-k}^{k} D_{q'q}^{(k)}(\hat{R}) \hat{T}_{q'}^{(k)} \hat{R}$$

Then have

$$\begin{aligned}
\hat{R} \hat{T}_q^{(k)} | j, m \rangle &= \sum_{q'=-k}^{k} D_{q'q}^{(k)}(\hat{R}) \hat{T}_{q'}^{(k)} \sum_{m'} | j, m' \rangle \langle j, m' | \hat{R} | j, m \rangle \\
&= \sum_{q'=-k}^{k} \sum_{m'} D_{q'q}^{(k)}(\hat{R}) D_{m'm}^{(j)}(\hat{R}) \hat{T}_{q'}^{(k)} | j, m' \rangle
\end{aligned}$$

(a) Spherical tensor operator of rank 1

The spherical tensor operator of rank 1 is related to the vector operator by the relation,

$$\hat{T}_1^{(1)} = -\frac{\hat{V}_x + i\hat{V}_y}{\sqrt{2}}, \qquad \hat{T}_0^{(1)} = \hat{V}_z, \qquad \hat{T}_{-1}^{(1)} = \frac{\hat{V}_x - i\hat{V}_y}{\sqrt{2}}$$

The vector operator $\hat{\mathbf{V}}$ satisfies the commutation relation.

$$[\hat{V}_i, \hat{J}_j] = i\hbar\varepsilon_{ijk}\hat{V}_k$$

Using this relation, we can show that

$$[\hat{J}_z, \hat{T}_1^{(1)}] = [\hat{J}_z, -\frac{\hat{V}_x + i\hat{V}_y}{\sqrt{2}}] = \frac{1}{\sqrt{2}}[\hat{V}_x + i\hat{V}_y, \hat{J}_z] = \frac{1}{\sqrt{2}}(-i\hbar\hat{V}_y - \hbar\hat{V}_x) = \hbar\hat{T}_1^{(1)}$$

$$[\hat{J}_z, \hat{T}_{-1}^{(1)}] = [\hat{J}_z, \frac{\hat{V}_x - i\hat{V}_y}{\sqrt{2}}] = -\frac{1}{\sqrt{2}}[\hat{V}_x - i\hat{V}_y, \hat{J}_z] = -\frac{1}{\sqrt{2}}(-i\hbar\hat{V}_y + \hbar\hat{V}_x) = \hbar\hat{T}_{-1}^{(1)}$$

$$[\hat{J}_z, \hat{T}_0^{(1)}] = [\hat{J}_z, \hat{V}_z] = 0$$

where

$$[\hat{V}_x, \hat{J}_z] = i\hbar\varepsilon_{132}\hat{V}_y = -i\hbar\hat{V}_y, \qquad [\hat{V}_y, \hat{J}_z] = i\hbar\varepsilon_{231}\hat{V}_x = i\hbar\hat{V}_x$$

(b) Spherical tensor operator of rank 2

Spherical tensor of rank 2

$$P_{2,0}(x,y,z) = r^2 Y_2^0(\theta,\phi) = \sqrt{\frac{5}{16\pi}}(3z^2 - r^2) = \sqrt{\frac{15}{8\pi}}\frac{[2z^2 - \frac{(x+iy)(x-iy)}{2} - \frac{(x-iy)(x+iy)}{2}]}{\sqrt{6}}$$

$$\hat{T}_0^{(2)} = \sqrt{\frac{15}{8\pi}}\frac{\hat{T}_1^{(1)}\hat{T}_{-1}^{(1)} + 2\hat{T}_0^{(1)2} + \hat{T}_{-1}^{(1)}\hat{T}_1^{(1)}}{\sqrt{6}}$$

$$P_{2,\pm 2}(x,y,z) = r^2 Y_2^{\pm 2}(\theta,\phi) = \sqrt{\frac{15}{16\pi}}(\frac{x \pm iy}{\sqrt{2}})^2$$

$$\hat{T}_{\pm 2}^{(2)} = \sqrt{\frac{15}{16\pi}}\left(\hat{T}_{\pm 1}^{(1)}\right)^2$$

$$P_{2,1}(x,y,z) = r^2 Y_2^1(\theta,\phi) = \sqrt{\frac{15}{8\pi}}\frac{z(x-iy) + (x-iy)z}{\sqrt{2}\sqrt{2}}$$

$$\hat{T}_{-1}^{(2)} = \sqrt{\frac{15}{8\pi}}\frac{\hat{T}_0^{(1)}\hat{T}_{-1}^{(1)} + \hat{T}_{-1}^{(1)}\hat{T}_0^{(1)}}{\sqrt{2}}$$

$$P_{2,-1}(x,y,z) = r^2 Y_2^{-1}(\theta,\phi) = -\sqrt{\frac{15}{8\pi}}\frac{z(x+iy)+(x+iy)z}{\sqrt{2}\sqrt{2}}$$

$$\hat{T}_1^{(2)} = \sqrt{\frac{15}{8\pi}}\frac{\hat{T}_0^{(1)}\hat{T}_1^{(1)}+\hat{T}_1^{(1)}\hat{T}_0^{(1)}}{\sqrt{2}}$$

5. Construction of new tensors: product of tensors

((**Theorem**))

Let $\hat{X}_{q_1}^{(k_1)}$ and $\hat{Z}_{q_2}^{(k_2)}$ be irreducible spherical tensors of rank k_1 and k_2, respectively. Then

$$\hat{T}_q^{(k)} = \sum_{q_1,q_2}\langle k_1,k_2;q_1,q_2|k_1,k_2;k,q\rangle \hat{X}_{q_1}^{(k_1)}\hat{Z}_{q_2}^{(k_2)}$$

is a spherical (irreducible) tensor of rank k. $\langle k_1,k_2;q_1,q_2|k_1,k_2;k,q\rangle$ is the Clebsch-Gordan coefficient.

((**Proof**))

$$\begin{aligned}
\hat{R}\hat{T}_q^{(k)}\hat{R}^+ &= \sum_{q_1,q_2}\langle k_1,k_2;q_1,q_2|k_1,k_2;k,q\rangle(\hat{R}\hat{X}_{q_1}^{(k_1)}\hat{R}^+)(\hat{R}\hat{Z}_{q_2}^{(k_2)}\hat{R}^+) \\
&= \sum_{q_1,q_2,q_1',q_2'}\langle k_1,k_2;q_1,q_2|k_1,k_2;k,q\rangle D_{q_1'q_1}^{(k_1)}(\hat{R})\hat{X}_{q_1'}^{(k_1)}D_{q_2'q_2}^{(k_2)}(\hat{R})\hat{Z}_{q_2'}^{(k_2)} \\
&= \sum_{\substack{q_1,q_2,q_1',q_2' \\ k'',q'',q'}}\langle k_1,k_2;q_1,q_2|k_1,k_2;k,q\rangle\langle k_1,k_2;q_1',q_2'|k_1,k_2;k'',q'\rangle\langle k_1,k_2;q_1,q_2|k_1,k_2;k'',q''\rangle D_{q'q''}^{(k'')}(\hat{R})\hat{X}_{q_1'}^{(k_1)}\hat{Z}_{q_2'}^{(k_2)} \\
&= \sum_{\substack{q_1',q_2' \\ k'',q'',q'}}\delta_{k,k''}\delta_{q,q''}\langle k_1,k_2;q_1',q_2'|k_1,k_2;k'',q'\rangle D_{q'q''}^{(k'')}(\hat{R})\hat{X}_{q_1'}^{(k_1)}\hat{Z}_{q_2'}^{(k_2)} \\
&= \sum_{q',q_1',q_2'}\langle k_1,k_2;q_1',q_2'|k_1,k_2;k,q'\rangle\hat{X}_{q_1'}^{(k_1)}\hat{Z}_{q_2'}^{(k_2)}D_{q'q}^{(k)}(\hat{R}) \\
&= \sum_{q'}D_{q'q}^{(k)}(\hat{R})T_{q'}^{(k)}
\end{aligned}$$

where

$$\hat{R}\hat{X}_{q_1}^{(k_1)}\hat{R}^+ = \sum_{q_1'}D_{q_1'q_1}^{(k_1)}(\hat{R})\hat{X}_{q_1'}^{(k_1)}$$

$$\hat{R}\hat{Z}_{q_2}^{(k_2)}\hat{R}^+ = \sum_{q_2'}D_{q_2'q_2}^{(k_2)}(\hat{R})\hat{Z}_{q_2'}^{(k_2)}$$

and **the Clebsch-Gordan series** given by

$$D^{(k_1)}_{q_1'q_1}(\hat{R})D^{(k_2)}_{q_2'q_2}(\hat{R}) = \sum_{k''q''q'}\langle k_1,k_2;q_1',q_2'|k_1,k_2;k'',q'\rangle\langle k_1,k_2;q_1,q_2|k_1,k_2;k'',q'\rangle D^{(k'')}_{q'q''}(\hat{R})$$

where

$$D^{(l)}_{m,m'}(\hat{R}) = \langle l,m|\hat{R}|l,m'\rangle$$

$$D_{k_1}\times D_{k_2} = D_{k_1+k_2} + D_{k_1+k_2-1} + ... + D_{|k_1-k_2|}$$

(The proof of this series will be given in the APPENDIX.

((**Example**))

We now consider the case,

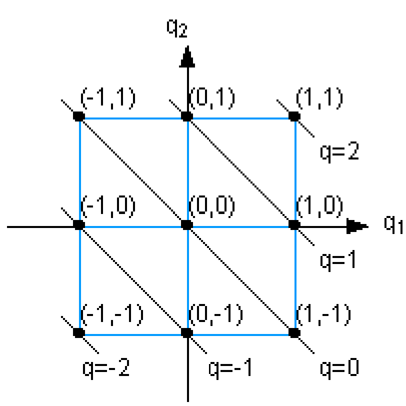
$$D_1\times D_1 = D_2 + D_1 + D_0$$

or

k = 2, 1, and 1.

<u>Tensor of rank 2</u>

k = 2,
q_1 = 1,0,-1, and q_2 = 1,0,-1, and



$$\hat{T}_2^{(2)} = \hat{X}_1^{(1)} Z_1^{(1)} = \hat{U}_1 \hat{V}_1 = \frac{1}{2}(\hat{U}_x + i\hat{U}_y)(\hat{V}_x + i\hat{V}_y)$$

$$\hat{T}_1^{(2)} = \frac{\hat{X}_1^{(1)} \hat{Z}_0^{(1)} + \hat{X}_0^{(1)} \hat{Z}_1^{(1)}}{\sqrt{2}} = \frac{\hat{U}_1 \hat{V}_0 + \hat{U}_0 \hat{V}_1}{\sqrt{2}} = -\left(\frac{\hat{U}_z \hat{V}_x + \hat{U}_x \hat{V}_z}{2}\right) - i\left(\frac{\hat{U}_y \hat{V}_z + \hat{U}_z \hat{V}_y}{2}\right)$$

$$\hat{T}_0^{(2)} = \frac{\hat{X}_1^{(1)} \hat{Z}_{-1}^{(1)} + 2\hat{X}_0^{(1)} \hat{Z}_0^{(1)} + \hat{X}_{-1}^{(1)} \hat{Z}_1^{(1)}}{\sqrt{6}} = \frac{\hat{U}_1 \hat{V}_{-1} + 2\hat{U}_0 \hat{V}_0 + \hat{U}_{-1} \hat{V}_1}{\sqrt{6}} = -\left(\frac{\hat{U}_x \hat{V}_x + \hat{U}_y \hat{V}_y - 2\hat{U}_z \hat{V}_z}{\sqrt{6}}\right)$$

$$\hat{T}_{-1}^{(2)} = \frac{\hat{X}_0^{(1)} \hat{Z}_{-1}^{(1)} + \hat{X}_{-1}^{(1)} \hat{Z}_0^{(1)}}{\sqrt{2}} = \frac{\hat{U}_0 \hat{V}_{-1} + \hat{U}_{-1} \hat{V}_1}{\sqrt{2}} = \left(\frac{\hat{U}_z \hat{V}_x + \hat{U}_x \hat{V}_z}{2}\right) - i\left(\frac{\hat{U}_y \hat{V}_z + \hat{U}_z \hat{V}_y}{2}\right)$$

$$\hat{T}_{-2}^{(2)} = \hat{X}_{-1}^{(1)} \hat{Z}_{-1}^{(1)} = \hat{U}_{-1} \hat{V}_{-1} = \frac{1}{2}(\hat{U}_x - i\hat{U}_y)(\hat{V}_x - i\hat{V}_y)$$

When $\hat{U}_i = \hat{V}_i = \hat{x}_i$ (in a special case),

$$\hat{T}_2^{(2)} = \frac{1}{2}(\hat{x} + i\hat{y})(\hat{x} + i\hat{y}) = \frac{1}{2}(\hat{x}^2 - \hat{y}^2) + i\hat{x}\hat{y}$$

$$\hat{T}_1^{(2)} = -\hat{x}\hat{z} - i\hat{y}\hat{z}$$

$$\hat{T}_0^{(2)} = -\left(\frac{\hat{x}^2 + \hat{y}^2 - 2\hat{z}^2}{\sqrt{6}}\right)$$

$$\hat{T}_{-1}^{(2)} = \hat{x}\hat{z} - i\hat{y}\hat{z}$$

$$\hat{T}_{-2}^{(2)} = \frac{1}{2}(\hat{x} + i\hat{y})(\hat{x} + i\hat{y}) = \frac{1}{2}(\hat{x}^2 - \hat{y}^2) - i\hat{x}\hat{y}$$

Therefore we have the following relations.

$$\hat{x}^2 - \hat{y}^2 = \hat{T}_2^{(2)} + \hat{T}_{-2}^{(2)}$$

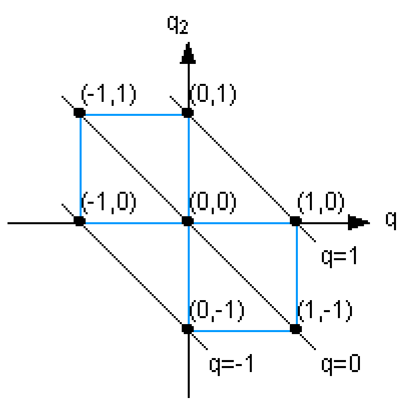
$$\hat{x}\hat{y} = \frac{\hat{T}_2^{(2)} - \hat{T}_{-2}^{(2)}}{2i}$$

$$\hat{y}\hat{z} = \frac{\hat{T}_1^{(2)} + \hat{T}_{-1}^{(2)}}{-2i}$$

$$\hat{x}\hat{z} = \frac{\hat{T}_1^{(2)} - \hat{T}_{-1}^{(2)}}{-2}$$

$$\left(\frac{\hat{x}^2 + \hat{y}^2 - 2\hat{z}^2}{\sqrt{6}}\right) = -\hat{T}_0^{(2)} =$$

Tensor of rank 1

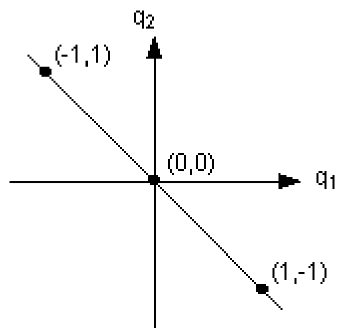


$$T_1^{(1)} = \frac{X_1^{(1)} Z_0^{(1)} - X_0^{(1)} Z_1^{(1)}}{\sqrt{2}} = \frac{U_1 V_0 - U_0 V_1}{\sqrt{2}}$$

$$T_0^{(1)} = \frac{X_1^{(1)} Z_{-1}^{(1)} - X_{-1}^{(1)} Z_1^{(1)}}{\sqrt{2}} = \frac{U_1 V_{-1} - U_{-1} V_1}{\sqrt{2}}$$

$$T_{-1}^{(1)} = \frac{X_0^{(1)} Z_{-1}^{(1)} - X_{-1}^{(1)} Z_0^{(1)}}{\sqrt{2}} = \frac{U_0 V_{-1} - U_{-1} V_0}{\sqrt{2}}$$

Tensor of rank 0



$$T_0^{(0)} = \frac{X_1^{(1)} Z_{-1}^{(1)} - X_0^{(1)} Z_0^{(1)} + X_{-1}^{(1)} Z_1^{(1)}}{\sqrt{3}} = \frac{U_1 V_{-1} - U_0 V_0 + U_{-1} V_1}{\sqrt{3}}$$

Tensor of rank 2

$$T_2^{(2)} = X_1^{(1)} Z_1^{(1)} = U_1 V_1$$

$$T_1^{(2)} = \frac{X_1^{(1)} Z_0^{(1)} + X_0^{(1)} Z_1^{(1)}}{\sqrt{2}} = \frac{U_1 V_0 + U_0 V_1}{\sqrt{2}}$$

$$T_0^{(2)} = \frac{X_1^{(1)} Z_{-1}^{(1)} + 2 X_0^{(1)} Z_0^{(1)} + X_{-1}^{(1)} Z_1^{(1)}}{\sqrt{6}} = \frac{U_1 V_{-1} + 2 U_0 V_0 + U_{-1} V_1}{\sqrt{6}}$$

$$T_{-1}^{(2)} = \frac{X_0^{(1)} Z_{-1}^{(1)} + X_{-1}^{(1)} Z_0^{(1)}}{\sqrt{2}} = \frac{U_0 V_{-1} + U_{-1} V_0}{\sqrt{2}}$$

$$T_{-2}^{(2)} = U_{-1} V_{-1}$$

((**Mathematica**))

```
Clear["Global`*"]; CCGG[{j1_, m1_}, {j2_, m2_}, {j_, m_}] :=
 Module[{s1},
  s1 = If[Abs[m1] ≤ j1 && Abs[m2] ≤ j2 && Abs[m] ≤ j,
    ClebschGordan[{j1, m1}, {j2, m2}, {j, m}], 0]];
CG[j1_, j2_, j_] :=
 Table[Sum[CCGG[{j1, k1}, {j2, k2}, {j, k1 + k2}] X[j1, k1] Z[j2, k2]
    KroneckerDelta [k1 + k2, m], {k1, -j1, j1}, {k2, -j2, j2}], {m, -j, j}];
CG[1, 1, 2]
```

$$\left\{X[1,-1]\,Z[1,-1],\ \frac{X[1,0]\,Z[1,-1]}{\sqrt{2}}+\frac{X[1,-1]\,Z[1,0]}{\sqrt{2}},\ \frac{X[1,1]\,Z[1,-1]}{\sqrt{6}}+\sqrt{\frac{2}{3}}\,X[1,0]\,Z[1,0]+\frac{X[1,-1]\,Z[1,1]}{\sqrt{6}},\ \frac{X[1,1]\,Z[1,0]}{\sqrt{2}}+\frac{X[1,0]\,Z[1,1]}{\sqrt{2}},\ X[1,1]\,Z[1,1]\right\}$$

```
CG[1, 1, 1]
```

$$\left\{\frac{X[1,0]\,Z[1,-1]}{\sqrt{2}}-\frac{X[1,-1]\,Z[1,0]}{\sqrt{2}},\ \frac{X[1,1]\,Z[1,-1]}{\sqrt{2}}-\frac{X[1,-1]\,Z[1,1]}{\sqrt{2}},\ \frac{X[1,1]\,Z[1,0]}{\sqrt{2}}-\frac{X[1,0]\,Z[1,1]}{\sqrt{2}}\right\}$$

```
CG[1, 1, 0]
```

$$\left\{\frac{X[1,1]\,Z[1,-1]}{\sqrt{3}}-\frac{X[1,0]\,Z[1,0]}{\sqrt{3}}+\frac{X[1,-1]\,Z[1,1]}{\sqrt{3}}\right\}$$

6. Tensor of rank zero (scalar)

We now construct the tensor of rank zero (scalar) by the product of two tensors of rank 1.

$$\begin{aligned}\hat{T}_{q=0}^{(k=0)} &= \sum_{q_1,q_2}\langle k_1=k,k_2=k;q_1,q_2|k_1=k,k_2=k;k=0,q=0\rangle \hat{X}_{q_1}^{(k_1=1)}\hat{Z}_{q_2}^{(k_2=1)} \\ &= \sum_{q_1}\langle k_1=k,k_2=k;q_1,-q_1|k_1=k,k_2=k;k=0,q=0\rangle \hat{X}_{q_1}^{(k)}\hat{Z}_{-q_1}^{(k)}\end{aligned}$$

Here we note that

$$\langle k_1=k,k_2=k;q_1,q_2|k_1=k,k_2=k;k=0,q=0\rangle \neq 0 \qquad \text{only if } q_1+q_2=0$$

and

$$\langle k_1=k,k_2=k;q_1,-q_1|k_1=k,k_2=k;k=0,q=0\rangle = -\frac{(-1)^{q_1}}{\sqrt{2k+1}}$$

Then we have

$$\hat{T}_{q=0}^{(k=0)} = -\frac{1}{\sqrt{2k+1}} \sum_{q_1} (-1)^{q_1} \hat{X}_{q_1}^{(k)} \hat{Z}_{-q_1}^{(k)}$$

which is the tensor of rank zero (a scalar).

((**Mathematica**))

```
Clear["Global`*"]; CCGG[{j1_, m1_}, {j2_, m2_}, {j_, m_}] :=
 Module[{s1},
  s1 = If[Abs[m1] ≤ j1 && Abs[m2] ≤ j2 && Abs[m] ≤ j,
    ClebschGordan[{j1, m1}, {j2, m2}, {j, m}], Null]];
CG[k_] := Table[{{k, q}, CCGG[{k, q}, {k, -q}, {0, 0}]}, {q, -k, k, 1}];
```

```
CG[1]
```

$\{\{\{1,-1\},\frac{1}{\sqrt{3}}\},\{\{1,0\},-\frac{1}{\sqrt{3}}\},\{\{1,1\},\frac{1}{\sqrt{3}}\}\}$

```
CG[2]
```

$\{\{\{2,-2\},\frac{1}{\sqrt{5}}\},\{\{2,-1\},-\frac{1}{\sqrt{5}}\},\{\{2,0\},\frac{1}{\sqrt{5}}\},\{\{2,1\},-\frac{1}{\sqrt{5}}\},\{\{2,2\},\frac{1}{\sqrt{5}}\}\}$

```
CG[3]
```

$\{\{\{3,-3\},\frac{1}{\sqrt{7}}\},\{\{3,-2\},-\frac{1}{\sqrt{7}}\},\{\{3,-1\},\frac{1}{\sqrt{7}}\},$
$\{\{3,0\},-\frac{1}{\sqrt{7}}\},\{\{3,1\},\frac{1}{\sqrt{7}}\},\{\{3,2\},-\frac{1}{\sqrt{7}}\},\{\{3,3\},\frac{1}{\sqrt{7}}\}\}$

```
CG[4]
```

$\{\{\{4,-4\},\frac{1}{3}\},\{\{4,-3\},-\frac{1}{3}\},\{\{4,-2\},\frac{1}{3}\},\{\{4,-1\},-\frac{1}{3}\},$
$\{\{4,0\},\frac{1}{3}\},\{\{4,1\},-\frac{1}{3}\},\{\{4,2\},\frac{1}{3}\},\{\{4,3\},-\frac{1}{3}\},\{\{4,4\},\frac{1}{3}\}\}$

7. Tensor operator: example

$$[\hat{V}_i, \hat{J}_j] = i\hbar \varepsilon_{ijk} \hat{V}_k$$

$$[\hat{V}_x, \hat{J}_x] = 0, [\hat{V}_x, \hat{J}_y] = i\hbar\hat{V}_z, [\hat{V}_x, \hat{J}_z] = -i\hbar\hat{V}_y$$

$$[\hat{V}_y, \hat{J}_x] = -i\hbar\hat{V}_z, [\hat{V}_y, \hat{J}_y] = 0, [\hat{V}_y, \hat{J}_z] = i\hbar\hat{V}_x$$

$$[\hat{V}_z, \hat{J}_1] = i\hbar\hat{V}_y, [\hat{V}_z, \hat{J}_y] = -i\hbar\hat{V}_1, [\hat{V}_z, \hat{J}_z] = 0$$

or

$$[\hat{J}_x, \hat{V}_x] = 0, [\hat{J}_x, \hat{V}_2] = i\hbar\hat{V}_z, [\hat{J}_x, \hat{V}_z] = -i\hbar\hat{V}_y$$

$$[\hat{J}_y, \hat{V}_x] = -i\hbar\hat{V}_z, [\hat{J}_y, \hat{V}_y] = 0, [\hat{J}_y, \hat{V}_z] = i\hbar\hat{V}_1$$

$$[\hat{J}_z, \hat{V}_x] = i\hbar\hat{V}_y, [\hat{J}_z, \hat{V}_y] = -i\hbar\hat{V}_x, [\hat{J}_z, \hat{V}_z] = 0$$

Here we introduce

$$\hat{V}_1 = -\frac{1}{\sqrt{2}}\hat{V}_+ = -\frac{1}{\sqrt{2}}(\hat{V}_x + i\hat{V}_y)$$

$$\hat{V}_0 = \hat{V}_z$$

$$\hat{V}_{-1} = \frac{1}{\sqrt{2}}\hat{V}_- = \frac{1}{\sqrt{2}}(\hat{V}_x - i\hat{V}_y)$$

It is possible and useful for many purposes to think of $\hat{V}_1, \hat{V}_0, \hat{V}_{-1}$ as forming three "operator eigenstates" $\hat{V}_1, \hat{V}_0, \hat{V}_{-1}$ of *j* having *j* = 1 and *m* = 1,0, amd -1.

$$[\hat{J}_+, \hat{V}_1] = [\hat{J}_z, \hat{V}_0] = [\hat{J}_-, \hat{V}_{-1}] = 0$$

$$[\hat{J}_\pm, \hat{V}_0] = \hbar\sqrt{2}\hat{V}_{\pm 1}, [\hat{J}_z, \hat{V}_{\pm 1}] = \pm\hbar\hat{V}_{\pm 1}$$

$$[\hat{J}_\pm, \hat{V}_{\mp 1}] = \hbar\sqrt{2}\hat{V}_0$$

This is compared with

$$\hat{J}_+|1,1\rangle = 0, \hat{J}_+|1,0\rangle = \sqrt{2}\hbar|1,1\rangle, \hat{J}_+|1,-1\rangle = \sqrt{2}\hbar|1,0\rangle,$$

$$\hat{J}_-|1,1\rangle = \sqrt{2}\hbar|1,0\rangle, \hat{J}_-|1,0\rangle = \sqrt{2}\hbar|1,-1\rangle, \hat{J}_-|1,-1\rangle = 0$$

$$\hat{J}_z|1,1\rangle = \hbar|1,1\rangle, \hat{J}_z|1,0\rangle = 0, \hat{J}_z|1,-1\rangle = -\hbar|1,-1\rangle$$

or

$$\hat{J}_+|1,1\rangle = 0, \hat{J}_z|1,0\rangle = 0, \hat{J}_-|1,-1\rangle = 0$$

$$\hat{J}_+|1,0\rangle = \sqrt{2}\hbar|1,1\rangle, \hat{J}_-|1,0\rangle = \sqrt{2}\hbar|1,-1\rangle,$$

$$\hat{J}_z|1,1\rangle = \hbar|1,1\rangle, \hat{J}_z|1,-1\rangle = -\hbar|1,-1\rangle$$

$$\hat{J}_+|1,-1\rangle = \sqrt{2}\hbar|1,0\rangle, \hat{J}_-|1,1\rangle = \sqrt{2}\hbar|1,0\rangle$$

---

8. Wigner and Eckart Theorem

$$[\hat{J}_z, T_q^{(k)}] = \sum_{q'=-k}^{k} \hat{T}_{q'}^{(k)} \langle k,q'|\hat{J}_z|k,q\rangle = \hbar q \hat{T}_q^{(k)} \qquad (3)$$

$$\langle \alpha'; j',m'|[\hat{J}_z, T_q^{(k)}]|\alpha; j,m\rangle = \hbar q \langle \alpha; j',m'|\hat{T}_q^{(k)}|\alpha; j,m\rangle$$

or

$$\hbar(m'-m-q)\langle \alpha'; j',m'|\hat{T}_q^{(k)}|\alpha; j,m\rangle = 0$$

Then we have

$$\langle \alpha'; j',m'|\hat{T}_q^{(k)}|\alpha; j,m\rangle = 0$$

unless

$$m'-m-q \neq 0$$

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

(a)

$$\langle \alpha'; j', m' | [\hat{J}_+, \hat{T}_q^{(k)}] | \alpha; j, m \rangle = \hbar\sqrt{(k-q)(k+q+1)} \langle \alpha; j', m' | \hat{T}_{q+1}^{(k)} | \alpha; j, m \rangle$$

or

$$\langle \alpha'; j', m' | \hat{J}_+ T_q^{(k)} - T_q^{(k)} \hat{J}_+ | \alpha; j, m \rangle = \hbar\sqrt{(k-q)(k+q+1)} \langle \alpha; j', m' | \hat{T}_{q+1}^{(k)} | \alpha; j, m \rangle$$

$$\langle \alpha'; j', m' | \hat{J}_+ \hat{T}_q^{(k)} | \alpha; j, m \rangle - \langle \alpha'; j', m' | \hat{T}_q^{(k)} \hat{J}_+ | \alpha; j, m \rangle = \hbar\sqrt{(k-q)(k+q+1)} \langle \alpha; j', m' | \hat{T}_{q+1}^{(k)} | \alpha; j, m \rangle$$

$$\begin{aligned}
&\sqrt{(j'+m')(j'-m'+1)} \langle \alpha'; j', m'-1 | \hat{T}_q^{(k)} | \alpha; j, m \rangle - \sqrt{(j-m)(j+m+1)} \langle \alpha'; j', m' | \hat{T}_q^{(k)} | \alpha; j, m+1 \rangle \\
&= \sqrt{(k-q)(k+q+1)} \langle \alpha; j', m' | \hat{T}_{q+1}^{(k)} | \alpha; j, m \rangle
\end{aligned}$$

(b)

$$\langle \alpha'; j', m' | [\hat{J}_-, \hat{T}_q^{(k)}] | \alpha; j, m \rangle = \hbar\sqrt{(k+q)(k-q+1)} \langle \alpha; j', m' | \hat{T}_{q-1}^{(k)} | \alpha; j, m \rangle$$

$$\langle \alpha'; j', m' | \hat{J}_- \hat{T}_q^{(k)} | \alpha; j, m \rangle - \langle \alpha'; j', m' | \hat{T}_q^{(k)} \hat{J}_- | \alpha; j, m \rangle = \hbar\sqrt{(k+q)(k-q+1)} \langle \alpha; j', m' | \hat{T}_{q-1}^{(k)} | \alpha; j, m \rangle$$

$$\begin{aligned}
&\sqrt{(j'-m')(j'+m'+1)} \langle \alpha'; j', m'+1 | \hat{T}_q^{(k)} | \alpha; j, m \rangle \\
&- \sqrt{(j+m)(j-m+1)} \langle \alpha'; j', m' | T_q^{(k)} | \alpha; j, m-1 \rangle \\
&= \sqrt{(k+q)(k-q+1)} \langle \alpha; j', m' | \hat{T}_{q+1}^{(k)} | \alpha; j, m \rangle
\end{aligned}$$

or

$$\begin{aligned}
\sqrt{(j'\pm m')(j'\mp m'+1)} \langle \alpha'; j', m'\mp 1 | T_q^{(k)} | \alpha; j, m \rangle &= \sqrt{(j\mp m)(j\pm m+1)} \langle \alpha'; j', m' | T_q^{(k)} | \alpha; j, m\pm 1 \rangle \\
&+ \sqrt{(k\mp q)(k\pm q+1)} \langle \alpha; j', m' | \hat{T}_{q\pm 1}^{(k)} | \alpha; j, m \rangle
\end{aligned}$$

We find the same recursion relations for the $\langle \alpha'; j', m' | \hat{T}_q^{(k)} | \alpha; j, m \rangle$ as we find for the Clebsch-Gordan coefficients $\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \rangle = \langle j, k; m, q | j, k; j', m' \rangle$

with

$j_1 = j$, $j_2 = k$, $m_1 = m$, $m_2 = q$, $j = j'$ $m = m'$

$$\sqrt{(j'\pm m')(j'\mp m'+1)}\langle j,k;m,q|j,k;j',m'\rangle$$
$$=\sqrt{(j\pm m)(j\mp m+1))}\langle j,k;m\mp 1,q|j_1,k;j',m'\mp 1\rangle$$
$$+\sqrt{(k\pm q)(k\mp q+1)}\langle j,k;m,q\mp 1|j,k;j',m'\mp 1\rangle$$

or
By changing by $\pm\to\mp$ and $\mp\to\pm$, and $m'\to m'\mp 1$ we have

$$\sqrt{(j'\pm m')(j'\mp m'+1)}\langle j,k;m,q|j,k;j',m'\mp 1\rangle$$
$$=\sqrt{(j\mp m)(j\pm m+1))}\langle j,k;m\pm 1,q|j_1,k;j',m'\rangle$$
$$+\sqrt{(k\mp q)(k\pm q+1)}\langle j,k;m,q\pm 1|j,k;j',m\rangle$$

Therefore the *m* behavior of the $\langle\alpha';j',m'|T_q^{(k)}|\alpha;j,m\rangle$ must be the same as that of the Clebsch-Gordan coefficients. We see that

$\langle\alpha';j',m'|\hat{T}_q^{(k)}|\alpha;j,m\rangle=\langle j,k;m,q|j,k;j',m'\rangle\times$ term independent of *m'*, *m*, and *q*.

or

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

(Wigner-Eckart theorem)

$\langle\alpha' j'\|\hat{T}_k\|\alpha j\rangle$ is the reduced matrix element, independent of *m'*, *m*, and *q*.

where

$$m'=m+q$$

$$j'=j+k,j+k-1,.......,|j-k|$$

((Note)) As the Wigner-Eckart theorem, one can use conventionally the form

$$\langle\alpha';j',m'|\hat{T}_q^{(k)}|\alpha;j,m\rangle=\langle j,k;m,q|j,k;j',m'\rangle\frac{\langle\alpha' j'\|\hat{T}^{(k)}\|\alpha j\rangle}{\sqrt{2j+1}}$$

The $\sqrt{2j+1}$ factor is arbitrary, but conventional. Here we use the formula which is used by Zettli.

((**Note**))

Recursion relation of the Clebsch-Gordan coefficients

$$\left| j_1, j_2; j, m \right\rangle = \sum_{m_1} \sum_{m_2} \left| j_1, j_2; m_1, m_2 \right\rangle \left\langle j_1, j_2; m_1, m_2 \right| j_1, j_2; j, m \rangle$$

where

$$(m - m_1 - m_2) \left\langle j_1, j_2; m_1, m_2 \right| j_1, j_2; j, m \rangle = 0$$

and

$$\begin{aligned}
&\sqrt{(j \mp m)(j \pm m + 1)} \left\langle j_1, j_2; m_1, m_2 \right| j_1, j_2; j, m \pm 1 \rangle \\
&= \sqrt{(j_1 \mp m_1 + 1)(j_1 \pm m_1)} \left\langle j_1, j_2; m_1 \mp 1, m_2 \right| j_1, j_2; j, m \rangle \\
&+ \sqrt{(j_2 \mp m_2 + 1)(j_2 \pm m_2)} \left\langle j_1, j_2; m_1, m_2 \mp 1 \right| j_1, j_2; j, m \rangle
\end{aligned}$$

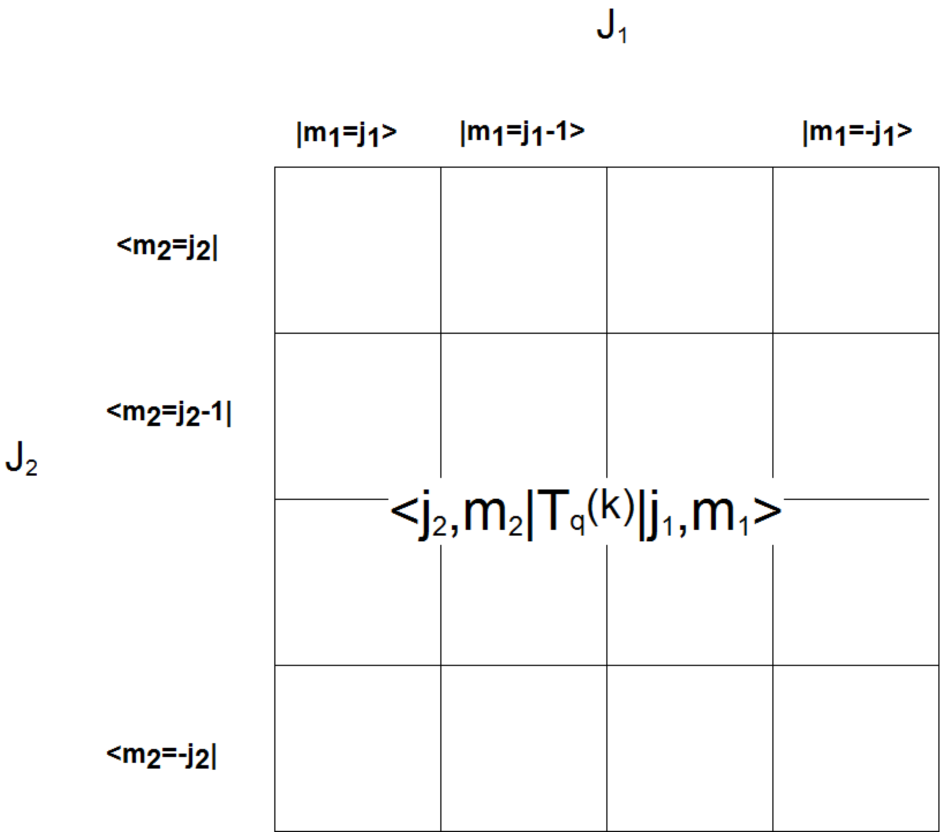
or

$$\begin{aligned}
&\sqrt{(j \pm m)(j \mp m + 1)} \left\langle j_1, j_2; m_1, m_2 \right| j_1, j_2; j, m \rangle \\
&= \sqrt{(j_1 \pm m_1)(j_1 \mp m_1 + 1))} \left\langle j_1, j_2; m_1 \mp 1, m_2 \right| j_1, j_2; j, m \mp 1 \rangle \\
&+ \sqrt{(j_2 \pm m_2)(j_2 \mp m_2 + 1)} \left\langle j_1, j_2; m_1, m_2 \mp 1 \right| j_1, j_2; j, m \mp 1 \rangle
\end{aligned}$$

9. Defintion of matrix element

We define the matrix element of the Clebsch-Gordon coefficient as

$$\left\langle \alpha'; j', m' \right| \hat{T}_{q=0}^{(k=0)} \left| \alpha; j, m \right\rangle = CCG[\{j', \{k, q\}, j]$$



where

$j' = j+k, j+k-1, \ldots\ldots, |j-k|.$

$q = k, k-1, \ldots, -k.$

10. Numerical calculation of matrix using Mathematica

```
Clear["Global`*"]; CCGG[{j1_, m1_}, {j2_, m2_}, {j_, m_}] :=
 Module[{s1},
  s1 = If[Abs[m1] ≤ j1 && Abs[m2] ≤ j2 && Abs[m] ≤ j,
    ClebschGordan[{j1, m1}, {j2, m2}, {j, m}], 0]];
CCG[j2_, {k1_, q1_}, j1_] :=
 Table[{{m1 + q1, m1}, CCGG[{j1, m1}, {k1, q1}, {j2, m1 + q1}]}, {m1, j1, -j1, -1}];
```

Using this program, one can get the table of the matrix elements of the tensor operator,

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

for given k, q, and j. Here the matrix can be obtained using the notation of matrix (mathematica)

$CCG[\{j', \{k, q\}, j]$

10 Example 1: Tensor of rank 0 (scalar)

$$\langle \alpha'; j', m' | \hat{T}_{q=0}^{(k=0)} | \alpha; j, m \rangle \neq 0$$

only if

$m' = m$ and $j' = j$

((**Example**))

$k = 0$, $q = 0$; $j = 0$, $j' = 0$

```
CCG[0, {0, 0}, 0]
{{{0, 0}, 1}}
```

$k = 0$, $q = 0$; $j = 1$, $j' = 1$

```
CCG[1, {0, 0}, 1]
{{{1, 1}, 1}, {{0, 0}, 1}, {{-1, -1}, 1}}
```

11. Example 2: Tensor of rank 1 (vector)

$$\langle \alpha'; j', m' | \hat{T}_{q}^{(k=1)} | \alpha; j, m \rangle \neq 0$$

only if

$m' = m + q$, $j' = j + 1, j, | j - 1 |$

(1)

$k = 1$, $q = 1$: $j = 0$, $j' = 1$

```
CCG[1, {1, 1}, 0]
{{{1, 0}, 1}}
```

$k = 1$, $q = 0$: $j = 0$, $j' = 1$

```
CCG[1, {1, 0}, 0]
```

$\{\{\{0, 0\}, 1\}\}$

$k = 1, q = -1$: $\quad j = 0, \quad j' = 1$

```
CCG[1, {1, -1}, 0]
```

$\{\{\{-1, 0\}, 1\}\}$

(2.1)

$k = 1, q = 1$: $\quad j = 1, \quad j' = 2$

```
CCG[2, {1, 1}, 1]
```

$\left\{\{\{2, 1\}, 1\}, \left\{\{1, 0\}, \frac{1}{\sqrt{2}}\right\}, \left\{\{0, -1\}, \frac{1}{\sqrt{6}}\right\}\right\}$

$k = 1, q = 0$: $\quad j = 1, \quad j' = 2$

```
CCG[2, {1, 0}, 1]
```

$\left\{\left\{\{1, 1\}, \frac{1}{\sqrt{2}}\right\}, \left\{\{0, 0\}, \sqrt{\frac{2}{3}}\right\}, \left\{\{-1, -1\}, \frac{1}{\sqrt{2}}\right\}\right\}$

$k = 1, q = -1$: $\quad j = 1, \quad j' = 2$

```
CCG[2, {1, -1}, 1]
```

$\left\{\left\{\{0, 1\}, \frac{1}{\sqrt{6}}\right\}, \left\{\{-1, 0\}, \frac{1}{\sqrt{2}}\right\}, \{\{-2, -1\}, 1\}\right\}$

(2.2)

$k = 1, q = 1$: $\quad j = 1, \quad j' = 1$

```
CCG[1, {1, 1}, 1]
```

$\left\{\{\{2, 1\}, \text{Null}\}, \left\{\{1, 0\}, -\frac{1}{\sqrt{2}}\right\}, \left\{\{0, -1\}, -\frac{1}{\sqrt{2}}\right\}\right\}$

$k = 1, q = 0$: $\quad j = 1, \quad j' = 1$

CCG[1, {1, 0}, 1]

$$\left\{\left\{\{1,\ 1\},\ \frac{1}{\sqrt{2}}\right\},\ \{\{0,\ 0\},\ 0\},\ \left\{\{-1,\ -1\},\ -\frac{1}{\sqrt{2}}\right\}\right\}$$

$k = 1, q = -1$: $j = 1$, $j'=1$

CCG[1, {1, -1}, 1]

$$\left\{\left\{\{0,\ 1\},\ \frac{1}{\sqrt{2}}\right\},\ \left\{\{-1,\ 0\},\ \frac{1}{\sqrt{2}}\right\},\ \{\{-2,\ -1\},\ \text{Null}\}\right\}$$

(2.3)

$k = 1, q = 1$: $j = 1$, $j'=0$

CCG[0, {1, 1}, 1]

$$\left\{\{\{2,\ 1\},\ \text{Null}\},\ \{\{1,\ 0\},\ \text{Null}\},\ \left\{\{0,\ -1\},\ \frac{1}{\sqrt{3}}\right\}\right\}$$

$k = 1, q = 0$: $j = 1$, $j'=0$

CCG[0, {1, 0}, 1]

$$\left\{\{\{1,\ 1\},\ \text{Null}\},\ \left\{\{0,\ 0\},\ -\frac{1}{\sqrt{3}}\right\},\ \{\{-1,\ -1\},\ \text{Null}\}\right\}$$

$k = 1, q = -1$: $j = 1$, $j'=0$

CCG[0, {1, -1}, 1]

$$\left\{\left\{\{0,\ 1\},\ \frac{1}{\sqrt{3}}\right\},\ \{\{-1,\ 0\},\ \text{Null}\},\ \{\{-2,\ -1\},\ \text{Null}\}\right\}$$

---

12. Parity operator

We consider the case when

$$\hat{T}_{+1}^{(1)} = \hat{V}_{+1} = -\frac{1}{\sqrt{2}}\hat{V}_{+} = -\frac{1}{\sqrt{2}}(\hat{V}_x + i\hat{V}_y)$$

$$\hat{T}_0^{(1)} = \hat{V}_0 = \hat{V}_z$$

$$\hat{T}_{-1}^{(1)} = \hat{V}_{-1} = \frac{1}{\sqrt{2}}\hat{V}_{-} = \frac{1}{\sqrt{2}}(\hat{V}_x - i\hat{V}_y)$$

Then we have

(a)

$$\langle \alpha'; j', m' | \hat{V}_x | \alpha; j, m \rangle = \langle \alpha'; j', m' | \frac{\hat{T}_{-1}^{(1)} - \hat{T}_1^{(1)}}{\sqrt{2}} | \alpha; j, m \rangle = 0$$

$$\langle \alpha'; j', m' | \hat{V}_y | \alpha; j, m \rangle = \langle \alpha'; j', m' | \frac{\hat{T}_{-1}^{(1)} + \hat{T}_1^{(1)}}{-\sqrt{2}i} | \alpha; j, m \rangle = 0$$

unless $m' = m \pm 1$ and $j' = j+1, j, |j-1|$

(b)

$$\langle \alpha'; j', m' | \hat{V}_z | \alpha; j, m \rangle = \langle \alpha'; j', m' | \hat{T}_0^{(1)} | \alpha; j, m \rangle = 0$$

unless $m' = m$ and $j' = j+1, j, |j-1|$

13. Selection rule for the rank 1 tensor (vector)

Spherical tensor of rank 1

$$T_1^{(1)} = -\frac{\hat{x} + i\hat{y}}{\sqrt{2}}$$

$$T_0^{(1)} = \hat{z}$$

$$T_{-1}^{(1)} = \frac{\hat{x} - i\hat{y}}{\sqrt{2}}$$

From Wigner-Eckart theorem

$$\langle n',l',m'|\hat{T}_q^{(1)}|n,l,m\rangle \neq 0 \text{ for } m' = m+q \text{ and for } l' = l+1, l, |l-1|.$$

where *l* is interger. For the parity operator, we have

$$\hat{\pi}\hat{T}_q^{(1)}\hat{\pi} = -\hat{T}_q^{(1)}$$

and

$$\hat{\pi}|n,l,m\rangle = (-1)^l|n,l,m\rangle, \qquad \langle n,l,m|\hat{\pi} = (-1)^l\langle n,l,m|$$

Thus the matrix element is equal to zero for $l' = l$, since

$$\langle n',l',m'|\hat{T}_q^{(2)}|n,l,m\rangle = -\langle n',l',m'|\hat{\pi}\hat{T}_q^{(2)}\hat{\pi}|n,l,m\rangle = (-1)^{l'+l-1}\langle n',l',m'|\hat{T}_q^{(2)}|n,l,m\rangle$$

Finally we have the selection rule

$$\langle n',l',m'|\hat{T}_q^{(1)}|n,l,m\rangle \neq 0 \text{ for } m' = m+q \text{ and for } l' - l = \pm 1$$

14. Selection rule for rank-2 tensor

Spherical tensor of rank 2

$$\hat{x}^2 - \hat{y}^2 = \hat{T}_2^{(2)} + \hat{T}_{-2}^{(2)}$$

$$\hat{x}\hat{y} = \frac{\hat{T}_2^{(2)} - \hat{T}_{-2}^{(2)}}{2i}$$

$$\hat{y}\hat{z} = \frac{\hat{T}_1^{(2)} + \hat{T}_{-1}^{(2)}}{-2i}$$

$$\hat{x}\hat{z} = \frac{\hat{T}_1^{(2)} - \hat{T}_{-1}^{(2)}}{-2}$$

$$\left(\frac{\hat{x}^2 + \hat{y}^2 - 2\hat{z}^2}{\sqrt{6}}\right) = -\hat{T}_0^{(2)}$$

From Wigner-Eckart theorem

$$\langle n',l',m'|\hat{T}_q^{(2)}|n,l,m\rangle \neq 0$$

for $m' = m + q$ and for $l' = l + 2, l + 1, l, |l - 1|, |l - 2|$. For the parity operator, we have

$$\hat{\pi}\hat{T}_q^{(2)}\hat{\pi} = \hat{T}_q^{(2)}$$

and

$$\hat{\pi}\left|n,l,m\right\rangle = (-1)^l \left|n,l,m\right\rangle, \qquad \left\langle n,l,m\right|\hat{\pi} = (-1)^l \left\langle n,l,m\right|$$

Thus the matrix element is equal to zero for $l' = l \pm 1$ since

$$\left\langle n',l',m'\right|\hat{T}_q^{(2)}\left|n,l,m\right\rangle = \left\langle n',l',m'\right|\hat{\pi}\hat{T}_q^{(2)}\hat{\pi}\left|n,l,m\right\rangle = (-1)^{l'+l}\left\langle n',l',m'\right|\hat{T}_q^{(2)}\left|n,l,m\right\rangle.$$

Finally we have the selection rule;

$$\left\langle n',l',m'\right|\hat{T}_q^{(1)}\left|n,l,m\right\rangle \neq 0 \text{ for } m' = m + q \text{ and for } l' - l = \pm 2, 0$$

15. Projection theorem (Eigner-Eckart theorem for a scalar product $\hat{\boldsymbol{J}} \cdot \hat{\boldsymbol{V}}$)
A.0 The projection theorem for the first rank tensor

$$\hat{\boldsymbol{J}} \cdot \boldsymbol{T}^{(1)} = \sum_q (-1)^q \hat{J}_q \hat{T}_{-q}^{(1)}$$

1. Decomposition theorem

$$\left\langle j',m'\right|\hat{T}_q^{(1)}\left| j,m\right\rangle = \frac{\left\langle j',m'\right|\hat{J}_q(\hat{\boldsymbol{J}} \cdot \boldsymbol{T}^{(1)})\left| j,m\right\rangle}{j(j+1)}\delta_{j,j'} \tag{1}$$

2. Factorization theorem

$$\left\langle j',m'\right|\hat{J}_q(\hat{\boldsymbol{J}} \cdot \boldsymbol{T}^{(1)})\left| j,m\right\rangle = \left\langle j',m'\right|\hat{J}_q\left| j,m\right\rangle < j \,\|\, \hat{\boldsymbol{J}} \cdot \boldsymbol{T}^{(1)} \,\|\, j >. \tag{2}$$

3. Decomposition theorem of the second kind (the projection theorem)

$$\left\langle j',m'\right|\hat{T}_q^{(1)}\left| j,m\right\rangle = \frac{\left\langle j',m'\right|\hat{J}_q\left| j,m\right\rangle < j \,\|\, \hat{\boldsymbol{J}} \cdot \boldsymbol{T}^{(1)} \,\|\, j >}{j(j+1)}\delta_{j,j'}. \tag{3}$$

((Proof of the theorem I))

$$M=\left\langle j',m'\right|\hat{J}_q(\hat{\boldsymbol{J}}\cdot\boldsymbol{T}^{(1)})\left| j,m\right\rangle=\sum_\mu(-1)^\mu\left\langle j',m'\right|\hat{J}_q(\hat{J}_\mu\hat{T}_{-\mu}{}^{(1)})\left| j,m\right\rangle$$

Here we use the commutation relation,

$$\hat{J}_\mu\hat{T}_{-\mu}{}^{(1)}=[\hat{J}_\mu,\hat{T}_{-\mu}{}^{(1)}]+\hat{T}_{-\mu}{}^{(1)}\hat{J}_\mu$$

Then we get

$$\begin{aligned}M&=\left\langle j',m'\right|\hat{J}_q(\hat{\boldsymbol{J}}\cdot\boldsymbol{T}^{(1)})\left| j,m\right\rangle\\&=\sum_\mu(-1)^\mu\left\langle j',m'\right|\hat{J}_q(\hat{T}_{-\mu}{}^{(1)}\hat{J}_\mu)\left| j,m\right\rangle+\sum_\mu(-1)^\mu\left\langle j',m'\right|\hat{J}_q([\hat{J}_\mu,\hat{T}_{-\mu}{}^{(1)}])\left| j,m\right\rangle\end{aligned}$$

Here we note that

$$[\hat{J}_\mu,T_q^{(k)}]=\sqrt{k(k+1)}\left\langle k,1;q,\mu\right| k,1;k,q+\mu\rangle\hat{T}_{q+\mu}^{(k)}$$

For $q=-\mu$ and $k=1$, we have

$$[\hat{J}_\mu,T_{-\mu}^{(1)}]=\sqrt{2}\left\langle 1,1;-\mu,\mu\right|1,1;k,0\rangle\hat{T}_0^{(1)}$$

Using this commutation relation, we calculate the second term defined by

$$\begin{aligned}\sum_\mu(-1)^\mu\left\langle j',m'\right|\hat{J}_q([\hat{J}_\mu,\hat{T}_{-\mu}{}^{(1)}])\left| j,m\right\rangle&=\sum_\mu(-1)^\mu\left\langle j',m'\right|\hat{J}_qT_0{}^{(1)}\left| j,m\right\rangle\left\langle 1,1;-\mu,\mu\right|1,1;1,0\mu\rangle\\&=\left\langle j',m'\right|\hat{J}_qT_0{}^{(1)}\left| j,m\right\rangle\sum_\mu(-1)^\mu\left\langle 1,1;-\mu,\mu\right|1,1;1,0\rangle=0\end{aligned}$$

(We check the final result using the Mathematica). Then we have

$$M=\sum_\mu(-1)^\mu\left\langle j',m'\right|\hat{J}_q\hat{T}_{-\mu}{}^{(1)}\hat{J}_\mu\left| j,m\right\rangle$$

We note that

$$\begin{aligned}\left\langle j',m'\right|\hat{J}_\mu\left| j,m\right\rangle&=\left\langle j,1;m,\mu\right| j,k=1;j',m'\rangle<j'\|\hat{\boldsymbol{J}}\|j>\\&=\delta_{j,j'}\delta_{m',m+\mu}\left\langle j,1;m,\mu\right| j,1;j,m+\mu\rangle<j\|\hat{\boldsymbol{J}}\|j>\\&=\delta_{j,j'}\delta_{m',m+\mu}\sqrt{j(j+1)}\left\langle j,1;m,\mu\right| j,1;j,m+\mu\rangle\end{aligned}$$

$$\langle j',m'|\hat{J}_q\hat{T}_{-\mu}{}^{(1)}\hat{J}_\mu|j,m\rangle = \langle j',m'|\hat{J}_q|j',m'-q\rangle\sum_{j'',m''}\langle j',m'-q|\hat{T}_{-\mu}{}^{(1)}|j'',m''\rangle\langle j'',m''|\hat{J}_\mu|j,m\rangle$$

$$= \langle j',m'|\hat{J}_q|j',m'-q\rangle\langle j',m'-q|\hat{T}_{-\mu}{}^{(1)}|j,m+\mu\rangle\langle j,m+\mu|\hat{J}_\mu|j,m\rangle$$

$$= \langle j',m'|\hat{J}_q|j',m'-q\rangle\langle j,m+\mu|\hat{J}_\mu|j,m\rangle\langle j',m'-q|\hat{T}_{-\mu}{}^{(1)}|j,m+\mu\rangle$$

$$= \delta_{m'm+q}\langle j',m'|\hat{J}_q|j',m'-q\rangle\langle j,m+\mu|\hat{J}_\mu|j,m\rangle\langle j',m|\hat{T}_{-\mu}{}^{(1)}|j,m+\mu\rangle$$

$$= \delta_{m'm+q}\langle j',m'|\hat{J}_q|j',m'-q\rangle\langle j,m+\mu|\hat{J}_\mu|j,m\rangle$$

$$\times < j,1;m+\mu,-\mu\,|\,j,1;j',m >< j'\|\hat{T}^{(1)}\|\,j >$$

$$= \delta_{m'm+q}\sqrt{j'(j'+1)}\sqrt{j(j+1)} < j'\|\hat{T}^{(1)}\|\,j > \langle j',1;m'-q,q|j',1;j',m'\rangle$$

$$\langle j,1;m+\mu,-\mu|j,1;j',m\rangle\langle j,1;m,\mu|j,1;j,m+\mu\rangle$$

Here we note that

$$(-1)^\mu\langle j,1;m,\mu|j,1;j,m+\mu\rangle = \langle j,1;m+\mu,-\mu|j,1;j,m\rangle$$

(see the proof of this equation below). The sum over μ is

$$\sum_\mu(-1)^\mu\langle j,1;m+\mu,-\mu|j,1;j',m\rangle\langle j,1;m,\mu|j,1;j,m+\mu\rangle = \sum_\mu\langle j,1;m+\mu,-\mu|j,1;j',m\rangle$$

$$\times\langle j,1;m+\mu,-\mu|j,1;j,m\rangle$$

$$= \delta_{j,j'}$$

(from the condition of orthogonality), where we use

$$\sum_{m_1,m_2}\langle j_1,j_2;m_1,m_2|j_1,j_2;j,m\rangle\langle j_1,j_2;m_1,m_2|j_1,j_2;j',m'\rangle = \delta_{j,j'}\delta_{m,m'}$$

$$\langle j',m'|\hat{T}_q^{(k)}|j,m\rangle = \delta_{m',m+q}\langle j,k;m,q|j,k;j',m'\rangle < j'\|\hat{T}^{(k)}\|\,j >,$$

$$\langle j',m'|\hat{J}_\mu|j,m\rangle = \delta_{j,j'}\delta_{m',m+\mu}\sqrt{j(j+1)}\langle j,1;m,\mu|j,1;j',m+\mu\rangle$$

Then

$$\langle j',m+q|\hat{J}_q\hat{T}_{-\mu}{}^{(1)}\hat{J}_\mu|j,m\rangle = [j(j+1)]\delta_{j,j'} < j'\|\hat{T}^{(1)}\|\,j > \langle j,1;m,q|j,1;j,m+q\rangle$$

Here we put

$$m' = m + q$$

we have the form such that

$$\langle j', m'|\hat{J}_q \hat{T}_{-\mu}^{(1)} \hat{J}_\mu | j, m\rangle = j(j+1)\delta_{j,j'} < j'\|\hat{T}^{(1)}\| j > \langle j,1; m,q | j,1; j',m'\rangle$$
$$= j(j+1)\delta_{j,j'} \langle j', m'|\hat{T}_q^{(1)}| j,m\rangle$$

Then we get the final result

$$\boxed{\langle j', m'|\hat{T}_q^{(1)}| j,m\rangle = \frac{\langle j',m'|\hat{J}_q(\hat{\boldsymbol{J}}\cdot \boldsymbol{T}^{(1)})| j,m\rangle}{j(j+1)}\delta_{j,j'}}$$

((**Note-1**))
Proof of

$$\langle j,1; m,\mu | j,1; j, m+\mu\rangle = (-1)^\mu \langle j,1; m+\mu, -\mu | j,1; j,m\rangle$$

$$\langle j, m+\mu|\hat{J}_\mu| j,m\rangle = \sqrt{j(j+1)}\langle j,1; m,\mu | j,1; j,m+\mu\rangle$$

When μ is changed into -μ,

$$\langle j, m-\mu|\hat{J}_{-\mu}| j,m\rangle = \sqrt{j(j+1)}\langle j,1; m,-\mu | j,1; j,m-\mu\rangle$$

When $m' = m - \mu$, or $m = m' + \mu$,

$$\langle j, m'|\hat{J}_{-\mu}| j,m'+\mu\rangle = \sqrt{j(j+1)}\langle j,1; m'+\mu,-\mu | j,1; j,m'\rangle$$

Replacing μ' into μ,

$$\langle j, m|\hat{J}_{-\mu}| j,m+\mu\rangle = \sqrt{j(j+1)}\langle j,1; m+\mu,-\mu | j,1; j,m\rangle$$

Here we note that

$$\hat{J}_\mu^{\,+} = (-1)^\mu \hat{J}_{-\mu}, \qquad \text{or} \qquad \hat{J}_{-\mu} = (-1)^\mu \hat{J}_\mu^{\,+}$$

Then we get

$$\langle j,m|\hat{J}_{-\mu}|j,m+\mu\rangle=(-1)^{\mu}\langle j,m|\hat{J}_{\mu}{}^{+}|j,m+\mu\rangle=\sqrt{j(j+1)}\langle j,1;m+\mu,-\mu|j,1;j,m\rangle$$

Then we have

$$\langle j,m|\hat{J}_{\mu}{}^{+}|j,m+\mu\rangle=\langle j,m+\mu|\hat{J}_{\mu}|j,m\rangle^{*}=(-1)^{\mu}\sqrt{j(j+1)}\langle j,1;m+\mu,-\mu|j,1;j,m\rangle$$

Since

$$\langle j,m+\mu|\hat{J}_{\mu}|j,m\rangle=\langle j,m+\mu|\hat{J}_{\mu}|j,m\rangle^{*}$$

from the definition, we finally obtain the relation

$$\langle j,m+\mu|\hat{J}_{\mu}|j,m\rangle=(-1)^{\mu}\sqrt{j(j+1)}\langle j,1;m+\mu,-\mu|j,1;j,m\rangle$$

or

$$\langle j,1;m,\mu|j,1;j,m+\mu\rangle=(-1)^{\mu}\langle j,1;m+\mu,-\mu|j,1;j,m\rangle$$

((**Note-2**))
We show that

$$\sum_{\mu}(-1)^{\mu}\langle 1,1;-\mu,\mu|1,1;1,0\rangle=0$$

using the Mathematica

((**Mathematica**)) We use the Mathematica to calculate the Clebsch-Gordan coefficient.

```
Clear["Global`*"];

ClebschGordan[{1, -1}, {1, 1}, {1, 0}]
```

$-\frac{1}{\sqrt{2}}$

```
ClebschGordan[{1, 1}, {1, -1}, {1, 0}]
```

$\frac{1}{\sqrt{2}}$

```
ClebschGordan[{1, 0}, {1, 0}, {1, 0}]
```

0

```
Sum[(-1)^μ ClebschGordan[{1, -μ}, {1, μ}, {1, 0}], {μ, -1, 1, 1}]
```

0

((**Proof of the theorem II**)

$$\langle j',m'|\hat{J}_q(\hat{\boldsymbol{J}}\cdot\boldsymbol{T}^{(1)})|j,m\rangle = \sum_{j'',m''}\langle j',m'|\hat{J}_q|j'',m''\rangle\langle j'',m''|\hat{\boldsymbol{J}}\cdot\boldsymbol{T}^{(1)}|j,m\rangle$$

We use the fact that $\hat{\boldsymbol{J}}\cdot\boldsymbol{T}^{(1)}$ is a zero-rank tensor and

$$\langle j'',m''|\hat{\boldsymbol{J}}\cdot\boldsymbol{T}^{(1)}|j,m\rangle = \delta_{j'',j}\delta_{m'',m} < j\,\|\hat{\boldsymbol{J}}\cdot\boldsymbol{T}^{(1)}\|\,j >$$

Then we have

$$\begin{aligned}\langle j',m'|\hat{J}_q(\hat{\boldsymbol{J}}\cdot\boldsymbol{T}^{(1)})|j,m\rangle &= \sum_{j'',m''}\langle j',m'|\hat{J}_q|j'',m''\rangle\delta_{j'',j}\delta_{m'',m} < j\,\|\hat{\boldsymbol{J}}\cdot\boldsymbol{T}^{(1)}\|\,j > \\ &= \langle j',m'|\hat{J}_q|j,m\rangle < j\,\|\hat{\boldsymbol{J}}\cdot\boldsymbol{T}^{(1)}\|\,j >\end{aligned}$$

((Proof of the theorem III))

$$\begin{aligned}\langle j',m'|\hat{T}_q^{(1)}|j,m\rangle &= \frac{\langle j',m'|\hat{J}_q(\hat{\boldsymbol{J}}\cdot\boldsymbol{T}^{(1)})|j,m\rangle}{j(j+1)}\delta_{j,j'} \\ &= \frac{\langle j',m'|\hat{J}_q|j,m\rangle < j\,\|\hat{\boldsymbol{J}}\cdot\boldsymbol{T}^{(1)}\|\,j >}{j(j+1)}\delta_{j,j'}\end{aligned}$$

---

16 Calculation of the reduced matrix $\langle j' \| \hat{\boldsymbol{J}}^2 \| j \rangle$

In the projection theorem

$$\langle j',m'|\hat{T}_q^{(1)}|j,m\rangle = \frac{\langle j',m'|\hat{J}_q|j,m\rangle < j \| \hat{\boldsymbol{J}}\cdot\boldsymbol{T}^{(1)} \| j >}{j(j+1)}\delta_{j,j'}$$

we put

$$\hat{T}_q^{(1)} = \hat{J}_q$$

Then we get

$$\langle j',m'|\hat{J}_q^{(1)}|j,m\rangle = \frac{\langle j',m'|\hat{J}_q|j,m\rangle < j \| \hat{\boldsymbol{J}}^2 \| j >}{j(j+1)}\delta_{j,j'}$$

or

$$< j' \| \hat{\boldsymbol{J}}^2 \| j >= \delta_{j,j'} j(j+1)$$

---

16 Calculation of the reduced matrix $\langle j \| \hat{\boldsymbol{J}} \| j \rangle$

In the Wigner-Eckart theorem,

$$\langle j,m'|\hat{T}_q^{(k=1)}|j,m\rangle = \langle j,k=1;m,q|j,k=1;j,m'\rangle\langle j\|\hat{T}^{(k=1)}\|j\rangle$$

we put

$$\hat{T}_q^{(k=1)} = \hat{J}_q$$

Then we get

$$\langle j,m'|\hat{J}_0|j,m\rangle = \langle j,k=1;m,q=0|j,k=1;j,m'\rangle\langle j\|\hat{\boldsymbol{J}}\|j\rangle$$

for $q = 0$. Here we note that

$$\langle j',m'|\hat{J}_0|j,m\rangle = m\hbar\delta_{m'm'}\delta_{j,j'}$$

$$\langle j,k=1;m,q=0|j,k=1;j,m'\rangle = \frac{m}{\sqrt{j(j+1)}}\delta_{m,m'}$$

Then we have

$$1 = \frac{1}{\sqrt{j(j+1)}} \langle j \| \hat{\boldsymbol{J}} \| j \rangle$$

or

$$\boxed{\langle j \| \hat{\boldsymbol{J}} \| j \rangle = \sqrt{j(j+1)}}$$

((**Proof**))

The proof of the formula

$$\langle j, k=1; m, q=0 | j, k=1; j, m \rangle = \frac{m}{\sqrt{j(j+1)}}$$

is given by Mathematica as follows.

((**Mathematica**))

```
Clear["Global`*"]; CCGG[{j1_, m1_}, {j2_, m2_}, {j_, m_}] :=
 Module[{s1},
  s1 = If[Abs[m1] ≤ j1 && Abs[m2] ≤ j2 && Abs[m] ≤ j,
    ClebschGordan[{j1, m1}, {j2, m2}, {j, m}], 0]];

j1 = 1;

Table[{m1, CCGG[{j1, m1}, {1, 0}, {j1, m1}], m1/Sqrt[j1 (j1 + 1)]}, {m1, j1, -j1, -1}]
```

$\left\{\left\{1, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right\}, \{0, 0, 0\}, \left\{-1, -\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}\right\}\right\}$

```
j1 = 2;

Table[{m1, CCGG[{j1, m1}, {1, 0}, {j1, m1}], m1/Sqrt[j1 (j1 + 1)]}, {m1, j1, -j1, -1}]
```

$\left\{\left\{2, \sqrt{\frac{2}{3}}, \sqrt{\frac{2}{3}}\right\}, \left\{1, \frac{1}{\sqrt{6}}, \frac{1}{\sqrt{6}}\right\}, \{0, 0, 0\}, \left\{-1, -\frac{1}{\sqrt{6}}, -\frac{1}{\sqrt{6}}\right\}, \left\{-2, -\sqrt{\frac{2}{3}}, -\sqrt{\frac{2}{3}}\right\}\right\}$

```
j1 = 3;

Table[{m1, CCGG[{j1, m1}, {1, 0}, {j1, m1}], m1/Sqrt[j1 (j1 + 1)]}, {m1, j1, -j1, -1}]
```

$\left\{\left\{3, \frac{\sqrt{3}}{2}, \frac{\sqrt{3}}{2}\right\}, \left\{2, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right\}, \left\{1, \frac{1}{2\sqrt{3}}, \frac{1}{2\sqrt{3}}\right\}, \{0, 0, 0\},$
$\left\{-1, -\frac{1}{2\sqrt{3}}, -\frac{1}{2\sqrt{3}}\right\}, \left\{-2, -\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}\right\}, \left\{-3, -\frac{\sqrt{3}}{2}, -\frac{\sqrt{3}}{2}\right\}\right\}$

18. Landè g-factor

The magnetic moment is defined by

$$\hat{\boldsymbol{\mu}} = -\frac{\mu_B}{\hbar}(\hat{\boldsymbol{L}} + 2\hat{\boldsymbol{S}})$$

The total angular momentum is

$$\hat{\boldsymbol{J}} = \hat{\boldsymbol{L}} + \hat{\boldsymbol{S}}$$

The expectation value of the *m*-th component of the magnetic moment m can be obtained from the projection theorem (decomposition theorem of the second kind, see Rose),

$$\langle j,m|\hat{\mu}_q|j,m\rangle = \frac{< j \| \hat{\boldsymbol{J}}\cdot\hat{\boldsymbol{\mu}} \| j >}{\hbar^2 j(j+1)}\langle j,m|\hat{J}_q|; j,m\rangle$$

Now we have

$$\hat{\boldsymbol{\mu}}\cdot\hat{\boldsymbol{J}} = -\frac{\mu_B}{\hbar}(\hat{\boldsymbol{L}} + 2\hat{\boldsymbol{S}})\cdot(\hat{\boldsymbol{L}} + \hat{\boldsymbol{S}}) = -\frac{\mu_B}{\hbar}(\hat{\boldsymbol{L}}^2 + 2\hat{\boldsymbol{S}}^2 + 3\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}})\cdot$$

and

$$\hat{\boldsymbol{J}}^2 = \hat{\boldsymbol{L}}^2 + \hat{\boldsymbol{S}}^2 + 2\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}$$

or

$$\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}} = \frac{\hat{\boldsymbol{J}}^2 - \hat{\boldsymbol{L}}^2 - \hat{\boldsymbol{S}}^2}{2}$$

Then we get

$$\hat{\boldsymbol{\mu}}\cdot\hat{\boldsymbol{J}} = \hat{\boldsymbol{J}}\cdot\hat{\boldsymbol{\mu}}\cdot = -\frac{\mu_B}{\hbar}[\hat{\boldsymbol{L}}^2 + 2\hat{\boldsymbol{S}}^2 + \frac{3}{2}(\hat{\boldsymbol{J}}^2 - \hat{\boldsymbol{L}}^2 - \hat{\boldsymbol{S}}^2)]\cdot$$

and

$$< j \| \hat{\boldsymbol{J}}\cdot\hat{\boldsymbol{\mu}} \| j >= -\frac{\mu_B}{\hbar}\hbar^2\{l(l+1) + 2s(s+1) + \frac{3}{2}[(j(j+1) - l(l+1) - s(s+1)]\}$$

Then the expectation value of the magnetic moment along the *z* axis is

$$\langle j,m|\hat{\mu}_0|j,m\rangle = \frac{<j\|\hat{\boldsymbol{J}}\cdot\hat{\boldsymbol{\mu}}\|j>}{\hbar^2 j(j+1)}\langle j,m|\hat{J}_0|j,m\rangle$$
$$= -\frac{\mu_B}{\hbar}\frac{m\hbar}{\hbar^2 j(j+1)}\hbar^2\{l(l+1)+2s(s+1)$$
$$+\frac{3}{2}[(j(j+1)-l(l+1)-s(s+1)]\}$$
$$= -\frac{m\mu_B}{2j(j+1)}[3(j(j+1)-l(l+1)+s(s+1)]$$

since $|j,m\rangle$ is a joint eigenstate of $\hat{\boldsymbol{J}}^2$, $\hat{\boldsymbol{L}}^2$, $\hat{\boldsymbol{S}}^2$, and $\hat{J}_0 = \hat{J}_z$ with eigenvalues $\hbar^2 j(j+1)$, $\hbar^2 l(l+1)$, $\hbar^2 s(s+1)$, and $\hbar m$, respectively.

Here we introduce the Landè g-factor as

$$\hat{\boldsymbol{\mu}} = -\frac{g_J\mu_B}{\hbar}\hat{\boldsymbol{J}}$$

Then we have

$$\langle j,m|\hat{\mu}_0|j,m\rangle = -\frac{g_J\mu_B}{\hbar}\langle j,m|\hat{J}_0|j,m\rangle = -\frac{g_J\mu_B}{\hbar}m\hbar = -mg_J\mu_B$$

and

$$g_J = \frac{3}{2} + \frac{s(s+1)-l(l+1)}{2j(j+1)}$$

19. The expectation value of S_z

Since

$$\hat{\boldsymbol{S}}\cdot\hat{\boldsymbol{J}}\cdot = \hat{\boldsymbol{S}}\cdot(\hat{\boldsymbol{L}}+\hat{\boldsymbol{S}}) = \hat{\boldsymbol{S}}^2 + \hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}} = \hat{\boldsymbol{S}}^2 + \frac{\hat{\boldsymbol{J}}^2-\hat{\boldsymbol{L}}^2-\hat{\boldsymbol{S}}^2}{2} = \frac{\hat{\boldsymbol{J}}^2-\hat{\boldsymbol{L}}^2+\hat{\boldsymbol{S}}^2}{2}$$

we get the expectation of S_z as

$$\left\langle j,m\left|\hat{S}_0\right|j,m\right\rangle = \frac{\left\langle j,m\right| < j\,\|\,\hat{\boldsymbol{J}}\cdot\hat{\boldsymbol{S}}\,\|\,j > \left|j,m\right\rangle}{\hbar^2 j(j+1)}\left\langle j,m\left|\hat{J}_0\right|;j,m\right\rangle$$
$$= \frac{m\hbar}{2\hbar^2 j(j+1)}\hbar^2[j(j+1)-l(l+1)+s(s+1)]$$
$$= \frac{m\hbar}{2}[1+\frac{s(s+1)-l(l+1)}{j(j+1)}]$$

where we use the projection theorem.

20. Spin-orbit interaction: example of equivalent operators

The idea of operator equivalents finds applications in many branches of physics. As one of typical examples, we consider the effect of the spin-orbit interaction.

$$H_{SO} = \sum_{i=1}^{N}\xi(\boldsymbol{r}_i)\hat{\boldsymbol{l}}_i\cdot\hat{\boldsymbol{s}}_i = \lambda\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}$$

where λ is the spin-orbit interaction constant. We use the equivalent operator

$$\left\langle j,m'\left|\hat{T}_q^{(1)}\right|j,m\right\rangle = \frac{\left\langle J,m'\left|\hat{J}_q\right|J,m\right\rangle}{\sqrt{j(j+1)}} < j\,\|\,\hat{T}^{(1)}\,\|\,j >$$

for the rank-1 tensor (vector): operator equivalents.

$$\left\langle LM_L';SM_S'\left|\xi(\boldsymbol{r}_i)\hat{\boldsymbol{l}}_i\cdot\hat{\boldsymbol{s}}_i\right|LM_L;S,M_S\right\rangle = [[\left\langle LM_L'\left|\hat{\boldsymbol{L}}\right|LM_L\right\rangle\frac{< L\,\|\,\xi(\boldsymbol{r}_i)\hat{\boldsymbol{l}}\,\|\,L >}{\sqrt{L(L+1)}}]\cdot[\left\langle SM_s'\left|\boldsymbol{S}\right|SM_s\right\rangle\frac{< S\,\|\,\hat{\boldsymbol{s}}_i\,\|\,S >}{\sqrt{S(S+1)}}]$$
$$= \left\langle L\left\|\xi(\boldsymbol{r}_i)\hat{\boldsymbol{l}}\right\|L\right\rangle\left\langle S\left\|\hat{\boldsymbol{s}}_i\right\|S\right\rangle\frac{\left\langle LM_L'\left|\hat{\boldsymbol{L}}\right|LM_L\right\rangle}{\sqrt{L(L+1)}}\cdot\frac{\left\langle SM_s'\left|\boldsymbol{S}\right|SM_s\right\rangle}{\sqrt{S(S+1)}}$$

If we sum over all the electrons (i) , we get

$$\left\langle LM_L';SM_S'\left|H_{SO}\right|LM_L;S,M_S\right\rangle = \left\langle LM_L';SM_S'\left|\sum_i\xi(\boldsymbol{r}_i)\hat{\boldsymbol{l}}_i\cdot\hat{\boldsymbol{s}}_i\right|LM_L;S,M_S\right\rangle$$
$$= \sum_i\left\langle L\left\|\xi(\boldsymbol{r}_i)\hat{\boldsymbol{l}}\right\|L\right\rangle\left\langle S\left\|\hat{\boldsymbol{s}}_i\right\|S\right\rangle\frac{\left\langle LM_L'\left|\hat{\boldsymbol{L}}\right|LM_L\right\rangle}{\sqrt{L(L+1)}}\cdot\frac{\left\langle SM_s'\left|\boldsymbol{S}\right|SM_s\right\rangle}{\sqrt{S(S+1)}}$$

Noting that

$$\langle LM_L';SM_S'|H_{SO}|LM_L;S,M_S\rangle = \langle LM_L';SM_S'|\lambda\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}}|LM_L;S,M_S\rangle$$
$$= \lambda\langle LM_L'|\hat{\boldsymbol{L}}|LM_L\rangle\cdot\langle SM_s'|\hat{\boldsymbol{S}}|SM_s\rangle$$

Then we have

$$\lambda\langle LM_L'|\hat{\boldsymbol{L}}|LM_L\rangle\cdot\langle SM_s'|\hat{\boldsymbol{S}}|SM_s\rangle = \sum_i \langle L\|\xi(\boldsymbol{r}_i)\hat{\boldsymbol{l}}\|L\rangle\langle S\|\hat{\boldsymbol{s}}_i\|S\rangle$$
$$\times\frac{\langle LM_L'|\hat{\boldsymbol{L}}|LM_L\rangle}{\sqrt{L(L+1)}}\cdot\frac{\langle SM_s'|\boldsymbol{S}|SM_s\rangle}{\sqrt{S(S+1)}}$$

or

$$\lambda = \sum_i \frac{\langle L\|\xi(\boldsymbol{r}_i)\hat{\boldsymbol{l}}\|L\rangle\langle S\|\hat{\boldsymbol{s}}_i\|S\rangle}{\sqrt{L(L+1)}\sqrt{S(S+1)}}$$

20. Magnetic form factor

Here we use the projection theorem,

$$\langle j',m'|\hat{\boldsymbol{V}}_q|j,m\rangle = \langle j',m'|\hat{\boldsymbol{J}}_q|j,m'\rangle\frac{< j\|\hat{\boldsymbol{J}}\cdot\hat{\boldsymbol{V}}\|j>}{\hbar^2 j(j+1)}$$

where $\hat{\boldsymbol{J}}\cdot\hat{\boldsymbol{V}}$ is a scalar so its expectation value is independent of *m*.

$$\hat{\boldsymbol{V}} = \sum_\nu e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_\nu}\hat{\boldsymbol{s}}_\nu = \sum_\nu f_\nu\hat{\boldsymbol{s}}_\nu \qquad\qquad \hat{\boldsymbol{J}} = \hat{\boldsymbol{S}}_{ld} = \sum_\nu \hat{\boldsymbol{s}}_\nu$$

where the atom site is denoted by $j = \{l, d\}$, and $\boldsymbol{\nu}$ is the vector connecting atom at the site $\{l, d\}$ and electrons surrounding the nucleus. We also put

$$f_\nu = e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_\nu},$$

for the simplicity. $\boldsymbol{\kappa}$ is the wave vector. $\hat{\boldsymbol{S}}_{ld}$ is the resultant spin determined from the Hund rule. Then we get

$$\hat{\boldsymbol{J}}\cdot\hat{\boldsymbol{V}} = \left(\sum_\nu f_\nu\hat{\boldsymbol{s}}_\nu\right)\cdot\boldsymbol{S}_{ld} = \boldsymbol{S}_{ld}\cdot\left(\sum_\nu f_\nu\hat{\boldsymbol{s}}_\nu\right).$$

Here we use the projection theorem,

$$\langle \lambda' | \sum_\nu f_\nu \hat{\boldsymbol{s}}_\nu | \lambda \rangle = \langle \lambda' | \hat{\boldsymbol{S}}_{ld} | \lambda \rangle \frac{< \lambda \| \boldsymbol{S}_{ld} \cdot \sum_\nu f_\nu \hat{\boldsymbol{s}}_\nu \| \lambda >}{\hbar^2 S(S+1)} \tag{1}$$
$$= F_d(\boldsymbol{\kappa}) \langle \lambda' | \hat{\boldsymbol{S}}_{ld} | \lambda \rangle$$

where

$$F_d(\boldsymbol{\kappa}) = \frac{< \lambda \| \boldsymbol{S}_{ld} \cdot \sum_\nu f_\nu \hat{\boldsymbol{s}}_\nu \| \lambda >}{\hbar^2 S(S+1)}$$

is called the magnetic form factor. It is obtained by the Fourier transform of the normalized spin density at the site j (or denoted by l, d).

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21. Quadrupole interaction

Using the Wigner-Eckart thorem, we get

$$\langle j, m' | \hat{Q}_q^{(k=2)} | j, m \rangle = \langle j, k=2; m, q | j, k=2; j, m' \rangle \langle j \| \hat{Q}^{(k=2)} \| j \rangle$$

for $\hat{T}_q^{(k=2)} = \hat{Q}_q^{(k=2)}$ (spherical tensor of rank-2)

and

$$\langle j, m' | \hat{Q}_{q=0}^{(k=2)} | j, m \rangle = \langle j, k=2; m, q=0 | j, k=2; j, m' \rangle \langle j \| \hat{Q}^{(k=2)} \| j \rangle$$

In this last equation we put $m' = j$ and $m = j$

$$\langle j, m' = j | \hat{Q}_{q=0}^{(k=2)} | j, m = j \rangle = \langle j, k=2; m=j, q=0 | j, k=2; j, m' = j \rangle \langle j \| \hat{Q}^{(k=2)} \| j \rangle$$

Then we get

$$\langle j \| \hat{Q}^{(k=2)} \| j \rangle = \frac{\langle j, m' = j | \hat{Q}_{q=0}^{(k=2)} | j, m = j \rangle}{\langle j, k=2; m=j, q=0 | j, k=2; j, m' = j \rangle} =$$

Using this relation, we have

$$\langle j, m' | \hat{Q}_q^{(k=2)} | j, m \rangle = \frac{\langle j, k=2; m, q | j, k=2; j, m' \rangle \langle j, m'=j | \hat{Q}_{q=0}^{(k=2)} | j, m=j \rangle}{\langle j, k=2; m=j, q=0 | j, k=2; j, m'=j \rangle}$$
$$= \frac{1}{2} eQ \frac{\langle j, k=2; m, q | j, k=2; j, m' \rangle}{\langle j, k=2; m=j, q=0 | j, k=2; j, m'=j \rangle}$$

where we define

$$\langle j, m'=j | \hat{Q}_{q=0}^{(k=2)} | j, m=j \rangle = \frac{1}{2} eQ$$

APPENDIX

1. Orthogonality condition

The CG coefficients form an unitary matrix. Furthermore, the matrix elements are taken to be real by convention. A real unitary matrix is orthogonal. We have the orthogonal condition.

$$\langle j_1, j_2, j, m | j_1, j_2, m_1, m_2 \rangle = \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \rangle^* = \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \rangle$$

Closure relation

$$\langle j_1, j_2; m_1, m_2 | j_1, j_2; m_1', m_2' \rangle = \sum_{j,m} \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \rangle \langle j_1, j_2; j, m | j_1, j_2; m_1', m_2' \rangle$$
$$= \sum_{j,m} \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \rangle \langle j_1, j_2; m_1', m_2' | j_1, j_2; j, m \rangle$$
$$= \delta_{m_1, m_1'} \delta_{m_2, m_2'}$$

or

$$\sum_{j,m} \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \rangle \langle j_1, j_2; m_1', m_2' | j_1, j_2; j, m \rangle = \delta_{m_1, m_1'} \delta_{m_2, m_2'}$$

Similarly,

$$\langle j_1, j_2; j, m | j_1, j_2; j', m' \rangle = \sum_{j,m} \langle j_1, j_2; j, m | j_1, j_2; m_1, m_2 \rangle \langle j_1, j_2; m_1, m_2 | j_1, j_2; j', m' \rangle$$
$$= \sum_{j,m} \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \rangle \langle j_1, j_2; m_1, m_2 | j_1, j_2; j', m' \rangle$$
$$= \delta_{j,j'} \delta_{m,m'}$$

or

$$\sum_{m_1,m_2} \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \rangle \langle j_1, j_2; m_1, m_2 | j_1, j_2; j', m' \rangle = \delta_{j,j'} \delta_{m,m'}$$

As a special case of this, we may set $j = j'$, $m' = m = m_1 + m_2$.

$$\sum_{\substack{m_1,m_2 \\ m=m_1+m_2}} \left| \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \rangle \right|^2 = 1$$

which is just the normalization condition of $| j_1, j_2; j, m \rangle$.

2. Clebsch-Gordon series

$$D^{(k_1)}_{q_1'q_1}(\hat{R}) D^{(k_2)}_{q_2'q_2}(\hat{R}) = \sum_{k''q''q'} \langle k_1, k_2; q_1', q_2' | k_1, k_2; k'', q' \rangle \langle k_1, k_2; q_1, q_2 | k_1, k_2; k'', q' \rangle D^{(k'')}_{q'q''}(\hat{R})$$

((**proof**)) Sakurai Modern Quantum Mechanics

$$D^{(j_1)}_{m_1m_1'}(\hat{R}) D^{(j_2)}_{m_2m_2'}(\hat{R}) = \sum_{j,m,m''} \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \rangle \langle j_1, j_2; m_1', m_2' | j_1, j_2; j, m' \rangle D^{(j)}_{mm'}(\hat{R}) \quad (1)$$

We start with the notation given by

$$D_{j_1} \times D_{j_2} = D_{j_1+j_2} + D_{j_1+j_2-1} + ... + D_{|j_1-j_2|}$$

This means that a similarity transformation must exist which reduces $D_{j_1} \times D_{j_2}$ to the block form

$$\begin{pmatrix} D_{|j_1-j_2|}(\hat{R}) & 0 & \cdots & 0 & 0 \\ 0 & D_{|j_1-j_2|+1}(\hat{R}) & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & D_{|j_1+j_2-1}(\hat{R}) & 0 \\ 0 & 0 & \cdots & 0 & D_{j_1+j_2}(\hat{R}) \end{pmatrix}$$

First we note that the left-hand side of Eq.(1) is the same as

$$\langle j_1, j_2; m_1, m_2 | \hat{R} | j_1, j_2; m_1', m_2' \rangle = \langle j_1, m_1 | \hat{R} | j_1, m_1' \rangle \langle j_2, m_2 | \hat{R} | j_2, m_2' \rangle = D^{(j_1)}_{m_1m_1'}(\hat{R}) D^{(j_2)}_{m_2m_2'}(\hat{R})$$

((Note)) This expression can be understood from the following consideration.

$$\hat{R}(\theta)=\hat{R}_y(\theta)=\exp(-\frac{i}{\hbar}\theta\hat{J}_y)=\exp[-\frac{i}{\hbar}\theta(\hat{J}_{1y}+\hat{J}_{2y})]=\exp(-\frac{i}{\hbar}\theta\hat{J}_{1y})\exp(-\frac{i}{\hbar}\theta\hat{J}_{2y})$$

$$\begin{aligned}&\langle j_1,j_2;m_1,m_2|\exp(-\frac{i}{\hbar}\theta\hat{J}_{1y})\exp(-\frac{i}{\hbar}\theta\hat{J}_{2y})|j_1,j_2;m_1',m_2'\rangle\\&=\langle j_1,m_1|\exp(-\frac{i}{\hbar}\theta\hat{J}_{1y})|j_1,m_1'\rangle\langle j_2,m_2|\exp(-\frac{i}{\hbar}\theta\hat{J}_{2y})|j_2,m_2'\rangle\\&=D^{(j_1)}_{m_1m_1'}(\theta)D^{(j_2)}_{m_2m_2'}(\theta)=D^{(j_1)}_{m_1m_1'}(\hat{R})D^{(j_2)}_{m_2m_2'}(\hat{R})\end{aligned}$$

This matrix element can be also calculated as

$$\begin{aligned}\langle j_1,j_2;m_1,m_2|\hat{R}|j_1,j_2;m_1',m_2'\rangle&=\sum_{j,m,j,m'}\langle j_1,j_2;m_1,m_2|j_1,j_2;j,m\rangle\langle j_1,j_2;j,m|\hat{R}|j_1,j_2;j',m'\rangle\\&\quad\times\langle j_1,j_2;j'm'|j_1,j_2;m_1'm_2'\rangle\\&=\sum_{j,m,j,m'}\langle j_1,j_2;m_1,m_2|j_1,j_2;j,m\rangle D^{(j)}_{mm'}(\hat{R})\delta_{j,j'}\\&\quad\times\langle j_1,j_2;j'm'|j_1,j_2;m_1'm_2'\rangle\\&=\sum_{j,m,m'}\langle j_1,j_2;m_1,m_2|j_1,j_2;j,m\rangle\langle j_1,j_2;j,m'|j_1,j_2;m_1'm_2'\rangle D^{(j)}_{mm'}(\hat{R})\\&=\sum_{j,m,m'}\langle j_1,j_2;m_1,m_2|j_1,j_2;j,m\rangle\langle j_1,j_2;m_1'm_2'|j_1,j_2;j,m\rangle D^{(j)}_{mm'}(\hat{R})\end{aligned}$$

using the closure relations. Note that all the Clebsch-Gordon coefficients are real.

3. Formula for tensor product

We define

$$\hat{T}^{(k)}(1)\cdot\hat{T}^{(k)}(2)=\sum_q(-1)^q\hat{T}_q^{(k)}(1)\hat{T}_{-q}^{(k)}(2)$$

which represents an interaction between two independent subsystems 1 and 2. Here we discuss the matrix element of the type

$$\langle j_1',j_2';j'm'|\hat{T}^{(k)}(1)\cdot\hat{T}^{(k)}(2)|j_1,j_2;jm\rangle$$

where $\hat{T}^{(k)}(1)$ is the tensor operator of the rank *k* for the subsystem 1 and $\hat{T}^{(k)}(2)$ is the tensor operator of the rank *k* for the subsystem 2. Here we note that

$$\left| j_1, j_2; j, m \right\rangle = \sum_{m_1, m_2} \left| j_1, j_2; m_1, m_2 \right\rangle \left\langle j_1, j_2; m_1, m_2 \,\middle|\, j_1, j_2; j, m \right\rangle$$

and

$$\left| j_1', j_2'; j', m' \right\rangle = \sum_{m_1', m_2'} \left| j_1', j_2'; m_1', m_2' \right\rangle \left\langle j_1', j_2'; m_1', m_2' \,\middle|\, j_1', j_2'; j', m' \right\rangle$$

By using these, the matrix elements becomes

$$\left\langle j_1', j_2'; j'm' \middle| \hat{T}^{(k)}(1) \cdot \hat{T}^{(k)}(2) \middle| j_1, j_2; jm \right\rangle = \sum_{\substack{q, m_1', m_2' \\ m_1, m_2}} (-1)^q \left\langle j_1', j_2'; m_1', m_2' \,\middle|\, j_1', j_2'; j', m' \right\rangle^* \left\langle j_1, j_2; m_1, m_2 \,\middle|\, j_1, j_2; j, m \right\rangle$$
$$\times \left\langle j_1', j_2'; m_1', m_2' \middle| \hat{T}_q^{(k)}(1) \hat{T}_{-q}^{(k)}(2) \middle| j_1, j_2; m_1, m_2 \right\rangle$$

Here we have

$$\left\langle j_1', j_2'; m_1', m_2' \middle| \hat{T}_q^{(k)}(1) \hat{T}_{-q}^{(k)}(2) \middle| j_1, j_2; m_1, m_2 \right\rangle = \left\langle j_1', m_1' \middle| \hat{T}_q^{(k)}(1) \middle| j_1, m_1 \right\rangle \left\langle j_2', m_2' \middle| \hat{T}_{-q}^{(k)}(2) \middle| j_2, m_2 \right\rangle$$

since two factors operate in separate decoupled systems. According to the Wigner-Eckart theorem,

$$\left\langle j_1', m_1' \middle| \hat{T}_q^{(k)}(1) \middle| j_1, m_1 \right\rangle = \left\langle j_1, k; m_1, q \,\middle|\, j_1, k; j_1', m_1' \right\rangle < j_1' \| \hat{T}^{(k)}(1) \| j_1 >$$

$$\left\langle j_2', m_2' \middle| \hat{T}_{-q}^{(k)}(2) \middle| j_2, m_2 \right\rangle = \left\langle j_2, k; m_2, -q \,\middle|\, j_2, k; j_2', m_2' \right\rangle < j_2' \| \hat{T}^{(k)}(1) \| j_2 >$$

Then we get

$$\left\langle j_1', j_2'; m_1', m_2' \middle| \hat{T}_q^{(k)}(1) \hat{T}_q^{(k)}(2) \middle| j_1, j_2; m_1, m_2 \right\rangle = \left\langle j_1, k; m_1, q \,\middle|\, j_1, k; j_1', m_1' \right\rangle \left\langle j_2, k; m_2, -q \,\middle|\, j_2, k; j_2', m_2' \right\rangle$$
$$< j_1' \| \hat{T}^{(k)}(1) \| j_1 >< j_2' \| \hat{T}^{(k)}(2) \| j_2 >$$

Using this relation, we have

$$\frac{\left\langle j_1', j_2'; j', m' \middle| \hat{T}_q^{(k)}(1)\hat{T}_{-q}^{(k)}(2) \middle| j_1, j_2; j, m \right\rangle}{< j_1' \| \hat{T}^{(k)}(1) \| j_1 >< j_2' \| \hat{T}^{(k)}(2) \| j_2 >} = \sum_{\substack{m_1', m_2' \\ m_1, m_2}} \left\langle j_1', j_2'; m_1', m_2' \middle| j_1', j_2'; j', m' \right\rangle^* \left\langle j_1, j_2; m_1, m_2 \middle| j_1, j_2; j, m \right\rangle$$

$$\times \left\langle j_1, k; m_1, q \middle| j_1, k; j_1', m_1' \right\rangle \left\langle j_2, k; m_2, -q \middle| j_2, k; j_2', m_2' \right\rangle$$

$$= \sum_{\substack{m_1', m_2' \\ m_1, m_2}} \left\langle j_1', j_2'; j', m' \middle| j_1', j_2'; m_1', m_2' \right\rangle \left\langle j_1, j_2; m_1, m_2 \middle| j_1, j_2; j, m \right\rangle$$

$$\times \left\langle j_1, k; m_1, q \middle| j_1, k; j_1', m_1' \right\rangle \left\langle j_2, k; m_2, -q \middle| j_2, k; j_2', m_2' \right\rangle$$

since

$$\left\langle j_1, j_2; m_1, m_2 \middle| j_1, j_2; j', m' \right\rangle^* = \left\langle j_1, j_2; j', m' \middle| j_1, j_2; m_1, m_2 \right\rangle$$

$$\frac{\left\langle j_1', j_2'; j', m' \middle| \hat{T}^{(k)}(1) \cdot \hat{T}^{(k)}(2) \middle| j_1, j_2; j, m \right\rangle}{< j_1' \| \hat{T}^{(k)}(1) \| j_1 >< j_2' \| \hat{T}^{(k)}(2) \| j_2 >} = \sum_{\substack{q, m_1', m_2' \\ m_1, m_2}} (-1)^q \left\langle j_1', j_2'; m_1', m_2' \middle| j_1', j_2'; j', m' \right\rangle^* \left\langle j_1, j_2; m_1, m_2 \middle| j_1, j_2; j, m \right\rangle$$

$$\times \left\langle j_1, k; m_1, q \middle| j_1, k; j_1', m_1' \right\rangle \left\langle j_2, k; m_2, -q \middle| j_2, k; j_2', m_2' \right\rangle$$

$$= \delta_{m,m'} \sum_{m_1, m_1'} (-1)^{m_1' - m_1} \left\langle j_1', j_2'; m_1', m' - m_1' \middle| j_1', j_2'; j', m' \right\rangle$$

$$\times \left\langle j_1, j_2; m_1, m - m_1 \middle| j_1, j_2; j, m \right\rangle \left\langle j_1, k; m_1, m_1' - m_1 \middle| j_1, k; j_1', m_1' \right\rangle$$

$$\times \left\langle j_2, k; m - m_1, m_1 - m_1' \middle| j_2, k; j_2', m - m_1' \right\rangle$$

We may also apply the Wigner-Eckart theorem to the entire matrix element

$$\left\langle j' m' \middle| \hat{T}^{(k)}(1) \cdot \hat{T}^{(k)}(2) \middle| j, m \right\rangle = \delta_{m,m'} \delta_{j,j'} \left\langle j, k = 0; m, q = 0 \middle| j, k = 0; j, m \right\rangle$$

$$< j \| \hat{T}^{(k)}(1) \cdot \hat{T}^{(k)}(2) \| j >$$

$$= \delta_{m,m'} \delta_{j,j'} < j \| \hat{T}^{(k)}(1) \cdot \hat{T}^{(k)}(2) \| j >$$

where

$$\left\langle j, k = 0; m, q = 0 \middle| j, k = 0; j, m \right\rangle = 1 .$$

Using the above two equations, we get

$$
\begin{aligned}
\left\langle j_1', j_2'; j'm' \middle| \hat{T}^{(k)}(1)\cdot\hat{T}^{(k)}(2) \middle| j_1, j_2; j, m \right\rangle &= \delta_{m,m'}\delta_{j,j'} < j_1' \| \hat{T}^{(k)}(1) \| j_1 >< j_2' \| \hat{T}^{(k)}(2) \| j_2 > \\
&\quad \sum_{m_1, m_1'} (-1)^{m_1'-m_1} \left\langle j_1', j_2'; m_1', m'-m_1' \middle| j_1', j_2'; j', m' \right\rangle \\
&\quad \times \left\langle j_1, j_2; m_1, m-m_1 \middle| j_1, j_2; j, m \right\rangle \left\langle j_1, k; m_1, m_1'-m_1 \middle| j_1, k; j_1', m_1' \right\rangle \\
&\quad \times \left\langle j_2, k; m-m_1, m_1 - m_1' \middle| j_2, k; j_2', m-m_1' \right\rangle \\
&= \delta_{m,m'}\delta_{j,j'} < j_1' \| \hat{T}^{(k)}(1) \| j_1 >< j_2' \| \hat{T}^{(k)}(2) \| j_2 > \\
&\quad \sum_{m_1, m_1'} (-1)^{m_1'-m_1} \left\langle j_1', j_2'; m_1', m'-m_1' \middle| j_1', j_2'; j', m' \right\rangle \\
&\quad \times \left\langle j_1, j_2; m_1, m-m_1 \middle| j_1, j_2; j, m \right\rangle \left\langle j_1, k; m_1, m_1'-m_1 \middle| j_1, k; j_1', m_1' \right\rangle \\
&\quad \times \left\langle j_2, k; m-m_1, m_1 - m_1' \middle| j_2, k; j_2', m-m_1' \right\rangle \\
&= \delta_{m,m'}\delta_{j,j'} (-1)^{j_1'+j_2-j} \times \sqrt{2j_1'+1}\sqrt{2j_2'+1} \\
&\quad < j_1' \| \hat{T}^{(k)}(1) \| j_1 >< j_2' \| \hat{T}^{(k)}(2) \| j_2 > W(j_1, j_2, j_1', j_2'; j, k)
\end{aligned}
$$

or

$$
\begin{aligned}
\left\langle j_1', j_2'; j'm' \middle| \hat{T}^{(k)}(1)\cdot\hat{T}^{(k)}(2) \middle| j_1, j_2; j, m \right\rangle &= \delta_{m,m'}\delta_{j,j'} (-1)^{j_1'+j_2-j} \times \sqrt{2j_1'+1}\sqrt{2j_2'+1} \\
&\quad < j_1' \| \hat{T}^{(k)}(1) \| j_1 >< j_2' \| \hat{T}^{(k)}(2) \| j_2 > W(j_1, j_2, j_1', j_2'; j, k)
\end{aligned}
$$

where the Racah coefficient *W* is defined by (Tinkham, Rose)

$$
\begin{aligned}
W(j_1, j_2, j_1', j_2'; j, k) &= \frac{(-1)^{-j_1'-j_2+j}}{\sqrt{(2j_1'+1)(2j_2'+1)}} \sum_{m_1, m_1'} (-1)^{m_1'-m_1} \left\langle j_1, j_2; m_1, m-m_1 \middle| j_1, j_2; j, m \right\rangle \\
&\quad \times \left\langle j_2, k; m-m_1, m_1 - m_1' \middle| j_2, k; j_2', m-m_1' \right\rangle \\
&\quad \times \left\langle j_1, k; m_1, m_1'-m_1 \middle| j_1, k; j_1', m_1' \right\rangle \\
&\quad \times \left\langle j_1', j_2'; m_1', m-m_1' \middle| j_1', j_2'; j, m \right\rangle
\end{aligned}
$$

A.5 Wigner 3*j* coefficient

The Clebsch-Gordan coefficients are sometimes expressed using the Wigner 3*j* symbol,

$$
\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix}
$$

Connection among these two is given by

$$\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle = (-1)^{j_1-j_2+m}\sqrt{2j+1}\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix}$$

or

$$\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{pmatrix} = (-1)^{m-j_1+j_2}\frac{\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, -m\rangle}{\sqrt{2j+1}}$$

They have the symmetry

$$\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle = (-1)^{j_1+j_2-j}\langle j_2, j_1; m_2, m_1 | j_2, j_2; j, m\rangle$$

A.6 Property of the Wigner 3j symmbol

We have that an even permutation of the column leaves the numerical value unchanged

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{pmatrix} j_2 & j_3 & j_1 \\ m_2 & m_3 & m_1 \end{pmatrix} = \begin{pmatrix} j_3 & j_1 & j_2 \\ m_3 & m_1 & m_2 \end{pmatrix}$$

An odd permutation is equivalent to multiplication by $(-1)^{j_1+j_2+j_3}$

$$\begin{aligned}(-1)^{j_1+j_2+j_3}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} &= \begin{pmatrix} j_2 & j_1 & j_3 \\ m_2 & m_1 & m_3 \end{pmatrix} \\ &= \begin{pmatrix} j_1 & j_3 & j_2 \\ m_1 & m_3 & m_2 \end{pmatrix} \\ &= \begin{pmatrix} j_3 & j_2 & j_1 \\ m_3 & m_2 & m_1 \end{pmatrix}\end{aligned}$$

We also have

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3}\begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix}$$

A7. The orthogonality property

$$\sum_{j,m}\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle\langle j_1, j_2; m_1', m_2' | j_1, j_2; j, m\rangle = \delta_{m_1,m_1'}\delta_{m_2,m_2'}$$

$$\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle = (-1)^{j_1-j_2+m}\sqrt{2j+1}\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix}$$

$$\langle j_1, j_2; m_1', m_2' | j_1, j_2; j, m\rangle = (-1)^{j_1-j_2+m}\sqrt{2j+1}\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix}$$

$$\begin{aligned}
\delta_{m_1,m_1'}\delta_{m_2,m_2'} &= \sum_{j,m}\langle j_1, j_2; j, m | j_1, j_2; m_1, m_2\rangle\langle j_1, j_2; m_1', m_2' | j_1, j_2; j, m\rangle \\
&= \sum_{j,m}(-1)^{j_1-j_2+m}\sqrt{2j+1}\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix}(-1)^{j_1-j_2+m}\sqrt{2j+1}\begin{pmatrix} j_1 & j_2 & j \\ m_1' & m_2' & -m \end{pmatrix} \\
&= \sum_{j,m}(-1)^{2j_1-2j_2+2m}(2j+1)\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix}\begin{pmatrix} j_1 & j_2 & j \\ m_1' & m_2' & -m \end{pmatrix} \\
&= \sum_{j,m}(2j+1)\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{pmatrix}\begin{pmatrix} j_1 & j_2 & j \\ m_1' & m_2' & m \end{pmatrix}
\end{aligned}$$

Similarly, we have

$$\begin{aligned}
\delta_{j,j'}\delta_{m,m'} &= \sum_{m_1,m_2}\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle\langle j_1, j_2; m_1, m_2 | j_1, j_2; j', m'\rangle \\
&= \sum_{m_1,m_2}(-1)^{j_1-j_2+m}\sqrt{2j+1}\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix}(-1)^{j_1-j_2+m'}\sqrt{2j'+1}\begin{pmatrix} j_1 & j_2 & j' \\ m_1 & m_2 & -m' \end{pmatrix} \\
&= (2j+1)\sum_{m_1,m_2}(-1)^{2j_1-2j_2+m+m'}\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix}\begin{pmatrix} j_1 & j_2 & j' \\ m_1 & m_2 & -m' \end{pmatrix} \\
&= (2j+1)\sum_{m_1,m_2}(-1)^{2j_1-2j_2+2m}\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix}\begin{pmatrix} j_1 & j_2 & j' \\ m_1 & m_2 & -m' \end{pmatrix} \\
&= (2j+1)\sum_{m_1,m_2}\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix}\begin{pmatrix} j_1 & j_2 & j' \\ m_1 & m_2 & -m' \end{pmatrix}
\end{aligned}$$

((Note))

$$(-1)^{2j_1-2j_2+2m} = 1$$

(a) Suppose that j_1=1/2 and j_2=1. j = 3/2 or 1/2. Then m is a half-integer. m = 3/2, 1/2, -1/2, or -3/2. Then j_1 - j_2 + m=integer.

(b) Suppose that j_1=1/2 and j_2=3/2. j = 2 or 1. Then m is an integer. m = 2, 1, 0, -1, -2. Then j_1 - j_2 + m=integer.

A.8 Mathematica for Wigner 3j coefficient

((**Mathematica**)) Calculation of the Wigner 3*j* coefficient

W3J[{j_1,m_1}m{j_2,m_2},{j_3,m_3}]$\rightarrow \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$

```
Clear["Global`*"]; W3J[{j1_, m1_}, {j2_, m2_}, {j_, m_}] :=
 Module[{s1},
  s1 = If[Abs[m1] ≤ j1 && Abs[m2] ≤ j2 && Abs[m] ≤ j,
    (-1)^(j1-j2-m)/Sqrt[2 j + 1] ClebschGordan[{j1, m1}, {j2, m2}, {j, -m}], Null]];
```

```
W3J[{2, 1}, {2, 1}, {2, -2}]
```

$-\sqrt{\frac{3}{35}}$

```
W3J[{3/2, 1/2}, {3/2, 1/2}, {2, -1}]
```

0

```
W3J[{2, 1}, {2, 1}, {3, -2}]
```

0

```
W3J[{4, 0}, {4, 0}, {0, 0}]
```

$\frac{1}{3}$

```
W3J[{3, 0}, {2, 0}, {3, 0}]
```

$\frac{2}{\sqrt{105}}$

```
W3J[{j, -m}, {0, 0}, {j, m}] // Simplify[#, Abs[m] ≤ j && Abs[m] ≤ j] &
```

$\frac{(-1)^{j-m}}{\sqrt{1+2j}}$

A.9 Matrix elements of vector operator

Spherical tensor of rank 1

$$T_1^{(1)} = -\frac{V_x + iV_y}{\sqrt{2}} = -\frac{V_+}{\sqrt{2}}$$

$$T_0^{(1)} = V_z$$

$$T_{-1}^{(1)} = \frac{V_x - iV_y}{\sqrt{2}} = \frac{V_-}{\sqrt{2}}$$

Using the Wigner-Eckart theorem, we have

$$\left\langle J', M' \left| \hat{T}_q^{(1)} \right| J, M \right\rangle = \left\langle J, 1; M, q \right| J, 1; J', M' \rangle \left\langle J' \left\| \hat{T}^{(k)} \right\| J \right\rangle$$

where

J'=J+1, J, J-1, $\qquad$ $M' = M+q$

For $q = 1$,

$$\begin{aligned}\left\langle J+1, M+1 \left| \hat{T}_1^{(1)} \right| J, M \right\rangle &= \left\langle J, 1; M, q=1 \right| J, 1; J+1, M+1 \rangle \left\langle J+1 \left\| \hat{T}^{(1)} \right\| J \right\rangle \\ &= (-1)^{2(J+M)} \sqrt{\frac{(1+J+M+1)(J+M+2)}{2(1+J)(1+2J)}} \left\langle J+1 \left\| \hat{T}^{(1)} \right\| J \right\rangle \\ &= \sqrt{\frac{(1+J+M+1)(J+M+2)}{2(1+J)(1+2J)}} \left\langle J+1 \left\| \hat{T}^{(1)} \right\| J \right\rangle\end{aligned}$$

$$\begin{aligned}\left\langle J, M+1 \left| \hat{T}_1^{(1)} \right| J, M \right\rangle &= \left\langle J, 1; M, q=1 \right| J, 1; J, M+1 \rangle \left\langle J \left\| \hat{T}^{(1)} \right\| J \right\rangle \\ &= -\sqrt{\frac{(J-M)(J+M+1)}{2J(J+1)}} \left\langle J \left\| \hat{T}^{(1)} \right\| J \right\rangle\end{aligned}$$

$$\begin{aligned}\left\langle J-1, M+1 \left| \hat{T}_1^{(1)} \right| J, M \right\rangle &= \left\langle J, 1; M, q=1 \right| J, 1; J-1, M+1 \rangle \left\langle J-1 \left\| \hat{T}^{(1)} \right\| J \right\rangle \\ &= \sqrt{\frac{(J-M)(J-M-1)}{2J(2J+1)}} \left\langle J-1 \left\| \hat{T}^{(1)} \right\| J \right\rangle\end{aligned}$$

For $q = 0$,

$$\left\langle J+1,M\left|\hat{T}_0^{(1)}\right|J,M\right\rangle = \left\langle J,1;M,q=0\right|J,1;J+1,M\right\rangle\left\langle J+1\left\|\hat{T}^{(1)}\right\|J\right\rangle$$

$$= (-1)^{2(J+M)}\sqrt{\frac{(J-M+1)(J+M+1)}{(2J+1)(J+1)}}\left\langle J+1\left\|\hat{T}^{(1)}\right\|J\right\rangle$$

$$= \sqrt{\frac{(J-M+1)(J+M+1)}{(2J+1)(J+1)}}\left\langle J+1\left\|\hat{T}^{(1)}\right\|J\right\rangle$$

$$\left\langle J,M\left|\hat{T}_0^{(1)}\right|J,M\right\rangle = \left\langle J,1;M,q=0\right|J,1;J,M\right\rangle\left\langle J\left\|\hat{T}^{(1)}\right\|J\right\rangle$$

$$= \frac{M}{\sqrt{J(J+1)}}\left\langle J\left\|\hat{T}^{(1)}\right\|J\right\rangle$$

$$\left\langle J-1,M\left|\hat{T}_0^{(1)}\right|J,M\right\rangle = \left\langle J,1;M,q=0\right|J,1;J-1,M\right\rangle\left\langle J-1\left\|\hat{T}^{(1)}\right\|J\right\rangle$$

$$= \sqrt{\frac{(J+M)(J-M)}{J(2J+1)}}\left\langle J-1\left\|\hat{T}^{(1)}\right\|J\right\rangle$$

For $q = -1$,

$$\left\langle J+1,M-1\left|\hat{T}_{-1}^{(1)}\right|J,M\right\rangle = \left\langle J,1;M,q=-1\right|J,1;J+1,M-1\right\rangle\left\langle J+1\left\|\hat{T}^{(1)}\right\|J\right\rangle$$

$$= (-1)^{2(J+M)}\sqrt{\frac{(J-M+1)(J-M+2)}{2(J+1)(2J+1)}}\left\langle J+1\left\|\hat{T}^{(1)}\right\|J\right\rangle$$

$$= \sqrt{\frac{(J-M+1)(J-M+2)}{2(J+1)(2J+1)}}\left\langle J+1\left\|\hat{T}^{(1)}\right\|J\right\rangle$$

$$\left\langle J,M-1\left|\hat{T}_{-1}^{(1)}\right|J,M\right\rangle = \left\langle J,1;M,q=-1\right|J,1;J,M-1\right\rangle\left\langle J\left\|\hat{T}^{(1)}\right\|J\right\rangle$$

$$= (-1)^{2(J+M)}\sqrt{\frac{(J+M)(J-M+1)}{2J(J+1)}}\left\langle J\left\|\hat{T}^{(1)}\right\|J\right\rangle$$

$$= \sqrt{\frac{(J+M)(J-M+1)}{2J(J+1)}}\left\langle J\left\|\hat{T}^{(1)}\right\|J\right\rangle$$

$$\left\langle J-1,M-1\left|\hat{T}_{-1}^{(1)}\right|J,M\right\rangle = \left\langle J,1;M,q=-1\right|J,1;J-1,M-1\right\rangle\left\langle J-1\left\|\hat{T}^{(1)}\right\|J\right\rangle$$

$$= \sqrt{\frac{(J+M)(J+M-1)}{2J(2J+1)}}\left\langle J-1\left\|\hat{T}^{(1)}\right\|J\right\rangle$$

Here we note that

$$(-1)^{2(J+M)} = 1$$

when J is either a positive integer or a half-integer.

A.10 Matrix elements of vector operator ($J' = J$)

We now calculate the matrix element with $J' = J$,

$$\langle J, M' | \hat{T}_q^{(1)} | J, M \rangle = \langle J, 1; M, q | J, 1; J, M' \rangle \langle J' \| \hat{T}^{(k)} \| J \rangle$$

where $M' = M + q$

For $q = 1$

$$\begin{aligned}
\langle J, M+1 | \hat{T}_1^{(1)} | J, M \rangle &= \langle J, 1; M, 1 | J, 1; J, M+1 \rangle \langle J \| \hat{T}^{(k)} \| J \rangle \\
&= -\frac{\sqrt{(J-M)(J+M+1)}}{\sqrt{2J(J+1)}} \langle J \| \hat{T}^{(k)} \| J \rangle \\
&= \langle J, M+1 | -\frac{\hat{J}_+}{\sqrt{2}} | J, M \rangle \frac{\langle J \| \hat{T}^{(k)} \| J \rangle}{\sqrt{J(J+1)}}
\end{aligned}$$

For q=0

$$\begin{aligned}
\langle J, M | \hat{T}_0^{(1)} | J, M \rangle &= \langle J, 1; M, 0 | J, 1; J, M \rangle \langle J \| \hat{T}^{(k)} \| J \rangle \\
&= \frac{M}{\sqrt{J(J+1)}} \langle J \| \hat{T}^{(k)} \| J \rangle \\
&= \langle J, M | \hat{J}_0 | J, M \rangle \frac{\langle J \| \hat{T}^{(k)} \| J \rangle}{\sqrt{J(J+1)}}
\end{aligned}$$

For q = -1

$$\begin{aligned}
\langle J, M-1 | \hat{T}_{-1}^{(1)} | J, M \rangle &= \langle J, 1; M, -1 | J, 1; J, M-1 \rangle \langle J \| \hat{T}^{(k)} \| J \rangle \\
&= (-1)^{2(J+M)} \frac{\sqrt{(J+M)(J-M+1)}}{\sqrt{2J(J+1)}} \langle J \| \hat{T}^{(k)} \| J \rangle \\
&= \langle J, M-1 | (-1)^{2(J+M)} \frac{\hat{J}_+}{\sqrt{2}} | J, M \rangle \frac{\langle J \| \hat{T}^{(k)} \| J \rangle}{\sqrt{J(J+1)}} \\
&= \langle J, M-1 | \frac{\hat{J}_+}{\sqrt{2}} | J, M \rangle \frac{\langle J \| \hat{T}^{(k)} \| J \rangle}{\sqrt{J(J+1)}}
\end{aligned}$$

where we use the relations

$$\langle J, M+1|\hat{J}_+|J, M\rangle = \sqrt{(J-M)(J+M+1)}$$

$$\langle J, M-1|\hat{J}_-|J, M\rangle = \sqrt{(J+M)(J-M+1)}$$

$$\langle J, M|\hat{J}_0|J, M\rangle = M|J, M\rangle$$

Here we note that

$$(-1)^{2(J+M)} = 1$$

when J is either a positive integer or a half-integer. Since

$$V_+ = -\sqrt{2}T_1^{(1)}$$

$$V_z = T_0^{(1)}$$

$$V_- = \sqrt{2}T_{-1}^{(1)}$$

we have

$$\langle J, M+1|\hat{V}_+|J, M\rangle = \langle J, M+1|\hat{J}_+|J, M\rangle \frac{\langle J\|\hat{\boldsymbol{V}}\|J\rangle}{\sqrt{J(J+1)}}$$

$$\langle J, M|\hat{V}_0|J, M\rangle = \langle J, M|\hat{J}_0|J, M\rangle \frac{\langle J\|\hat{\boldsymbol{V}}\|J\rangle}{\sqrt{J(J+1)}}$$

$$\langle J, M-1|\hat{V}_-|J, M\rangle = \langle J, M-1|\hat{J}_-|J, M\rangle \frac{\langle J\|\hat{\boldsymbol{V}}\|J\rangle}{\sqrt{J(J+1)}}$$

A.11 Operator equivalents

We start with

$$\langle J, M'|\hat{T}_q^{(1)}|J, M\rangle = \langle J,1;M,q|J,1;J,M'\rangle\langle J'\|\hat{T}^{(1)}\|J\rangle$$

Suppose that $\hat{T}_q^{(1)} = \hat{J}_q$. Then we get

$$\langle J,M'|\hat{J}_q|J,M\rangle = \langle J,1;M,q|J,1;J,M'\rangle\langle J'\|\hat{\boldsymbol{J}}\|J\rangle$$

or

$$\langle J,M+1|\hat{J}_1|J,M\rangle = \langle J,1;M,1|J,1;J,M+1\rangle\langle J'\|\hat{\boldsymbol{J}}\|J\rangle$$

$$\langle J,M|\hat{J}_0|J,M\rangle = \langle J,1;M,0|J,1;J,M\rangle\langle J'\|\hat{\boldsymbol{J}}\|J\rangle$$

$$\langle J,M-1|\hat{J}_{-1}|J,M\rangle = \langle J,1;M,-1|J,1;J,M-1\rangle\langle J'\|\hat{\boldsymbol{J}}\|J\rangle$$

From the above equations we have the following relations

$$\frac{\langle J,M'|\hat{T}_q^{(1)}|J,M\rangle}{\langle J,M'|\hat{J}_q|J,M\rangle} = \frac{\langle J,1;M,q|J,1;J,M'\rangle\langle J'\|\hat{T}^{(1)}\|J\rangle}{\langle J,1;M,q|J,1;J,M'\rangle\langle J'\|\hat{\boldsymbol{J}}\|J\rangle} = \frac{\langle J'\|\hat{T}^{(1)}\|J\rangle}{\langle J'\|\hat{\boldsymbol{J}}\|J\rangle}$$

or

$$\langle J,M'|\hat{T}_q^{(1)}|J,M\rangle = \langle J,M'|\hat{J}_q|J,M\rangle\frac{\langle J\|\hat{T}^{(1)}\|J\rangle}{\langle J\|\hat{\boldsymbol{J}}\|J\rangle} = \frac{\langle J,M'|\hat{J}_q|J,M\rangle}{\sqrt{j(j+1)}}\langle J\|\hat{T}^{(1)}\|J\rangle$$

In other words, $\hat{T}_q^{(1)}$ may be replaced by $c\hat{J}_q$, the angular operator times a constant *c*.

$$\hat{T}_q^{(1)} = c\hat{J}_q$$

A.12 Calculation of the scalar product

$$\hat{\boldsymbol{V}}\cdot\hat{\boldsymbol{W}} = -\hat{V}_-\hat{W}_+ + \hat{V}_0\hat{W}_0 - \hat{V}_+\hat{W}_-$$

$$\begin{aligned}\langle J,M|\hat{V}_+\hat{W}_-|J,M\rangle &= \sum_{M'}\langle J,M|\hat{V}_+|J,M'\rangle\langle J,M'|\hat{W}_-|J,M\rangle \\ &= \langle J,M|\hat{V}_+|J,M-1\rangle\langle J,M-1|\hat{W}_-|J,M\rangle \\ &= \langle J,M|\hat{J}_+|J,M-1\rangle\langle J,M-1|\hat{J}_-|J,M\rangle\frac{\langle J\|\hat{\boldsymbol{V}}\|J\rangle}{\sqrt{J(J+1)}}\frac{\langle J\|\hat{\boldsymbol{W}}\|J\rangle}{\sqrt{J(J+1)}}\end{aligned}$$

$$\langle J,M|\hat{V}_{-}\hat{W}_{+}|J,M\rangle = \sum_{M'}\langle J,M|\hat{V}_{-}|J,M'\rangle\langle J,M'|\hat{W}_{+}|J,M\rangle$$
$$= \langle J,M|\hat{V}_{-}|J,M+1\rangle\langle J,M+1|\hat{W}_{+}|J,M\rangle$$
$$= \langle J,M|\hat{J}_{-}|J,M+1\rangle\langle J,M+1|\hat{J}_{-}|J,M\rangle \frac{\langle J\|\hat{\boldsymbol{V}}\|J\rangle}{\sqrt{J(J+1)}}\frac{\langle J\|\hat{\boldsymbol{W}}\|J\rangle}{\sqrt{J(J+1)}}$$

$$\langle J,M|\hat{V}_{0}\hat{W}_{0}|J,M\rangle = \sum_{M'}\langle J,M|\hat{V}_{0}|J,M'\rangle\langle J,M'|\hat{W}_{0}|J,M\rangle$$
$$= \langle J,M|\hat{V}_{0}|J,M\rangle\langle J,M|\hat{W}_{0}|J,M\rangle$$
$$= \langle J,M|\hat{J}_{0}|J,M\rangle\langle J,M|\hat{J}_{0}|J,M\rangle \frac{\langle J\|\hat{\boldsymbol{V}}\|J\rangle}{\sqrt{J(J+1)}}\frac{\langle J\|\hat{\boldsymbol{W}}\|J\rangle}{\sqrt{J(J+1)}}$$

((**Mathematica**))

```
Clear["Global`*"];

ClebschGordan[{J, M}, {1, 1}, {J, M + 1}] // FullSimplify[#, {2 J > 1}] &
```

$$-\frac{\sqrt{\frac{(J-M)(1+J+M)}{J(1+J)}}}{\sqrt{2}}$$

```
ClebschGordan[{J, M}, {1, 0}, {J, M}] // FullSimplify[#, {2 J > 1}] &
```

$$\frac{M}{\sqrt{J(1+J)}}$$

```
ClebschGordan[{J, M}, {1, -1}, {J, M - 1}] // FullSimplify[#, {2 J > 1}] &
```

$$\frac{(-1)^{2(J+M)}\sqrt{\frac{J+J^2+M-M^2}{J+J^2}}}{\sqrt{2}}$$

```
J + J^2 + M - M^2 // Factor
```

$(1+J-M)(J+M)$

A.13

$$(-1)^{m_1'-m_1}\langle j_1', j_2'; m_1', m'-m_1' | j_1', j_2'; j', m'\rangle \times \langle j_1, j_2; m_1, m-m_1 | j_1, j_2; j, m\rangle$$
$$\langle j_1, k; m_1, m_1'-m_1 | j_1, k; j_1', m_1'\rangle \times \langle j_2, k; m-m_1, m_1-m_1' | j_2, k; j_2', m-m_1'\rangle$$
$$= (-1)^{m_1'-m_1}(-1)^{j_1'-j_2'+m'}\sqrt{2j'+1}\begin{pmatrix} j_1' & j_2' & j' \\ m_1' & m'-m_1' & -m' \end{pmatrix}(-1)^{j_1-j_2+m}\sqrt{2j+1}\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m-m_1 & -m \end{pmatrix}$$
$$\times(-1)^{j_1-k+m_1'}\sqrt{2j_1'+1}\begin{pmatrix} j_1 & k & j_1' \\ m_1 & m_1'-m_1 & -m_1' \end{pmatrix}(-1)^{j_2-k+m-m_1'}\sqrt{2j_2'+1}\begin{pmatrix} j_2 & k & j_2' \\ m-m_1 & m_1-m_1' & -m+m_1' \end{pmatrix}$$
$$= (-1)^{2j_1-2k+j_1'-j_2'+2m-m_1+m'+m_1'}\sqrt{2j'+1}\sqrt{2j+1}\sqrt{2j_1'+1}\sqrt{2j_2'+1}$$
$$\times\begin{pmatrix} j_1' & j_2' & j' \\ m_1' & m'-m_1' & -m' \end{pmatrix}\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m-m_1 & -m \end{pmatrix}$$
$$\times\begin{pmatrix} j_1 & k & j_1' \\ m_1 & m_1'-m_1 & -m_1' \end{pmatrix}\begin{pmatrix} j_2 & k & j_2' \\ m-m_1 & m_1-m_1' & -m+m_1' \end{pmatrix}$$

(Wigner-Eckart theorem)

Appendix (Tinkham)

$$V_1 = -\left(\frac{V_x + iV_y}{\sqrt{2}}\right) = -\frac{V_+}{\sqrt{2}} \qquad \boldsymbol{e}_1 = -\left(\frac{\boldsymbol{e}_x + i\boldsymbol{e}_y}{\sqrt{2}}\right)$$

$$V_0 = V_z \qquad \boldsymbol{e}_0 = \boldsymbol{e}_z$$

$$V_{-1} = \left(\frac{V_x - iV_y}{\sqrt{2}}\right) = \frac{V_-}{\sqrt{2}} \qquad \boldsymbol{e}_{-1} = \left(\frac{\boldsymbol{e}_x - i\boldsymbol{e}_y}{\sqrt{2}}\right)$$

where

$$\boldsymbol{e}_\mu \cdot \boldsymbol{e}_\nu = (-1)^\mu \delta_{\mu,-\nu}$$

Then the vector $\boldsymbol{V}$ can be expresses by

$$\boldsymbol{V} = V_x\boldsymbol{e}_x + V_y\boldsymbol{e}_y + V_z e_z = -V_{-1}\boldsymbol{e}_1 + V_0\boldsymbol{e}_0 - V_1\boldsymbol{e}_{-1} = \sum_\mu (-1)^\mu V_{-\mu}\boldsymbol{e}_\mu$$

The scalar product of two vectors has the form

$$
\begin{aligned}
\boldsymbol{V}\cdot\boldsymbol{W} &= \sum_{\mu,\nu}(-1)^{\mu+\nu}V_{-\mu}\boldsymbol{e}_{\mu}\cdot W_{-\nu}\boldsymbol{e}_{\nu} \\
&= \sum_{\mu,\nu}(-1)^{\mu+\nu}V_{-\mu}W_{-\nu}(-1)^{\mu}\delta_{\mu,-\nu} \\
&= \sum_{\mu}(-1)^{\mu}V_{-\mu}W_{\mu} \\
&= -V_{-1}W_{1}+V_{0}W_{0}-V_{1}W_{-1} \\
&= -V_{-}W_{+}+V_{0}W_{0}-V_{+}W_{-}
\end{aligned}
$$

Appendix Spherical Harmonics as rotator matrices

Using the relation

$$
|\Re\boldsymbol{r}\rangle = \hat{R}|\boldsymbol{r}\rangle
$$

$$
\begin{aligned}
|\boldsymbol{n}\rangle &= |\Re\boldsymbol{r}\rangle \\
&= \hat{R}|\boldsymbol{e}_{z}\rangle \\
&= \hat{R}_{z}(\phi)\hat{R}_{y}(\theta)|\boldsymbol{e}_{z}\rangle \\
&= \sum_{m'}\hat{R}_{z}(\phi)\hat{R}_{y}(\theta)|lm'\rangle\langle lm'|\boldsymbol{e}_{z}\rangle
\end{aligned}
$$

Then

$$
\langle lm|\boldsymbol{n}\rangle = \sum_{m'}\langle lm|\hat{R}_{z}(\phi)\hat{R}_{y}(\theta)|lm'\rangle\langle lm'|\boldsymbol{e}_{z}\rangle
$$

Here note that

$$
\langle\boldsymbol{n}|lm\rangle = Y_{\ell}^{m}(\boldsymbol{n}) = Y_{\ell}^{m}(\theta,\phi)
$$

or

$$
\langle lm|\boldsymbol{n}\rangle = [Y_{\ell}^{m}(\theta,\phi)]^{*}
$$

$\langle lm|\boldsymbol{e}_{z}\rangle = [Y_{\ell}^{m}(\theta,\phi)]^{*}$ evaluated at $\theta = 0$ with ϕ undetermined. At $\theta = 0$, $Y_{\ell}^{m}(\theta,\phi)$ is known to vanish for $m\neq 0$. Then we get

$$\langle lm|\boldsymbol{e}_z\rangle = [Y_\ell^m(\theta=0,\phi)]^*\delta_{m,0}$$
$$= \sqrt{\frac{2\ell+1}{4\pi}}P_\ell(\cos\theta=1)\delta_{m,0}$$
$$= \sqrt{\frac{2\ell+1}{4\pi}}\delta_{m,0}$$

$$[Y_\ell^m(\theta,\phi)]^* = \sum_{m'}\langle lm|\hat{R}_z(\phi)\hat{R}_y(\theta)|lm'\rangle\langle lm'|\boldsymbol{e}_z\rangle$$
$$= \sqrt{\frac{2\ell+1}{4\pi}}\sum_{m'}\langle lm|\hat{R}_z(\phi)\hat{R}_y(\theta)|lm'\rangle\delta_{m',0} = \sqrt{\frac{2\ell+1}{4\pi}}\langle lm|\hat{R}_z(\phi)\hat{R}_y(\theta)|l0\rangle$$

or

$$\langle lm|\hat{R}_z(\phi)\hat{R}_y(\theta)|l0\rangle = \sqrt{\frac{4\pi}{2\ell+1}}[Y_\ell^m(\theta,\phi)]^*$$

Since

$$\hat{R}_z(\phi) = \exp[-\frac{i}{\hbar}\hat{J}_z\phi]$$

we have

$$\langle lm|\hat{R}_z(\phi)\hat{R}_y(\theta)|l0\rangle = \langle lm|\exp[-\frac{i}{\hbar}\hat{J}_z\phi]\hat{R}_y(\theta)|l0\rangle = e^{-im\phi}\langle lm|\hat{R}_y(\theta)|l0\rangle$$

or

$$e^{-im\phi}\langle lm|\hat{R}_y(\theta)|l0\rangle = \sqrt{\frac{4\pi}{2\ell+1}}[Y_\ell^m(\theta,\phi)]^*$$

or

$$\langle lm|\hat{R}_y(\theta)|l0\rangle = e^{im\phi}\sqrt{\frac{4\pi}{2\ell+1}}[Y_\ell^m(\theta,\phi)]^*$$

Important formula

Wigner-Eckart theorem

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

$$\langle j_1', j_2'; j' m' | \hat{T}^{(k)}(1) \cdot \hat{T}^{(k)}(2) | j_1, j_2; j, m \rangle = \delta_{m,m'} \delta_{j,j'} (-1)^{j_1' + j_2 - j} \times \sqrt{2 j_1' + 1} \sqrt{2 j_2' + 1}$$
$$< j_1' \| \hat{T}^{(k)}(1) \| j_1 >< j_2' \| \hat{T}^{(k)}(2) \| j_2 > W(j_1, j_2, j_1', j_2'; j, k)$$

Equivalent operator:

$$\langle j, m' | \hat{T}_q^{(1)} | j, m \rangle = \frac{\langle J, m' | \hat{J}_q | J, m \rangle}{\sqrt{j(j+1)}} < j \| \hat{T}^{(1)} \| j >$$

1. Decomposition theorem

$$\langle j', m' | \hat{T}_q^{(1)} | j, m \rangle = \frac{\langle j', m' | \hat{J}_q (\hat{\boldsymbol{J}} \cdot \boldsymbol{T}^{(1)}) | j, m \rangle}{j(j+1)} \delta_{j,j'} \tag{1}$$

2. Factorization theorem

$$\langle j', m' | \hat{J}_q (\hat{\boldsymbol{J}} \cdot \boldsymbol{T}^{(1)}) | j, m \rangle = \langle j', m' | \hat{J}_q | j, m \rangle < j \| \hat{\boldsymbol{J}} \cdot \boldsymbol{T}^{(1)} \| j > . \tag{2}$$

3. Decomposition theorem of the second kind (the projection theorem)

$$\langle j', m' | \hat{T}_q^{(1)} | j, m \rangle = \frac{\langle j', m' | \hat{J}_q | j, m \rangle < j \| \hat{\boldsymbol{J}} \cdot \boldsymbol{T}^{(1)} \| j >}{j(j+1)} \delta_{j,j'} .$$

Formula

$$\begin{aligned}
[\hat{J}_\mu, T_q^{(k)}] &= \sum_{q'=-k}^{k} \hat{T}_{q'}^{(k)} \langle k, q' | \hat{J}_\mu | k, q \rangle \\
&= \sum_{q'=-k}^{k} \hat{T}_{q'}^{(k)} \langle k, 1; q, \mu | k, 1; k, q' \rangle < k \| \hat{\boldsymbol{J}} \| k > \\
&= \langle k, 1; q, \mu | k, 1; k, q + \mu \rangle < k \| \hat{\boldsymbol{J}} \| k > \hat{T}_{q+\mu}^{(k)} \\
&= \sqrt{k(k+1)} \langle k, 1; q, \mu | k, 1; k, q + \mu \rangle \hat{T}_{q+\mu}^{(k)}
\end{aligned}$$

where we use the Wigner-Eckart theoren

$$\langle j', m' | \hat{T}_q^{(k)} | j, m \rangle = \langle j, k; m, q | j, k; j', m' \rangle < j' \| \hat{T}^{(k)} \| j >$$

For $k = 1$ and $q = \mu$,

$$\langle j',m'|\hat{J}_\mu|j,m\rangle = \langle j,k=1;m,q=\mu|j,k=1;j',m'\rangle < j'\|\hat{\boldsymbol{J}}\|j >$$
$$= \delta_{j,j'}\delta_{m',m+\mu}\sqrt{j(j+1)}\langle j,1;m,\mu|j,1;j,m+\mu\rangle$$

$$\langle j,1;m,\mu|j,1;j,m+\mu\rangle = (-1)^\mu\langle j,1;m+\mu,-\mu|j,1;j,m\rangle$$

REFERENCES

M. Tinkham, Group Theory and Quantum Mechanics (McGraHill Book Company, New York, 1964).

J.J. Sakurai

Inui

A.R. Edmonds, Angular Momentum in Quantum Mechanics, 2nd edition, Princeton University Press, 1960.

Slichter

M.E. Rose, Elementary theory of angular momentum

E. Balcar and S.W. Lovesey, Introduction to the Graphical Theory of Angular Momentum (Springer, Berlin, 2009).

W.J. Thompson Angular momentum, An illustrated guide to Rotational Symmetries for Physical Systems

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Formula

$$\langle j',m'|\hat{J}_\mu|j,m\rangle = \langle j,1;m,\mu|j,k=1;j',m'\rangle < j'\|\hat{\boldsymbol{J}}\|j >$$
$$=\delta_{j,j'}\delta_{m',m+\mu}\langle j,1;m,\mu|j,1;j,m+\mu\rangle < j\|\hat{\boldsymbol{J}}\|j >$$
$$=\delta_{j,j'}\delta_{m',m+\mu}\sqrt{j(j+1)}\langle j,1;m,\mu|j,1;j',m+\mu\rangle$$

$$\langle j',m'|\hat{T}_q^{(k)}|j,m\rangle = \delta_{m',m+q}\langle j,k;m,q|j,k;j',m'\rangle\langle j'\|\hat{T}^{(k)}\|j\rangle$$

$$[\hat{J}_\mu,T_q^{(k)}] = \sqrt{k(k+1)}\langle k,1;q,\mu|k,1;k,q+\mu\rangle\hat{T}_{q+\mu}^{(k)}$$

$$[\hat{J}_\mu,T_{-\mu}^{(1)}] = \sqrt{2}\langle 1,1;-\mu,\mu|1,1;k,0\rangle\hat{T}_0^{(1)}$$

$$(-1)^\mu\langle j,1;m,\mu|j,1;j,m+\mu\rangle = \langle j,1;m+\mu,-\mu|j,1;j,m\rangle$$

$$< j' \| \hat{\boldsymbol{J}}^2 \| j >= \delta_{j,j'} j(j+1)$$

$$\hat{\boldsymbol{J}} \cdot \boldsymbol{T}^{(1)} = \sum_q (-1)^q \hat{J}_q \hat{T}_{-q}{}^{(1)}$$

$$\langle j, k=1; m, q=0 | j, k=1; j, m' \rangle = \frac{m}{\sqrt{j(j+1)}} \delta_{m,m'}$$

$$\langle j \| \hat{\boldsymbol{J}} \| j \rangle = \sqrt{j(j+1)}$$

The construction of tensor with rank k

$$\hat{T}_q^{(k)} = \sum_{q_1,q_2} \langle k_1, k_2; q_1, q_2 | k_1, k_2; k, q \rangle \hat{X}_{q_1}^{(k_1)} \hat{Z}_{q_2}^{(k_2)}$$

Decomposition theorem

$$\langle j', m' | \hat{T}_q{}^{(1)} | j, m \rangle = \frac{\langle j', m' | \hat{J}_q (\hat{\boldsymbol{J}} \cdot \boldsymbol{T}^{(1)}) | j, m \rangle}{j(j+1)} \delta_{j,j'}$$

Factorization theorem

$$\langle j', m' | \hat{J}_q (\hat{\boldsymbol{J}} \cdot \boldsymbol{T}^{(1)}) | j, m \rangle = \langle j', m' | \hat{J}_q | j, m \rangle < j \| \hat{\boldsymbol{J}} \cdot \boldsymbol{T}^{(1)} \| j > .$$

Decomposition theorem of the second kind (the projection theorem)

$$\langle j', m' | \hat{T}_q{}^{(1)} | j, m \rangle = \frac{\langle j', m' | \hat{J}_q | j, m \rangle < j \| \hat{\boldsymbol{J}} \cdot \boldsymbol{T}^{(1)} \| j >}{j(j+1)} \delta_{j,j'} .$$

$$\hat{T}^{(k)}(1) \cdot \hat{T}^{(k)}(2) = \sum_q (-1)^q \hat{T}_q{}^{(k)}(1) \hat{T}_{-q}{}^{(k)}(2)$$

$$\begin{aligned} \langle j_1', j_2'; j' m' | \hat{T}^{(k)}(1) \cdot \hat{T}^{(k)}(2) | j_1, j_2; j, m \rangle &= \delta_{m,m'} \delta_{j,j'} (-1)^{j_1' + j_2 - j} \times \sqrt{2 j_1' + 1} \sqrt{2 j_2' + 1} \\ &< j_1' \| \hat{T}^{(k)}(1) \| j_1 >< j_2' \| \hat{T}^{(k)}(2) \| j_2 > W(j_1, j_2, j_1', j_2'; j, k) \end{aligned}$$

Equivalent operator

$$\langle J,M'|\hat{T}_q^{(1)}|J,M\rangle = \langle J,M'|\hat{J}_q|J,M\rangle \frac{\langle J\|\hat{T}^{(k)}\|J\rangle}{\langle J\|\hat{\boldsymbol{J}}\|J\rangle} = \frac{\langle J,M'|\hat{J}_q|J,M\rangle}{\sqrt{j(j+1)}}\langle J\|\hat{T}^{(k)}\|J\rangle$$

Nuclear quadrupole fioeld
(Yosida)

The nucleus is not just a point, but has a finite size. If we define the nuclear charge distribution function $\rho(\boldsymbol{r})$ and the electrostatic potential due to the electrons around the nucleus by $V(\boldsymbol{r})$.

$$H = \int \rho(\boldsymbol{r})V(\boldsymbol{r})d\boldsymbol{r},$$

where d$\boldsymbol{r}$ denotes the volume elements. Expanding $V(\boldsymbol{r})$ about the origin, we get

$$H = ZeV_0 + \sum_j P_j (\frac{\partial V}{\partial x_j})_0 + \frac{1}{2}\sum_{j,k} Q_{jk}'(\frac{\partial^2 V}{\partial x_j \partial x_k})_0 + \ldots$$

Here Ze, P_j and Q_{jk}' are defined by

$$Ze = \int \rho(\boldsymbol{r})d\boldsymbol{r} \qquad \text{(nuclear charge)}$$

$$P_j = \int \rho(\boldsymbol{r})x_j d\boldsymbol{r} \qquad \text{(electric dipole moment)}$$

$$Q_{jk}' = \int \rho(\boldsymbol{r})x_j x_k d\boldsymbol{r} \qquad \text{(electric quadrupole moment)}$$

The electric dipole moment P_j vanishes if the nuclear charge distribution has inversion symmetry with respect to the origin, as is assumed here. The first term is the energy of the nucleus when the nucleus is regarded as a point charge. Neglecting this term, we get

$$H_Q = H - ZeV_0 = \frac{1}{2}\sum_{j,k} Q_{jk}'V_{jk}$$

where

$$V_{jk} = (\frac{\partial^2 V}{\partial x_j \partial x_k})_0$$

The Hamiltonian H_Q is the interaction of electric field gradient and the quadrupole moment. We introduce the traceless tensor as

$$Q_{jk}=3Q_{jk}'-\delta_{jk}\sum_i Q_{ii}'=\begin{pmatrix} 3Q_{11}'-\sum_i Q_{ii}' & 3Q_{12}' & 3Q_{13}' \\ 3Q_{21}' & 3Q_{22}'-\sum_i Q_{ii}' & 3Q_{23}' \\ 3Q_{31}' & 3Q_{32}' & 3Q_{33}'-\sum_i Q_{ii}' \end{pmatrix}$$

Then we get

$$H_Q=\frac{1}{6}\sum_{j,k}Q_{jk}V_{jk}+\frac{1}{6}\left(\sum_i Q_{ii}'\right)\left(\sum_j V_{jj}\right)$$

with

$$Q_{jk}=\int\rho(\boldsymbol{r})(3x_jx_k-\delta_{jk}\boldsymbol{r}^2)d\boldsymbol{r}$$

Suppose that

$$\rho(\boldsymbol{r})=\sum_i e\delta(\boldsymbol{r}-\boldsymbol{r}_i)$$

Then we have

$$Q_{jk}=\sum_i e(3x_{ij}x_{ik}-\delta_{jk}\boldsymbol{r}_i^{\,2})$$

((**Slichter**))

We are in general concerned only with thr ground state of a nucleus or perhaps with an excited state when the excited state is sufficiently long-lived. The eigenstate of nucleus are characterized by the state $|I,m\rangle$ with $m = I, I\text{-}1, I\text{-}2,\ldots,\text{-}I$ ($2I+1$ states). Then we need only the matrix elements of the quadrupole operator,

$$\langle I,m'|\hat{Q}_{jk}|I,m\rangle$$

According to the Wigner-Eckart theorem these can be shown to obey the equation

$$\langle I,m'|\hat{Q}_{jk}|I,m\rangle=c\langle I,m'|\frac{3}{2}(\hat{I}_\alpha\hat{I}_\beta+\hat{I}_\beta\hat{I}_\alpha)-\delta_{\alpha\beta}\boldsymbol{I}^2|I,m\rangle$$

where c is a constant. We will show you later how to derive this form.

The Hamiltonian is then given by

$$H_Q = \frac{eQ}{6I(2I-1)} \sum_{\alpha,\beta} V_{\alpha\beta} [\frac{3}{2}(\hat{I}_\alpha \hat{I}_\beta + \hat{I}_\beta \hat{I}_\alpha) - \delta_{\alpha\beta} \boldsymbol{I}^2]$$

We choose a set of principal axes such that

$$V_{\alpha\beta} = 0 \qquad \text{for } \alpha \neq \beta$$

Then we get a simplified Hamiltonian

$$H_Q = \frac{eQ}{6I(2I-1)} [V_{xx}(3\hat{I}_x{}^2 - \boldsymbol{I}^2) + V_{yy}(3\hat{I}_y{}^2 - \boldsymbol{I}^2) + V_{zz}(3\hat{I}_z{}^2 - \boldsymbol{I}^2)].$$

Since

$$V_{xx} + V_{yy} + V_{zz} = 0 \qquad \text{(from the Laplace's equation)}$$

we have

$$H_Q = \frac{eQ}{4I(2I-1)} [V_{zz}(3\hat{I}_z{}^2 - \boldsymbol{I}^2) + (V_{xx} - V_{yy})(\hat{I}_x{}^2 - \hat{I}_y{}^2)]$$

We define

$$eq = V_{zz}$$

$$\eta = \frac{V_{xx} - V_{yy}}{V_{zz}}$$

where η is called the asymmetry parameter and q is called the field gradient. then we have

$$H_Q = \frac{e^2 qQ}{4I(2I-1)} [(3\hat{I}_z{}^2 - \boldsymbol{I}^2) + \eta)(\hat{I}_x{}^2 - \hat{I}_y{}^2)].$$

((**Equivalent operator**))

$$\hat{T}_2^{(2)} = \hat{U}_1{}^2 = \frac{1}{2}\hat{U}_+{}^2$$

$$\hat{T}_1^{(2)} = \frac{\hat{U}_1\hat{U}_0 + \hat{U}_0\hat{U}_1}{\sqrt{2}} = -\frac{1}{2}(\hat{U}_+\hat{U}_0 + \hat{U}_0\hat{U}_+)$$

$$\hat{T}_0^{(2)} = \frac{\hat{U}_1\hat{U}_{-1} + 2\hat{U}_0\hat{U}_0 + \hat{U}_{-1}\hat{U}_1}{\sqrt{6}} = \frac{-\dfrac{(\hat{U}_+\hat{U}_- + \hat{U}_-\hat{U}_+)}{2} + 2\hat{U}_0{}^2}{\sqrt{6}}$$

$$\hat{T}_{-1}^{(2)} = \frac{\hat{U}_0\hat{U}_{-1} + \hat{U}_{-1}\hat{U}_1}{\sqrt{2}} = \frac{1}{2}(\hat{U}_-\hat{U}_0 + \hat{U}_0\hat{U}_-)$$

$$\hat{T}_{-2}^{(2)} = \hat{U}_{-1}\hat{U}_{-1} = \frac{1}{2}\hat{U}_-{}^2$$

$$\hat{T}_2^{(2)} = \frac{\hat{I}_+{}^2}{2} = \frac{1}{2}(\hat{I}_x + i\hat{I}_y)(\hat{I}_x + i\hat{I}_y) = \frac{\hat{I}_x{}^2 - \hat{I}_y{}^2}{2} + i\frac{(\hat{I}_x\hat{I}_y + \hat{I}_y\hat{I}_x)}{2}$$

$$\hat{T}_1^{(2)} = -\left(\frac{\hat{I}_+\hat{I}_0 + \hat{I}_0\hat{I}_+}{2}\right) = -\left(\frac{\hat{I}_z\hat{I}_x + \hat{I}_x\hat{I}_z}{2}\right) - i\left(\frac{\hat{I}_y\hat{I}_z + \hat{I}_z\hat{I}_y}{2}\right)$$

$$\hat{T}_0^{(2)} = \frac{-\left(\dfrac{\hat{I}_+\hat{I}_- + \hat{I}_-\hat{I}_+}{2}\right) + 2\hat{I}_0{}^2}{\sqrt{6}} = \frac{2\hat{I}_z{}^2 - (\hat{I}_x{}^2 + \hat{I}_y{}^2)}{\sqrt{6}}$$

$$\hat{T}_{-1}^{(2)} = \frac{\hat{I}_0\hat{I}_- + \hat{I}_-\hat{I}_0}{2} = \left(\frac{\hat{I}_z\hat{I}_x + \hat{I}_x\hat{I}_z}{2}\right) - i\left(\frac{\hat{I}_y\hat{I}_z + \hat{I}_z\hat{I}_y}{2}\right)$$

$$\hat{T}_{-2}^{(2)} = \frac{\hat{I}_-{}^2}{2} = \frac{1}{2}(\hat{I}_x - i\hat{I}_y)(\hat{I}_x - i\hat{I}_y) = \left(\frac{\hat{I}_x{}^2 - \hat{I}_y{}^2}{2}\right) - i\frac{(\hat{I}_x\hat{I}_y + \hat{I}_y\hat{I}_x)}{2}$$

or

$$\hat{I}_x\hat{I}_y + \hat{I}_y\hat{I}_x = -i(\hat{T}_2^{(2)} - \hat{T}_{-2}^{(2)})$$

$$-\hat{I}_x{}^2-\hat{I}_y{}^2+2\hat{I}_z{}^2=\sqrt{6}\hat{T}_0^{(2)}$$

$$\hat{I}_z\hat{I}_x+\hat{I}_x\hat{I}_z=i(\hat{T}_{-1}^{(2)}-\hat{T}_1^{(2)})$$

The operator equivalent
Thompson p.321

(a)

$$\langle I,m|T_{q=0}{}^{(k=2)}|I,m\rangle=\langle I,k=2;m,q=0|I,k=2;I,m\rangle<I\,\|\,T^{(k=2)}\,\|\,I>$$
$$=\frac{3m^2-I(I+1)}{\sqrt{I(1+I)(2I-1)(2I+3)}}<I\,\|\,T^{(k=2)}\,\|\,I>$$

$$\langle I,m|\frac{-\left(\dfrac{\hat{I}_+\hat{I}_-+\hat{I}_-\hat{I}_+}{2}\right)+2\hat{I}_0{}^2}{\sqrt{6}}|I,m\rangle=\frac{1}{\sqrt{6}}[-\frac{(I-m+1)(I+m)}{2}+2m^2+$$
$$-\frac{(I+m+1)(I-m)}{2}]$$
$$=\frac{1}{\sqrt{6}}[3m^2-I(I+1)]$$

where

$$\langle I,m+1|\hat{I}_+|I,m\rangle=\sqrt{(I-m)(I+m+1)}$$
$$\langle I,m|\hat{I}_+|I,m-1\rangle=\sqrt{(I-m+1)(I+m)}$$

$$\langle I,m-1|\hat{I}_-|I,m\rangle=\sqrt{(I+m)(I-m+1)}$$
$$\langle I,m|\hat{I}_-|I,m+1\rangle=\sqrt{(I+m+1)(I-m)}$$

Then we have

$$\langle I,m|T_{q=0}{}^{(k=2)}|I,m\rangle=\frac{\langle I,m|-\left(\dfrac{\hat{I}_+\hat{I}_-+\hat{I}_-\hat{I}_+}{2}\right)+2\hat{I}_0{}^2|I,m\rangle}{\sqrt{I(1+I)(2I-1)(2I+3)}}<I\,\|\,T^{(k=2)}\,\|\,I>$$

The atomic spectroscopic quadrupole moment Q is defined by

$$Q = \langle I, I | T_{q=0}{}^{(k=2)} | I, I \rangle$$
$$= \frac{3I^2 - I(I+1)}{\sqrt{I(1+I)(2I-1)(2I+3)}} < I \| T^{(k=2)} \| I >$$
$$= \sqrt{\frac{I(2I-1)}{(I+1)(2I+3)}} < I \| T^{(k=2)} \| I >$$

which is consistent with vanishing matrix elements for $I = 0$ and $I = 1/2$.

$$< I \| T^{(k=2)} \| I >= \sqrt{\frac{(I+1)(2I+3)}{I(2I-1)}} Q$$

Suppose that

$$\langle I, m | \hat{T}_{q=0}^{(2)} | I, m \rangle = c \langle I, m | 3\hat{I}_z{}^2 - \boldsymbol{I}^2 | I, m \rangle = c[3m^2 - I(I+1)]$$

((**Equivalent operator**))

Then we have

$$\langle I, m | T_{q=0}{}^{(k=2)} | I, m \rangle = \frac{3m^2 - I(I+1)}{\sqrt{I(1+I)(2I-1)(2I+3)}} < I \| T^{(k=2)} \| I >$$
$$= \frac{3m^2 - I(I+1)}{I(2I-1)} Q$$

(b)

$$\langle I, m+2 | T_{q=2}{}^{(k=2)} | I, m \rangle = \langle I, k=2; m, q=2 | I, k=2; I, m+2 \rangle < I \| T^{(k=2)} \| I >$$
$$= \sqrt{\frac{3}{2}} \frac{\sqrt{(I-m-1)(I-m)(I+m+1)(I+m+2)}}{\sqrt{I(1+I)(2I-1)(2I+3)}} < I \| T^{(k=2)} \| I >$$

and

$$\langle I, m+2 | \hat{I}_+{}^2 | I, m \rangle = \sum_{m'} \langle I, m+2 | \hat{I}_+ | I, m' \rangle \langle I, m' | \hat{I}_+ | I, m \rangle$$
$$= \langle I, m+2 | \hat{I}_+ | I, m+1 \rangle \langle I, m+1 | \hat{I}_+ | I, m \rangle$$
$$= \sqrt{(I-m-1)(I-m)(I+m+1)(I+m+2)}$$

Then we have

$$\left\langle I,m+2\middle|T_{q=2}{}^{(k=2)}\middle|I,m\right\rangle = \sqrt{6}\,\frac{\left\langle I,m+2\middle|\frac{\hat{I}_+{}^2}{2}\middle|I,m\right\rangle}{\sqrt{I(1+I)(2I-1)(2I+3)}} < I\,\|\,T^{(k=2)}\,\|\,I >$$

(c)

$$\left\langle I,m+1\middle|T_{q=1}{}^{(k=2)}\middle|I,m\right\rangle = \left\langle I,k=2;m,q=1\middle|I,k=2;I,m+1\right\rangle < I\,\|\,T^{(k=2)}\,\|\,I >$$
$$= -\sqrt{\frac{3}{2}}\,\frac{\sqrt{(I-m)(I+m+1)}}{\sqrt{I(1+I)(2I-1)(2I+3)}}(2m+1) < I\,\|\,T^{(k=2)}\,\|\,I >$$

$$\left\langle I,m-1\middle|-\frac{\hat{I}_-\hat{I}_0+\hat{I}_0\hat{I}_-}{\sqrt{2}}\middle|I,m\right\rangle = -\frac{1}{\sqrt{2}}[m\left\langle I,m-1\middle|\hat{I}_-\middle|I,m\right\rangle + (m-1)\left\langle I,m-1\middle|\hat{I}_-\middle|I,m\right\rangle]$$
$$= -\frac{1}{\sqrt{2}}(2m-1)\left\langle I,m-1\middle|\hat{I}_-\middle|I,m\right\rangle$$
$$= -\frac{1}{\sqrt{2}}(2m-1)\sqrt{(I-m+1)(I+m)}$$

Then

$$\left\langle I,m+1\middle|T_{q=1}{}^{(k=2)}\middle|I,m\right\rangle = \sqrt{3}\,\frac{\left\langle I,m-1\middle|-\frac{\hat{I}_-\hat{I}_0+\hat{I}_0\hat{I}_-}{\sqrt{2}}\middle|I,m\right\rangle}{\sqrt{I(1+I)(2I-1)(2I+3)}} < I\,\|\,T^{(k=2)}\,\|\,I >$$

(d)

$$\left\langle I,m-1\middle|T_{q=-1}{}^{(k=2)}\middle|I,m\right\rangle = \left\langle I,k=2;m,q=-1\middle|I,k=2;I,m-1\right\rangle < I\,\|\,T^{(k=2)}\,\|\,I >$$
$$= (-1)^{2(I+m)}\sqrt{\frac{3}{2}}\,\frac{\sqrt{(I-m+1)(I+m)}}{\sqrt{I(1+I)(2I-1)(2I+3)}}(2m-1) < I\,\|\,T^{(k=2)}\,\|\,I >$$

$$\left\langle I,m-1\middle|\frac{\hat{I}_-\hat{I}_0+\hat{I}_0\hat{I}_-}{\sqrt{2}}\middle|I,m\right\rangle = \frac{1}{\sqrt{2}}[m\left\langle I,m-1\middle|\hat{I}_-\middle|I,m\right\rangle + (m-1)\left\langle I,m-1\middle|\hat{I}_-\middle|I,m\right\rangle]$$
$$= \frac{1}{\sqrt{2}}(2m-1)\left\langle I,m-1\middle|\hat{I}_-\middle|I,m\right\rangle$$
$$= \frac{1}{\sqrt{2}}(2m-1)\sqrt{(I-m+1)(I+m)}$$

or

$$\langle I,m-1|T_{q=-1}^{(k=2)}|I,m\rangle=(-1)^{2(I+m)}\sqrt{3}\frac{\langle I,m-1|\frac{\hat{I}_-\hat{I}_0+\hat{I}_0\hat{I}_-}{\sqrt{2}}|I,m\rangle}{\sqrt{I(1+I)(2I-1)(2I+3)}}<I\|T^{(k=2)}\|I>$$

(e)

$$\langle I,m-2|T_{q=-2}^{(k=2)}|I,m\rangle=\langle I,k=2;m,q=-2|I,k=2;I,m-2\rangle<I\|T^{(k=2)}\|I>$$

$$=(-1)^{2(I+m)}\sqrt{\frac{3}{2}}\frac{\sqrt{(I+m-1)(I-m+2)(I+m)(I-m+1)}}{\sqrt{I(1+I)(2I-1)(2I+3)}}<I\|T^{(k=2)}\|I>$$

and

$$\begin{aligned}\langle I,m-2|\hat{I}_-^{\,2}|I,m\rangle&=\sum_{m'}\langle I,m-2|\hat{I}_-|I,m'\rangle\langle I,m'|\hat{I}_-|I,m\rangle\\&=\langle I,m-2|\hat{I}_-|I,m-1\rangle\langle I,m-1|\hat{I}_-|I,m\rangle\\&=\sqrt{(I+m-1)(I-m+2)(I+m)(I-m+1)}\end{aligned}$$

or

$$\langle I,m-2|T_{q=-2}^{(k=2)}|I,m\rangle=(-1)^{2(I+m)}\sqrt{6}\frac{\langle I,m-2|\frac{\hat{I}_-^{\,2}}{2}|I,m\rangle}{\sqrt{I(1+I)(2I-1)(2I+3)}}<I\|T^{(k=2)}\|I>$$

where we use the relations

$$\langle I,m+1|\hat{I}_+|I,m\rangle=\sqrt{(I-m)(I+m+1)}$$

$$\langle I,m-1|\hat{I}_-|I,m\rangle=\sqrt{(I+m)(I-m+1)}$$

$$\langle I,m|\hat{I}_0|I,m\rangle=m$$

((**Mathematica**))

Claculation of the Clebsch-Gordan coefficients for the rank 2 tensors

```
Clear["Global`*"];

ClebschGordan[{J, m}, {2, 2}, {J, m + 2}] // FullSimplify[#, {J > 1}] &
```

$$\sqrt{\frac{3}{2}}\sqrt{\frac{(-1+J-m)(J-m)(1+J+m)(2+J+m)}{J(1+J)(-1+2J)(3+2J)}}$$

```
ClebschGordan[{J, m}, {2, 1}, {J, m + 1}] // FullSimplify[#, {J > 1}] &
```

$$-\sqrt{\frac{3}{2}}\sqrt{\frac{(J-m)(1+J+m)}{J(-3+J(1+4J(2+J)))}}\,(1+2m)$$

```
ClebschGordan[{J, m}, {2, 0}, {J, m}] // FullSimplify[#, {J > 1}] &
```

$$\frac{-J(1+J)+3m^2}{\sqrt{J(-3+J(1+4J(2+J)))}}$$

```
ClebschGordan[{J, m}, {2, -1}, {J, m - 1}] // FullSimplify[#, {J > 1}] &
```

$$(-1)^{2(J+m)}\sqrt{\frac{3}{2}}\sqrt{\frac{(1+J-m)(J+m)}{J(-3+J(1+4J(2+J)))}}\,(-1+2m)$$

```
ClebschGordan[{J, m}, {2, -2}, {J, m - 2}] // FullSimplify[#, {J > 1}] &
```

$$(-1)^{2(J+m)}\sqrt{\frac{3}{2}}\sqrt{\frac{(1+J-m)(2+J-m)(-1+J+m)(J+m)}{J(1+J)(-1+2J)(3+2J)}}$$

```
(-3 + J (1 + 4 J (2 + J))) // Factor
```

$$(1+J)(-1+2J)(3+2J)$$

$$\hat{T}_2^{(2)} = \hat{U}_1{}^2 = \frac{1}{2}\hat{U}_+{}^2$$

$$\hat{T}_1^{(2)} = \frac{\hat{U}_1\hat{U}_0 + \hat{U}_0\hat{U}_1}{\sqrt{2}} = -\frac{1}{2}(\hat{U}_+\hat{U}_0 + \hat{U}_0\hat{U}_+)$$

$$\hat{T}_0^{(2)} = \frac{\hat{U}_1\hat{U}_{-1} + 2\hat{U}_0\hat{U}_0 + \hat{U}_{-1}\hat{U}_1}{\sqrt{6}} = \frac{-\dfrac{(\hat{U}_+\hat{U}_- + \hat{U}_-\hat{U}_+)}{2} + 2\hat{U}_0{}^2}{\sqrt{6}}$$

$$\hat{T}_{-1}^{(2)} = \frac{\hat{U}_0\hat{U}_{-1} + \hat{U}_{-1}\hat{U}_1}{\sqrt{2}} = \frac{1}{2}(\hat{U}_-\hat{U}_0 + \hat{U}_0\hat{U}_-)$$

$$\hat{T}_{-2}^{(2)} = \hat{U}_{-1}\hat{U}_{-1} = \frac{1}{2}\hat{U}_-{}^2$$

where

$$\hat{U}_1 = -\frac{\hat{U}_x + i\hat{U}_y}{\sqrt{2}} = -\frac{\hat{U}_+}{\sqrt{2}}, \qquad \hat{U}_0 = \hat{U}_z, \qquad \hat{U}_{-1} = \frac{\hat{U}_-}{\sqrt{2}}$$

---

or

$$\hat{I}_x\hat{I}_y + \hat{I}_y\hat{I}_x = -i(\hat{T}_2^{(2)} - \hat{T}_{-2}^{(2)})$$

$$-\hat{I}_x{}^2 - \hat{I}_y{}^2 + 2\hat{I}_z{}^2 = \sqrt{6}\hat{T}_0^{(2)}$$

$$\hat{I}_z\hat{I}_x + \hat{I}_x\hat{I}_z = i(\hat{T}_{-1}^{(2)} - \hat{T}_1^{(2)})$$

Comment

$$\hat{T}(i)_{q=0}^{k=2} = (2\hat{z}_i{}^2 - \hat{x}_i{}^2 - \hat{y}_i{}^2)$$

Wigner-Eckart theorem

$$\langle I', m' | \hat{T}(i)_{q=0}^{k=2} | I, m \rangle = \langle I, k=2; m, q=0 | I, k=2; I', m' \rangle < I' \| \hat{T}(i)^{k=2} \| I >$$

$$\left\langle I',m'\middle|\sum_i \hat{T}(i)^{k=2}_{q=0}\middle|I,m\right\rangle = \left\langle I,k=2;m,q=0\middle|I,k=2;I',m'\right\rangle \sum_i < I' \| \hat{T}(i)^{k=2} \| I >$$

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The last term of the right-hand side is independent of *m* and *m*'.