Tensors

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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.

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

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

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

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

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 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.

2 Example

(a) When $\hat{V} = \hat{\boldsymbol{J}}$,

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

(b) When $\hat{V} = \hat{\boldsymbol{r}}$, $\hat{J}_j = \hat{L}_j$

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

(c) When $\hat{V} = \hat{\boldsymbol{p}}$, $\hat{J}_j = \hat{L}_j$

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

3 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 $\Re$.

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

or

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

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

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

where $\hat{U}_i$ and $\hat{V}_i$ are the components of ordinary 3D vector operators. There are nine components: 1+3+5 = 9. The trouble with a Cartesian tensor like $\hat{T}_{ij} = \hat{U}_i\hat{V}_j$ is that it is reducible. It can be decomposed into the three parts.

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

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

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

There are 3 independent components.

$$T_a = \begin{pmatrix} 0 & T_{a12} & T_{a13} \\ -T_{a12} & 0 & T_{a23} \\ -T_{a13} & -T_{a23} & 0 \end{pmatrix}$$

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

$$T_s = \begin{pmatrix} T_{s11} & T_{s12} & T_{s13} \\ T_{s12} & T_{s22} & T_{s23} \\ T_{s13} & T_{s23} & T_{s33} \end{pmatrix}$$

with $T_{s11}+T_{s22}+T_{s33}=0$. In conclusion, the tensor $\hat{T}_{ij}=\hat{U}_i\hat{V}_j$ can be decomposed into spherical tensors of rank 0, 1, and 2.

rank 0 →	$j=0$,	(1 component)
rank 1	$j=1$,	(3 component)
rank 2	$j=2$,	(5 component)

4 Spherical tensor: definition

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

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

The quantity

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

is a homogeneous polynomial of order *l*.

5 Spherical tensor of rank 1

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)

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

which leads to

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

(ii)

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

which leads to

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

(iii)

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

which leads to

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

6 Spherical tensor of rank 2

(i)

$$P_{2,0}(x,y,z) = r^2 Y_2^0(\theta,\phi) = \sqrt{\frac{5}{16\pi}}(3z^2 - r^2)$$

$$= \sqrt{\frac{15}{8\pi}} \frac{[2z^2 - \frac{(x+iy)(x-iy)}{2} - \frac{(x-iy)(x+iy)}{2}]}{\sqrt{6}}$$

which leads to

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

(iii)

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

which leads to

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

(iv)

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

which leads to

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

(v)

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

which leads to

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

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

7 Spherical tensor under rotation

We consider how

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

transforms under rotation. Using the relations

$$|\boldsymbol{n}'\rangle = \hat{R}|\boldsymbol{n}\rangle, \qquad \langle\boldsymbol{n}'| = \langle\boldsymbol{n}|\hat{R}^+$$

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

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

we have

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

where

$$Y_l^m(\boldsymbol{n}) = \langle\boldsymbol{n}|l,m\rangle,$$

and

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

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

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

((**Note**))

In classical theory, the average *A* changes into A'

$$A \to A'$$

under the rotation operator. In quantum mechanics, this can be expressed by

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

where

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

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

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

where

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

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

or

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

with $q = k, k\text{-}1,\ldots, \text{-}k$. The switching of $\hat{R} \to \hat{R}^{+}$ in Eq.(1) leads to another expression

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

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

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

or

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

or

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

For $\boldsymbol{n} = \boldsymbol{e}_{x}, \boldsymbol{e}_{y}, \boldsymbol{e}_{z}$

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

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

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

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

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

We now consider

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

This equation is rewritten as

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

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

((**Note**))

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 $\hat{\boldsymbol{V}}$ 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

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

8 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, where

$$\langle k_1, k_2; q_1, q_2 | k_1, k_2; k, q \rangle$$

is the Clebsch-Gordan (CG) coefficient.

((**Proof**))

$$
\begin{aligned}
\hat{R}\hat{T}_q^{(k)}\hat{R}^+ &= \sum_{q_1,q_2}\langle k_1,k_2;q_1,q_2|k_1,k_2;k,q\rangle(\hat{R}\hat{X}_{q_1}^{(k_1)}\hat{R}^+)(\hat{R}\hat{Z}_{q_2}^{(k_2)}\hat{R}^+) \\
&= \sum_{q_1,q_2,q_1',q_2'}\langle k_1,k_2;q_1,q_2|k_1,k_2;k,q\rangle D_{q_1q_1'}^{(k_1)}(\hat{R})\hat{X}_{q_1'}^{(k_1)}D_{q_2q_2'}^{(k_2)}(\hat{R})\hat{Z}_{q_2'}^{(k_2)} \\
&= \sum_{\substack{q_1,q_2,q_1',q_2' \\ k'',q'',q'}}\langle k_1,k_2;q_1,q_2|k_1,k_2;k,q\rangle\langle k_1,k_2;q_1',q_2'|k_1,k_2;k'',q'\rangle\langle k_1,k_2;q_1,q_2|k_1,k_2;k'',q''\rangle D_{q'q''}^{(k'')}(\hat{R})\hat{X}_{q_1'}^{(k_1)}\hat{Z}_{q_2'}^{(k_2)} \\
&= \sum_{\substack{q_1',q_2' \\ k'',q'',q'}}\delta_{k,k''}\delta_{q,q''}\langle k_1,k_2;q_1',q_2'|k_1,k_2;k'',q'\rangle D_{q'q''}^{(k'')}(\hat{R})\hat{X}_{q_1'}^{(k_1)}\hat{Z}_{q_2'}^{(k_2)} \\
&= \sum_{q',q_1',q_2'}\langle k_1,k_2;q_1',q_2'|k_1,k_2;k,q'\rangle\hat{X}_{q_1'}^{(k_1)}\hat{Z}_{q_2'}^{(k_2)}D_{q'q}^{(k)}(\hat{R}) \\
&= \sum_{q'}D_{q'q}^{(k)}(\hat{R})T_{q'}^{(k)}
\end{aligned}
$$

where

$$\hat{R}\hat{X}_{q_1}^{(k_1)}\hat{R}^+ = \sum_{q_1'}D_{q_1q_1'}^{(k_1)}(\hat{R})\hat{X}_{q_1'}^{(k_1)}$$

$$\hat{R}\hat{Z}_{q_2}^{(k_2)}\hat{R}^+ = \sum_{q_2'}D_{q_2q_2'}^{(k_2)}(\hat{R})\hat{Z}_{q_2'}^{(k_2)}$$

$$D_{q_1q_1'}^{(k_1)}(\hat{R})D_{q_2q_2'}^{(k_2)}(\hat{R}) = \sum_{k''q''q'}\langle k_1,k_2;q_1',q_2'|k_1,k_2;k'',q'\rangle\langle k_1,k_2;q_1,q_2|k_1,k_2;k'',q'\rangle D_{q'q''}^{(k'')}(\hat{R})$$

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

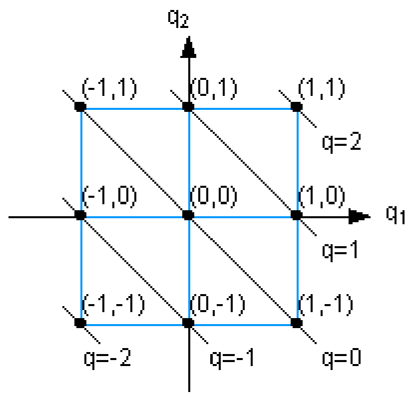
9 Tensor of rank 2

In the case of

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

we consider the case k = 2 for k_1=1 (q_1 = 1, 0, -1), and k_2 = 1 (q_2 = 1, 0, -1):

$$D_1\times D_1 \to D_2$$



We use the values of CG.

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

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

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

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

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

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

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

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

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

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

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

Therefore we have the following relations.

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

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

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

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

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

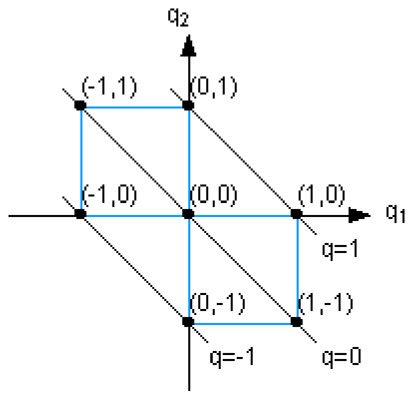
((Note)) we use the commutation relations;

$[\hat{x}, \hat{y}] = 0$, $[\hat{y}, \hat{z}] = 0$, and $[\hat{z}, \hat{x}] = 0$

10 Tensor of rank 1

We consider the case $k = 1$ for $k_1=1$ ($q_1 = 1, 0, -1$), and $k_2 = 1$ ($q_2 = 1, 0, -1$):

$$D_1 \times D_1 \to D_1$$



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

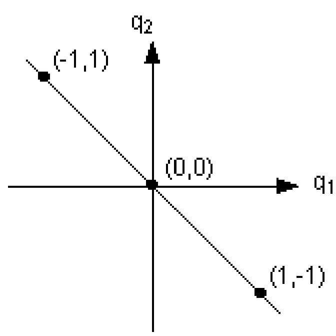
$$T_0^{(1)} = \frac{X_1^{(1)} Z_{-1}^{(1)} - X_{-1}^{(1)} Z_1^{(1)}}{\sqrt{2}} = \frac{U_1 V_{-1} - U_{-1} V_1}{\sqrt{2}}$$

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

11 Tensor of rank 0

We consider the case $k = 0$ for $k_1=1$ ($q_1 = 1, 0, -1$), and $k_2 = 1$ ($q_2 = 1, 0, -1$):

$$D_1 \times D_1 \rightarrow D_0$$



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

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