Vector and Tensor operators in quantum mechanics

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We discuss the properties of vector and tensor operators under rotations in quantum mechanics. We use the analogy from the classical physics, where vector and tensor of a quantity with three components that transforms by definition like

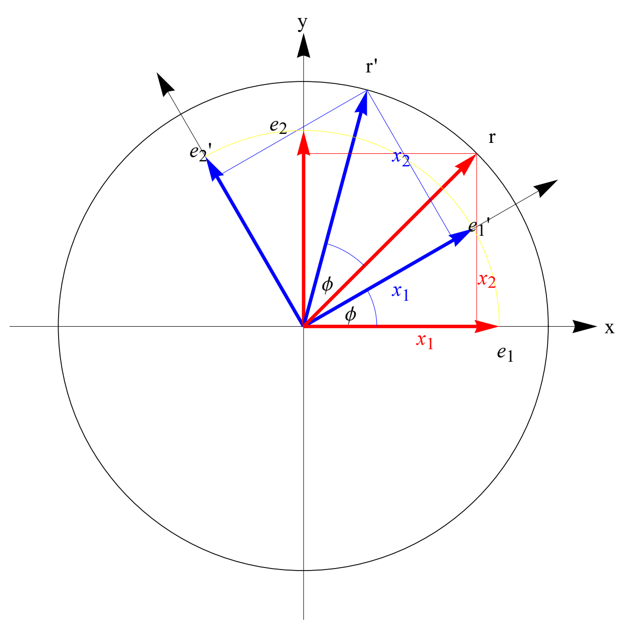
$$V_i' = \sum_j \Re_{ij} V_j \qquad\qquad T_{ij}' = \sum_{k,l} \Re_{ik} \Re_{jl} T_{ikl}$$

under rotation. First I will present a brief review in the case of classical physics. After that the properties of vector and tensor operators under rotation in quantum mechanics. The irreducible spherical tensor operators are introduced based on the rotation operators. The Cartesian tensors are decomposed into irreducible spherical tensors. The Wigner – Eckart theorem will be discussed elsewhere.

1. Definition of vector in classical physics

(i) 2D rotation

Suppose that the vector $\boldsymbol{r}$ is rotated through θ (counter-clock wise) around the z axis. The position vector $\boldsymbol{r}$ is changed into $\boldsymbol{r}'$ in the same orthogonal basis $\{\boldsymbol{e}_1, \boldsymbol{e}_2\}$.



In this Fig, we have

$$\boldsymbol{e}_1 \cdot \boldsymbol{e}_1' = \cos\phi \qquad \mathbf{e}_2 \cdot \mathbf{e}_1' = \sin\phi$$
$$\boldsymbol{e}_1 \cdot \boldsymbol{e}_2' = -\sin\phi\,, \qquad \mathbf{e}_2 \cdot \mathbf{e}_2' = \cos\phi$$

We define $\boldsymbol{r}$ and $\boldsymbol{r}'$ as

$$\boldsymbol{r}' = x_1'\boldsymbol{e}_1 + x_2'\boldsymbol{e}_2 = x_1\boldsymbol{e}_1' + x_2\boldsymbol{e}_2',$$

and

$$\boldsymbol{r} = x_1\boldsymbol{e}_1 + x_2\boldsymbol{e}_2.$$

Using the relation

$$\boldsymbol{e}_1 \cdot \boldsymbol{r}' = \boldsymbol{e}_1 \cdot (x_1'\boldsymbol{e}_1 + x_2'\boldsymbol{e}_2) = \boldsymbol{e}_1 \cdot (x_1\boldsymbol{e}_1' + x_2\boldsymbol{e}_2')$$
$$\boldsymbol{e}_2 \cdot \boldsymbol{r}' = \boldsymbol{e}_2 \cdot (x_1'\boldsymbol{e}_1 + x_2'\boldsymbol{e}_2) = \boldsymbol{e}_2 \cdot (x_1\boldsymbol{e}_1' + x_2\boldsymbol{e}_2')$$

we have

$$x_1' = \mathbf{e}_1 \cdot (x_1\mathbf{e}_1' + x_2\mathbf{e}_2') = x_1\cos\phi - x_2\sin\phi$$
$$x_2' = \mathbf{e}_2 \cdot (x_1\mathbf{e}_1' + x_2\mathbf{e}_2') = x_1\sin\phi + x_2\cos\phi$$

or

$$\begin{pmatrix} x_1' \\ x_2' \end{pmatrix} = \Re(\phi)\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \Re_{11} & \Re_{12} \\ \Re_{21} & \Re_{22} \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

where

$$\Re_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j'$$

(ii) 3D rotation

Next we discuss the three-dimensional (3D) case,

$$\boldsymbol{r} = \sum_{j=1}^{3} x_j\boldsymbol{e}_j, \qquad \boldsymbol{r}' = \sum_{j=1}^{3} x_j'\boldsymbol{e}_j = \sum_{j=1}^{3} x_j\boldsymbol{e}_j'$$

Note that

$$\boldsymbol{e}_i = \sum_j (\boldsymbol{e}_i \cdot \boldsymbol{e}_j')\boldsymbol{e}_j' = \sum_j \Re_{ij}\boldsymbol{e}_j'$$

$$\boldsymbol{e}_i' = \sum_j (\boldsymbol{e}_i' \cdot \boldsymbol{e}_j)\boldsymbol{e}_j = \sum_j (\boldsymbol{e}_j \cdot \boldsymbol{e}_i')\boldsymbol{e}_j = \sum_j \Re_{ji}\boldsymbol{e}_j$$

where

$$\Re_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j'$$

Then we get

$$\boldsymbol{r}' = \sum_{i=1}^{3} x_i' \boldsymbol{e}_i = \sum_{j=1}^{3} x_j \boldsymbol{e}_j' = \sum_{j=1}^{3} x_j \sum_i \Re_{ij} \boldsymbol{e}_i = \sum_{i,j} \Re_{ij} x_j \boldsymbol{e}_i$$

or

$$x_i' = \sum_j \Re_{ij} x_j$$

or

$$\boldsymbol{r}' = \begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix} = \Re_z(\phi)\boldsymbol{r} = \begin{pmatrix} \Re_{11} & \Re_{12} & \Re_{13} \\ \Re_{21} & \Re_{22} & \Re_{23} \\ \Re_{31} & \Re_{32} & \Re_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

where

$$\Re_z(\phi) = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Using the relation $\boldsymbol{r}' = \Re_z(\phi)\boldsymbol{r}$, we can write down

$$\boldsymbol{r}' = \Re_z(\phi)\boldsymbol{r} = \Re_z(\phi)(\sum_{j=1}^{3} x_j \boldsymbol{e}_j) = \sum_{j=1}^{3} x_j \Re_z(\phi) \boldsymbol{e}_j = \sum_{j=1}^{3} x_j \boldsymbol{e}_j'$$

where

$$\Re_z(\phi)\boldsymbol{e}_j = \boldsymbol{e}_j', \qquad \boldsymbol{e}_i \cdot \Re_z(\phi)\boldsymbol{e}_j = \boldsymbol{e}_i \cdot \boldsymbol{e}_j' = \Re_{ij}$$

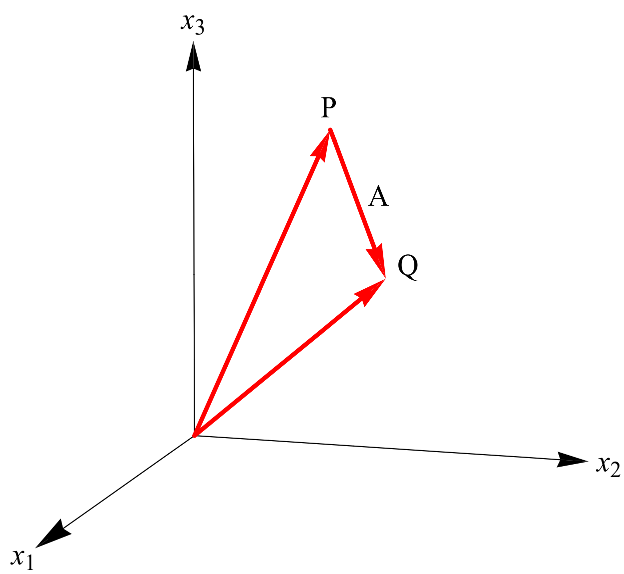
We note that

$$\sum_i \Re_{ij} \Re_{ik} = \sum_i (\boldsymbol{e}_i \cdot \boldsymbol{e}_j')(\boldsymbol{e}_i \cdot \boldsymbol{e}_k') = \boldsymbol{e}_j' \cdot \boldsymbol{e}_k' = \delta_{j,k}$$

since

$$\boldsymbol{e}_j' = \sum_i (\boldsymbol{e}_i \cdot \boldsymbol{e}_j') \boldsymbol{e}_i \qquad \text{(formula)}$$

Now we consider more general case in order to get the definition of vector.



Suppose that

$$\overrightarrow{OP} = \sum_i y_i \boldsymbol{e}_i , \qquad \overrightarrow{OP'} = \sum_i y_i' \boldsymbol{e}_i = \sum_i y_i \boldsymbol{e}_i'$$

$$\overrightarrow{OQ} = \sum_i z_i \boldsymbol{e}_i , \qquad \overrightarrow{OQ'} = \sum_i z_i' \boldsymbol{e}_i = \sum_i z_i \boldsymbol{e}_i'$$

Then we have

$$\boldsymbol{A} = \overrightarrow{PQ} = \overrightarrow{OQ} - \overrightarrow{OP} = \sum_i (z_i - y_i) \boldsymbol{e}_i$$

$$\begin{aligned} \boldsymbol{A}' &= \overrightarrow{P'Q'} = \overrightarrow{OQ'} - \overrightarrow{OP'} \\ &= \sum_i (z_i' - y_i') \boldsymbol{e}_i \\ &= \sum_i (z_i - y_i) \boldsymbol{e}_i' \end{aligned}$$

Since

$$\boldsymbol{e}_j' = \sum_i (\boldsymbol{e}_i \cdot \boldsymbol{e}_j') \boldsymbol{e}_i = \sum_j \Re_{ij} \boldsymbol{e}_i ,$$

the expression of $\boldsymbol{A}$ can be rewritten as

$$\sum_i (z_i' - y_i')\boldsymbol{e}_i = \sum_j (z_j - y_j)\boldsymbol{e}_j' = \sum_{i,j} (z_i - y_i)\Re_{ij}\boldsymbol{e}_i \ .$$

Therefore we get

$$z_i' - y_i' = \sum_j \Re_{ij}(z_j - y_j) \ .$$

Since the component of $\boldsymbol{A}$ is given by

$A_i = z_i - y_i$, and $A_i' = z_i' - y_i'$

in the old and new co-ordinate systems, we can write

$$A_i' = \sum_j R_{ij} A_j \ .$$

We note that

$$\sum_i A_i' \boldsymbol{e}_i = \sum_i A_i \boldsymbol{e}_j'$$

In summary, under the rotation of the co-ordinate system, the components of the vector are transformed through

$$A_i' = \sum_j \Re_{ij} A_j$$

where the vector is a tensor of rank 1. Similarly, the components of the tensor are transformed through

$$T_{ij}' = \sum_j \Re_{ik} \Re_{jl} T_{kl} ,$$ for the tensor of rank 2

and

$$T_{ijk}' = \sum_j \Re_{il} \Re_{jm} \Re_{kn} T_{lmn}$$ for the tensor of rank 3

((Note)) The scalar (tensor of rank 0) is invariant under the rotation.

$$\boldsymbol{A}'\cdot\boldsymbol{B}' = \sum_{i,j} A_i B_j (\boldsymbol{e}_i'\cdot\boldsymbol{e}_j') = \sum_{i,j} A_i B_j \delta_{i,j} = \sum_i A_i B_i = \boldsymbol{A}\cdot\boldsymbol{B}$$

2. Vector operators in quantum mechanics

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

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

Note that $\Re$ is the rotation matrix. For the rotation by the angle θ around the z axis

$$\Re_z(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix},, \qquad a_z(\theta) = \Re_z(-\theta) = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

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 $\hat{\boldsymbol{V}}$ 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

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

((**Note**))
We show that

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

From the relation

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

we get

$$\begin{aligned}
\sum_i \hat{V}_i \Re_{ik} &= \sum_{i,j} \Re_{ij}\Re_{ik}\hat{R}\hat{V}_j\hat{R}^+ \\
&= \sum_j \hat{R}\hat{V}_j\hat{R}^+ \sum_i \Re_{ij}\Re_{ik} \\
&= \sum_j \delta_{jk}\hat{R}\hat{V}_j\hat{R}^+ \\
&= \hat{R}\hat{V}_k\hat{R}^+
\end{aligned}$$

or

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

We now consider a special case, infinitesimal rotation.

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

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

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

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

where

$$\hat{V}_1 = \hat{V}_x, \qquad \hat{V}_2 = \hat{V}_y, \qquad \hat{V}_3 = \hat{V}_z$$

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

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

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

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

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 ε_{ijk}. =0.

((**Example**))

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

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

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 $\hat{\boldsymbol{A}} = \hat{\boldsymbol{r}}$,

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

((**Mathematica**))

Signature[i,j,k], which is equal to the Levi-Civita ε_{ijk}.

((**Note**)) Speherical component
We define the spherical components as

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

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

We note that

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

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

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

We introduce the operators as

$$\hat{V}_{\pm} = \hat{V}_x \pm i\hat{V}_y , \qquad \hat{J}_{\pm} = \hat{J}_x \pm i\hat{J}_y$$

Using the above relation, we get

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

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

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

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

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

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

These relations in turn can be shown to lead to

$$[V_+,\hat{J}_z]=-\hbar\hat{V}_+, \qquad [V_-,\hat{J}_z]=\hbar\hat{V}_-$$

$$[\hat{V}_+,\hat{J}_+]=0, \qquad [\hat{V}_-,\hat{J}_-]=0,$$

$$[\hat{V}_+,\hat{J}_-]=2\hbar\hat{V}_z, \qquad [\hat{V}_-,\hat{J}_+]=-2\hbar\hat{V}_z,$$

Using the above relations, we get

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

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

$$[J_{-1},\hat{V}_{+1}]=\sqrt{2}\hbar\hat{V}_0, \qquad [\hat{J}_+,\hat{V}_{-1}]=\sqrt{2}\hbar\hat{V}_0,$$

These satisfy the following relations

$$[\hat{J}_z,\hat{V}_q]=\hbar q\hat{V}_q$$

$$[\hat{J}_\pm,\hat{V}_q]=\hbar\sqrt{2-q(q\pm1)}\hat{V}_{q\pm1}$$

where $q = 0,\ \pm1$.

3. Example for the spin 1/2 system

We discuss the validity of the above formula for the spin 1/2 system.

The angular momentum operator

$$\hat{J}_x=\frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \qquad \hat{J}_y=\frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \qquad \hat{J}_z=\frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

The rotation operator

$$\hat{R}_x(\theta) = \exp(-\frac{i}{\hbar}\hat{J}_x\theta) = \begin{pmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix},$$

$$\hat{R}_y(\theta) = \exp(-\frac{i}{\hbar}\hat{J}_y\theta) = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}$$

$$\hat{R}_z(\theta) = \exp(-\frac{i}{\hbar}\hat{J}_z\theta) = \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}$$

$$\hat{R}_z^{+}(\theta)\hat{J}_x\hat{R}_z(\theta) = \frac{\hbar}{2}\begin{pmatrix} 0 & e^{i\theta} \\ e^{-i\theta} & 0 \end{pmatrix}$$

$$\hat{R}_z^{+}(\theta)\hat{J}_y\hat{R}_z(\theta) = \frac{\hbar}{2}\begin{pmatrix} 0 & -ie^{i\theta} \\ ie^{-i\theta} & 0 \end{pmatrix}$$

$$\hat{R}_z^{+}(\theta)\hat{J}_z\hat{R}_z(\theta) = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The rotation matrix:

$$\Re_z(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$$\hat{R}_z^{+}(\theta)\hat{J}_x\hat{R}_z(\theta) = \Re_{11}\hat{J}_x + \Re_{12}\hat{J}_y + \Re_{13}\hat{J}_z = \frac{\hbar}{2}\begin{pmatrix} 0 & e^{i\theta} \\ e^{-i\theta} & 0 \end{pmatrix}$$

$$\hat{R}_z^{+}(\theta)\hat{J}_y\hat{R}_z(\theta) = \Re_{21}\hat{J}_x + \Re_{22}\hat{J}_y + \Re_{23}\hat{J}_z = \frac{\hbar}{2}\begin{pmatrix} 0 & -ie^{i\theta} \\ ie^{-i\theta} & 0 \end{pmatrix}$$

$$\hat{R}_z^{+}(\theta)\hat{J}_z\hat{R}_z(\theta) = \Re_{31}\hat{J}_x + \Re_{32}\hat{J}_y + \Re_{33}\hat{J}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

4. Example for the spin 1 system

The angular momentum operator

$$\hat{J}_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \hat{J}_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \qquad \hat{J}_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

The rotation operator

$$\hat{R}_x(\theta) = \exp(-\frac{i}{\hbar}\hat{J}_x\theta) = \begin{pmatrix} \frac{1+\cos\theta}{2} & -\frac{i\sin\theta}{\sqrt{2}} & \frac{-1+\cos\theta}{2} \\ -\frac{i\sin\theta}{\sqrt{2}} & \cos\theta & -\frac{i\sin\theta}{\sqrt{2}} \\ \frac{-1+\cos\theta}{2} & -\frac{i\sin\theta}{\sqrt{2}} & \frac{1+\cos\theta}{2} \end{pmatrix},$$

$$\hat{R}_y(\theta) = \exp(-\frac{i}{\hbar}\hat{J}_y\theta) = \begin{pmatrix} \frac{1+\cos\theta}{2} & -\frac{\sin\theta}{\sqrt{2}} & \frac{1-\cos\theta}{2} \\ \frac{\sin\theta}{\sqrt{2}} & \cos\theta & -\frac{\sin\theta}{\sqrt{2}} \\ \frac{1-\cos\theta}{2} & \frac{\sin\theta}{\sqrt{2}} & \frac{1+\cos\theta}{2} \end{pmatrix}$$

$$\hat{R}_z(\theta) = \exp(-\frac{i}{\hbar}\hat{J}_z\theta) = \begin{pmatrix} e^{-i\theta} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\theta} \end{pmatrix}$$

$$\hat{R}_z^{+}(\theta)\hat{J}_x\hat{R}_z(\theta) = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & e^{i\theta} & 0 \\ e^{-i\theta} & 0 & e^{i\theta} \\ 0 & e^{-i\theta} & 0 \end{pmatrix}$$

$$\hat{R}_z^{+}(\theta)\hat{J}_y\hat{R}_z(\theta) = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -ie^{i\theta} & 0 \\ ie^{-i\theta} & 0 & -ie^{i\theta} \\ 0 & ie^{-i\theta} & 0 \end{pmatrix}$$

$$\hat{R}_z^{+}(\theta)\hat{J}_z\hat{R}_z(\theta) = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

The rotation matrix:

$$\Re_z(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\hat{R}_z^{\ +}(\theta)\hat{J}_x\hat{R}_z(\theta) = \Re_{11}\hat{J}_x + \Re_{12}\hat{J}_y + \Re_{13}\hat{J}_z = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & e^{i\theta} & 0 \\ e^{-i\theta} & 0 & e^{i\theta} \\ 0 & e^{-i\theta} & 0 \end{pmatrix}$$

$$\hat{R}_z^{\ +}(\theta)\hat{J}_y\hat{R}_z(\theta) = \Re_{21}\hat{J}_x + \Re_{22}\hat{J}_y + \Re_{23}\hat{J}_z = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -ie^{i\theta} & 0 \\ ie^{-i\theta} & 0 & -ie^{i\theta} \\ 0 & ie^{-i\theta} & 0 \end{pmatrix}$$

$$\hat{R}_z^{\ +}(\theta)\hat{J}_z\hat{R}_z(\theta) = \Re_{31}\hat{J}_x + \Re_{32}\hat{J}_y + \Re_{33}\hat{J}_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

4 Scalar (tensor of rank zero)

The scalar is invariant under the rotation. In quantum mechanics, we may write

$$\langle\psi'|\hat{\boldsymbol{A}}|\psi'\rangle \cdot \boldsymbol{B}' = \langle\psi|\hat{\boldsymbol{A}}|\psi\rangle.\boldsymbol{B}$$

where $\boldsymbol{B}$ denotes an arbitrary vector and also rotates with the system into the vector $\boldsymbol{B}'$. This can be rewritten as

$$(\hat{R}^+\hat{\boldsymbol{A}}\hat{R}) \cdot \boldsymbol{B}' = \hat{\boldsymbol{A}} \cdot \boldsymbol{B}$$

or

$$\hat{\boldsymbol{A}} \cdot \boldsymbol{B}' = \hat{R}\hat{\boldsymbol{A}}\hat{R}^+ \cdot \boldsymbol{B}$$

Then we have

$$\sum_i \hat{A}_i B_i' = \sum_j (\hat{R}\hat{A}_j\hat{R}^+) B_j$$

Using the relation

$$B_i' = \sum_j \Re_{ij} B_j$$

we get

$$\sum_j (\sum_i \hat{A}_i \Re_{ij}) B_j = \sum_j (\hat{R}\hat{A}_j \hat{R}^+) B_j$$

or

$$\hat{R}\hat{A}_j \hat{R}^+ = \sum_i \hat{A}_i \Re_{ij}$$

5. 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 $\hat{\boldsymbol{U}}$ 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. This Cartesian tensor 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 (corresponding to $j = 0$)

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 (corresponding to $j = 1$).

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

where

$$\hat{A}_{ij} = \frac{\hat{U}_i \hat{V}_j - \hat{U}_j \hat{V}_i}{2}$$

The third term is a 3x3 symmetric traceless tensor with 5 independent components (=6-1), where 1 comes from the traceless condition (corresponding to $j = 2$).

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

with $S_{11} + S_{22} + S_{33} = 0$, where

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

In conclusion, the Cartesian tensor $\hat{T}_{ij} = \hat{U}_i \hat{V}_j$ can be decomposed into irreducible spherical tensors of rank 0, 1, and 2. The Cartesian tensors are not very suitable for studying transformations under rotations, because they are reducible whenever their rank exceeds 1. It is therefore interesting to consider irreducible spherical tensors.

7. Irreducible 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 $Y_l^m(\theta, \phi) = Y_l^m(\boldsymbol{n})$, 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).

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

where

$$Y_l^m(\boldsymbol{n}) \to Y_{l=k}^{m=q}(\hat{\boldsymbol{V}}) = T_k^q(\hat{\boldsymbol{V}})$$

The quantity

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

is a homogeneous polynomial of order l.

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.

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

$$\left|\boldsymbol{n}'\right\rangle = \hat{R}\left|\boldsymbol{n}\right\rangle = \left|\Re\boldsymbol{n}\right\rangle$$

$$\left\langle\boldsymbol{n}'\right| = \left\langle\boldsymbol{n}\right|\hat{R}^{+} = \left\langle\Re\boldsymbol{n}\right|$$

Using the closure relation,

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

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

or

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

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

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

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

from the relation

$$Y_l^m(\boldsymbol{n}') \to \hat{R}^{+}Y_l^m(\hat{\boldsymbol{V}})\hat{R}, \qquad Y_l^{m'}(\boldsymbol{n}) \to Y_l^{m'}(\hat{\boldsymbol{V}})$$

We define a spherical tensor operator of rank k as a set of $2k+1$, $\hat{T}_q^{(k)}$, $q = k, k-1,\ldots, -k$ 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

$$\hat{T}_q^{(k)} = Y_{l=k}^{m=q}(\hat{\mathbf{V}}) \qquad [q = k, k\text{-}1, \ldots.., \text{-}k\text{+}1, \text{-}k; (2k\text{+}1) \text{ components})]$$

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

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

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

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

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

In general, we have

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

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

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

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

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

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

where

$$\hat{J}_\pm | k, q \rangle = \hbar \sqrt{(k \mp q)(k \pm q + 1)} | k, q \pm 1 \rangle$$

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 $\hat{\boldsymbol{V}}$ 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

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

((**Note**))
Using

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

the vector operator $\hat{\boldsymbol{V}}$ van be expressed as

$$\hat{\boldsymbol{V}} = \hat{V}_x\boldsymbol{e}_x + \hat{V}_y\boldsymbol{e}_y + \hat{V}_z\boldsymbol{e}_z = -\hat{V}_{-1}\boldsymbol{u}_1 + \hat{V}_0\boldsymbol{u}_0 - V_1\boldsymbol{u}_{-1} = \sum_{\mu=-1}^{1}(-1)^{\mu}\hat{V}_{-\mu}\boldsymbol{u}_{\mu}$$

where

$$\boldsymbol{u}_1 = -\frac{\boldsymbol{e}_x + i\boldsymbol{e}_y}{\sqrt{2}}, \qquad \boldsymbol{u}_{-1} = \frac{\boldsymbol{e}_x - i\boldsymbol{e}_y}{\sqrt{2}}, \qquad \boldsymbol{u}_0 = \boldsymbol{e}_z.$$

The orthonormality relation of these new unit vectors is

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

Thus the ordinary scalar product of two vectors has the form

$$\hat{\boldsymbol{V}}\cdot\hat{\boldsymbol{W}}=\sum_{\mu,\mu'}(-1)^{\mu+\mu'}\hat{V}_{-\mu}W_{-\mu'}(\boldsymbol{u}_{\mu}\cdot\boldsymbol{u}_{\mu'})$$
$$=\sum_{\mu,}(-1)^{\mu}\hat{V}_{-\mu}W_{\mu}$$
$$=\hat{V}_0\hat{W}_0-(\hat{V}_{+1}\hat{W}_{-1}+\hat{V}_{-1}\hat{W}_{+1})$$

(b) Spherical tensor operator of rank 2

Spherical tensor of rank 2

(i)

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

which corresponds to

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

(ii)

$$P_{2,\pm2}(x,y,z)=r^2Y_2^{\pm2}(\theta,\phi)=\sqrt{\frac{15}{16\pi}}(\frac{x\pm iy}{\sqrt{2}})^2$$

which corresponds to

$$\hat{T}_{\pm2}^{(2)}=\sqrt{\frac{15}{16\pi}}\left(\hat{T}_{\pm1}^{(1)}\right)^2$$

(iii)

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

which corresponds to

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

(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 corresponds to

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

8 Product of tensors (CG)

((**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

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

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

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

(Clebsch-Gordan series)

where

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

or

$$k'' = k_1+k_2, k_1+k_2-1, ..., |k_1-k_2|.$$

Orthogonality of the Clebsch-Gordan coefficient

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

and

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

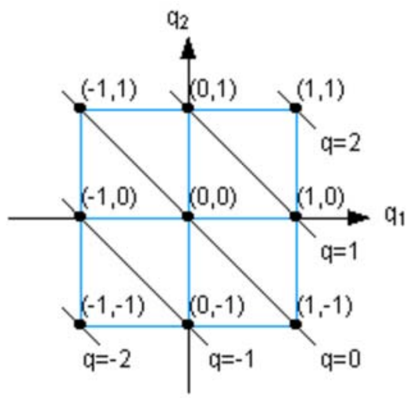
9 Tensor of rank 2 from CG

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.

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

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

$$\hat{T}_0^{(2)} = \frac{\hat{X}_1^{(1)}\hat{Z}_{-1}^{(1)} + 2\hat{X}_0^{(1)}\hat{Z}_0^{(1)} + \hat{X}_{-1}^{(1)}\hat{Z}_1^{(1)}}{\sqrt{6}}$$
$$= \frac{\hat{U}_1\hat{V}_{-1} + 2\hat{U}_0\hat{V}_0 + \hat{U}_{-1}\hat{V}_1}{\sqrt{6}}$$
$$= -\left(\frac{\hat{U}_x\hat{V}_x + \hat{U}_y\hat{V}_y - 2\hat{U}_z\hat{V}_z}{\sqrt{6}}\right)$$
$$= -\frac{1}{\sqrt{6}}(\hat{\mathbf{U}}\cdot\hat{\mathbf{V}} - 3\hat{U}_z\hat{V}_z)$$

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

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

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.

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

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

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

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

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

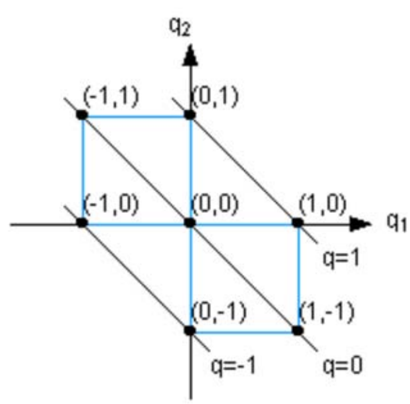
((**Note**)) We use the commutation relations;

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

10 Tensor of rank 1 from CG

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

$$D_1 \times D_1 \to D_1$$



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

$$= \frac{\hat{U}_1 \hat{V}_0 - \hat{U}_0 \hat{V}_1}{\sqrt{2}}$$

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

$$= \frac{1}{2}(\hat{\mathbf{U}} \times \hat{\mathbf{V}})_y + \frac{1}{2i}(\hat{\mathbf{U}} \times \hat{\mathbf{V}})_x$$

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

$$= \frac{\hat{U}_1 \hat{V}_{-1} - \hat{U}_{-1} \hat{V}_1}{\sqrt{2}}$$

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

$$= -\frac{1}{\sqrt{2} i}(\hat{\mathbf{U}} \times \hat{\mathbf{V}})_z$$

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

$$= \frac{\hat{U}_0 \hat{V}_{-1} - \hat{U}_{-1} \hat{V}_0}{\sqrt{2}}$$

$$= \frac{1}{2}(U_z V_x - U_x V_z) - \frac{(\hat{U}_y \hat{V}_z - \hat{U}_z \hat{V}_y)}{2i}$$

$$= \frac{1}{2}(\hat{\mathbf{U}} \times \hat{\mathbf{V}})_y - \frac{1}{2i}(\hat{\mathbf{U}} \times \hat{\mathbf{V}})_x$$

This tensors can be written in terms of its Cartesian components as

$$T_1^{(1)} = -\frac{1}{\sqrt{2}}(C_x + iC_y), \qquad T_{-1}^{(1)} = \frac{1}{\sqrt{2}}(C_x - iC_y)$$

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

Then we get

$$\frac{T_1^{(1)} - T_{-1}^{(1)}}{\sqrt{2}} = -C_x = \frac{(\hat{\mathbf{U}} \times \hat{\mathbf{V}})_x}{\sqrt{2} i}$$

$$\frac{T_1^{(1)} + T_{-1}^{(1)}}{\sqrt{2}i} = -C_y = \frac{(\hat{\boldsymbol{U}} \times \hat{\boldsymbol{V}})_y}{\sqrt{2}i}$$

$$-T_0^{(1)} = -C_z = \frac{(\hat{\boldsymbol{U}} \times \hat{\boldsymbol{V}})_z}{\sqrt{2}i}$$

leading to

$$C_x = i\frac{(\hat{\boldsymbol{U}} \times \hat{\boldsymbol{V}})_x}{\sqrt{2}}, \qquad C_y = i\frac{(\hat{\boldsymbol{U}} \times \hat{\boldsymbol{V}})_y}{\sqrt{2}}, \qquad C_z = i\frac{(\hat{\boldsymbol{U}} \times \hat{\boldsymbol{V}})_z}{\sqrt{2}}$$

or

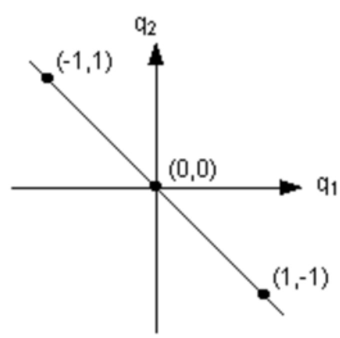
$$\boldsymbol{C} = i\frac{(\hat{\boldsymbol{U}} \times \hat{\boldsymbol{V}})}{\sqrt{2}}$$

This is, up to a factor, nothing but the ordinary vector product.

11 Tensor of rank 0 from CG

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

$$D_1 \times D_1 \rightarrow D_0$$



$$\begin{aligned} T_0^{(0)} &= \frac{X_1^{(1)} Z_{-1}^{(1)} - X_0^{(1)} Z_0^{(1)} + X_{-1}^{(1)} Z_1^{(1)}}{\sqrt{3}} \\ &= \frac{U_1 V_{-1} - U_0 V_0 + U_{-1} V_1}{\sqrt{3}} \\ &= -\frac{1}{\sqrt{3}} (\boldsymbol{U} \cdot \boldsymbol{V}) \end{aligned}$$

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APPENDIX

We consider the rotation operator for the angular momentum $J = \hbar$.

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

We calculate $\hat{R}^+\hat{J}_i\hat{R}$ for i = 1 (*x*), 2 (*y*), and 3(*z*), and compare these with $\sum_j \Re_{ij}\hat{J}_j$

$$\Re_z = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Here we present the calculation for J = 3/2 using the Mathematica program.

((**Mathematica**))

Matrices j = 3/2

```
Clear["Global`*"]; j = 3 / 2;
exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};
Jx[j_, n_, m_] := ħ/2 Sqrt[(j - m) (j + m + 1)] KroneckerDelta[n, m + 1] +
   ħ/2 Sqrt[(j + m) (j - m + 1)] KroneckerDelta[n, m - 1];
Jy[j_, n_, m_] := -ħ/2 ⅈ Sqrt[(j - m) (j + m + 1)] KroneckerDelta[n, m + 1] +
   ħ/2 ⅈ Sqrt[(j + m) (j - m + 1)] KroneckerDelta[n, m - 1];
Jz[j_, n_, m_] := ħ m KroneckerDelta[n, m];
Jx = Table[Jx[j, n, m], {n, j, -j, -1}, {m, j, -j, -1}];
Jy = Table[Jy[j, n, m], {n, j, -j, -1}, {m, j, -j, -1}];
Jz = Table[Jz[j, n, m], {n, j, -j, -1}, {m, j, -j, -1}];

Jx // MatrixForm
```

$$\begin{pmatrix} 0 & \frac{\sqrt{3}\,\hbar}{2} & 0 & 0 \\ \frac{\sqrt{3}\,\hbar}{2} & 0 & \hbar & 0 \\ 0 & \hbar & 0 & \frac{\sqrt{3}\,\hbar}{2} \\ 0 & 0 & \frac{\sqrt{3}\,\hbar}{2} & 0 \end{pmatrix}$$

```
Jy // MatrixForm
```

$$\begin{pmatrix} 0 & -\frac{1}{2} i \sqrt{3}\, \hbar & 0 & 0 \\ \frac{1}{2} i \sqrt{3}\, \hbar & 0 & -i \hbar & 0 \\ 0 & i \hbar & 0 & -\frac{1}{2} i \sqrt{3}\, \hbar \\ 0 & 0 & \frac{1}{2} i \sqrt{3}\, \hbar & 0 \end{pmatrix}$$

```
Jz // MatrixForm
```

$$\begin{pmatrix} \frac{3\hbar}{2} & 0 & 0 & 0 \\ 0 & \frac{\hbar}{2} & 0 & 0 \\ 0 & 0 & -\frac{\hbar}{2} & 0 \\ 0 & 0 & 0 & -\frac{3\hbar}{2} \end{pmatrix}$$

Rotation around the z axis

$$\text{A1z} = \left(\text{MatrixExp}\left[\frac{i}{\hbar}\, \text{Jz}\, \theta\right]\right).\text{Jx}.\left(\text{MatrixExp}\left[-\frac{i}{\hbar}\, \text{Jz}\, \theta\right]\right) \text{ // Simplify;}$$

```
A1z // MatrixForm
```

$$\begin{pmatrix} 0 & \frac{1}{2}\sqrt{3}\, e^{i\theta} \hbar & 0 & 0 \\ \frac{1}{2}\sqrt{3}\, e^{-i\theta} \hbar & 0 & e^{i\theta} \hbar & 0 \\ 0 & e^{-i\theta} \hbar & 0 & \frac{1}{2}\sqrt{3}\, e^{i\theta} \hbar \\ 0 & 0 & \frac{1}{2}\sqrt{3}\, e^{-i\theta} \hbar & 0 \end{pmatrix}$$

```
A2z = MatrixExp[(i/ħ) Jz θ].Jy.MatrixExp[-(i/ħ) Jz θ] // Simplify;
A2z // MatrixForm
```

$$\begin{pmatrix} 0 & -\frac{1}{2} i \sqrt{3}\, e^{i\theta} \hbar & 0 & 0 \\ \frac{1}{2} i \sqrt{3}\, e^{-i\theta} \hbar & 0 & -i\, e^{i\theta} \hbar & 0 \\ 0 & i\, e^{-i\theta} \hbar & 0 & -\frac{1}{2} i \sqrt{3}\, e^{i\theta} \hbar \\ 0 & 0 & \frac{1}{2} i \sqrt{3}\, e^{-i\theta} \hbar & 0 \end{pmatrix}$$

```
A3z = MatrixExp[(i/ħ) Jz θ].Jz.MatrixExp[-(i/ħ) Jz θ] // Simplify;
A3z // MatrixForm
```

$$\begin{pmatrix} \frac{3\hbar}{2} & 0 & 0 & 0 \\ 0 & \frac{\hbar}{2} & 0 & 0 \\ 0 & 0 & -\frac{\hbar}{2} & 0 \\ 0 & 0 & 0 & -\frac{3\hbar}{2} \end{pmatrix}$$

```
Mz = RotationMatrix[θ, {0, 0, 1}]
```

```
{{Cos[θ], -Sin[θ], 0}, {Sin[θ], Cos[θ], 0}, {0, 0, 1}}
```

```
Mz // MatrixForm
```

$$\begin{pmatrix} \cos[\theta] & -\sin[\theta] & 0 \\ \sin[\theta] & \cos[\theta] & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

```
B1z = Mz[[1, 1]] Jx + Mz[[1, 2]] Jy + Mz[[1, 3]] Jz // FullSimplify;
B2z = Mz[[2, 1]] Jx + Mz[[2, 2]] Jy + Mz[[2, 3]] Jz // FullSimplify;
B3z = Mz[[3, 1]] Jx + Mz[[3, 2]] Jy + Mz[[3, 3]] Jz // FullSimplify;
A1z - B1z // Simplify
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
A2z - B2z // FullSimplify
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
A3z - B3z // FullSimplify
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```

Rotation around the y axis

$$A1y = \left(\text{MatrixExp}\left[\frac{i}{\hbar}\,Jy\,\theta\right]\right).Jx.\left(\text{MatrixExp}\left[-\frac{i}{\hbar}\,Jy\,\theta\right]\right) \text{ // Simplify;}$$

```
A1y // MatrixForm
```

$$\begin{pmatrix} \frac{3}{2}\hbar\,\text{Sin}[\theta] & \frac{1}{2}\sqrt{3}\,\hbar\,\text{Cos}[\theta] & 0 & 0 \\ \frac{1}{2}\sqrt{3}\,\hbar\,\text{Cos}[\theta] & \frac{1}{2}\hbar\,\text{Sin}[\theta] & \hbar\,\text{Cos}[\theta] & 0 \\ 0 & \hbar\,\text{Cos}[\theta] & -\frac{1}{2}\hbar\,\text{Sin}[\theta] & \frac{1}{2}\sqrt{3}\,\hbar\,\text{Cos}[\theta] \\ 0 & 0 & \frac{1}{2}\sqrt{3}\,\hbar\,\text{Cos}[\theta] & -\frac{3}{2}\hbar\,\text{Sin}[\theta] \end{pmatrix}$$

```
A2y = MatrixExp[ⅈ/ℏ Jy θ].Jy.MatrixExp[-ⅈ/ℏ Jy θ] // Simplify;
A2y // MatrixForm
```

$$\begin{pmatrix} 0 & -\frac{1}{2} i \sqrt{3}\, \hbar & 0 & 0 \\ \frac{1}{2} i \sqrt{3}\, \hbar & 0 & -i \hbar & 0 \\ 0 & i \hbar & 0 & -\frac{1}{2} i \sqrt{3}\, \hbar \\ 0 & 0 & \frac{1}{2} i \sqrt{3}\, \hbar & 0 \end{pmatrix}$$

```
A3y = MatrixExp[ⅈ/ℏ Jy θ].Jz.MatrixExp[-ⅈ/ℏ Jy θ] // Simplify;
A3y // MatrixForm
```

$$\begin{pmatrix} \frac{3}{2} \hbar \,\mathrm{Cos}[\theta] & -\frac{1}{2} \sqrt{3}\, \hbar \,\mathrm{Sin}[\theta] & 0 & 0 \\ -\frac{1}{2} \sqrt{3}\, \hbar \,\mathrm{Sin}[\theta] & \frac{1}{2} \hbar \,\mathrm{Cos}[\theta] & -\hbar \,\mathrm{Sin}[\theta] & 0 \\ 0 & -\hbar \,\mathrm{Sin}[\theta] & -\frac{1}{2} \hbar \,\mathrm{Cos}[\theta] & -\frac{1}{2} \sqrt{3}\, \hbar \,\mathrm{Sin}[\theta] \\ 0 & 0 & -\frac{1}{2} \sqrt{3}\, \hbar \,\mathrm{Sin}[\theta] & -\frac{3}{2} \hbar \,\mathrm{Cos}[\theta] \end{pmatrix}$$

```
My = RotationMatrix[θ, {0, 1, 0}]; My // MatrixForm
```

$$\begin{pmatrix} \mathrm{Cos}[\theta] & 0 & \mathrm{Sin}[\theta] \\ 0 & 1 & 0 \\ -\mathrm{Sin}[\theta] & 0 & \mathrm{Cos}[\theta] \end{pmatrix}$$

```
B1y = My[[1, 1]] Jx + M[y[1, 2]] Jy + My[[1, 3]] Jz // FullSimplify;
B2y = My[[2, 1]] Jx + My[[2, 2]] Jy + My[[2, 3]] Jz // FullSimplify;
B3y = My[[3, 1]] Jx + My[[3, 2]] Jy + My[[3, 3]] Jz // FullSimplify;
A1y - B1y // Simplify
```

$$\left\{\left\{0, \frac{1}{2} i \sqrt{3}\, \hbar\, M[y[1,2]], 0, 0\right\}, \left\{-\frac{1}{2} i \sqrt{3}\, \hbar\, M[y[1,2]], 0, i \hbar\, M[y[1,2]], 0\right\}, \left\{0, -i \hbar\, M[y[1,2]], 0, \frac{1}{2} i \sqrt{3}\, \hbar\, M[y[1,2]]\right\}, \left\{0, 0, -\frac{1}{2} i \sqrt{3}\, \hbar\, M[y[1,2]], 0\right\}\right\}$$

```
A2y - B2y // FullSimplify
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
A3y - B3y // FullSimplify
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```

Rotation around the x axis

$$A1x = \left(\text{MatrixExp}\left[\frac{i}{\hbar} Jx\, \theta\right]\right).Jx.\left(\text{MatrixExp}\left[-\frac{i}{\hbar} Jx\, \theta\right]\right) \text{ // Simplify;}$$

```
A1x // MatrixForm
```

$$\begin{pmatrix} 0 & \frac{\sqrt{3}\,\hbar}{2} & 0 & 0 \\ \frac{\sqrt{3}\,\hbar}{2} & 0 & \hbar & 0 \\ 0 & \hbar & 0 & \frac{\sqrt{3}\,\hbar}{2} \\ 0 & 0 & \frac{\sqrt{3}\,\hbar}{2} & 0 \end{pmatrix}$$

```
A2x = MatrixExp[ⅈ/ℏ Jx θ].Jy.MatrixExp[-ⅈ/ℏ Jx θ] // Simplify;
A2x // MatrixForm
```

$$\begin{pmatrix} -\frac{3}{2}\hbar\,\mathrm{Sin}[\theta] & -\frac{1}{2} i\sqrt{3}\,\hbar\,\mathrm{Cos}[\theta] & 0 & 0 \\ \frac{1}{2} i\sqrt{3}\,\hbar\,\mathrm{Cos}[\theta] & -\frac{1}{2}\hbar\,\mathrm{Sin}[\theta] & -i\,\hbar\,\mathrm{Cos}[\theta] & 0 \\ 0 & i\,\hbar\,\mathrm{Cos}[\theta] & \frac{1}{2}\hbar\,\mathrm{Sin}[\theta] & -\frac{1}{2} i\sqrt{3}\,\hbar\,\mathrm{Cos}[\theta] \\ 0 & 0 & \frac{1}{2} i\sqrt{3}\,\hbar\,\mathrm{Cos}[\theta] & \frac{3}{2}\hbar\,\mathrm{Sin}[\theta] \end{pmatrix}$$

```
A3x = MatrixExp[ⅈ/ℏ Jx θ].Jz.MatrixExp[-ⅈ/ℏ Jx θ] // Simplify;
A3x // MatrixForm
```

$$\begin{pmatrix} \frac{3}{2}\hbar\,\mathrm{Cos}[\theta] & -\frac{1}{2} i\sqrt{3}\,\hbar\,\mathrm{Sin}[\theta] & 0 & 0 \\ \frac{1}{2} i\sqrt{3}\,\hbar\,\mathrm{Sin}[\theta] & \frac{1}{2}\hbar\,\mathrm{Cos}[\theta] & -i\,\hbar\,\mathrm{Sin}[\theta] & 0 \\ 0 & i\,\hbar\,\mathrm{Sin}[\theta] & -\frac{1}{2}\hbar\,\mathrm{Cos}[\theta] & -\frac{1}{2} i\sqrt{3}\,\hbar\,\mathrm{Sin}[\theta] \\ 0 & 0 & \frac{1}{2} i\sqrt{3}\,\hbar\,\mathrm{Sin}[\theta] & -\frac{3}{2}\hbar\,\mathrm{Cos}[\theta] \end{pmatrix}$$

```
Mx = RotationMatrix[θ, {1, 0, 0}]; Mx // MatrixForm
```

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \mathrm{Cos}[\theta] & -\mathrm{Sin}[\theta] \\ 0 & \mathrm{Sin}[\theta] & \mathrm{Cos}[\theta] \end{pmatrix}$$

```
B1x = Mx[[1, 1]] Jx + Mx[[1, 2]] Jy + Mx[[1, 3]] Jz // FullSimplify;

B2x = Mx[[2, 1]] Jx + Mx[[2, 2]] Jy + Mx[[2, 3]] Jz // FullSimplify;

B3x = Mx[[3, 1]] Jx + Mx[[3, 2]] Jy + Mx[[3, 3]] Jz // FullSimplify;

A1x - B1x // Simplify

{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

A2x - B2x // FullSimplify

{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

A3x - B3x // FullSimplify

{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```