# 31

# Spherical Tensor Operators

From the previous discussion, it is clear it would be advantageous to give vectors, such as $\vec{r}$, not in Cartesian component, but in spherical component form. Recalling

$$\begin{pmatrix} rY_{1+1} \\ rY_{10} \\ rY_{1-1} \end{pmatrix} = \sqrt{\frac{3}{4\pi}} \times \begin{pmatrix} -\frac{1}{\sqrt{2}} r \sin\theta e^{+i\phi} \\ r\cos\theta \\ +\frac{1}{\sqrt{2}} r \sin\theta e^{-i\phi} \end{pmatrix} = \sqrt{\frac{3}{4\pi}} \times \begin{pmatrix} -\frac{1}{\sqrt{2}}(x+iy) \\ z \\ +\frac{1}{\sqrt{2}}(x-iy) \end{pmatrix},$$

it will be useful to write the vector $\vec{r}$ in terms of the spherical components $(r_{+1}, r_0, r_{-1})$, with

$$r_{+1} = -\tfrac{1}{\sqrt{2}}(x+iy), \qquad r_0 = z, \qquad r_{-1} = +\tfrac{1}{\sqrt{2}}(x-iy). \tag{1}$$

Note, in particular, the differences between $r_{+1}$ and $r_+ = (x+iy)$, and $r_{-1}$ and $r_- = (x-iy)$. Before generalizing this vector result to higher rank tensor components in spherical form, let us look at second rank tensors, $T_{ij}$, in Cartesian component form. Write the general second rank tensor in terms of a symmetric, traceless part, $S_{ij}$, an antisymmetric part, $A_{ij}$, and the trace $\sum_\alpha T_{\alpha\alpha}$.

$$\begin{aligned} T_{ij} &= \Big(\tfrac{1}{2}(T_{ij}+T_{ji}) - \tfrac{1}{3}\delta_{ij}\sum_\alpha T_{\alpha\alpha}\Big) + \tfrac{1}{2}(T_{ij}-T_{ji}) + \tfrac{1}{3}\delta_{ij}\sum_\alpha T_{\alpha\alpha} \\ &= S_{ij} + A_{ij} + \tfrac{1}{3}\delta_{ij}\sum_\alpha T_{\alpha\alpha}, \end{aligned} \tag{2}$$

where $S_{ij} = S_{ji}$ and $\sum_\alpha S_{\alpha\alpha} = 0$, and $A_{ij} = -A_{ji}$. Under this decomposition of the nine components of the tensor, the $9 \times 9$ rotation matrix $O_{ij,\alpha\beta}$ that gives the rotated tensor components $T'_{ij}$ in terms of the original $T_{\alpha\beta}$ via

$$T'_{ij} = \sum_{\alpha,\beta} O_{ij,\alpha\beta} T_{\alpha\beta} \tag{3}$$

will split into three submatrices. The five independent components of the traceless, symmetric tensor, $S_{ij}$, transform only among themselves. The three components of the antisymmmetric tensor, $A_{ij}$, will transform only among themselves, and the trace of the tensor is a rotationally invariant quantity. The five independent components of $S_{ij}$ transform like the five components of a spherical harmonic, $Y_{2m}$. The three components of $A_{ij}$ transform like the three components of a vector. We can see this at once if we build the tensor $T_{ij}$ from two vectors $(x, y, z)$ and $(X, Y, Z)$, with $A_{12} = (xY - yX)$, $A_{31} = (zX - xZ)$, and $A_{23} = (yZ - zY)$, where these are the $z$, $y$, and $x$ components of the vector product $\vec{r} \times \vec{R}$. The trace of the tensor transforms like the spherical harmonic $Y_{00}$. We have thus succeeded in finding second rank tensor components that transform like spherical harmonics, with $l = 2$, 1, and 0. As we go to higher rank tensors, this type of decomposition will become more difficult. For example, the 27 components of a third rank tensor will have 10 totally symmetric components. These components could be split further into seven components that transform like spherical harmonics, with $l = 3$, and three components that transform like the three components of a spherical harmonic, with $l = 1$. A single, totally antisymmetric tensor component exists, which is rotationally invariant; i.e., it transforms like a $Y_{00}$. The 16 remaining components of mixed symmetry could be split into two sets of five components that transform like spherical harmonics with $l = 2$ and two sets of three components that transform like spherical harmonics, with $l = 1$.

# A Definition: Spherical Tensors

The set of $(2k + 1)$ components of a spherical tensor $T^k_q$ with $q = +k, (k - 1), \ldots, -k$ and $k =$ integer or $\frac{1}{2}$-integer are a set of $(2k + 1)$ operators that under rotations transform like the components of an angular momentum eigenfunction, $\psi_{kq}$. Recalling $O_{\text{rot.}} = ROR^{-1}$,

$$(T^k_q)_{\text{rot.}} = R(\alpha, \beta, \gamma)T^k_q R^{-1}(\alpha, \beta, \gamma) = \sum_{\nu=-k}^{k} T^k_\nu D^{k*}_{\nu q}(\alpha, \beta, \gamma). \tag{4}$$

# B Alternative Definition

The components of a spherical tensor can also be defined through their commutator relations with the components of the total angular momentum vector of the system on which the tensor components act. In particular,

$$\begin{aligned} [J_0, T^k_q] &= qT^k_q, \\ [J_\pm, T^k_q] &= \sqrt{(k \mp q)(k \pm q + 1)}\,T^k_{(q\pm 1)}, \end{aligned} \tag{5}$$

where this definition essentially just involves infinitesimal rotation operators in place of the finite rotation operators of eq. (4). Let $R$ correspond to an infinitesimal rotation about the $z, x, y$ axes. For example, with

$$R = e^{-i\alpha J_z}, \qquad \text{and with} \qquad \alpha \ll 1, \tag{6}$$

we get

$$\begin{aligned} RT_q^k R^{-1} &= (1 - i\alpha J_z + \cdots)T_q^k(1 + i\alpha J_z + \cdots) = T_q^k - i\alpha[J_z, T_q^k] + \cdots \\ &= \sum_\nu D_{\nu q}^{k*} T_q^k = \delta_{\nu q}(1 - i\alpha q + \cdots)T_q^k, \end{aligned} \tag{7}$$

where we have used

$$D_{\nu q}^{k*} = \langle k\nu | e^{-i\alpha J_z} | kq \rangle = \delta_{\nu q}(1 - i\alpha q + \cdots), \tag{8}$$

thus leading to the first relation, $[J_z, T_q^k] = qT_q^k$. Similarly, combining infinitesimal rotations about the $x$ and $y$ axes, we are lead to the remaining two relations of eq. (5). We can use these relations to show the $r_q$ of eq.(1) are spherical tensor components of rank $k = 1$. We can build higher rank spherical tensors from spherical vectors like these by a build-up process.

## C Build-up Process

If $V_{q_1}^{k_1}$ and $U_{q_2}^{k_2}$ are spherical tensors, $T_q^k$, defined by

$$T_q^k = \sum_{q_1,(q_2)} V_{q_1}^{k_1} U_{q_2}^{k_2} \langle k_1 q_1 k_2 q_2 | kq \rangle, \tag{9}$$

are spherical tensors of rank $k$. This relation follows from

$$\begin{aligned} RT_q^k R^{-1} &= \sum_{q_1,q_2} RV_{q_1}^{k_1} R^{-1} RU_{q_2}^{k_2} R^{-1} \langle k_1 q_1 k_2 q_2 | kq \rangle \\ &= \sum_{q_1,q_2} \sum_{q_1',q_2'} V_{q_1'}^{k_1} U_{q_2'}^{k_2} D_{q_1' q_1}^{k_1 *} D_{q_2' q_2}^{k_2 *} \langle k_1 q_1 k_2 q_2 | kq \rangle \\ &= \sum_j \sum_{q_1' q_2'} V_{q_1'}^{k_1} U_{q_2'}^{k_2} \Big( \sum_{q_1 q_2} \langle k_1 q_1 k_2 q_2 | kq \rangle \langle k_1 q_1 k_2 q_2 | jq \rangle \Big) \langle k_1 q_1' k_2 q_2' | jq' \rangle D_{q'q}^{j*} \\ &= \sum_j \sum_{q_1' q_2'} V_{q_1'}^{k_1} U_{q_2'}^{k_2} \Big( \delta_{jk} \Big) \langle k_1 q_1' k_2 q_2' | jq' \rangle D_{q'q}^{j*} \\ &= \sum_{q_1' q_2'} V_{q_1'}^{k_1} U_{q_2'}^{k_2} \langle k_1 q_1' k_2 q_2' | kq' \rangle D_{q'q}^{k*} = \sum_{q'} T_{q'}^k D_{q'q}^{k*}. \end{aligned} \tag{10}$$

We shall often also use the shorthand notation

$$T_q^k = \sum_{q_1,(q_2)} V_{q_1}^{k_1} U_{q_2}^{k_2} \langle k_1 q_1 k_2 q_2 | kq \rangle \equiv [V^{k_1} \times U^{k_2}]_q^k. \tag{11}$$

Let us now use this build-up process to construct tensors from two vectors each of spherical rank, $l = 1$. Let us choose the coordinate vector of eq. (1), with $r_q = (r_{+1}, r_0, r_{-1})$, and as our second vector, the momentum vector with spherical components $p_q = (p_{+1}, p_0, p_{-1})$, and let us construct the spherical tensors

$$T_q^k = \sum_{q_1 q_2} r_{q_1} p_{q_2} \langle 1q_1 1q_2 | kq \rangle, \tag{12}$$

with $k = 0, 1, 2$. With $k = 0$, using

$$\langle 1q_1 1 - q_1 | 00 \rangle = \frac{1}{\sqrt{3}}(-1)^{1-q_1}, \tag{13}$$

we get

$$\begin{aligned} T_0^0 &= -\frac{1}{\sqrt{3}} \sum_q (-1)^q r_{+q} p_{-q} = -\frac{1}{\sqrt{3}} (\vec{r} \cdot \vec{p}) \\ &= -\frac{1}{\sqrt{3}} \Big( \tfrac{1}{2}(x + iy)(p_x - ip_y) + \tfrac{1}{2}(x - iy)(p_x + ip_y) + zp_z \Big). \end{aligned} \tag{14}$$

Note,

$$(\vec{r} \cdot \vec{p}) = \sum_q (-1)^q r_q^1 p_{-q}^1. \tag{15}$$

We can now generalize this scalar product to the more general scalar product of two tensors of rank $k$,

$$(T^k \cdot T^k) = \sum_m (-1)^m T_m^k T_{-m}^k. \tag{16}$$

We shall continue by constructing next the coupled spherical tensor operator, constructed from the vectors $\vec{r}$ and $\vec{p}$ to make the spherical tensor of rank $l = 1$,

$$T_q^1 = [r^1 \times p^1]_q^1. \tag{17}$$

$$\begin{aligned} T_{+1}^1 &= \langle 1110 | 11 \rangle r_{+1} p_0 + \langle 1011 | 11 \rangle r_0 p_{+1} \\ &= \tfrac{1}{\sqrt{2}} r_{+1} p_0 + (-\tfrac{1}{\sqrt{2}}) r_0 p_{+1} \\ &= -\tfrac{1}{2}(x + iy) p_z + \tfrac{1}{2} z (p_x + ip_y) = \tfrac{i}{\sqrt{2}} \Big( -\tfrac{1}{\sqrt{2}} (L_x + iL_y) \Big). \end{aligned} \tag{18}$$

In general,

$$[r^1 \times p^1]_m^1 = \tfrac{i}{\sqrt{2}} L_m, \qquad \text{with} \quad m = +1, 0, -1. \tag{19}$$

Also, in general,

$$\begin{aligned} [V^1 \times U^1]_{+1}^1 &= \tfrac{1}{2}(V_0 U_+ - V_+ U_0), \\ [V^1 \times U^1]_0^1 &= -\tfrac{1}{2\sqrt{2}}(V_+ U_- - V_- U_+), \\ [V^1 \times U^1]_{-1}^1 &= \tfrac{1}{2}(V_0 U_- - V_- U_0), \end{aligned} \tag{20}$$

where $V_+ = (V_x + iV_y)$, $V_- = (V_x - iV_y)$. Note again the difference from the spherical components $V_{+1} = -\frac{1}{\sqrt{2}} V_+$ and $V_{-1} = +\frac{1}{\sqrt{2}} V_-$. Finally, we build a spherical tensor of rank $l = 2$ from two vectors. The results for the five components are

$$[V^1 \times U^1]_{+2}^2 = \tfrac{1}{2} V_+ U_+,$$

$$
\begin{aligned}
[V^1 \times U^1]^2_{+1} &= -\tfrac{1}{2}(V_0 U_+ + V_+ U_0), \\
[V^1 \times U^1]^2_0 &= -\frac{1}{\sqrt{6}}\Big[\tfrac{1}{2}(V_+ U_- + V_- U_+) - 2V_0 U_0\Big], \\
[V^1 \times U^1]^2_{-1} &= \tfrac{1}{2}(V_0 U_- + V_- U_0), \\
[V^1 \times U^1]^2_{-2} &= \tfrac{1}{2} V_- U_-. \qquad (21)
\end{aligned}
$$