Notes: Tensor Operators

Ben Baragiola

I. VECTORS

We are already familiar with the concept of a vector, but let's review vector properties to refresh ourselves. A 3-component Cartesian vector is

$$\mathbf{v} = v_x \mathbf{e}_x + v_y \mathbf{e}_y + v_z \mathbf{e}_z. \tag{1}$$

Operationally, what makes this a vector is the way it transforms under rotations. General rotations can be specified by Euler angles, but for the sake of simplicity we will consider a rotation by θ around the z-axis, which is represented in the Cartesian basis by the matrix

$$R_z(\theta) = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{2}$$

We use this matrix to rotate $\mathbf{v}$ into a the new, rotated vector denoted by $\mathbf{v}' = v'_x \mathbf{e}_x + v'_y \mathbf{e}_y + v'_z \mathbf{e}_z$. We will use the explicit for of the rotation matrix to write the elements of $\mathbf{v}'$ in terms of those of $\mathbf{v}$ and the angle θ.

$$\mathbf{v}' = R_z(\theta)\mathbf{v} = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = \begin{pmatrix} \cos\theta v_x + \sin\theta v_y \\ -\sin\theta v_x + \cos\theta v_y \\ v_z \end{pmatrix} = \begin{pmatrix} v'_x \\ v'_y \\ v'_z \end{pmatrix}. \tag{3}$$

By definition, the components of a vector transform like

$$v'_i = \sum_j R_{ij} v_j. \tag{4}$$

Let's verify that according to this definition our $\mathbf{v}$ is a vector:

$$v'_x = \sum_j R_{xj} v_j = R_{xx} v_x + R_{xy} v_y + R_{xz} v_z \tag{5}$$

$$= \cos\theta v_x + \sin\theta v_y \tag{6}$$

and one can similarly check the other components to verify that indeed $\mathbf{v}$ is a vector. In quantum mechanics, the rotation *operator* is

$$\mathcal{D}(\mathbf{n}, \theta) = e^{-i\hat{\mathbf{J}}\cdot\mathbf{n}\theta} \tag{7}$$

where $\mathbf{n}$ is the unit vector about which the rotation occurs, and $\hat{\mathbf{J}}$ is the angular momentum **vector operator**, which has operator components that transform according to Eq. (4). A vector operator $\hat{\mathbf{V}}$ is rotated in the following way

$$\mathcal{D}(\mathbf{n}, \theta)^\dagger \hat{\mathbf{V}} \mathcal{D}(\mathbf{n}, \theta) = \sum_j R_{ij} \hat{V}_j \tag{8}$$

To evaluate this, we make use of a property of vector operators

$$[\hat{V}_i, \hat{J}_i] = i\epsilon_{ijk}\hbar \hat{V}_k \tag{9}$$

and the Hadamard lemma

$$e^X Y e^{-X} = Y + [X, Y] + \frac{1}{2!}[X, [X, Y]] + ... \tag{10}$$

Writing out a couple terms in the series for the instructive case of $\mathbf{n} \cdot \hat{\mathbf{J}} = \hat{J}_z$, we recognize quickly that

$$e^{i\hat{J}_z\theta} \hat{V}_x e^{-i\hat{J}_z\theta} = \cos\theta \hat{V}_x + \sin\theta V_y \tag{11}$$

with similar, expected transformations for the other components of $\hat{\mathbf{V}}$.

II. TENSORS

Classically, tensors are defined by the way they transform under rotations. We are primarily concerned with tensors of rank 0 (scalars), rank 1 (vectors), and of rank 2 and we will restrict the discussion to this subset. Scalars do not transform under rotations, vectors transform according to Eq. (4), and rank 2 tensors transform according to

$$T'_{ij} = \sum_{i'j'} R_{ii'} R_{jj'} T_{i'j'}. \tag{12}$$

Rank 2 tensors have two sets of indices each which runs from 1 to 3, so there are nine components. For this reason, they are often represented as matrices. Given a rank 2 tensor $\overleftrightarrow{T}$, let's compute an element of a rotated tensor $\overleftrightarrow{T}'$ where the rotation matrix is around the z-axis as above.

$$\begin{aligned} T'_{xx} =& \sum_{i'j'} R_{xi'} R_{xj'} T_{i'j'} & (13) \\ =& R_{xx}R_{xx}T_{xx} + R_{xx}R_{xy}T_{xy} + R_{xx}R_{xz}T_{xz} \\ &+ R_{xy}R_{xx}T_{yx} + R_{xy}R_{xy}T_{yy} + R_{xy}R_{xz}T_{yz} \\ &+ R_{xz}R_{xx}T_{zx} + R_{xz}R_{xy}T_{zy} + R_{xz}R_{xz}T_{zz} \\ =& \cos^2\theta T_{xx} + \cos\theta\sin\theta(T_{xy} + T_{yx}) + \sin^2 T_{yy} & (14) \end{aligned}$$

Clearly, calculating all 9 elements would be exhaustive but exhausting.

A. Cartesian Tensors

Two vectors, $\mathbf{v}$ and $\mathbf{w}$, expressed in the Cartesian basis $(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$ can be used to create a rank 2 Cartesian tensor $\overleftrightarrow{T}$. It is formed as the *dyad* of the two vectors

$$T_{ij} \equiv v_i w_j \tag{15}$$

and can be expressed as a 3×3 matrix

$$\overleftrightarrow{T} = \begin{pmatrix} v_x w_x & v_x w_y & v_x w_z \\ v_y w_x & v_y w_y & v_y w_z \\ v_z w_x & v_z w_y & v_z w_z \end{pmatrix}. \tag{16}$$

Dyadic Cartesian tensors, such as $\overleftrightarrow{T}$, can be decomposed into *irreducible representations* in the following way

$$\begin{aligned} T_{ij} &= T^{(0)}_{ij} + T^{(1)}_{ij} + T^{(2)}_{ij} & (17) \\ &= \frac{(\mathbf{v}\cdot\mathbf{w})}{3}\delta_{ij} + \frac{(v_i w_j - v_j w_i)}{2} + \left(\frac{v_i w_j + v_j w_i}{2} - \frac{\mathbf{v}\cdot\mathbf{w}}{3}\delta_{ij}\right). & (18) \end{aligned}$$

Each of these irreducible representations has particular properties.

$\overleftrightarrow{T}^{(0)}$ is a rank 0 tensor and transforms under rotations like a scalar. In our matrix representation, it can also be written as the trace of the full, reducible tensor $\overleftrightarrow{T}$

$$T^{(0)} = \frac{1}{3}\,\mathrm{Tr}(\overleftrightarrow{T}) \cdot \mathbb{1} = \frac{1}{3}\begin{pmatrix} \mathbf{v}\cdot\mathbf{w} & 0 & 0 \\ 0 & \mathbf{v}\cdot\mathbf{w} & 0 \\ 0 & 0 & \mathbf{v}\cdot\mathbf{w} \end{pmatrix} \tag{19}$$

where $\mathbf{v}\cdot\mathbf{w} = v_x w_x + v_y w_y + v_z w_z$. $\overleftrightarrow{T}^{(0)}$ has only one independent component.

$\overleftrightarrow{T}^{(1)}$ is a rank 1 tensor and transforms under rotations like a vector. It can be represented as a vector (cross) product $T^{(1)}_{ij} = \frac{1}{2}\epsilon_{ijk}(\mathbf{v}\times\mathbf{w})_k$ and has a matrix representation

$$\overleftrightarrow{T}^{(1)} = \frac{1}{2}\begin{pmatrix} 0 & (v_x w_y - v_y w_x) & (v_x w_z - v_z w_x) \\ -(v_x w_y - v_y w_x) & 0 & (v_y w_z - v_z w_y) \\ -(v_x w_z - v_z w_x) & -(v_y w_z - v_z w_y) & 0 \end{pmatrix}. \tag{20}$$

$\overleftrightarrow{T}^{(1)}$ has three independent components. $\overleftrightarrow{T}^{(2)}$ is a rank 2 tensor and transforms according to Eq. (12). It has the following form in our matrix representation

$$\overleftrightarrow{T}^{(2)} = \begin{pmatrix} v_x w_x - \frac{\mathbf{v}\cdot\mathbf{w}}{3} & \frac{(v_x w_y + v_y w_x)}{2} & \frac{(v_x w_z + v_z w_x)}{2} \\ -\frac{(v_x w_y + v_y w_x)}{2} & v_y w_y - \frac{\mathbf{v}\cdot\mathbf{w}}{3} & \frac{(v_y w_z + v_z w_y)}{2} \\ -\frac{(v_x w_z + v_z w_x)}{2} & -\frac{(v_y w_z + v_z w_y)}{2} & v_z w_z - \frac{\mathbf{v}\cdot\mathbf{w}}{3} \end{pmatrix}. \tag{21}$$

Due to the fact that they are antisymmetric and traceless, $\mathrm{Tr}(\overleftrightarrow{T}^{(2)}) = 0$, irreducible rank 2 tensors have 5 independent entries.

Notice that the number of independent components of $\overleftrightarrow{T}$ is equal to the number of independent components of $\overleftrightarrow{T}^{(0)} + \overleftrightarrow{T}^{(1)} + \overleftrightarrow{T}^{(2)} : 3 \times 3 = 1 + 3 + 5$. In addition, each of the irreducible representations transforms like angular momentum according to its number of independent components.

B. Spherical Tensors

The fact that Cartesian tensors are reducible prompts us to seek out an irreducible set of tensors. A useful set of these are the **spherical tensors**.

1. Spherical Basis

Spherical tensors are defined on a set of basis vectors defined as follows

$$\mathbf{e}_{\pm} = \frac{\mp(\mathbf{e}_x + i\mathbf{e}_y)}{\sqrt{2}}, \qquad \mathbf{e}_0 = \mathbf{e}_z. \tag{22}$$

and we use the letter q to designate an arbitrary spherical basis element. The fact that these are complex will lead to some definitions that may seem strange at first, but arise only to maintain the familiar properties of Cartesian space. The components of a vector $\mathbf{A}$ in the spherical basis are

$$A_q = \mathbf{e}_q \cdot \mathbf{A} \tag{23}$$

so that $\mathbf{A}$ may be decomposed in the spherical basis as

$$\mathbf{A} = \sum_q A_q e_q^* = \sum_q (-1)^q A_q e_{-q} = A_+ \mathbf{e}_+^* + A_0 \mathbf{e}_0 + A_- \mathbf{e}_-^*. \tag{24}$$

The dot product of two vectors has a form that seems unfamiliar, but preserves the norm of a vector $|\mathbf{A}|^2$:

$$\mathbf{A} \cdot \mathbf{B} = -A_+ B_- + A_0 B_0 - A_- B_+ = \sum_q (-1)^q A_q B_{-q} \tag{25}$$

2. Spherical Harmonics

An example of irreducible spherical tensors that will prove quite useful are the spherical harmonics. Recalling the definition of spherical harmonics as the angular representation of the $|l, m\rangle$ angular momentum eigenstates:

$$Y_l^m(\theta, \phi) = \langle \theta, \phi | l, m \rangle = \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} P_l^m(\cos\theta) e^{im\phi} \tag{26}$$

Spherical harmonics are irreducible and transform like tensors of rank k=l, where m indexes the number of unique elements.

C. Formal Definition of Spherical Tensor Operators

Motivated by the above discussion, we define a spherical tensor operator of rank k as a set of 2k+1 operators

$$\hat{T}_q^{(k)} \qquad q = k, k-1 ... -k+1, -k \tag{27}$$

which transform among themselves like 2j+1 angular momentum eigenstates $|j = k, m = q\rangle$ (and thus like spherical harmonics) according to

$$\mathcal{D}(\mathbf{n},\theta)^\dagger \hat{T}_q^{(k)} \mathcal{D}(\mathbf{n},\theta) = \sum_{q'=-k}^{k} \mathcal{D}_{q,q'}^{(k)*}(\theta) T_{q'}^{(k)} \tag{28}$$

where

$$\mathcal{D}_{q,q'}^{(k)*}(\theta) = \langle k, q'| e^{-i\mathbf{n}\cdot\hat{\mathbf{J}}_\mathbf{k}} |k, q\rangle. \tag{29}$$

Now, we are prepared to represent a dyad formed from two vectors **v** and **w** (written in the spherical basis) in terms of irreducible spherical tensors:

$$T_0^{(0)} = \frac{-\mathbf{v}\cdot\mathbf{w}}{2} = \frac{1}{3}(v_1 w_{-1} + v_0 w_0 + v_{-1} w_1) \tag{30}$$

$$T_q^{(1)} = \frac{-(\mathbf{v}\times\mathbf{w})_q}{i\sqrt{2}} \tag{31}$$

$$T_{\pm 2}^{(2)} = v_{\pm 1} w_{\pm 1} \tag{32}$$

$$T_{\pm 1}^{(2)} = \frac{1}{\sqrt{2}}(v_{\pm 1} w_0 + v_0 w_{\pm 1}) \tag{33}$$

$$T_0^{(2)} = \frac{1}{\sqrt{6}}(v_1 w_{-1} + 2 v_0 w_0 + v_{-1} w_1) \tag{34}$$

D. Wigner Eckhart Theorem

Given a spherical tensor operator $T_q^{(k)}$, the Wigner-Eckhart theorem states:

$$\langle \alpha'; j', m'| T_q^{(k)} |\alpha; j, m\rangle = \langle \alpha'; j' || T_q^{(k)} || \alpha; j\rangle \langle j' m' | kq; jm\rangle. \tag{35}$$

Essentially, the theorem says that it is possible to factor the matrix element into a *reduced matrix element* which is independent of m (and thus of any specific geometry) and a Clebsch-Gordan coefficient. The CG coefficients determine the **selection rules**

$$m' = m + q \qquad \text{and} \qquad |j - k| \le j' \le j + k. \tag{36}$$

III. THE DIPOLE OPERATOR

The motivation for the previous sections has been to arrive at a place where we are prepared to discuss the dipole operator $\hat{\mathbf{d}}$ which shows up in the dipole Hamiltonian for the interaction between an atom and an electric field.

$$H_{AF} = -\hat{\mathbf{d}}\cdot\mathbf{E} \tag{37}$$

The dipole operator is related to the position operator $\hat{\mathbf{r}}$ through the charge of the electron:

$$\hat{\mathbf{d}} = -e\hat{\mathbf{r}}. \tag{38}$$

we write down those corresponding to $l = \{0, 1, 2\}$ as they are irreducible representations of corresponding rank:

$$Y_0^0 = \frac{1}{4\pi} \tag{39}$$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos\theta \tag{40}$$

$$Y_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}} \sin\theta e^{\pm i\phi} \tag{41}$$

$$Y_2^0 = \sqrt{\frac{5}{16\pi}} (3\cos^2 - 1) \tag{42}$$

$$Y_2^{\pm 1} = \mp\sqrt{\frac{5}{16\pi}} \sin\theta \cos\theta e^{\pm i\phi} \tag{43}$$

$$Y_2^{\pm 2} = \sqrt{\frac{5}{32\pi}} \sin^2\theta e^{\pm 2i\phi}. \tag{44}$$

Now, we see that the position vector

$$\mathbf{r} = r_x \mathbf{e}_x + r_y \mathbf{e}_y + r_z \mathbf{e}_z \tag{45}$$

$$= r \sin\theta \cos\phi \mathbf{e}_x + r \sin\theta \sin\phi \mathbf{e}_y + r \cos\theta \mathbf{e}_z \tag{46}$$

can be written in the spherical basis (and thus as spherical harmonics):

$$\mathbf{r} = -\frac{r}{\sqrt{2}} \sin\theta e^{i\phi} \mathbf{e}_+^* + r\cos\theta \mathbf{e}_0 + \frac{r}{\sqrt{2}} \sin\theta e^{-i\phi} \mathbf{e}_-^* \tag{47}$$

$$= r\sqrt{\frac{4\pi}{3}} (Y_1^1 \mathbf{e}_+^* + Y_1^0 \mathbf{e}_0 + Y_1^{-1} \mathbf{e}_-^*) \tag{48}$$

with individual components

$$r_q = r\sqrt{\frac{4\pi}{3}} Y_1^q. \tag{49}$$