Comparison of Cartesian and Spherical Vector Operators PhL 1.23.08

See Section 6 for summary of results, then Section 7 for d and D functions.

1. Derivation of the commutation relations for a Cartesian vector operator.

Let **J** = operator and J = 3x3 Cartesian generator matrices. Let

$$R = R_{\hat{\mathbf{n}}}(\theta) \equiv \exp(-i\theta\hat{\mathbf{n}}\bullet\mathbf{J})$$
$$\mathsf{R} = \mathsf{R}_{\hat{\mathbf{n}}}(\theta) \equiv \exp(-i\theta\hat{\mathbf{n}}\bullet\mathsf{J})$$

Then if **V** is a Cartesian vector operator, it must transform as follows:

$$R\mathbf{V}R^{-1} = \mathsf{R}^{-1}\,\mathbf{V}$$

[See "confusion about rotation operators.doc" for details related to this entire section.]

If we apply this to the operator **V** = **J** and examine the first order term in a θ expansion, we learn that

$$[J_i]_{jk} = -i\,\varepsilon_{ijk}$$ // see "confusion about rotation operators.doc "

Then considering this same small rotation for a general vector operator **V**, we learn that

$$[J_i, V_j] = -[J_i V]_j = -[J_i]_{jk}V_k = i\varepsilon_{ijk}V_k$$

so our final result is

$$[J_i, V_j] = i\varepsilon_{ijk}V_k$$

Since **J** itself is an example of a vector operator, we get $[J_i, J_j] = i\varepsilon_{ijk}J_k$.

2. Commutation Relations for a Spherical Operator

In contrast, for a spherical vector operator we have: (j=1)

$$[J_+ , V_{1,m}] = \sqrt{2-m(m+1)}\; V_{1,m+1}$$
$$[J_- , V_{1,m}] = \sqrt{2-m(m-1)}\; V_{1,m-1}$$
$$[J_z , V_{1,m}] = m\, V_{1,m}$$

This is just an example of an irreducible tensor operator, see for example Tinkham bottom p 130.

By adding and subtracting the first two lines, we find that (but I never used these results)

$$[J_x , V_{1,m}] = (1/2)\ \{\sqrt{2\text{-}m(m+1)}\ V_{1,m+1} + \sqrt{2\text{-}m(m-1)}\ V_{1,m-1}\}$$
$$[J_y , V_{1,m}] = (1/2i)\ \{\sqrt{2\text{-}m(m+1)}\ V_{1,m+1} - \sqrt{2\text{-}m(m-1)}\ V_{1,m-1}\}$$
$$[J_z , V_{1,m}] = m\ V_{1,m}$$

3. How do we relate the $V_{1,m}$ to the V_i ? Let's start by *assuming* this:

$$V_{1,0} = V_z$$
$$V_{1,1} = a(V_x + iV_y)$$
$$V_{1,-1} = b(V_x - iV_y)$$

which we can invert to get

$$V_x = (1/2)\ [\ V_{1,1}/a + V_{1,-1}/b\ ]$$
$$V_y = (1/2i)\ [\ V_{1,1}/a - V_{1,-1}/b\ ]$$
$$V_z = V_{1,0}$$

Now define a matrix U such that $V_{1,m} = U_{mk}V_k$. We know that

$$U := \begin{bmatrix} a & Ia & 0 \\ 0 & 0 & 1 \\ b & -Ib & 0 \end{bmatrix}$$

We want U to be unitary which means $U^\dagger U = 1$. If we have Maple compute $U^\dagger$ (called htranspose(U)), we can then multiply and see what we get. When we do this, the conclusion is that U is unitary as long as we have $|a|^2 = |b|^2 = 1/2$. But this does not determine the phase or sign of these numbers, too bad.

4. Here is a way to compute a and b. Start with $[J_i, V_j] = i\varepsilon_{ijk}V_k$. Make linear combinations to find that

$$[J_\pm, V_j] = [\ i\varepsilon_{xjk} \mp \varepsilon_{yjk}]V_k$$

Next, set j=x and insert $V_x = (1/2)\ [\ V_{1,1}/a + V_{1,-1}/b\ ]$ on the left. Then write out as

$$(1/2a)\ [J_\pm, V_{1,1}] + (1/2b)[J_\pm, V_{1,-1}] = \mp\ \varepsilon_{yxk}V_k = \mp\ \varepsilon_{yxz}V_z = \pm\ V_z = \pm V_{1,0}$$

Now go off separately using the spherical operator commutator rules to compute that

$$[J_+, V_{1,1}] = 0$$
$$[J_-, V_{1,1}] = \sqrt{2}\ V_{1,0}$$

$[J_+, V_{1,-1}] = \sqrt{2}\, V_{1,0}$
$[J_-, V_{1,-1}] = 0$

Now from just above we had

$$(1/2a)\,[J_\pm, V_{1,1}] + (1/2b)[J_\pm, V_{1,-1}] = \pm V_{1,0}$$

The upper sign equation says this:

$$(1/2a)\,0 + (1/2b)\sqrt{2}\, V_{1,0} = +V_{1,0} \quad \Rightarrow \quad b = 1/\sqrt{2} \qquad 1/b = \sqrt{2}$$

The lower sign equation says this

$$(1/2a)\,\sqrt{2}\, V_{1,0} + (1/2b)0 = -V_{1,0} \quad \Rightarrow \quad a = -1/\sqrt{2} \qquad 1/a = -\sqrt{2}$$

So if we choose $b = 1/\sqrt{2}$ and $a = -1/\sqrt{2}$, then the two sets of commutators are at least consistent, though we have not proved yet they are completely compatible. At this point then we know this:

$V_{1,0} = V_z$
$V_{1,1} = -1/\sqrt{2}\,(V_x + iV_y)$
$V_{1,-1} = 1/\sqrt{2}\,(V_x - iV_y)$

(which agrees exactly with Tinkham top page 126) which we can invert to get

$V_x = -(1/\sqrt{2})\,[\,V_{1,1} - V_{1,-1}\,]$
$V_y = -(1/\sqrt{2}\, i)\,[\,V_{1,1} + V_{1,-1}\,]$
$V_z = V_{1,0}$

5. Proof that the Cartesian commutators imply the spherical commutators. Now let's start with the Cartesian commutators and prove the spherical ones. We already saw that, starting with the Cartesian commutators, we had

$$[J_\pm, V_j] = [\, i\varepsilon_{xjk} \mp \varepsilon_{yjk}]V_k$$
$$[J_z, V_j] = i\varepsilon_{zjk}V_k$$

which we can write out as:

$$[J_\pm, V_x] = \mp\, \varepsilon_{yxz}]V_z = \pm\, V_z = \pm V_{1,0}$$
$$[J_\pm, V_y] = i\varepsilon_{xyz}V_z = +\, i\, V_z = +i\, V_{1,0}$$
$$[J_\pm, V_z] = [\, i\varepsilon_{xzk} \mp \varepsilon_{yzk}]V_k = i\varepsilon_{xzy}V_y \mp \varepsilon_{yzx}V_x = -\, i\, V_y \mp V_x = \mp(V_x \pm iV_y)$$

$$\text{so } [J_+, V_z] = -(V_x + iV_y) = +\sqrt{2}\, V_{1,1}$$
$$[J_-, V_z] = +(V_x - iV_y) = +\sqrt{2}\, V_{1,-1}$$

which we summarize here

$$[J_\pm, V_x] = \pm V_{1,0}$$
$$[J_\pm, V_y] = +i\, V_{1,0}$$
$$[J_\pm, V_z] = +\sqrt{2}\, V_{1,\pm 1}$$

We want to show ALL the spherical commutators, and here they all are:

$$[J_+, V_{1,m}] = \sqrt{2\text{-}m(m+1)}\, V_{1,m+1}$$
$$[J_-, V_{1,m}] = \sqrt{2\text{-}m(m-1)}\, V_{1,m-1}$$
$$[J_z, V_{1,m}] = m\, V_{1,m}$$

and now we write them all out

1 $[J_+, V_{1,1}] = 0$
2 $[J_-, V_{1,1}] = \sqrt{2}\, V_{1,0}$

3 $[J_+, V_{1,-1}] = \sqrt{2}\, V_{1,0}$
4 $[J_-, V_{1,-1}] = 0$

5 $[J_+, V_{1,0}] = \sqrt{2}\, V_{1,1}$
6 $[J_-, V_{1,0}] = \sqrt{2}\, V_{1,-1}$

7 $[J_z, V_{1,m}] = m\, V_{1,m}$

Now we prove each one of these to be true:

1. $[J_+, V_{1,1}] = [J_+, -1/\sqrt{2}\,(V_x + iV_y)] = -1/\sqrt{2}\ \ [J_+, V_x + iV_y] = (-1/\sqrt{2})\,\{ V_{1,0} + i\, iV_{1,0} \} = 0$

2. $[J_-, V_{1,1}] = [J_-, -1/\sqrt{2}\,(V_x + iV_y)] = -1/\sqrt{2}\,[J_-, V_x + iV_y] = (-1/\sqrt{2})\{ - V_{1,0} + i\ i\, V_{1,0}\} = \sqrt{2}\, V_{1,0}$

3. $[J_+, V_{1,-1}] = [J_+, 1/\sqrt{2}\,(V_x - iV_y)] = 1/\sqrt{2}\ \ [J_+, V_x - iV_y] = (1/\sqrt{2})\,\{ V_{1,0} - i\, iV_{1,0} \} = \sqrt{2}\, V_{1,0}$

4. $[J_-, V_{1,-1}] = [J_-, 1/\sqrt{2}\,(V_x - iV_y)] = 1/\sqrt{2}\,[J_-, V_x - iV_y] = (1/\sqrt{2})\{ - V_{1,0} - i\ i\, V_{1,0}\} = 0$

5. $[J_+, V_{1,0}] = [J_+, V_z] = +\sqrt{2}\, V_{1,1}$

6. $[J_-, V_{1,0}] = [J_-, V_z] = \sqrt{2}\, V_{1,-1}$

7a. $[J_z , V_{1,1}] = [J_z , -1/\sqrt{2}\,(V_x + iV_y)] = -1/\sqrt{2}\;\; [J_z, V_x + iV_y] = (-1/\sqrt{2})\,\{ iV_y + i\,[-iV_x] \}$
$= (-1/\sqrt{2})\{V_x + iV_y\} = + V_{1,1}$

7b. $[J_z , V_{1,-1}] = [J_z , 1/\sqrt{2}\,(V_x - iV_y)] = 1/\sqrt{2}\;\; [J_z, V_x - iV_y] = (1/\sqrt{2})\,\{ iV_y - i\,[-iV_x] \}$
$= (1/\sqrt{2})\{-V_x + iV_y\} = -(1/\sqrt{2})\{V_x - iV_y\} = - V_{1,-1}$

7c. $[J_z , V_{1,0}] = [J_z , V_z] = 0.$

6. Summary of all of the above:

The commutation relations for the Cartesian vector operator is given by (indices = x,y or z)

$[J_i, V_j] = i\varepsilon_{ijk} V_k$ // for proof see section 1 above,

The commutation relations for the Spherical vector operator is given by (m = 1, 0 and -1)

$[J_+ , V_{1,m}] = \sqrt{2\text{-}m(m+1)}\; V_{1,m+1}$
$[J_- , V_{1,m}] = \sqrt{2\text{-}m(m-1)}\; V_{1,m-1}$
$[J_z , V_{1,m}] = m\, V_{1,m}$

The two sets of commutators agree with each other if we assume this relationship between the two sets of vector operators:

$V_{1,0} = V_z$
$V_{1,1} = -1/\sqrt{2}\,(V_x + iV_y)$
$V_{1,-1} = 1/\sqrt{2}\,(V_x - iV_y)$

(which agrees exactly with Tinkham top page 126) which we can invert to get

$V_x = -(1/\sqrt{2})\;[\, V_{1,1} - V_{1,-1}\,]$
$V_y = -(1/\sqrt{2}\, i)\,[\, V_{1,1} + V_{1,-1}\,]$
$V_z = V_{1,0}$

Now define a matrix U such that $V_{1,m} = U_{mk} V_k$. We know that

$$U := \begin{bmatrix} a & Ia & 0 \\ 0 & 0 & 1 \\ b & -Ib & 0 \end{bmatrix}$$

where I means i, and where $a = -1/\sqrt{2}$ and $b = 1/\sqrt{2}$. This matrix is unitary since $U^{\dagger}U = 1$ so we can claim that our two sets of vector operators are connected by this unitary transformation. We can write this out as

$$U = \begin{pmatrix} -\frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 \end{pmatrix}$$

In our demonstration of these facts claimed above, we ran into the following commutators which to some degree cross over between the two sets of operators, and some do not:

$$[J_{\pm}, V_j] = [\, i\varepsilon_{xjk} \mp \varepsilon_{yjk}]V_k$$

$$[J_{\pm}, V_x] = \pm V_{1,0}$$
$$[J_{\pm}, V_y] = +i\, V_{1,0}$$
$$[J_{\pm}, V_z] = +\sqrt{2}\, V_{1,\pm 1}$$

1 $[J_{+}, V_{1,1}] = 0$
2 $[J_{-}, V_{1,1}] = \sqrt{2}\, V_{1,0}$

3 $[J_{+}, V_{1,-1}] = \sqrt{2}\, V_{1,0}$
4 $[J_{-}, V_{1,-1}] = 0$

5 $[J_{+}, V_{1,0}] = \sqrt{2}\, V_{1,1}$
6 $[J_{-}, V_{1,0}] = \sqrt{2}\, V_{1,-1}$

7 $[J_z\, , V_{1,m}] = m\, V_{1,m}$

7. Connection between the Cartesian rotation matrices and the D and d functions .

In the Cartesian basis, the rotation matrix is given as $R = R_{\hat{n}}(\theta) \equiv \exp(-i\theta\hat{\mathbf{n}}\bullet J)$ where $[J_i]_{jk} = -i\, \varepsilon_{ijk}$. But in the Spherical Basis, we express the same rotation in Euler Angles α,β,γ and the rotation matrix is then given by $D^{(1)}(\alpha,\beta,\gamma)$ as shown on Tinkham page 111. Although I have not followed through on the details, one would make this guess:

$D^{(1)}(\alpha,\beta,\gamma) = u\, R\, u^{-1}$ where u is some unitary matrix

Let's show that this is in fact the case. We have,

$$D^{(1)}(\alpha,\beta,\gamma)_{m'm} = \langle 1m'|\, R_z(\alpha)R_y(\beta)R_z(\gamma)|1m\rangle = \exp(-im'\alpha - im\gamma)\, \langle 1m'|\, R_y(\beta)|1m\rangle$$

We can make these state relations:

$V_{1,m} = U_{mk} V_k$ meaning that $\langle 1,m \mid V\rangle = U_{mk} \langle k|V\rangle$ or

$|1,m\rangle = U_{mk}^{*} |k\rangle = |k\rangle U_{km} \Rightarrow \langle k|1,m\rangle = U_{km} \Rightarrow \langle 1,m|k\rangle = U_{km}^{*} = U^{\dagger}_{mk}$

We then have $D^{(1)}(0,\beta,0)_{m'm} = d^{(1)}(\beta)_{m'm} = \langle 1m'| R_y(\beta)|1m\rangle$

$= \langle 1m'|k\rangle\langle k| R_y(\beta)|j\rangle\langle j|1m\rangle = U^{\dagger}_{m'k} \langle k| R_y(\beta)|j\rangle U_{jm}$

$= U^{\dagger}_{m'k} R_y(\beta)_{kj} U_{jm} = [U^{\dagger} R_y(\beta) U]_{m'm}$

The conclusion is that

$d^{(1)}(\beta) = U^{-1} R_y(\beta) U$

$D^{(1)}(\alpha,\beta,\gamma) = U^{-1} R_z(\alpha) R_y(\beta) R_z(\gamma) U$

and similarly,

$R_y(\beta) = U d^{(1)}(\beta) U^{-1}$

$R_z(\alpha) R_y(\beta) R_z(\gamma) = U D^{(1)}(\alpha,\beta,\gamma) U^{-1}$

I don't think this is of any immediate use to me, but a good fact to understand.