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On the summations involving Wigner rotation matrix elements

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Two new methods to evaluate the sums over magnetic quantum numbers, together with Wigner rotation matrix elements, are formulated. The first is the coupling method which makes use of the coupling of Wigner rotation matrix elements. This method gives rise to a closed form for any kind of summation that involves a product of *two* Wigner rotation matrix elements. The second method is the equivalent operator method, for which a closed form is also obtained and easily implemented on the computer. A few examples are presented, and possible extensions are indicated. The formulae obtained are useful for the study of the angular distribution of the photofragments of diatomic and symmetric-top molecules caused by electric-dipole, electric-quadrupole and two-photon radiative transitions.

1. Introduction

Recently, we discussed [5,6] a number of summations involving Wigner rotation matrix elements which are needed for the angular distribution of photofragments caused by dissociative electric-dipole, electric-quadrupole and two-photon radiative transitions. The basic method previously employed involved the use of the recurrence relations of the Wigner rotation matrix elements. In the following, we report two alternative methods: (i) the coupling operator method [4,7], and (ii) the equivalent operator method. As illustrations, we shall use these methods to perform three kinds of summations.

2. The coupling method

From the coupling rule of the Wigner rotation matrix elements, we obtain the first kind of summation [4,7]:

$$\sum_m (-)^m \begin{pmatrix} j & j & j_3 \\ m & \overline{m} & 0 \end{pmatrix} \left|d^j_{m'm}(\beta)\right|^2 = (-)^{m'} \begin{pmatrix} j & j & j_3 \\ m & \overline{m} & 0 \end{pmatrix} P_{j_3}(\cos\beta), \qquad (1)$$

where $\binom{\cdots}{\cdots}$ are Wigner $3-j$ symbols, $P_j(\cos\beta)$ is a Legendre polynomial, and $j_3 = 0, 1, 2, \ldots, 2j$. This closed form is useful in dealing with the following prototypical summation:

$$\sum_m m^k \left|d^j_{m'm}(\beta)\right|^2, \tag{2}$$

for which k can assume the values $0, 1, 2, \ldots, 2j$. From equation (1) it is found that

$$\sum_m m^2 \left|d^j_{m'm}(\beta)\right|^2 = \frac{1}{3} j(j+1) - \frac{1}{3}\left[j(j+1) - 3m'^2\right] P_2(\cos\beta), \tag{2a}$$

$$\sum_m m^3 \left|d^j_{m'm}(\beta)\right|^2 = \frac{1}{5}(3j^2+3j-1)m' \cos\beta - \frac{1}{5}\left[(3j^2+3j-1) - 5m'^2\right] m' P_3(\cos\beta), \tag{2b}$$

$$\begin{aligned}\sum_m m^4 \left|d^j_{m'm}(\beta)\right|^2 &= \frac{1}{15} j(j+1)(3j^2+3j-1) \\ &\quad - \frac{1}{21}(6j^2+6j-5)\left[j(j+1) - 3m'^2\right] P_2(\cos\beta) \\ &\quad + \frac{1}{35}\left[3j(j+1)(j+2)(j-1) - 5(6j^2+6j-5)m'^2 + 35m'^4\right] \\ &\quad \times P_4(\cos\beta),\end{aligned} \tag{2c}$$

$$\begin{aligned}&\sum_m \left\{15j^2(j+1)^2 - 50j(j+1) - 70j(j+1)m^2 + 63m^4 + 105m^2 + 12\right\} \\ &\quad \times m\left|d^j_{m'm}(\beta)\right|^2 = \left\{15j^2(j+1)^2 - 50j(j+1) - 70j(j+1)m'^2\right. \\ &\qquad \left. + 63m'^4 + 105m'^2 + 12\right\} m' P_5(\cos\beta)\end{aligned} \tag{2d}$$

and

$$\begin{aligned}&\sum_m \left\{-5j^3(j+1)^3 + 105j^2(j+1)^2 m^2 - 315j(j+1)m^4 + 231m^6 + 40j^2(j+1)^2\right. \\ &\quad \left. - 525j(j+1)m^2 + 735m^4 - 60j(j+1) + 294m^2\right\} \left|d^j_{m'm}(\beta)\right|^2 \\ &= \left\{-5j^3(j+1)^3 + 105j^2(j+1)^2 m'^2 - 315j(j+1)m'^4 + 231m'^6 + 40j^2(j+1)^2\right. \\ &\quad \left. - 525j(j+1)m'^2 + 735m'^4 - 60j(j+1) + 294m'^2\right\} P_6(\cos\beta).\end{aligned} \tag{2e}$$

Equations (2d) and (2e) can be reduced to the following closed forms:

$$\begin{aligned}\sum_m m^5 \left|d^j_{m'm}(\beta)\right|^2 &= \frac{1}{63}\left\{\left[15j^2(j+1)^2 - 50j(j+1) + 12\right]\right. \\ &\quad \left. - 35\left[2j(j+1) - 3\right] m'^2 + 63m'^4\right\} m' P_5(\cos\beta) \\ &\quad + \frac{1}{9}\left[2j(j+1) - 3\right]\left\{(3j^2+3j-1)m' P_1(\cos\beta)\right.\end{aligned}$$

$$- \big[(3j^2+3j-1) - 5m'^2\big] m' P_3(\cos\beta)\big\}$$
$$- \frac{1}{63}\big[15j^2(j+1)^2 - 50j(j+1) + 12\big] m' P_1(\cos\beta) \quad \text{(3a)}$$

and

$$\sum_m m^6 \big|d^j_{m'm}(\beta)\big|^2 = \frac{1}{21} j(j+1)(3j^4+6j^3-3j+1)$$
$$- \frac{1}{21}\big[j(j+1) - 3m'^2\big]\big[5j(j+1)(j-1)(j+2)+7\big] P_2(\cos\beta)$$
$$+ \frac{1}{77}\big[3j(j+1)-7\big]\big[3j(j+1)(j-1)(j+2)$$
$$- 5(6j^2+6j-5)m'^2 + 35m'^4\big] P_4(\cos\beta)$$
$$+ \frac{1}{231}\big\{-5(j-2)(j-1)j(j+1)(j+2)(j+3)$$
$$+ 21\big[5j^2(j+1)^2 - 25j(j+1) + 14\big] m'^2$$
$$- 105\big[3j(j+1)-7\big] m'^4 + 231m'^6\big\} P_6(\cos\beta), \quad \text{(3b)}$$

respectively.

The coupling rule may also be used to obtain the second kind of summation:

$$\sum_m (-)^m \begin{pmatrix} j+k & j-k & j_3 \\ \overline{m} & m & 0 \end{pmatrix} d^{j+k}_{m'm}(\beta) d^{j-k}_{m'm}(\beta)$$
$$= (-)^{m'} \begin{pmatrix} j+k & j-k & j_3 \\ \overline{m}' & m' & 0 \end{pmatrix} P_{j_3}(\cos\beta), \quad \text{(4)}$$

where $j_3 = 2k, 2k+1, \ldots, 2j$ and $k = 0, 1/2, 1, \ldots, j$. This equation can be reduced to [4,7]

$$\sum_m \sum_L (-)^{L-m} \sqrt{\big[(j+k)^2 - m^2\big]\big[(j-k)^2 - m^2\big]} \binom{2k+j_3}{L} \binom{2j-j_3}{j+k+m-L}$$
$$\times \binom{j_3-2k}{j_3-L} d^{j+k}_{m'm}(\beta) d^{j-k}_{m'm}(\beta)$$
$$= \sum_L (-)^{L-m'} \sqrt{\big[(j+k)^2 - m'^2\big]\big[(j-k)^2 - m'^2\big]} \binom{2k+j_3}{L} \binom{2j-j_3}{j+k+m'-L}$$
$$\times \binom{j_3-2k}{j_3-L} P_{j_3}(\cos\beta), \quad \text{(5)}$$

where $\binom{\cdots}{\cdots}$ are binomial coefficients.

A third kind of summation that can be obtained by this coupling method is

$$\sum_m (-)^m \begin{pmatrix} j+k & j & j_3 \\ \overline{m} & m & 0 \end{pmatrix} d^{j+k}_{m'm}(\beta) d^j_{m'm}(\beta) = (-)^{m'} \begin{pmatrix} j+k & j & j_3 \\ \overline{m}' & m' & 0 \end{pmatrix} P_{j_3}(\cos\beta). \tag{6}$$

In summary, the general coupling form is given by [4,2]

$$\sum_{m_1}\sum_{m_2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} D^{j_1}_{m'_1 m_1}(\alpha\beta\gamma) D^{j_2}_{m'_2 m_2}(\alpha\beta\gamma) = \begin{pmatrix} j_1 & j_2 & j_3 \\ m'_1 & m'_2 & m'_3 \end{pmatrix} D^{j_3^*}_{m'_3 m_3}(\alpha\beta\gamma), \tag{7}$$

where

$$D^j_{m'm}(\alpha\beta\gamma) \equiv \mathrm{e}^{\mathrm{i}m'\alpha} d^j_{m'm}(\beta) \mathrm{e}^{\mathrm{i}m\gamma}. \tag{8}$$

3. The equivalent operator method

We shall deal with the first kind of summation by using the so-called equivalent operator method. From the definition [3,5]

$$d^j_{m'm}(\beta) \equiv \langle jm' | \mathrm{e}^{\mathrm{i}\beta J_y} | jm \rangle, \tag{9}$$

we begin by deriving an equality. For two noncommuting operators A and B, we have, by using the Baker–Campbell–Hausdorff identity, followed by the Taylor expansion,

$$B' = \mathrm{e}^{\mathrm{i}\lambda A} B \mathrm{e}^{-\mathrm{i}\lambda A} = \mathrm{e}^{\mathrm{i}\lambda \mathcal{A}} B = \sum_{k=0}^{\infty} \frac{(\mathrm{i}\lambda)^k}{k!} \mathcal{A}^k B, \tag{10}$$

in which $\mathcal{A}^k B$ denotes the kth degree nested commutator,

$$\mathcal{A}^k B = \big[A, \big[A, [A, \ldots [A, B], \ldots]\big]\big]. \tag{11}$$

Under a similarity transformation, $A = A^\dagger$, and the operators B and B' are said to be equivalent. For example, the Cartesian components of a rotational angular momentum obey the commutation relations

$$[J_x, J_y] = \mathrm{i}J_z, \qquad [J_y, J_z] = \mathrm{i}J_x, \qquad [J_z, J_x] = \mathrm{i}J_y. \tag{12}$$

Using equation (10), we have the equivalent-operator equality

$$\mathrm{e}^{\mathrm{i}\alpha J_x} J_z \mathrm{e}^{-\mathrm{i}\alpha J_x} = J_z \cos\alpha + J_y \sin\alpha, \tag{13}$$

where α is the angle of rotation with respect to the x-axis.

Similarly, we may obtain a useful equivalent-operator equality

$$\mathrm{e}^{\mathrm{i}\beta J_y} J_z \mathrm{e}^{-\mathrm{i}\beta J_y} = J_z \cos\beta - J_x \sin\beta. \tag{14}$$

An alternative geometrical interpretation of equations (10), (13) and (14) is given in the appendix. Here, the similarity transformation of J_z has been reduced to explicit forms which are more convenient for operating upon rotational wave functions.

We now give examples of the usefulness of equation (14) for the evaluation of summations of the first kind.

Example (1)

$$\begin{aligned}\sum_m m\left|d^j_{m'm}(\beta)\right|^2 &= \sum_m \left\langle jm'\middle|\mathrm{e}^{\mathrm{i}\beta J_y} J_z\middle|jm\right\rangle\left\langle jm\middle|\mathrm{e}^{-\mathrm{i}\beta J_y}\middle|jm'\right\rangle \\ &= \left\langle jm'\middle|\mathrm{e}^{\mathrm{i}\beta J_y} J_z \mathrm{e}^{-\mathrm{i}\beta J_y}\middle|jm'\right\rangle \\ &= \left\langle jm'\middle|J_z\cos\beta - J_x\sin\beta\middle|jm'\right\rangle = m'\cos\beta. \end{aligned}\tag{15}$$

Here, we have used the resolution of the identity for the jth irreducible vector space of $O^+(3)$, viz.

$$\sum_m |jm\rangle\langle jm| = 1, \tag{16a}$$

along with the identities

$$J_x = \frac{1}{2}(J_+ + J_-) \quad \text{and} \quad \langle jm'|J_\pm|jm'\rangle = 0. \tag{16b}$$

Example (2)

$$\begin{aligned}\sum_m m^2\left|d^j_{m'm}(\beta)\right|^2 &= \left\langle jm'\middle|(J_z\cos\beta - J_x\sin\beta)^2\middle|jm'\right\rangle \\ &= \frac{1}{2}j(j+1)\sin^2\beta + \frac{m'^2}{2}(3\cos\beta - 1). \end{aligned}\tag{17}$$

Example (3)

$$\begin{aligned}\sum_m m^3\left|d^j_{m'm}(\beta)\right|^2 &= \left\langle jm'\middle|(J_z\cos\beta - J_x\sin\beta)^3\middle|jm'\right\rangle \\ &= m'^3\cos\beta + \frac{m'}{2}\sin^2\beta\cos\beta\left[3j(j+1) - 5m'^2 - 1\right]. \end{aligned}\tag{18}$$

Equations (15), (17) and (18) agree with the results obtained by using the recurrence relations [4,5,7]. We note that for the equivalent operator method the powers of the expression $(J_z \cos\beta - J_x \sin\beta)$ are expressible as a symmetric sum, i.e.,

$$(J_z \cos\beta - J_x \sin\beta)^n = \sum_{k=0}^{n} (-)^k \{(J_z \cos\beta)^{n-k}(J_x \sin\beta)^k\}, \tag{19}$$

where the brackets occurring in the right-hand side indicate the symmetric sum of the product contained therein. Notice that in the previous section we have considered the angular momentum operators and the functions, $\sin\beta$ and $\cos\beta$ to be independent of each other. Thus, they commute and we may write equation (19) as

$$(J_z \cos\beta - J_x \sin\beta)^n = \sum_{k=0}^{n} (\cos\beta)^k (-\sin\beta)^{n-k} \{J_x^{n-k} J_z^k\}. \tag{20}$$

For each given term in the summation on the right-hand side there are $n!/(k!(n-k)!)$ terms that arise from the expansion of the symmetric sum. It is convenient to have an expression for this expansion. By induction,

$$\begin{aligned}
\{J_x^{n-1} J_z\} &= \sum_{r_1=0}^{n-1} \left(J_x^{r_1} J_z\right) J_x^{n-1-r_1}, \\
\{J_x^{n-2} J_z^2\} &= \sum_{r_1=0}^{n-2} \left(J_x^{r_1} J_z\right) \sum_{r_2=0}^{n-2-r_1} \left(J_x^{r_2} J_z\right) J_x^{n-2-r_1-r_2}, \\
&\vdots \\
\{J_x^{n-k} J_z^k\} &= \sum_{r_1=0}^{n-k} \left(J_x^{r_1} J_z\right) \sum_{r_2=0}^{n-k-\sigma(1)} \left(J_x^{r_2} J_z\right) \sum_{r_3=0}^{n-k-\sigma(2)} \left(J_x^{r_3} J_z\right) \\
&\quad \times \sum_{r_k=0}^{n-k-\sigma(k-1)} \left(J_x^{k} J_z^{r}\right) J_x^{n-k-\sigma(k)},
\end{aligned} \tag{21}$$

in which

$$\sigma(k) = \sum_{i=1}^{k} r_i. \tag{22}$$

In order to evaluate the various types of summations, we have need only of the diagonal parts of the symmetric sums. Since J_z is already a diagonal operator in the basis $\{|jm\rangle\}$, it behooves us to consider the diagonal parts of powers of J_x. For an operator J_x^p, diagonal parts arise solely from $p =$ even integer $= 2q$, and we may express them as

$$\left(J_x^{2q}\right)_{\text{diag}} = \frac{1}{2^{2q}} \{J_+^q J_-^q\}, \tag{23}$$

by making use of equation (16b). Thus, we are interested in the determination of equation (20) in the form

$$\begin{aligned}\big[(J_z\cos\beta - J_x\sin\beta)^n\big]_{\rm diag} &= \sum_{k=0}^{n}(\cos\beta)^k(-\sin\beta)^{n-k}\big\{\big(J_x^{n-k}\big)_{\rm diag}J_z^k\big\}\\ &= \sum_{k=0}^{n}{}'(\cos\beta)^k\left(-\frac{\sin\beta}{2}\right)^{n-k}\big\{\big\{J_+^{(n-k)/2}J_-^{(n-k)/2}\big\}J_z^k\big\},\end{aligned} \tag{24}$$

where the sum is restricted to those values of k for which $n-k$ is an even integer.

The symmetric sum may be easily evaluated from equation (21). The replacements $k=q,\ n=2q,\ J_x=J_+$ and $J_z=J_-$ in that equation lead one to

$$\begin{aligned}\big\{J_+^qJ_-^q\big\} &= \sum_{s_1=0}^{q}\big(J_+^{s_1}J_-\big)\sum_{s_2=0}^{q-\sigma(1)}\big(J_+^{s_2}J_-\big)\sum_{s_3=0}^{q-\sigma(2)}\big(J_+^{s_3}J_-\big)\\ &\quad\times\sum_{s_q=0}^{q-\sigma(k-1)}\big(J_+^{s_q}J_-\big)J_+^{q-\sigma(k)}.\end{aligned} \tag{25}$$

To determine the matrix elements we make use of the well-known stepping formulae

$$J_\pm^k|jm\rangle = \sqrt{\frac{(j\mp m)!(j\pm m+k)!}{(j\pm m)!(j\mp m-k)!}}\,|j,m\pm k\rangle. \tag{26}$$

First, we evaluate

$$J_+^{q-\sigma(k)}|jm\rangle = \sqrt{\frac{(j-m)![j+m+q-\sigma(q)]!}{(j+m)![j-m-q+\sigma(q)]!}}\,\big|j,m+q-\sigma(q)\big\rangle, \tag{27}$$

and then

$$J_+^sJ_-|jm'\rangle = \frac{(j-m'+1)!}{(j+m'-1)!}\sqrt{\frac{(j+m')!(j+m'+s-1)!}{(j-m')!(j-m'-s+1)!}}\,|j,m'+s-1\rangle. \tag{28}$$

We utilize these two formulae to obtain

$$\begin{aligned}\big\langle jm\big|\big\{J_+^qJ_-^q\big\}\big|jm\big\rangle &= \sum_{s_1=0}^{q}\frac{[j-m+\sigma(1)]!}{[j+m-\sigma(1)]!}\sqrt{\frac{[j+m-\sigma(1)+1]!(j+m)!}{[j-m+\sigma(1)-1]!(j-m)!}}\\ &\quad\times\sum_{s_2=0}^{q-\sigma(1)}\frac{[j-m+\sigma(2)-1]!}{[j+m-\sigma(2)+1]!}\\ &\quad\times\sqrt{\frac{[j+m-\sigma(2)+2]![j+m-\sigma(1)+1]!}{[j-m+\sigma(2)-2]!(j-m+\sigma(1)-1]!}}\end{aligned}$$

$$\begin{aligned}
&\vdots \\
&\times \sum_{s_l=0}^{q-\sigma(l-1)} \frac{[j-m+\sigma(l)-l+1]!}{[j+m-\sigma(l)+l-1]!} \\
&\times \sqrt{\frac{[j+m-\sigma(l)+l]![j+m-\sigma(l-1)+l-1]!}{[j-m+\sigma(l)-l]!(j-m+\sigma(l-1)-l+1]!}} \\
&\vdots \\
&\times \sum_{s_q=0}^{q-\sigma(q-1)} \big[j+m-\sigma(q)+q\big]\big[j-m+\sigma(q)-q+1\big] \\
&\times \sqrt{\frac{(j-m)![j+m-\sigma(q-1)+q-1]!}{(j+m)!(j-m+\sigma(q-1)-q+1]!}}, \qquad (29)
\end{aligned}$$

where the σ's are given by equation (22). The usage of this result is straightforward. It is, of course, valid for $q > 0$. For $q = 0$, the symmetric sum $\{J_+^0 J_-^0\}$ is simply 1.

With equation (29) in hand, the desired matrix elements of the diagonal parts, $[(J_z \cos\beta - J_x \sin\beta)^n]_{\text{diag}}$, are quite simple to evaluate, since all operators in equation (24) are diagonal and, therefore, commute. Thus, we may write it as

$$\begin{aligned}
&\langle jm \big| (J_z \cos\beta - J_x \sin\beta)^n \big| jm \rangle \\
&= \sum_{k=0}^{n}{}' (m\cos\beta)^k \left(-\frac{\sin\beta}{2}\right)^{n-k} \langle jm \big| \big\{ J_+^{(n-k)/2} J_-^{(n-k)/2} \big\} \big| jm \rangle. \qquad (30)
\end{aligned}$$

The advantage of having a closed analytical form for this expression is apparent: it is readily implemented on the computer.

Finally, it should be noted that, since Wigner rotation elements are related to the spherical harmonics by

$$D^j_{m'0}(\alpha\beta\gamma) = \sqrt{\frac{4\pi}{2j+1}} Y^*_{jm'}(\beta\alpha) = (-)^{m'} \sqrt{\frac{4\pi}{2j+1}} Y_{j\overline{m}'}(\beta\alpha), \qquad (31)$$

all of the summations over $d^j_{m'm}(\beta)$ can be easily reduced to summations over spherical harmonics $Y_{j\overline{m}'}(\beta\alpha)$ by setting $m = 0$.

Appendix

The geometric view of equations (10), (13) and (14) can be discussed as follows. Using the convention of a right-handed system of coordinates, let us consider rotating a given position vector **r** of components (x, y, z) about an axis **n** by angle ϕ, thereby yielding **r**′ (cf. figure 1). That is, $\mathbf{r}' = \mathbf{R}(\phi, \mathbf{n})\mathbf{r}$, where **n** makes an angle θ with **r**. For the convenience of discussion, we compare the scalar components with their vector

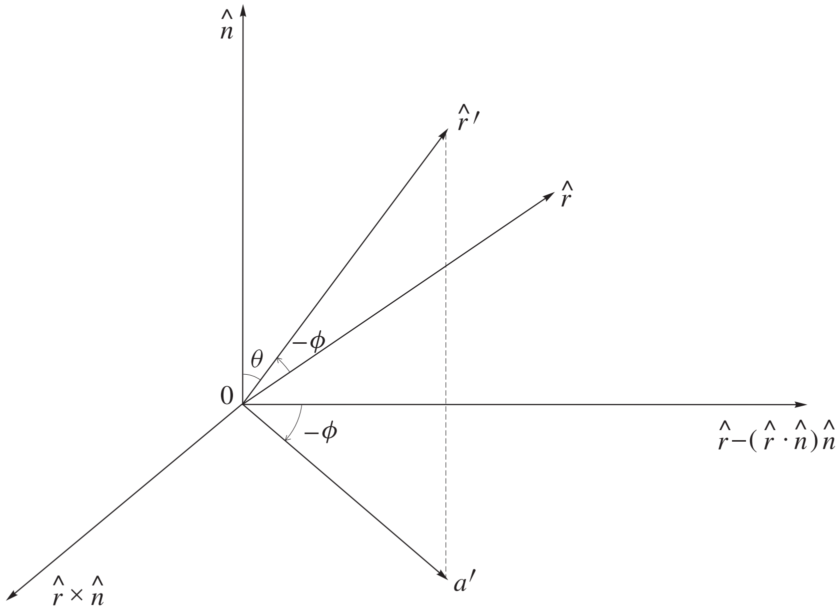

Figure 1.

directions after the rotation. To visualize the relative positions of $\mathbf{r}$ and $\mathbf{r}'$, we take $\mathbf{n}$ to be the z-axis and the y-axis to be the common plane of $\mathbf{n}$ and $\mathbf{r}$ before rotation through angle ϕ. The x-axis will be perpendicular to $\mathbf{n}$ and $\mathbf{r}$ (and y).

For vector $\mathbf{r}'$:

scalar components	vector direction
$x' = -r' \sin\theta \cos\phi$,	$\mathbf{r} \times \mathbf{n}$,
$y' = r' \sin\theta \cos\phi$,	$\mathbf{r} - (\mathbf{r} \cdot \mathbf{n})\mathbf{n}$,
$z' = r' \cos\theta$,	$(\mathbf{r} \cdot \mathbf{n})\mathbf{n}$,

and $\overline{0a'} = r' \sin\theta$, $\mathbf{r} \times \mathbf{n} = -\overline{0a'} \sin\phi$, $\mathbf{r} - (\mathbf{r} \cdot \mathbf{n})\mathbf{n} = \overline{0a'} \cos\phi$. Therefore, we obtain $\mathbf{0a}'$ in terms of $\mathbf{r} \times \mathbf{n}$ and $\mathbf{r} - (\mathbf{r} \cdot \mathbf{n})\mathbf{n}$, i.e.,

$$\mathbf{0a}' = (\mathbf{r} \times \mathbf{n}) \sin\phi + \big(\mathbf{r} - (\mathbf{r} \cdot \mathbf{n})\mathbf{n}\big) \cos\phi.$$

Finally, we have

$$\mathbf{r}' = \mathbf{R}(\phi, \mathbf{n})\mathbf{r} = (\mathbf{r} \cdot \mathbf{n})\mathbf{n} + (\mathbf{n} \times \mathbf{r}) \sin\phi + \big(\mathbf{r} - (\mathbf{r} \cdot \mathbf{n})\mathbf{n}\big) \cos\phi. \tag{A.1}$$

This result is obtained by rotating the vector $\mathbf{r}$. If the rotation were effected upon the coordinates (i.e., ϕ is replaced by $-\phi$), the result would be

$$\mathbf{r}' = (\mathbf{r} \cdot \mathbf{n})\mathbf{n} - (\mathbf{n} \times \mathbf{r}) \sin\phi + \big(\mathbf{r} - (\mathbf{r} \cdot \mathbf{n})\mathbf{n}\big) \cos\phi. \tag{A.2}$$

Since the rotational angular momentum transforms as a vector under rotation, we, therefore, have the following similarity transformation upon replacing the vector **r** by **J**:

$$\mathbf{J}' = \mathrm{e}^{-\mathrm{i}\phi\,\mathbf{n}\cdot\mathbf{J}}\mathbf{J}\,\mathrm{e}^{\mathrm{i}\phi\,\mathbf{n}\cdot\mathbf{J}} = (\mathbf{J}\cdot\mathbf{n})\mathbf{n} - (\mathbf{n}\times\mathbf{J})\sin\phi + \bigl(\mathbf{J} - (\mathbf{J}\cdot\mathbf{n})\mathbf{n}\bigr)\cos\phi. \tag{A.3}$$

This rotation of the coordinate system follows the convention of Rose [8], Brink and Satchler [2] and Biedenharn and Louck [1]. In contrast,

$$\mathbf{J}' = \mathrm{e}^{\mathrm{i}\phi\,\mathbf{n}\cdot\mathbf{J}}\mathbf{J}\,\mathrm{e}^{-\mathrm{i}\phi\,\mathbf{n}\cdot\mathbf{J}} = (\mathbf{J}\cdot\mathbf{n})\mathbf{n} + (\mathbf{n}\times\mathbf{J})\sin\phi + \bigl(\mathbf{J} - (\mathbf{J}\cdot\mathbf{n})\mathbf{n}\bigr)\cos\phi \tag{A.4}$$

represents a rotation of the physical system. For example,

$$\mathrm{e}^{\mathrm{i}\phi J_z}J_y\,\mathrm{e}^{-\mathrm{i}\phi J_z} = J_y\cos\phi + J_x\sin\phi, \tag{A.5}$$

where $\mathbf{n}\cdot\mathbf{J} = J_n = J_z$ and $J_x = J_y = 0$. Edmonds [3] uses this latter convention.

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