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Note

On the Calculation of Rotation Matrices

The matrix elements $d^j_{k,m} \equiv d^j(\pi/2)_{k,m}$ play an essential role in the construction of symmetry-adapted functions for the octahedral group (1). In a recent paper, Fox and Krohn (2) perform the evaluation of these elements by a recursion formula in which j and one of the subscripts are fixed. In the present note we propose an improved recursion relation to facilitate computation of the $d^j_{k,m}$ matrix elements. As this relation involves only integers, we eliminate cumulative roundoff errors (implicit in the method of Ref. (2)) arising from the introduction of a new irrational number with each recursive step.

Wigner's formula for the $d^j_{k,m}$ matrix elements (3) can be written, using combinational numbers, as

$$d^j_{k,m} = \frac{(-1)^{k-m}}{2^j} \frac{\binom{2j}{j+m}^{1/2}}{\binom{2j}{j+k}^{1/2}} \sum_\nu (-1)^\nu \binom{j+m}{\nu}\binom{j-m}{j-k-\nu}. \tag{1}$$

We now introduce the quantities $\omega^j(k, m)$ defined by

$$\omega^j(k, m) = (-1)^{k-m} \sum_\nu (-1)^\nu \binom{j+m}{\nu}\binom{j-m}{j-k-\nu}, \tag{2}$$

where ν takes those values for which the factorial terms in the binomial coefficients are positive.

Using the particular value of Eq. (2),

$$\omega^j(k, m) = \binom{2j}{j+k} \qquad \text{for} \quad m = j, \tag{3}$$

Eq. (1) can be written in the more convenient form:

$$d^j_{k,m} = \frac{1}{2^j} \frac{\{\omega^j(m, j)\}^{1/2}}{\{\omega^j(k, j)\}^{1/2}} \omega^j(k, m). \tag{4}$$

Applying the known symmetry relation $d^j_{k,m} = (-1)^{k-m} d^j_{m,k}$ to the preceding equation, we immediately obtain

$$\omega^j(k, m)\, \omega^j(m, j) = (-1)^{k-m} \omega^j(m, k)\, \omega^j(k, j). \tag{5}$$

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Therefore, we can transform Eq. (2) into

$$d^j_{k,m} = \frac{1}{2^j} \mid \omega^j(k, m)\, \omega^j(m, k)|^{1/2} \operatorname{sign}\{\omega^j(k, m)\}, \tag{6}$$

where the bars indicate absolute value.

In an actual computation of the set of all independent $d^j_{k,m}$'s with the same j, Eq. (4) is more convenient than Eq. (6) since we need only calculate l(or $j - \frac{1}{2}$) square roots. If Eq. (6) were used, we would need $l(l + 1)/2$ (or $\{j^2 - \frac{1}{4}\}/2$) *square* roots. On the other hand, when we want to test and check computational results, Eq. (6) appears easy to handle.

In order to obtain recursion relations between the $\omega^j(k, m)$ quantities, we define a generating functional of these matrix elements:

$$\sum_{k=-j}^{j} \omega^j(k, m)\, t^{j-k} = (t - 1)^{j-m}\, (t + 1)^{j+m}. \tag{7}$$

Writing this equation for m and $m + 1$, we directly obtain the simple recursion formula

$$\omega^j(k + 1, m + 1) = \omega^j(k, m) + \omega^j(k + 1, m) + \omega^j(k, m + 1). \tag{8}$$

The starting value given by Eq. (3), together with

$$\omega^j(j, m) = (-1)^{j-m} \qquad \text{for} \quad k = j, \tag{9}$$

can be used to perform the iteration of the $\omega^j(k, m)$ through Eq. (8).

Using Eqs. (3), (4), (8), and (9) we are able to compute all quantities $\omega^j(k, m)$ for $0 \leqslant k, m \leqslant j$. The remaining values can be calculated from the symmetry relations

$$\begin{aligned} \omega^j(k, m) &= (-1)^{j-k}\omega^j(k, -m) \\ &= (-1)^{j-m}\omega^j(-k, m), \end{aligned} \tag{10}$$

obtained by putting $\nu = j \pm k - \mu$ in Eq. (2).

When j can only take on integral values, quite convenient starting values can be obtained by writing Eq. (7) in the form

$$\sum_{k=-l}^{l} \omega^l(k, 0)\, t^{l-k} = (t^2 - 1)^l. \tag{11}$$

Comparing terms of the same order in t, we have

$$\omega^l(k, 0) = 0 \qquad \text{for} \quad l + k \text{ odd}, \tag{12}$$

$$\omega^l(k, 0) = (-1)^{(l+k)/2} \binom{l}{(l + k)/2} \qquad \text{for} \quad l + k \text{ even}. \tag{13}$$

Calculations of the $d^l_{k,m}$ matrix elements have been implemented using Eqs. (4), (8), (9), (12), (13), and the symmetry relation $d^l_{m,k} = (-1)^{m-k} d^l_{k,m}$, in Fortran IV language in an IBM 370/145.

All computed values of $d^l_{k,m}$ for $0 \leqslant l \leqslant 56$ using double-precision arithmetic are obtained in 9 sec. They show a maximum orthogonality error equal to 280×2^{-56}, i.e., they are obtained with 16 significant figures. The accuracy decreases for $l > 56$, as might be expected due to the computer precision.

References

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