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A NOTE ON THE CALCULATION OF THE MATRIX ELEMENTS OF THE ROTATION GROUP

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CONTENTS

A recurrence relation is given for the calculation of the matrix elements of representatives of odd dimensionality of the rotation group, which is simpler than some previously suggested. Reference is given to some extensive tables that have been computed by means of the scheme described in the paper and which are available.

1. Introduction

The matrix representations of finite rotations are required in a variety of physical problems and several methods have been proposed for their calculation. This is so because their general expression (see Wigner 1959) is difficult to handle on a desk computer and unsuitable for an electronic one, since it gives the matrix elements as an expansion with awkward coefficients. Altmann (1957) provided some simple recurrence relations for the latter, which allowed the hand calculation of the representations of lower order for particular values of the rotation angles, whereas for higher orders and general angles they were used to write a programme for an electronic computer (Cohan 1958).

The procedure mentioned proved adequate in the cases for which it was used. However, McIntosh (1960) has recently suggested that a more effective method could be built around certain recurrence relations between the matrix elements of the rotation group that have been given by Gel'fand & Shapiro (1956). The superiority of this method over the one we used before depends on the fact that the recurrence relations are between the matrix elements themselves, rather than between the coefficients in their expansion. McIntosh suggests a way in which the relations given by Gel'fand & Shapiro could be used, but he does not provide numerical results. We shall show in this note that a recurrence relation more convenient than that of Gel'fand & Shapiro can be derived and we shall give a systematic procedure for its use. Also, we shall report on a programme for an electronic computer that has been written to exploit the new relations, and on extensive tables that are now available as a result.

We must stress that the whole of this note will deal with representations of the rotation group of odd dimensionality only. Edmonds (1957) gives a recurrence relation that can be used for representations of even dimension (half-integral angular momentum).

2. Basic formulae

We shall follow exactly the notation used by Altmann (1957). The normalized spherical harmonics are†

$$Y_l^m(\theta,\phi) = \sqrt{\left(\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}\right)}\,P_l^m(\cos\theta)\,\mathrm{e}^{\mathrm{i}m\phi}. \tag{1}$$

The matrix representatives $D^{(l)}(\mathscr{R})$ of a rotation $\mathscr{R}$ are defined by the relation

$$\mathscr{R}Y_l^m = \sum_{m'} Y_l^{m'}D^{(l)}(\mathscr{R})_{m'm}. \tag{2}$$

In order to obtain the matrix elements that appear in (2) the rotations are expressed in terms of their Euler angles α, β, γ and their form is well known:

$$D^{(l)}(\mathscr{R})_{m'm} = C_{m'm}\,\mathrm{e}^{\mathrm{i}m'\gamma}\,\mathrm{e}^{\mathrm{i}m\alpha}\,d^{(l)}(\beta)_{m'm}, \tag{3}$$

where

$$C_{m'm} = \mathrm{i}^{|m'|+m'}\,\mathrm{i}^{|m|+m}, \tag{4}$$

$$d^{(l)}(\beta)_{m'm} = \sqrt{[(l+m)!\,(l-m)!\,(l+m')!\,(l-m')!]}\,S^{(l)}_{m'm}(\beta). \tag{5}$$

In this last expression,

$$S^{(l)}_{m'm}(\beta) = \sum_{r=0}^{r_m} \mathscr{C}^{(l)}_{\mu\nu}(r)\cos^{\nu-\mu+2r}\tfrac{1}{2}\beta\,\sin^{2l-(\nu-\mu+2r)}\tfrac{1}{2}\beta, \tag{6}$$

where

$$\left.\begin{aligned}\mu &= \min(l-m', l+m),\\ \nu &= \max(l-m', l+m),\\ r_m &= \min(\mu, 2l-\nu),\end{aligned}\right\} \tag{7}$$

$$\mathscr{C}^{(l)}_{\mu\nu}(r) = \frac{(-1)^{\mu-r}}{(\nu-\mu+r)!\,r!\,(\mu-r)!\,(2l-\nu-r)!}. \tag{8}$$

For tabulation purposes it is often convenient to work with unnormalized spherical harmonics $\mathscr{Y}_l^m(\theta,\phi) = P_l^m(\cos\theta)\exp(\mathrm{i}m\phi)$, so as not to lose significant figures. When the unnormalized functions are used as bases for the representations in an expression formally identical to (2), new matrix representatives must be defined which shall be denoted by $\mathscr{D}^{(l)}(\mathscr{R})_{m'm}$. These are given by the expression

$$\mathscr{D}^{(l)}(\mathscr{R})_{m'm} = C_{m'm}\,\mathrm{e}^{\mathrm{i}m'\gamma}\,\mathrm{e}^{\mathrm{i}m\alpha}\,\mathscr{S}^{(l)}_{m'm}(\beta), \tag{9}$$

where

$$\mathscr{S}^{(l)}_{m'm}(\beta) = (l+|m|)!\,(l-|m'|)!\,S^{(l)}_{m'm}(\beta). \tag{10}$$

The quantities $S^{(l)}_{m'm}(\beta)$ satisfy important symmetry relations

$$S^{(l)}_{ab}(\beta) = S^{(l)}_{-b,-a}(\beta) = (-1)^{a+b}\,S^{(l)}_{ba}(\beta). \tag{11}$$

Hence

$$S^{(l)}_{-a,b}(\beta) = (-1)^{a+b}\,S^{(l)}_{a,-b}(\beta). \tag{12}$$

It can be seen that the coefficients $d^{(l)}(\beta)_{m'm}$ satisfy exactly the same relations and that similar properties are possessed by the $\mathscr{S}^{(l)}_{m'm}(\beta)$. The only difference in this latter case is that the last term in (11) must be multiplied by

$$(l+|b|)!\,(l-|a|)!/(l+|a|)!\,(l-|b|)!.$$

† It should be noticed that we do not include in our definition the phase factor $(-1)^m$ (for $m \geqslant 0$) which is now always used in the treatment of angular momentum. The necessary changes in our formulae to include this factor are very easily made.

These symmetry relations are important because they allow us to limit ourselves to the range $-l \leqslant m \leqslant l$, $|m| \leqslant m' \leqslant l$ when calculating the quantities $S^{(l)}_{m'm}(\beta)$, $d^{(l)}(\beta)_{m'm}$ and $\mathscr{S}^{(l)}_{m'm}(\beta)$. It can be seen, by drawing a diagram with m as abscissae and m' as ordinates, that these conditions determine a domain in the (m, m') plane in the form of an isosceles triangle, the two equal sides of which are along the diagonals of the first and second quadrant, respectively.

3. The recurrence relations

We shall first consider the calculation of the quantities $\mathscr{S}^{(l)}_{m'm}(\beta)$. In the region of the (m, m') plane described at the end of the last section, we have $\mu = l-m'$, $\nu = l+m$ and $r_m = l-m'$, as follows from (7). Hence, from equations (10) and (6)

$$\mathscr{S}^{(l)}_{m'm}(\beta) = (l+|m|)!\,(l-m')!\sum_{r=0}^{l-m'} \frac{(-1)^{l-m'-r}\cos^{m+m'+2r}\tfrac{1}{2}\beta\,\sin^{2l-(m+m'+2r)}\tfrac{1}{2}\beta}{(m+m'+r)!\,r!\,(l-m'-r)!\,(l-m-r)!}. \tag{13}$$

The summation in (13) can be expressed in terms of the hypergeometric function† (see Morse & Feshbach 1953, p. 542)

$$\mathscr{S}^{(l)}_{m'm}(\beta) = \frac{(-1)^{l-m'}\,(l+m)!}{(m+m')!\,(l-|m|)!}\cot^{m+m'}\tfrac{1}{2}\beta\,\sin^{2l}\tfrac{1}{2}\beta\,F(m'-l, m-l; m+m'+1; -\cot^2\tfrac{1}{2}\beta). \tag{14}$$

As is well known, the hypergeometric function can be expressed for certain particular values of its parameters in terms of Jacobi polynomials:

$$F(-n, p+n; q; z) \equiv J_n(p, q; z), \tag{15}$$

whenever n is a positive integer (the degree of the Jacobi polynomial) and $q > 0$ (see Morse & Feshbach 1953, p. 780). Equation (14) now takes the form‡

$$\mathscr{S}^{(l)}_{m'm}(\beta) = \frac{(-1)^{l-m'}\,(l+m)!}{(m+m')!\,(l-|m|)!}\cot^{m+m'}\tfrac{1}{2}\beta\,\sin^{2l}\tfrac{1}{2}\beta\,J_{l-m'}(-2l+m+m', 1+m+m'; -\cot^2\tfrac{1}{2}\beta). \tag{16}$$

It is convenient to introduce some new polynomials of degree m in $\cot^2\tfrac{1}{2}\beta$, $G^{(l)}_{m'm}(\beta)$, which are related to the Jacobi polynomials as follows

$$G^{(l)}_{m'm}(\beta) = \frac{(-1)^{l-m'}\,(l+m)!}{(m'+m)!}\cot^{2(m+m'-l)}\tfrac{1}{2}\beta\,J_{l-m'}(-2l+m+m', 1+m+m'; -\cot^2\tfrac{1}{2}\beta). \tag{17}$$

With this notation, equation (16) takes the form

$$\mathscr{S}^{(l)}_{m'm}(\beta) = \frac{1}{(l-|m|)!}\cot^{2l-m-m'}\tfrac{1}{2}\beta\,\sin^{2l}\tfrac{1}{2}\beta\,G^{(l)}_{m'm}(\beta). \tag{18}$$

We can now make use of the following recurrence relation for the Jacobi polynomials (see Morse & Feshbach 1953, p. 781)

$$zJ_n(p, q; z) = \frac{q-1}{2n+p}[J_n(p-1, q-1; z) - J_{n+1}(p-1, q-1; z)] \tag{19}$$

† It might be useful to notice that expression (14) is valid not only for the triangular domain under discussion in the (m, m') plane, but also for the remainder of the first quadrant.

‡ Similar expressions of the matrix elements of the rotation group in terms of the Jacobi polynomials are well known and can be found in the references given. It should be noticed, nevertheless, that whereas our Jacobi polynomials are given in terms of $\cot^2\tfrac{1}{2}\beta$, previous expressions involve $\cos\beta$.

to obtain a similar relation for the polynomials $G^{(l)}_{m'm}(\beta)$

$$G^{(l)}_{m'-1,m}(\beta) = (m'-m)\,G^{(l)}_{m'm}(\beta)-(l+m)\,G^{(l)}_{m',m-1}(\beta). \tag{20}$$

In order to use this recurrence relation we must possess starting values of $G^{(l)}_{m'm}(\beta)$ for a particular value of m' and all m. These can be very easily obtained when m' is given its highest value, $m' = l$:

$$G^{(l)}_{lm}(\beta) = \cot^{2m}\tfrac{1}{2}\beta, \tag{21}$$

as follows immediately from (17), because $J_0 = 1$.

A systematic procedure for the calculation can now be described. Equation (21) is first used to provide the top row of our triangle in the (m, m') plane and the recurrence relation (20) will yield very quickly the successive rows of the $G^{(l)}_{m'm}(\beta)$. As a check, the last value of $G^{(l)}$ obtained can be compared with the one directly calculated from the expression

$$G^{(l)}_{00}(\beta) = l!\sec^{2l}\tfrac{1}{2}\beta P_l(\cos\beta), \tag{22}$$

which follows from the hypergeometric function that corresponds to the Legendre polynomial $P_l(\cos\beta)$. Once the G's are calculated, the $\mathscr{S}$'s are obtained from (18) and the $\mathscr{D}$'s from (9). If the d's are required they can be obtained directly from the $\mathscr{S}$'s by the relation

$$d^{(l)}(\beta)_{m'm} = \sqrt{\left(\frac{(l-|m|)!}{(l+|m|)!}\,\frac{(l+|m'|)!}{(l-|m'|)!}\right)}\,\mathscr{S}^{(l)}_{m'm}(\beta), \tag{23}$$

which follows from (5) and (10).

The method described is probably the quickest and safest if a desk computer is used, because of the extreme simplicity of the recurrence relation (20). On an electronic computer this is no advantage and it is better to work with direct recurrence relations, and starting values, for the $\mathscr{S}$'s or d's. These, which follow from (20) and (21), are

$$\mathscr{S}^{(l)}_{m'-1,m}(\beta) = (m'-m)\cot\tfrac{1}{2}\beta\,\mathscr{S}^{(l)}_{m'm}(\beta)-(l+m)\,(l+m+1)\,\mathscr{S}^{(l)}_{m',m-1}(\beta) \quad (m>0), \tag{24}$$

$$\mathscr{S}^{(l)}_{m'-1,m}(\beta) = (m'-m)\cot\tfrac{1}{2}\beta\,\mathscr{S}^{(l)}_{m'm}(\beta)-\mathscr{S}^{(l)}_{m',m-1}(\beta) \quad (m\leqslant 0), \tag{25}$$

with starting values
$$\mathscr{S}^{(l)}_{lm}(\beta) = \frac{1}{(l-|m|)!}\cot^{l+m}\tfrac{1}{2}\beta\,\sin^{2l}\tfrac{1}{2}\beta, \tag{26}$$

and
$$\sqrt{[(l+m')\,(l-m'+1)]}\,d^{(l)}(\beta)_{m'-1,m} = (m'-m)\cot\tfrac{1}{2}\beta\,d^{(l)}(\beta)_{m'm} -\sqrt{[(l+m)\,(l-m+1)]}\,d^{(l)}(\beta)_{m',m-1}, \tag{27}$$

with starting values
$$d^{(l)}(\beta)_{lm} = \sqrt{\frac{(2l)!}{(l+m)!\,(l-m)!}}\cot^{l+m}\tfrac{1}{2}\beta\,\sin^{2l}\tfrac{1}{2}\beta. \tag{28}$$

It should be noticed that, when computing the $\mathscr{S}$'s, two recurrence relations are required to cover the basic domain.

4. The particular case $\beta = \frac{1}{2}\pi$

The case $\beta = \frac{1}{2}\pi$ merits special attention for two reasons. First, as shown by Wigner, the matrix representatives for an arbitrary β can be obtained in terms of those for $\beta = \frac{1}{2}\pi$ (see Edmonds 1957, § 4·5). Secondly, it is always possible to choose axes in such a way that the β angle for all rotations in all crystallographic point groups takes no values other than 0, π, or $\frac{1}{2}\pi$ (Altmann 1957). In the first two cases the calculation of the matrix elements is trivial and, as we shall see, it is much simplified when $\beta = \frac{1}{2}\pi$. This is so because of the following facts:

(i) There exists now an extra symmetry relation for the functions $\mathscr{S}^{(l)}_{m'm}(\beta)$, namely

$$\mathscr{S}^{(l)}_{m',-m}(\tfrac{1}{2}\pi) = (-1)^{l+m'}\,\mathscr{S}^{(l)}_{m'm}(\tfrac{1}{2}\pi) \tag{29}$$

(Altmann 1957), which cuts down by one-half the basic domain of computation in the (m, m') plane.

(ii) The starting value given by (21) is now $G^{(l)}_{lm}(\frac{1}{2}\pi) = 1$.

(iii) The values $\mathscr{S}^{(l)}_{0m}(\frac{1}{2}\pi)$ and $\mathscr{S}^{(l)}_{m0}(\frac{1}{2}\pi)$ vanish if $(l-m)$ is odd, and this provides a very powerful intermediate check besides the final one already mentioned. The proof of this result is as follows: Let us take $m \geqslant 0$, because negative m's can be handled later by means of (29). Then, from (14),

$$\mathscr{S}^{(l)}_{m'm}(\tfrac{1}{2}\pi) = \frac{(-1)^{l-m'}(l+m)!}{2^l(m+m')!\,(l-m)!}F(m'-l, m-l;\, m+m'+1;\, -1). \tag{30}$$

The hypergeometric function that appears in (30) can be expressed by means of a relation due to Gauss (see Erdélyi, Magnus, Oberhettinger & Tricomi 1953, p. 104)

$$F(a, b;\, 1+a-b;\, -1) = 2^{-a}\frac{\Gamma(1+a-b)\,\Gamma(\frac{1}{2})}{\Gamma(1-b+\frac{1}{2}a)\,\Gamma[\frac{1}{2}(1+a)]}. \tag{31}$$

If we take $m = 0$ we see, on comparing the parameters of the hypergeometric functions that appear in (30) and (31), that the latter is applicable for all m' in the calculation of $\mathscr{S}^{(l)}_{m'0}(\frac{1}{2}\pi)$ as given by (30). The appropriate substitutions give

$$\mathscr{S}^{(l)}_{m'0}(\tfrac{1}{2}\pi) = \frac{(-1)^{l-m'}\sqrt{\pi}}{2^{m'}}\,\frac{1}{\Gamma[1+\frac{1}{2}(l+m')\,\Gamma[\frac{1}{2}-\frac{1}{2}(l-m')]} \tag{32}$$

and the expression on the right-hand side is zero whenever $l-m'$ is odd. In the same manner, or through the use of relations (11), the vanishing of $\mathscr{S}^{(l)}_{0m}(\frac{1}{2}\pi)$ for $l-m$ odd can also be proved.

5. Calculations and tables

A program has been written for the Mercury computer to calculate the coefficients $d^{(l)}(\beta)_{m'm}$. The only data required are β and the maximum value of l. The program uses the recurrence relation (27) and prints out all coefficients in the basic domain for each l required. Tables of $d^{(l)}(\frac{1}{2}\pi)_{m'm}$ have been compiled for values of all l up to $l = 20$ and have been deposited with the Royal Society and the Library of Congress (Bradley 1961).

Values up to $l = 12$ have been obtained accurately for $G^{(l)}(\frac{1}{2}\pi)_{m'm}$ using a desk machine and between the two sets of tables there is agreement to eight significant figures (the accuracy of the output routine used in the program: the computations were carried out with sixteen figures). The zeros, obtained along the axes in the (m, m') plane for higher values of l, indicate that the same accuracy is present up to $l = 20$.

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