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j symbols and jm factors for all dihedral and cyclic groups

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Abstract. The methodology of earlier papers by Butler and Wybourne is used to obtain algebraic formulae for $6j$ symbols of the double dihedral and cyclic groups and the $3jm$ factors for all possible imbeddings: $D_m \supset D_n$ and $D_m \supset C_n$. The usual $3jm$ symbols of angular momentum theory, that is for $SO_3 \supset SO_2$, do not have a phase choice which allows their factorisation into $SO_3 \supset D_\infty$ and $D_\infty \supset SO_2$ $3jm$ factors. We derive the change of phase necessary for factorisation, thus obtaining a relation between $SO_3 \supset D_\infty$ factors and the $SO_3 \supset SO_2$ $3jm$ symbols of standard angular momentum theory. The use of maximal imbeddings has removed the multiplicity problems encountered by other methods.

1. Introduction

The properties of j symbols and jm factors were reviewed and extended recently (Butler 1975). Emphasis was placed on the phase choices, symmetries and factorisation properties of these coefficients for groups which are not simply reducible. The review was followed by a paper on the methodology of computation of the coefficients using character theory alone (Butler and Wybourne 1976a, hereafter referred to as I). These methods were used for SO_3 and for the embedding $SO_3 \supset SO_2$ (Butler, hereafter referred to as II). They were also used to calculate the $6j$ symbols for the tetrahedral group and some $3jm$ factors for the chain $SO_3 \supset T \supset C_3$ (Butler and Wybourne 1976b, hereafter referred to as III). The reader is referred to I for notation and definitions.

In this paper formulae for the $6j$ symbols of arbitrary finite and infinite dihedral double groups are obtained. We also show how to calculate $3jm$ factors for the branchings $SO_3 \supset D_\infty$, $D_\infty \supset D_n$, $D_\infty \supset C_\infty = SO_2$, $D_{mn} \supset D_n$, $D_n \supset C_n$, $D_{odd} \supset C_2$, $C_{mn} \supset C_n$.

The $6j$ symbols and $3jm$ factors of various groups are essential for the application of the Wigner–Eckart theorem to various physical problems. Racah (1949) showed that it is possible to factor coupling coefficients for group chains. To obtain greatest benefit from Racah's factorisation lemma, one should ensure that all possible intermediate groups have been included, so that at each step one has a maximal subgroup. Intermediate subgroups have sometimes been overlooked. For instance, the existence of the intermediate group D_∞ in the chain $SO_3 \supset D_\infty \supset D_n$ solves the so-called multiplicity problem (Bickerstaff and Wybourne 1976, Patera and Winternitz 1973) encountered in attempting to go straight from SO_3 to D_n. The factorisation introduced in the $3jm$ symbols of angular momentum, by noting the existence of D_∞ in $SO_3 \supset D_\infty \supset SO_2$, gives a ready formula for the $SO_3 \supset D_\infty$ $3jm$ factors used in the above problem. Thus our results are more general than other calculations (see, for example, Golding and Newmarch 1977, Harnung and Schäffer 1972, Kibler and Grenet 1977). A

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minor modification of the $SO_3 \supset SO_2$ phase choices is required before the symbols factorise.

A book is being prepared which tabulates j symbols for all point groups and jm factors for all point group branchings (Butler 1979). A computer program exists to perform these tabulations, enabling the results of this paper to be checked easily.

2. The structure of the dihedral groups

The finite dihedral group D_n consists of the identity; $(n-1)$ rotations about the z axis by multiples of $2\pi/n$, $\exp(iJ_z 2m\pi/n)$, or C_n^m in Hammermesh's (1962) notation; and n twofold rotations about axes perpendicular to the z axis, $C_2(\phi)$ or C_2. The infinite dihedral group has an infinite number of elements of the latter types. We label the groups D_∞, D_n, D_{even} and D_{odd} for the infinite, finite, even and odd dihedral groups respectively.

The double dihedral groups include, in addition to the single-valued elements, a basic spin operator R, and all elements of the form AR where A is a member of the single group. We follow Hamermesh's (1962 § 9.7) definitions of double-valued rotations and their inverses which lead to the classes shown in the tables. Other authors, for example Koster *et al* (1963), use different definitions but this only affects the labelling of the classes.

The representation structure of the dihedral groups is also given in the tables. By including the spin irreps of the dihedral groups (equivalently, all the true irreps of the double dihedral groups) the irrep structures of D_{even}, D_{odd} and D_∞ are seen to be very similar. The reductions of products of irreps are easily deduced from the character tables by elementary character theory.

We have chosen to label irreps by a system analogous to the usual SO_3 and SO_2 labels, i.e. integers and half-integers. In D_∞ there are two one-dimensional irreps, the identity which we label 0^+, and another, 0^-.

If a and b are any two-dimensional irreps of D_∞ (i.e. $a, b \geq \frac{1}{2}$) then

$$0^- \times 0^- = 0^+ \tag{2.1}$$

$$0^- \times a = a \tag{2.2}$$

$$a \times b = (a+b) + |a-b| \qquad \text{for } a \neq b \tag{2.3}$$

$$a \times a = 0^+ + 0^- + (2a). \tag{2.4}$$

In the last product $2a$ and 0^+ are in the symmetric part of the product if a is integer and $2a$ and 0^- are in the symmetric part if a is half-integer.

In D_n the rules are the same, except for the following changes. When $a+b=\frac{1}{2}n$ we have two one-dimensional irreps $+\frac{1}{2}n$ and $-\frac{1}{2}n$, and if $a+b>\frac{1}{2}n$ the irrep $(a+b)$ becomes $[n-(a+b)]$. In addition, there are the special cases

$$(\pm\tfrac{1}{2}n)\times(\pm\tfrac{1}{2}n) = \begin{cases} 0^+ & \text{for } n \text{ even} \\ 0^- & \text{for } n \text{ odd} \end{cases} \tag{2.5}$$

$$(\pm\tfrac{1}{2}n)\times(\mp\tfrac{1}{2}n) = \begin{cases} 0^- & \text{for } n \text{ even} \\ 0^+ & \text{for } n \text{ odd.} \end{cases} \tag{2.6}$$

In (2.5) 0^+ is the symmetric part and there is no antisymmetric part.

Table 1. Character table for D_n with n odd. Where the n elements $C_2(\phi)$, $\phi = k\pi/n$, $0 \leq k < n$ form a single class and where $\theta = 2\pi k/n$, $0 < k < \frac{1}{2}n$ giving $(n-1)$ classes containing two elements each.

Class	E	R	$C_2(\phi)$	$C_2(\phi)R$	$\exp(iJ_z\theta)$ $\exp(-iJ_z\theta)R$	$\exp(iJ_z\theta)R$ $\exp(-iJ_z\theta)$
Number of elements in class	1	1	n	n	2	2
Irrep:						
0^+	1	1	1	1	1	1
0^-	1	1	−1	−1	1	1
$\frac{1}{2}$	2	−2	0	0	$2\cos\frac{1}{2}\theta$	$-2\cos\frac{1}{2}\theta$
1	2	2	0	0	$2\cos\theta$	$2\cos\theta$
$\frac{3}{2}$	2	−2	0	0	$2\cos\frac{3}{2}\theta$	$-2\cos\frac{3}{2}\theta$
⋮						
$\frac{1}{2}(n-1)$	2	2	0	0	$2\cos\frac{1}{2}(n-1)\theta$	$-2\cos\frac{1}{2}(n-1)\theta$
$+\frac{1}{2}n$	1	−1	i	−i	$(-)^k$	$(-)^{k+1}$
$-\frac{1}{2}n$	1	−1	−i	i	$(-)^k$	$(-)^{k+1}$

Table 2. Character table for D_n with n even. Where the n elements $C_2(\phi)$, $C_2(\phi)R$, $\phi = (2k+1)\pi/n$, $0 \leq k < n$ form one class; the n elements $C_2(\psi)$, $C_2(\psi)R$, $\psi = 2k\pi/n$, $0 \leq k < n$ form another; and where $\theta = l2\pi/n$, $0 < l < \frac{1}{2}n$ gives $(n-2)$ classes of two elements each.

Class	E	R	$C_2(\psi)$ $C_2(\psi)R$	$C_2(\phi)$ $C_2(\phi)R$	$\exp(iJ_z\theta)$ $\exp(-iJ_z\theta)R$	$\exp(iJ_z\theta)R$ $\exp(-iJ_z\theta)$	$\exp(iJ_z\pi)$ $\exp(iJ_z\pi)R$
Number of elements in	1	1	n	n	2	2	2
Irrep:							
0^+	1	1	1	1	1	1	1
0^-	1	1	−1	−1	1	1	1
$\frac{1}{2}$	2	−2	0	0	$2\cos\frac{1}{2}\theta$	$-2\cos\frac{1}{2}\theta$	$2\cos\frac{1}{2}\pi$
1	2	2	0	0	$2\cos\theta$	$2\cos\theta$	$2\cos\pi$
$\frac{3}{2}$	2	−2	0	0	$2\cos\frac{3}{2}$	$-2\cos\frac{3}{2}$	$2\cos\frac{3}{2}\pi$
⋮							
$\frac{1}{2}(n-1)$	2	−2	0	0	$2\cos\frac{1}{2}(n-1)\theta$	$-2\cos\frac{1}{2}(n-1)\theta$	$2\cos\frac{1}{2}(n-1)\pi$
$+\frac{1}{2}n$	1	1	1	−1	$(-)^l$	$(-)^l$	1
$-\frac{1}{2}n$	1	1	−1	1	$(-)^l$	$(-)^l$	1

Table 3. Character table for D_∞. Where all $C_2(\phi)$ and $C_2(\phi)R$, $0 \leq \phi < \pi$, form one class; and $0 < \phi < \pi$ gives a continuum of classes with 2 elements each.

Class	E	R	$C_2(\phi)$ $C_2(\phi)R$	$\exp(iJ_z\theta)$ $\exp(-iJ_z\theta)$	$\exp(iJ_z\theta)R$ $\exp(-iJ_z\theta)R$	$\exp(iJ_z\pi)$ $\exp(iJ_z\pi)R$
Number of elements in	1	1	∞	2	2	2
Irrep:						
0^+	1	1	1	1	1	1
0^-	1	1	−1	1	1	1
$\frac{1}{2}$	2	−2	0	$2\cos\frac{1}{2}\theta$	$-2\cos\frac{1}{2}\theta$	$2\cos\frac{1}{2}\pi$
1	2	2	0	$2\cos\theta$	$2\cos\theta$	$2\cos\pi$
$\frac{3}{2}$	2	−2	0	$2\cos\frac{3}{2}\theta$	$-2\cos\frac{3}{2}\theta$	$2\cos\frac{3}{2}\pi$
⋮						

Some $3j$ symbols $\{\lambda_1\lambda_2\lambda_3\}$ are fixed by the symmetric products while others may be chosen arbitrarily (Butler 1975, § 6). In D_∞ and D_{even} the choice $(-)^{j(\lambda_1)+j(\lambda_2)+j(\lambda_3)}$ where $j(\lambda_i)$ is the power (I, § 4) of irrep λ_i (and is equal to the modulus of the label except for $j(0^-)=1$) is useful because then there is no sign change under odd permutations of columns in a $6j$ symbol (see equation (16) of I). Note that D_∞ and D_{even} are simply reducible but D_{odd} is not. Wigner (1940) showed that such a choice may be used in simply reducible groups.

For D_{odd} $3j$'s of the form $\{a, a, b\}$ with $a \neq 0^+ \neq b$ must be positive, but we use the above choice in all but this case because in practice only a few $6j$ symbols of D_{odd} do change sign with this choice, and they are imaginary.

Thus we have the $3j$ symbols

$$\begin{aligned} &D_\infty, D_n: \{aa0^-\} = (-)^{2a+1} \\ &\{aa0^+\} = (-)^{2a} \\ &\{abc\} = (-)^{a+b+c} \end{aligned} \tag{2.7}$$

unless $a=b$ or $b=c$, when the sign is $(+)$, and

$$\begin{aligned} &D_n,\ n \text{ even}: \{\pm\tfrac{1}{2}n \pm\tfrac{1}{2}n 0^+\} = +1 \\ &\qquad \{\pm\tfrac{1}{2}n \mp\tfrac{1}{2}0^-\} = -1 \\ &D_n,\ n \text{ odd}: \{\pm\tfrac{1}{2}n \pm\tfrac{1}{2}n 0^-\} = +1 \\ &\qquad \{\pm\tfrac{1}{2}n \mp\tfrac{1}{2}n 0^+\} = -1. \end{aligned} \tag{2.8}$$

3. $6j$ symbols of D_∞

Our derivations follow the methods of I, II and III. Any $6j$ containing the identity irrep (0^+) may be evaluated by using equation (17) of I.

The primitive $6j$'s (those containing $\frac{1}{2}$; I § 4) are restricted by equations (14)–(19) of I. There are, however, choices of phase to be made, one for each non-primitive triad. We choose the phase of the coupling $(a, b+\frac{1}{2}, a+b+\frac{1}{2})$ relative to $(b, a+\frac{1}{2}, a+b+\frac{1}{2})$, and to the primitive couplings $(\frac{1}{2}, a, a+\frac{1}{2})$ and $(\frac{1}{2}, b, b+\frac{1}{2})$, by choosing

$$\begin{Bmatrix} a & b+\frac{1}{2} & a+b+\frac{1}{2} \\ b & a+\frac{1}{2} & \frac{1}{2} \end{Bmatrix} = \tfrac{1}{2}(-)^{2a+2b+1} \tag{3.1}$$

when $a \geqslant b \neq 0^\pm$ This choice has the advantage that the same formula applies for $b \geqslant a$. It follows that for $a, b \neq 0^+$

$$\begin{Bmatrix} a+b & a & b \\ a-\frac{1}{2} & a+b-\frac{1}{2} & \frac{1}{2} \end{Bmatrix} = \tfrac{1}{2}(-)^{2a+2b} \tag{3.2}$$

If we consider $6j$'s containing no $0^\pm$'s arranged so that the largest entry is in the top left corner and the next largest movable entry is on its immediate right, the possible forms are restricted by the appropriate Kronecker products (triads) (see I, equations (14)–(16), III, equation (3)) to

$$\begin{Bmatrix} a+b & a & b \\ a-c & a+b-c & c \end{Bmatrix} \quad \text{and} \quad \begin{Bmatrix} a+b & a & b \\ a+b & a & b \end{Bmatrix}.$$

Equation (18) of I easily shows that the first form has modulus of $\frac{1}{2}$ and a little calculation shows that the second form is zero. (This was used in the calculation of the primitives above.) The general $6j$ can be determined directly by using equation (20) of I to show that

$$\begin{Bmatrix} a+b & a & b \\ a-c & a+b-c & c \end{Bmatrix} = +\begin{Bmatrix} a+b & a & b \\ a-(c-\frac{1}{2}) & a+b-(c-\frac{1}{2}) & c-\frac{1}{2} \end{Bmatrix}$$

$$= \begin{Bmatrix} a+b & a & b \\ a-\frac{1}{2} & a+b-\frac{1}{2} & \frac{1}{2} \end{Bmatrix}$$

$$= \tfrac{1}{2}(-)^{2a+2b}. \tag{3.3}$$

$6j$ symbols containing 0^- must be treated as special cases, relating them via equation (19) of I. We choose

$$\begin{Bmatrix} a+b & a & b \\ 0^- & b & a \end{Bmatrix} = \tfrac{1}{2}(-)^{2a+2b} \tag{3.4}$$

for $a > b \geqslant \frac{1}{2}$. The same phase can be shown to apply for $a \leqslant b$ and we can also obtain

$$\begin{Bmatrix} a+b & a & b \\ a & a+b & 0^- \end{Bmatrix} = \tfrac{1}{2}(-)^{2a+2b+1} \tag{3.5}$$

$$\begin{Bmatrix} a & a & 0^- \\ a & a & 0^- \end{Bmatrix} = \tfrac{1}{2}(-)^{2a} \tag{3.6}$$

$$\begin{Bmatrix} 0^+ & 0^- & 0^- \\ 0^+ & 0^- & 0^- \end{Bmatrix} = \begin{Bmatrix} 0^+ & 0^- & 0^- \\ 0^- & 0^+ & 0^+ \end{Bmatrix} = 1. \tag{3.7}$$

4. 6*j* symbols of D_n

Most of the irreps, triads and $6j$ symbols of D_n are simply a subset of those of D_∞, so our D_∞ calculations are valid for most of the $6j$'s of D_n. The additional triads are of the form

$$(\pm\tfrac{1}{2}n \quad a \quad \tfrac{1}{2}n-a) \tag{4.1}$$

and

$$(a+b \quad \tfrac{1}{2}n-a \quad \tfrac{1}{2}n-b). \tag{4.2}$$

The phase choices associated with the first set of triads may be fixed by the choice

$$\begin{Bmatrix} \pm\frac{1}{2}n & a & b \\ a-\frac{1}{2} & \frac{1}{2}n-\frac{1}{2} & \frac{1}{2} \end{Bmatrix} = \tfrac{1}{2}(-)^n \qquad \text{for } a \geqslant b > \tfrac{1}{2}. \tag{4.3}$$

In order to fix the phase choice associated with the second 'special' triad (4.2) one must be careful to choose a form of $6j$ which does not vanish and does not contain the triad twice. Choosing the phases of all

$$\begin{Bmatrix} a+b & \frac{1}{2}n-a & \frac{1}{2}n-b \\ \frac{1}{2}n-a-\frac{1}{2} & a+b+\frac{1}{2} & \frac{1}{2} \end{Bmatrix} \qquad \text{for } \tfrac{1}{2}n > a+b \geqslant \tfrac{1}{2}n-b \tag{4.4}$$

fixes the rest of the phase relationships. If $a+b+\frac{1}{2} < \frac{1}{2}n$ the $6j$ is real and may be chosen consistent with the 'general pattern' below. If $a+b+\frac{1}{2} = \frac{1}{2}n$ and n is odd the $6j$ is imaginary. For n even it is real, but changes sign for $\pm\frac{1}{2}n$. The remaining $6j$'s are calculated using equations (19) and (20) of I.

We summarize the values for the non-trivial $6j$ symbols for the dihedral groups.

There is a general pattern for $6j$ symbols of dihedral groups which do not contain one-dimensional irreps or triads of the form of (4.2). Except for some vanishing $6j$ symbols,

$$\begin{Bmatrix} a & b & c \\ a & b & c \end{Bmatrix} = 0 \qquad \text{for } D_\infty \text{ and } D_n \tag{4.5}$$

$$\begin{Bmatrix} a & \frac{1}{2}n-a & \frac{1}{2}n-2a \\ \frac{1}{2}n-a & a & 2a \end{Bmatrix} = 0 \qquad \text{for } D_n, \tag{4.6}$$

the modulus is $\frac{1}{2}$ and their phase depends on the triads containing the largest element. The largest element belongs to two triads and the $6j$ has a phase equal to the $3j$ symbol for each triad. Occasionally, for n odd, the two $3j$ symbols have different phases. In this case the $6j$ is positive. This only happens when either triad contains two equal irreps, e.g.

$$\begin{Bmatrix} 2a & \frac{1}{2}n-a & \frac{1}{2}n-a \\ b & c & d \end{Bmatrix} = \tfrac{1}{2} \qquad \text{for } D_n. \tag{4.7}$$

Most of the non-trivial $6j$ symbols containing one-dimensional irreps are tabulated below. Those containing a triad of the form $(a+b\ \frac{1}{2}n-a\ \frac{1}{2}n-b)$ are easy to calculate but difficult to summarise.

For D_∞ or D_n:

$$\begin{Bmatrix} a+b & b & a \\ b & a+b & 0^- \end{Bmatrix} = \tfrac{1}{2}(-)^{2a+2b+1} \tag{4.8}$$

$$\begin{Bmatrix} a+b & b & a \\ 0^- & a & b \end{Bmatrix} = \tfrac{1}{2}(-)^{2a+2b} \tag{4.9}$$

$$\begin{Bmatrix} a & a & 0^- \\ a & a & 0^- \end{Bmatrix} = \tfrac{1}{2}(-)^{2a}. \tag{4.10}$$

For D_n:

$$\begin{Bmatrix} \pm\frac{1}{2}n & a & b \\ \pm\frac{1}{2}n & a & b \end{Bmatrix} = \tfrac{1}{2}(-)^{2a} \tag{4.11}$$

$$\begin{Bmatrix} +\frac{1}{2}n & a & b \\ -\frac{1}{2}n & a & b \end{Bmatrix} = \tfrac{1}{2}(-)^{2a+1} \tag{4.12}$$

$$\begin{Bmatrix} \pm\frac{1}{2}n & \frac{1}{2}n-2a & 2a \\ a & a & \frac{1}{2}n-a \end{Bmatrix} = \tfrac{1}{2}(-)^{n} \tag{4.13}$$

$$\begin{Bmatrix} +\frac{1}{2}n & \pm\frac{1}{2}n & 0^- \\ \frac{1}{2}n-a & \frac{1}{2}n-a & a \end{Bmatrix} = \frac{1}{\sqrt{2}}(-)^{n+1} \tag{4.14}$$

(note: use $\pm$ as n is odd/even)

$$\begin{Bmatrix} \pm\frac{1}{2}n & \frac{1}{2}n-a & a \\ 0^- & a & \frac{1}{2}n-a \end{Bmatrix} = \tfrac{1}{2}(-)^{n} \tag{4.15}$$

$$\begin{Bmatrix} +\frac{1}{2}n & \pm\frac{1}{2}n & 0^- \\ +\frac{1}{2}n & -\frac{1}{2}n & 0^- \end{Bmatrix} = \pm 1 \tag{4.16}$$

(note: use $\pm$ as n is odd/even).

The number of special cases makes it difficult to construct tables by hand using the above results. Butler (1979) will include tabulations of $6j$ symbols for D_∞ and for D_n, with $n \leqslant 6$.

5. The branchings $D_\infty \supset D_n$ and $D_{mn} \supset D_n$

The branching rules for $D_\infty \supset D_n$ are

$$\begin{aligned}
&0^+ \to 0^+\\
&0^- \to 0^-\\
&\tfrac{1}{2} \to \tfrac{1}{2}\\
&\cdots\\
&(\tfrac{1}{2}n - \tfrac{1}{2}) \to (\tfrac{1}{2}n - \tfrac{1}{2})\\
&\tfrac{1}{2}n \to (+\tfrac{1}{2}n) + (-\tfrac{1}{2}n)\\
&(\tfrac{1}{2}n + \tfrac{1}{2}) \to (\tfrac{1}{2}n - \tfrac{1}{2})\\
&\cdots\\
&(n - \tfrac{1}{2}) \to \tfrac{1}{2}\\
&n \to 0^+ + 0^-\\
&(n + \tfrac{1}{2}) \to \tfrac{1}{2}\\
&\cdots
\end{aligned} \tag{5.1}$$

All $2jm$ factors for $D_\infty \supset D_n$ can be chosen to be positive because orthogonal irreps contain orthogonal irreps and the symplectic irreps contain symplectic or quasisymplectic irreps (see equation (31) of I). It is advantageous to choose some $2jm$'s negative when the subgroup is D_{odd} so that all primitive $3jm$'s may be chosen real. Choose all $2jm$'s $(A)_{aa^*}$ negative for A in one of the ranges $\frac{1}{2}(4k+1)n < A < \frac{1}{2}(4k+3)n$, k integer, and positive otherwise. The norms of the primitive $3jm$ factors can be found from equations (35) and (36) of I. Most primitives involve a free phase choice for there is one for each ket $|Aa\rangle$. All primitive $3jm$ factors not involving $\pm\frac{1}{2}n$ may be chosen positive if the columns are appropriately ordered. If a and $a \pm \frac{1}{2}$ are two-dimensional irreps of D_n then

$$\begin{pmatrix} A+\frac{1}{2} & A & \frac{1}{2} \\ a \pm \frac{1}{2} & a & \frac{1}{2} \end{pmatrix} = 1. \tag{5.2}$$

There are the special cases involving $0^\pm$:

$$\begin{pmatrix} 0^- & \frac{1}{2} & \frac{1}{2} \\ 0^- & \frac{1}{2} & \frac{1}{2} \end{pmatrix} = 1 \qquad \begin{pmatrix} A \pm \frac{1}{2} & A & \frac{1}{2} \\ 0^+ & \frac{1}{2} & \frac{1}{2} \end{pmatrix} = \frac{1}{\sqrt{2}}$$
$$\begin{pmatrix} A+\frac{1}{2} & A & \frac{1}{2} \\ 0^- & \frac{1}{2} & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} A+\frac{1}{2} & A & \frac{1}{2} \\ \frac{1}{2} & 0^- & \frac{1}{2} \end{pmatrix} = \frac{1}{\sqrt{2}}. \tag{5.3}$$

The orthogonality relations ((35) and (36) of I) and the complex conjugation symmetries ((38) of I)) restrict the primitive $3jm$ factors involving $\pm\frac{1}{2}n$:

$$\begin{pmatrix} A & A-\frac{1}{2} & \frac{1}{2} \\ \pm\frac{1}{2}n & \frac{1}{2}n - \frac{1}{2} & \frac{1}{2} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} A+\frac{1}{2} & A & \frac{1}{2} \\ \frac{1}{2}n - \frac{1}{2} & \pm\frac{1}{2}n & \frac{1}{2} \end{pmatrix}. \tag{5.4}$$

If n is odd, $-\frac{1}{2}n = (+\frac{1}{2}n)^*$ and there is only one choice for the four cases of (5.4), while for n even there are independent choices for $+\frac{1}{2}n$ and $-\frac{1}{2}n$. We may choose

$$\begin{pmatrix} A & A-\frac{1}{2} & \frac{1}{2} \\ +\frac{1}{2}n & \frac{1}{2}n-\frac{1}{2} & \frac{1}{2} \end{pmatrix} = \frac{1}{\sqrt{2}} \qquad \text{for } n \text{ odd} \tag{5.5}$$

$$\begin{pmatrix} A & A-\frac{1}{2} & \frac{1}{2} \\ +\frac{1}{2}n & \frac{1}{2}n-\frac{1}{2} & \frac{1}{2} \end{pmatrix} = \frac{1}{\sqrt{2}} \qquad \text{for } n \text{ odd} \tag{5.6}$$

and

$$\begin{pmatrix} A+\frac{1}{2} & A & \frac{1}{2} \\ \frac{1}{2}n-\frac{1}{2} & \pm\frac{1}{2}n & \frac{1}{2} \end{pmatrix} = \pm\frac{1}{\sqrt{2}} \qquad \text{for } n \text{ even.} \tag{5.7}$$

Complex conjugation gives

$$\begin{pmatrix} A & A-\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2}n & \frac{1}{2}n-\frac{1}{2} & \frac{1}{2} \end{pmatrix} = \frac{1}{\sqrt{2}}(A-\tfrac{1}{2})_{\frac{1}{2}n-\frac{1}{2},n-\frac{1}{2}} \qquad \text{for } n \text{ odd} \tag{5.8}$$

and

$$\begin{pmatrix} A+\frac{1}{2} & A & \frac{1}{2} \\ \frac{1}{2}n-\frac{1}{2} & -\frac{1}{2}n & \frac{1}{2} \end{pmatrix} = \frac{1}{\sqrt{2}}(A+\tfrac{1}{2})_{\frac{1}{2}n-\frac{1}{2},n-\frac{1}{2}} \qquad \text{for } n \text{ odd} \tag{5.9}$$

since

$$(A)_{+\frac{1}{2}n\,-\frac{1}{2}n} = (\tfrac{1}{2})_{\frac{1}{2}\frac{1}{2}} = 1.$$

The remaining $3jm$ factors are calculated using equation (40) of I. With these choices only $3jm$'s with both n odd and containing triads of the form $(a+b \quad \frac{1}{2}n-a \quad \frac{1}{2}n-b)$ are imaginary.

The branching rules for $D_{mn} \supset D_n$ are the same as those for $D_\infty \supset D_n$ except for the special cases

$$\begin{aligned} \pm\tfrac{1}{2}mn &\to 0^{\pm} && m \text{ even} \\ &\to \pm\tfrac{1}{2}n && m \text{ odd.} \end{aligned} \tag{5.10}$$

The $2jm$ factors are chosen in the same way as the $D_\infty \supset D_n$ ones. It follows that the primitive $3jm$ factors for $D_{mn} \supset D_n$ are the same as $D_\infty \supset D_n$ except for m even when

$$\begin{pmatrix} \pm\frac{1}{2}mn & \frac{1}{2}mn-\frac{1}{2} & \frac{1}{2} \\ 0^{\pm} & \frac{1}{2} & \frac{1}{2} \end{pmatrix} = 1 \tag{5.11}$$

and for m odd when

$$\begin{aligned} \begin{pmatrix} \pm\frac{1}{2}mn & \frac{1}{2}mn-\frac{1}{2} & \frac{1}{2} \\ \pm\frac{1}{2}n & \frac{1}{2}n-\frac{1}{2} & \frac{1}{2} \end{pmatrix} &= 1 && \text{if } (\tfrac{1}{2}mn-\tfrac{1}{2})_{\frac{1}{2}(n-1)\frac{1}{2}(n-1)} = +1 \\ &= \pm 1 && \text{if } (\tfrac{1}{2}mn-\tfrac{1}{2})_{\frac{1}{2}(n-1)\frac{1}{2}(n-1)} = -1. \end{aligned} \tag{5.12}$$

The general $3jm$ factors are again calculated using equation (40) of I.

With the above choices, a $D_\infty - D_n - 3jm$ involving $\pm\frac{1}{2}n$ is not always equal to a product of $D_\infty - D_{mn}$ and $D_{mn} - D_n - 3jm$'s. Such chains may be chosen to factorise by making different choices in equations (5.5) and (5.6) but alternative factorisations (i.e. alternative intermediate groups) will not give the same results in general. For example, it is not difficult (but rather tedious) to show that no choice of phases exists such that the $3jm$'s for $D_\infty \supset D_{18} \supset D_6 \supset D_3$, $D_\infty \supset D_{18} \supset D_9 \supset D_3$, and $D_\infty \supset D_{12} \supset D_6 \supset D_3$ simultaneously factorise.

6. The chains $D_\infty \supset C_\infty$ and $D_n \supset C_n$

The *jm* factors in these chains are easily deduced in the same manner as the *jm* factors of the previous section. Note that, since $SO_2(=C_\infty)$ and C_n are Abelian, their irreps are one-dimensional. This means that all non-vanishing $3j$ and $6j$ symbols are $+1$ as are all $3jm$ factors in all possible imbeddings (see III).

For the cyclic subgroups of the dihedral groups the relevant branching rules are:

$D_\infty \supset C_\infty(=SO_2)$:

$$\begin{aligned} &a \to (+a)+(-a) \\ &0^+ \to 0 \\ &0^- \to 0 \end{aligned} \tag{6.1}$$

$D_n \supset C_n$:

$$\begin{aligned} &a \to (+a)+(-a) \\ &0^+ \to 0 \\ &0^- \to 0 \\ &+\tfrac{1}{2}n \to \tfrac{1}{2}n \\ &-\tfrac{1}{2}n \to \tfrac{1}{2}n \end{aligned} \tag{6.2}$$

$D_{odd} \supset C_2$:

$$\begin{aligned} &0^+ \to 0 \\ &0^- \to 0 \\ &\tfrac{1}{2} \to (+\tfrac{1}{2})+(-\tfrac{1}{2}) \\ &1 \to 0+1 \\ &\tfrac{3}{2} \to (+\tfrac{1}{2})+(-\tfrac{1}{2}) \\ &\\ &(+\tfrac{1}{2}n) \to (+\tfrac{1}{2}) \\ &(-\tfrac{1}{2}n) \to (-\tfrac{1}{2}). \end{aligned} \tag{6.3}$$

For $D_\infty \supset C_\infty$ the $2jm$ factors can be chosen:

$$(a)_{b-b} = (-)^{a-b} \qquad (0^-)_{00} = -1 \tag{6.4}$$

(note that $b = \pm a$).

An appropriate choice for the primitive $3jm$ factors for $D_\infty \supset C_\infty$ and a recoupling gives

$$\begin{pmatrix} a+b & a & b \\ a+b & -a & -b \end{pmatrix} = \frac{1}{\sqrt{2}}(-)^{2b} \tag{6.5}$$

$$\begin{pmatrix} a & a & 0^{\pm} \\ a & -a & 0 \end{pmatrix} = \frac{1}{\sqrt{2}}. \tag{6.6}$$

This $D_\infty \supset C_\infty$ phase choice is chosen because D_∞ is simply reducible (Wigner 1940), and use of this choice means all $3jm$ factors of $D_\infty \supset C_\infty$ and all $6j$ symbols of D_∞ are real. The reader will note that the choice of $3j$ symbols in (2.7) and the choice of $2jm$ factors in (6.4) leads to the following symmetry of the $3jm$ factor. Under either interchange of columns, or conjugating the irreps (changing the sign of the bottom line), the new $3jm$ factor is related to the old $3jm$ by + or − as the sum of the elements of the top line is even or odd (counting 0^- as 1). This is Wigner's (1940) result.

These formulae do not work for $D_n \supset C_n$, because D_{odd} is not simply reducible, but with appropriate choices the $3jm$ factors for $D_{even} \supset C_{even}$ are all real. (Tables are available and will be published: Butler 1979).

7. $3jm$ factors for $SO_3 \supset D_\infty$

The branching $SO_3 \supset SO_2$ has been studied extensively; see II for references and Rotenburg *et al* (1959) for tables. Unfortunately, although the group D_∞ belongs in the chain $SO_3 \supset D_\infty \supset SO_2$, the free phases in the Racah–Wigner algebra for $SO_3 \supset SO_2$ have not been chosen to allow factorisation. (We call the standard choice the *JM* basis choice.) The conflict can be seen from the symmetries of the following $3jm$ symbol of $SO_3 \supset SO_2$ and the corresponding $3jm$ factors for $SO_3 \supset D_\infty$ and $D_\infty \supset SO_2$ steps.

We have

$$\begin{pmatrix} 2 & 1 & 1 \\ -1 & 0 & 1 \end{pmatrix}_M^J = (2)_{1-1}(1)_{00}(1)_{1-1}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 0 & -1 \end{pmatrix}_M^{*J} \tag{7.1}$$

where the standard choices of $2jm$ $(J)_{M-M} = (-)^{J-M}$ give the standard result

$$\begin{pmatrix} 2 & 1 & 1 \\ -1 & 0 & 1 \end{pmatrix}_M^J = \begin{pmatrix} 2 & 1 & 1 \\ 1 & 0 & -1 \end{pmatrix}_M^J \tag{7.2}$$

In the $SO_3 \supset D_\infty \supset SO_2$ basis we have the factorisations

$$\begin{pmatrix} 2 & 1 & 1 \\ -1 & 0 & 1 \end{pmatrix}_{SO_2}^{SO_3} = \begin{pmatrix} 2 & 1 & 1 \\ 1 & 0^- & 1 \end{pmatrix}_{D_\infty}^{SO_3} \begin{pmatrix} 1 & 0^- & 1 \\ -1 & 0 & 1 \end{pmatrix}_{SO_2}^{D_\infty} \tag{7.3}$$

$$\begin{pmatrix} 2 & 1 & 1 \\ 1 & 0 & -1 \end{pmatrix}_{SO_2}^{SO_3} = \begin{pmatrix} 2 & 1 & 1 \\ 1 & 0^- & 1 \end{pmatrix}_{D_\infty}^{SO_3} \begin{pmatrix} 1 & 0^- & 1 \\ 1 & 0 & -1 \end{pmatrix}_{SO_2}^{D_\infty} \tag{7.4}$$

The $3jm$ factors for $SO_3 \supset D_\infty$ are identical in (7.3) and (7.4). The $3jm$ factors for $D_\infty \supset SO_2$ are related by the interchange of columns 1 and 3. The phase ($3j$ symbol) which arises is fixed by the occurrence of 0^- in the product of $1(D_\infty)$ with itself; this is negative (Butler 1975, § 6). This shows that the $SO_3 \supset D_\infty \supset SO_2$ basis is different from the standard *JM* basis.

The discrepancy in the two bases can be traced to the number of free phases in the Racah–Wigner algebra. In the example, the *JM* basis regards the kets $|21\rangle$ and $|2-1\rangle$ as unrelated, the relation being fixed by phase choices during the calculation (such as by the phases of the ladder operators $J_\pm = \mp(J_x \pm iJ_y)$). The $SO_3 \supset D_\infty \supset SO_2$ basis does not have this freedom, for the relation between $|211\rangle$ and $|21-1\rangle$ is forced to be the same as the relation between $|111\rangle$ and $|11-1\rangle$.

The $SO_3 \supset D_\infty$ $3jm$ factors follow from the usual arguments. It is possible to choose all $2jm$ factors positive and the primitive $3jm$ factors as

$$\begin{pmatrix} J+\frac{1}{2} & J & \frac{1}{2} \\ a\pm\frac{1}{2} & a & \frac{1}{2} \end{pmatrix} = \left(\frac{2J\pm 2a+2}{(2J+1)(2J+2)}\right)^{1/2} \tag{7.5}$$

$$\begin{pmatrix} J+\frac{1}{2} & J & \frac{1}{2} \\ 0^{\pm} & \frac{1}{2} & \frac{1}{2} \end{pmatrix} = \frac{1}{(2J+2)^{1/2}} \tag{7.6}$$

$$\begin{pmatrix} J+\frac{1}{2} & J & \frac{1}{2} \\ \frac{1}{2} & 0^{\pm} & \frac{1}{2} \end{pmatrix} = (-)^{J}\frac{1}{(2J+1)^{1/2}} \tag{7.7}$$

where $0^{\pm}$ occurs as $J+\frac{1}{2}$ (or J) is even or odd.

The primitive $3jm$ factors are all that are necessary to calculate the transformation coefficients between the JM and $SO_3 \supset D_\infty \supset SO_2$ bases (Butler 1975, § 11).

A recursive calculation shows that if

$${}_{D_\infty}\langle 000\,|\,00\rangle_{SO_2} = {}_{D_\infty}\langle \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\,|\,\tfrac{1}{2}\tfrac{1}{2}\rangle_{SO_2} = 1 \tag{7.8}$$

then

$$\langle Jaa\,|\,Ja\rangle = (-)^{J-a} \tag{7.9}$$

$$\langle Ja-a\,|\,J-a\rangle = 1 \tag{7.10}$$

where $a>0$, and for J even or odd,

$$\langle J0^{\pm}0\,|\,J0\rangle = 1. \tag{7.11}$$

Now that we have the transformation from the usual JM basis to the more symmetric $SO_3 \supset D_\infty \supset SO_2$ basis we may factorise the $SO_3 \supset SO_2$ chain at the D_∞ level and obtain the $SO_3 \supset D_\infty$ $3jm$ factors as

$$\begin{pmatrix} J_1 & J_2 & J_3 \\ a+b & a & b \end{pmatrix}^{SO_3}_{D_\infty} = 2^{1/2}(-)^{J_1-a+b}\begin{pmatrix} J_1 & J_2 & J_3 \\ a+b & -a & -b \end{pmatrix}^{J}_{M} \tag{7.12}$$

$$\begin{pmatrix} J_1 & J_2 & J_3 \\ a & a & 0^{\pm} \end{pmatrix}^{SO_3}_{D_\infty} = 2^{1/2}(-)^{J_1-a}\begin{pmatrix} J_1 & J_2 & J_3 \\ a & -a & 0 \end{pmatrix}^{J}_{M} \tag{7.13}$$

8. Conclusion

We have shown that all j and jm factors, for all dihedral and cyclic groups and for all possible imbeddings involving them, can be calculated using character theory alone.

A second important aspect of our work has been the use made of the factorisation of jm symbols for chains of groups. Direct use was made of this in § 7, where we derived a simple expression for the $SO_3 - D_\infty - 3jm$ factors in terms of the $SO_3 - SO_2 - 3jm$ symbol of angular momentum. The use of D_∞ to make $SO_3 \supset D_n$ more nearly maximal removes the multiplicity problems encountered by other authors.

References

Bickerstaff R P and Wybourne B G 1976 *J. Phys. A: Math. Gen.* **9** 1051–67

Butler P H 1975 *Trans. R. Soc.* A **277** 545–85

—— 1976 *Int. J. Quantum Chem.* **10** 699–713

—— 1979 *Point Group Symmetry Applications, Methods and Tables* (New York: Plenum).
Butler P H and Wybourne B G 1976a *Int. J. Quantum Chem.* **10** 581–98
—— 1976b *Int. J. Quantum Chem.* **10** 615–28
Golding R M and Newmarch J D 1977 *Molec. Phys.* **33** 1301–18
Hamermesh M 1962 *Group Theory* (Reading, Mass: Addison-Wesley)
Harnung S E and Schäffer C E 1972 *Structure and Bonding* **12** 201–55
Kibler M R and Grenet G 1977 *Int. J. Quantum Chem.* **11** 359–79
Koster G, Dimmock J, Wheeler R and Statz H 1963 *Properties of the Thirty-Two Point Groups* (MIT, Cambridge, Mass: MIT Press)
Patera J and Winternitz P 1973 *J. Math. Phys.* **14** 1130–9
Racah 1949 *Phys. Rev.* **76** 1352–65
Rotenberg M, Bivins R, Metropolis N and Wooten J K 1959 The 3*j* and 6*j* Symbols (Cambridge, Mass: Technology Press)
Wigner 1940 *Quantum Theory of Angular Momentum* eds L C Biedenharn and H Van Dam (New York, London: Academic) (published 1965)