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Calculation of primitive 6-j symbols

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Abstract. The 6-j symbols of a group are independent of the subgroup chain chosen to define the basis states. We present an improved algorithm for calculating the primitive 6-j symbols for a compact group with a faithful irrep by recursive building up using only the Kronecker product rules and the general properties of 6-j. Previously one has sometimes needed to search for the useful equations by systematically trying all equations which involve unknown 6-j. We show that the primitive 6-j may all be easily solved in terms of a subclass, the core 6-j. We discuss how the core 6-j can usually be solved, proving that the method is complete for SO_3. We conjecture that the algorithm is complete for all groups.

1. Introduction

There continues to be interest in finding improved methods for calculating 3-jm and 6-j symbols for various groups, because of the use of many different groups in quantum mechanics. Some recent examples of such calculations are Chen *et al* (1985) for the space groups, Haase and Dirl (1986) for the symmetric groups, Judd (1986, 1987), Judd *et al* (1986) and Pluhar *et al* (1986) for the classical groups, Raynal and Conte (1985) for the point groups and Zeng (1987) for OSp(1, 2).

Most authors have calculated 3-jm from explicitly symmetrised basis functions and then calculated 6-j from the 3-jm. Using such an approach, a basis choice for the partners of each irrep must be made to calculate the 3-jm, even though the 6-j are totally independent of such a choice. However when calculating 6-j, an alternative and more direct approach is to use the Biedenharn-Elliott, the Racah backcoupling and the orthonormality relations of 6-j, relations which are valid for all compact groups (see Derome and Sharp 1965, Butler 1975). As well as these generally valid relations, we require specific information about the group, specifically the product rules and plethysms (or symmetrised powers) of the irreps. An early example of such a calculation is the demonstration (Butler 1976) that the Racah formula for the 6-j of SO_3 can be obtained directly from the product rules of SO_3. If one requires 3-jm, a basis choice can then be made using the appropriate subgroups, and the general 3-jm can be calculated from this information and the 6-j of the group and subgroup. Complete tables for all point groups (up to $j=8$) have been calculated by this means (Butler 1981) and we have further improved upon that algorithm for all non-primitive transformation factors in a previous paper (Searle and Butler 1988).

Judd *et al* (1986) emphasise that calculating multiplicity-free 6-j for a general compact group is a relatively simple extension of the methods for SO_3. Our preceding paper showed that the calculation of non-primitive 6-j symbols with multiplicity may be carried out essentially as for the multiplicity-free case once the primitive symbols have been chosen. This paper will consider the calculation of primitive 6-*j* by placing them into various classes, and recursing downward until we reach a core 6-*j*. The calculation of the core 6-*j* includes calculation of basis 6-*j* which requires the choice of the free phases in the 6-*j* algebra and the separation of the coupling multiplicities.

The present study grew out of a request by Hamer (see Hamer *et al* 1986) for some 6-*j* of SU_3 involving irreps up to power five. The ALGOL program used by Butler (1981) for calculating 6-*j* and 3-*jm* of the point groups, and used by Bickerstaff *et al* (1982) for some 6-*j* of SU_3 and SU_6, was found to be unnecessarily indirect. It required more intermediate steps than were necessary and included the calculation of 6-*j* outside the range of interest. This arises partly because SU_3 contains the case $\{1\}\times\{1\}\supset\{1\}^*$, a case which does not occur when the primitive irrep is symplectic and indeed occurs only rarely amongst the classical groups. Our attempts to avoid the need to calculate 6-*j* outside Hamer's range of interest led us to the present algorithm.

Section 2 reviews the definitions needed in this paper. Section 3 discusses the number and occurrence of phase choices available in the 6-*j* part of the Racah–Wigner algebra, results due to Derome (1966) and used by him to make certain advantageous phase choices in the symmetry relations. In § 4 we categorise a subset of the 6-*j* as the basis set of 6-*j*. This basis set may be used to fix all the free phases and multiplicity separations of the 6-*j* algebra. Section 5 splits the primitive 6-*j* into various subclasses and shows how to solve for 6-*j* in some of the classes in terms of 6-*j* of a class of core 6-*j*. All the basis 6-*j* belong to the core subclass. It is the discovery of this classification and the consequential use of the recursion relations that is the central result of this paper. Our building-up method in the past has always provided sufficient relations for the 6-*j* of all the various groups we have studied. However one has sometimes needed to search for the useful equations by the tedious method of systematically trying all equations which involve the unknown 6-*j*. Section 5 proves that the primitive 6-*j* may all be written in terms of the core subclass. As noted above, this class of core 6-*j* includes all basis 6-*j*, and in § 6 we discuss how 6-*j* in this class can usually be solved.

The problem of calculating the core 6-*j* remains partly open. The group SO_3 is special in having one irrep of each power, and this allows us to prove completeness for SO_3. Likewise explicit calculation shows that the 6-*j* for all the point groups and SU_3 are readily calculated by the present algorithm.

2. Definitions and reviews

Derome and Sharp (1965) introduced the matrix $m(\pi, \lambda_1\lambda_2\lambda_3)$, indexed by coupling multiplicity labels, to describe the symmetries under column permutations, π, of a 3-*jm* symbol involving the irreps $\lambda_1\lambda_2\lambda_3$ of a compact group. The same paper introduced a generalisation of the 6-*j* symbols of angular momentum that give the remaining information on recoupling transformations in the Racah–Wigner algebra. Butler (1975) gives a review of the Racah–Wigner algebra for the case of a general compact group, while Butler (1981) gives an account of the definitions and results appropriate to those couplings, such as those within the point groups, that have a simple permutation symmetry. (The more general case occurs when the coupling of three identical irreps to a scalar is said to be of mixed symmetry, the three irreps of the threefold coupling transforming amongst themselves as the irrep [21] of the symmetric group S_3.) The above references show that the familiar methods of angular momentum theory apply to any compact group subject to the generalisations required when: (i) an irrep λ is not unitarily equivalent to its complex conjugate λ^*; (ii) when a coupling of the three irreps $\lambda_1\lambda_2\lambda_3$ gives the scalar irrep more than once; (iii) when mixed symmetry couplings occur.

As in our previous work (Butler 1981, Searle and Butler 1988) we use the concept of the power $p(\lambda)=k$ of an irrep λ, where $(\varepsilon+\varepsilon^*)^k \supset \lambda$ and ε is the primitive irrep, to define a partial ordering: we say that $\lambda <_p \mu$ if $p(\lambda)<p(\mu)$. The ordering of irreps is then arbitrarily completed ensuring only that λ and λ^* are contiguous irreps.

A triad $\lambda_1\lambda_2\lambda_3 r$ is defined to exist if $\lambda_1\times\lambda_2\times\lambda_3$ contains the scalar at least r times. The triad is said to be in standard order if $\lambda_1 \geqslant \lambda_2 \geqslant \lambda_3$. For the purposes of the classification we must define a partial ordering between two triads $\lambda_a\lambda_b\lambda_c r$, $\mu_a\mu_b\mu_c s$ by writing them in standard order $\lambda_1\lambda_2\lambda_3 r$ and $\mu_1\mu_2\mu_3 s$, and saying that $\lambda_1\lambda_2\lambda_3 r <_p \mu_1\mu_2\mu_3 s$ if $p(\lambda_2)+p(\lambda_3)<p(\mu_2)+p(\mu_3)$. This ordering differs from the one used by us for tabulation purposes. The present partial ordering ($<_p$) is to be completed by basing the further ordering on the completed ordering of the irreps. Further, a triad is in standard form if it is in both standard order and $\lambda_1\lambda_2\lambda_3 r<\lambda_1^*\lambda_2^*\lambda_3^* r$ in the completed ordering.

In addition to using these orderings, we classify triads by the power of their smallest irrep. A trivial triad contains the scalar irrep and is of the form $\lambda^*\lambda 0$, while a primitive triad contains an irrep of power one, that is, ε or ε^* (but we do not include the $\varepsilon^*\varepsilon 0$ triad). In the following we will often use ε_1, ε_2, etc, to denote an irrep of power one (either ε or ε^*). A triad is said to be stretched if $p(\lambda_1)=p(\lambda_2)+p(\lambda_3)$ when in standard order. For all the (double covered) point groups, all symmetric groups and all simple compact Lie groups, these triads are of multiplicity one if ε is chosen as the lowest-dimensional faithful irrep. For most of these groups the sets of primitive and stretched primitive triads are identical. However, for four of the above groups, namely SU_3, E_6, E_8 and G_2, the stretched primitive set is smaller because the non-stretched coupling $\varepsilon\times\varepsilon\supset\varepsilon^*$ occurs (if spinor irreps are excluded and the vector irrep is chosen as the primitive irrep such products also occur for some point groups, for all SO_n and for S_n). We will often write a stretched primitive triad in the standard form as $\lambda\bar{\lambda}\varepsilon_1$, since there is no multiplicity, and we use the notation $\bar{\lambda}$ to indicate any irrep of power $p(\lambda)-1$ contained in either of the products, $\lambda^*\times\varepsilon^*$ or $\lambda^*\times\varepsilon$.

In similar fashion to the definition of triads, a trivial 6-*j* is defined as a 6-*j* that contains the scalar irrep. A primitive 6-*j* does not contain 0 but does contain ε or ε^* and hence contains at least two primitive triads. A core 6-*j* is a certain kind of primitive 6-*j* and will be defined in § 5.

3. The phase factor matrices

Derome (1966) exploited the unitary freedom in the multiplicity space of a coupling coefficient to analyse the possible structures of the permutation matrices $m(\pi, \lambda_1\lambda_2\lambda_3)$. If $\lambda_1\lambda_2\lambda_3$ couple together to give n copies of the scalar irrep, so that there are n non-vanishing triads $\lambda_1\lambda_2\lambda_3 r$, then there is a $n\times n$ unitary matrix $K(\lambda_1\lambda_2\lambda_3)$ describing the transformation between one set of coupling coefficients with a given set of phases and multiplicity separations, and another such set. For each triple $\lambda_1\lambda_2\lambda_3$ in standard order, there are up to twelve distinct phase freedom matrices, K, one for each of the six orders and one for each complex conjugate triple. One of the principal results of Derome (1966) was to show how to exploit the phase freedom matrices to select simple values of the elements of the matrix $m(\pi, \lambda_1\lambda_2\lambda_3)$. We call the matrix elements the 3-j and write them as $\{\lambda_1\lambda_2\lambda_3\}_{rs}$.

Except for mixed symmetry couplings, the 3-j may be chosen (or fixed, depending on the case) as diagonal in rs, ± 1 for interchanges ($+1$ for cyclic permutations) and independent of the order of the triad (Butler 1975). This choice leaves us the freedom of choosing one phase freedom matrix $K(\lambda_1\lambda_2\lambda_3)$ for each ordered triple $\lambda_1\lambda_2\lambda_3$. If any two of the irreps in the triple are identical, the phase freedom matrix is not totally free but is restricted to being block diagonal with respect to the permutation symmetry type. Butler (1975) also chooses the Derome and Sharp (1965) A matrix to be unity, hence fixing the relationship of $K(\lambda_1^*\lambda_2^*\lambda_3^*)$ to $K(\lambda_1\lambda_2\lambda_3)^*$. (Bickerstaff and Damhus (1985) argue that a unit choice for A may not be the most propitious choice; however the actual choice does not affect the results of this paper.) Any choice of a standard form for the m and A matrices fix the relationship of the up to twelve distinct phase freedom matrices K. In the following sections we may therefore consider the matrix $K(\lambda_1\lambda_2\lambda_3)$ free if and only if the triple $\lambda_1\lambda_2\lambda_3$ is in standard form.

The above discussion looked at the coupling phase freedom. A similar argument applies to the branching phase freedoms which occur in the 3-jm part of the Racah–Wigner algebra. Bickerstaff (1984) and Bickerstaff and Damhus (1985) discuss conditions on the choice (or lack) of reality of coupling coefficients. However the coupling and branching phase choices are not always the only choices one must make within the Racah–Wigner algebra. Reid and Butler (1980, 1982) show that additional phases can occur for some group–subgroup pairs, phases that are related in some way to the orientation of the subgroup H within the group G. These orientation phases occur since certain basis kets are not fixed by the 3-jm algebra, and involve special cases of the branching rules. It is possible that the product rules $\lambda_1 \times \lambda_2 \supset \lambda_3$ contain similar choices since they are equivalent to a branching $G \times G \supset G$. However, we have found no evidence that such phases occur in the 6-j algebra of any of the groups we have studied.

4. The basis 6-j

Two alternative choices of the phase and multiplicity separation in a 6-j symbol are related by four coupling phase freedom matrices in the following manner:

$$\begin{Bmatrix} \lambda_1 & \lambda_2 & \lambda_3 \\ \mu_1 & \mu_2 & \mu_3 \end{Bmatrix}^{\mathrm{alt}}_{s_1s_2s_3s_4} = K(\lambda_1\mu_2^*\mu_3)^{s_1}{}_{r_1}K(\mu_1\lambda_2\mu_3^*)^{s_2}{}_{r_2}K(\mu_1^*\mu_2\lambda_3)^{s_3}{}_{r_3}K(\lambda_1^*\lambda_2^*\lambda_3^*)^{s_4}{}_{r_4} \times \begin{Bmatrix} \lambda_1 & \lambda_2 & \lambda_3 \\ \mu_1 & \mu_2 & \mu_3 \end{Bmatrix}_{r_1r_2r_3r_4}. \tag{4.1}$$

The non-primitive 6-j have previously been shown (Searle and Butler 1988) to be totally dependent on the primitive 6-j and hence contain no freedom at all. This means that the freedom allowed by the K matrices is only constrained by choices of primitive 6-j.

Each irrep in a 6-j occurs in two triads. As we build up our 6-j we will at some time try to solve for a 6-j which contains an irrep, λ, that has not previously been used. Since this irrep occurs in two triads, we have two new free phase matrices arising, one for each triad. We are allowed to choose the phase of the 6-j if the two triads are distinct. Such a phase choice results in the choice of (part of—if there is multiplicity) one of the two free K matrices involving λ with respect to (part of) the other and with respect to the K matrices of the other two triads in the 6-j. This process occurs for every triad that has the irreps λ or λ^* as the largest irrep, resulting in all the phases being chosen with respect to the one matrix K that is still free. We arbitrarily choose the triad that has the free phase matrix to be one of the stretched primitive triads $\lambda\bar{\lambda}\varepsilon_1$ for the irrep λ. This matrix $K(\lambda\bar{\lambda}\varepsilon_1)$ cannot be fixed within the 6-j algebra (Bickerstaff 1981) and the triad is known as the basis triad for the pair λ, λ^*. Those 6-j for which a phase is chosen are said to be the basis 6-j corresponding to those triads whose phase they fix. This selection process occurs once for every irrep λ (or pair λ, λ^*) where $\lambda > \varepsilon$. In groups where $\varepsilon \times \varepsilon \supset \varepsilon^*$ we find that the phase matrix of the triad $\varepsilon\varepsilon\varepsilon$ cannot be fixed by the algebra either, so that the primitive irrep has a basis triad in these few cases.

For each triad $\lambda\alpha\beta r_4$ where $p(\beta) > 1$ and where the triad is in standard form, we will select as the basis 6-j the 'least' of the 6-j in the form

$$\begin{Bmatrix} \lambda & \alpha & \beta \\ \beta' & \varepsilon_1 & \lambda' \end{Bmatrix}_{r_1r_2r_3r_4}. \tag{4.2}$$

We define this 'least' 6-j by choosing $\varepsilon_1 = \varepsilon$ and the irreps β' and λ' to be as small as possible in the following manner. Sometimes there is more than one irrep β' of power $p(\beta) - 1$ that can be used. In a similar way several λ' (and r_2) may occur. We select the smallest irrep β' for which the power of λ' is a minimum, and the smallest irrep λ' of this minimum power and where the 6-j is non-zero (see § 6). Finally ε^* may be used instead of ε if it allows irreps of smaller power to be chosen. Usually the resulting basis 6-j is of the form

$$\begin{Bmatrix} \lambda & \alpha & \beta \\ \bar{\beta} & \varepsilon & \bar{\lambda} \end{Bmatrix}_{r_1r_2r_3r_4}$$

and has two non-primitive triads $\lambda\alpha\beta r_4$, $\bar{\lambda}^*\alpha\bar{\beta}r_2$.

When more than one irrep $\bar{\lambda}$ exists for a given λ, then there is more than one primitive triad for the irrep (of the form $\lambda\bar{\lambda}\varepsilon$ or $\lambda\bar{\lambda}\varepsilon^*$). Any one of these triads can be chosen basis. We choose the one with the smallest $\bar{\lambda}$. The remaining primitive triads give rise to corresponding basis 6-j. If we choose $\beta' = \bar{\beta}$ as in the form above we will find that $\bar{\beta} = 0$. We cannot choose this as a basis 6-j as this is a trivial 6-j with no freedom of phase. For most groups the smallest useful value for β' is one of the power two irreps. We choose the smallest value of λ' that results in distinct triads involving λ, thus ensuring that there is sufficient freedom in the 6-j for it to be basis. The resulting basis 6-j is of the form

$$\begin{Bmatrix} \lambda & \bar{\lambda} & \varepsilon_1 \\ 2 & \varepsilon_2 & \bar{\lambda}_b \end{Bmatrix}_{r_1r_2r_3r_4} \tag{4.3}$$

where $\lambda\bar{\lambda}_b\varepsilon_2^*$ is the triad chosen as basis for λ. For those few groups where $\varepsilon\varepsilon\varepsilon$ is a triad, triads of the form $\lambda\alpha\varepsilon_1$ occur where $p(\alpha) = p(\lambda)$ or $p(\alpha) = p(\lambda) - 1$. In either case we have always found a suitable $\beta' = \varepsilon_3$ and $\lambda' = \bar{\lambda}$ to give a basis 6-j of the form

$$\begin{Bmatrix} \lambda & \alpha & \varepsilon_1 \\ \varepsilon_3 & \varepsilon_2 & \bar{\lambda} \end{Bmatrix}_{r_1r_2r_3r_4}. \tag{4.4}$$

5. Primitive 6-*j* symbols

In this section we classify all primitive 6-*j* into various forms determined by the number and the position of the primitive irreps. We then use the Racah backcoupling and Biedenharn-Elliott equations as recursion relations to relate any primitive 6-*j* to 6-*j* in one particular form and primitive 6-*j* involving only smaller triads.

Consider first the primitive 6-*j* with at least one non-primitive triad. In order to classify these 6-*j* we use symmetry relations to rearrange the 6-*j* so that the largest non-primitive triad $\lambda\alpha\beta r_4$ is in standard order and in the top row. For those primitive 6-*j* with two primitive triads (so two triads are non-primitive) we obtain a 6-*j* in one of three general forms, depending on the position in the bottom row of the primitive irrep. The primitive 6-*j* with one non-primitive triad can be rearranged to have two primitive irreps in the bottom row. Those 6-*j* with a primitive irrep in column 2 will be defined as core 6-*j*,

$$\begin{Bmatrix} \lambda & \alpha & \beta \\ \beta' & \varepsilon_1 & \lambda' \end{Bmatrix}_{r_1r_2r_3r_4} \begin{Bmatrix} \lambda & \alpha & \beta \\ \beta' & \varepsilon_1 & \varepsilon_2 \end{Bmatrix}_{r_1r_2r_3r_4} \begin{Bmatrix} \lambda & \alpha & \beta \\ \varepsilon_2 & \varepsilon_1 & \lambda' \end{Bmatrix}_{r_1r_2r_3r_4} \tag{5.1}$$

while the others are not:

$$\begin{Bmatrix} \lambda & \alpha & \beta \\ \alpha' & \lambda' & \varepsilon_1 \end{Bmatrix}_{r_1r_2r_3r_4} \begin{Bmatrix} \lambda & \alpha & \beta \\ \varepsilon_2 & \lambda' & \varepsilon_1 \end{Bmatrix}_{r_1r_2r_3r_4} \tag{5.2}$$

$$\begin{Bmatrix} \lambda & \alpha & \beta \\ \varepsilon_1 & \beta' & \alpha' \end{Bmatrix}_{r_1r_2r_3r_4}. \tag{5.3}$$

In (5.1), (5.2) and (5.3) the coupling conditions restrict the powers of α', β' and λ' to be within one of the powers of α, β and λ respectively.

All other primitive 6-*j* contain four primitive triads and may be related by the symmetry relations to one of the following:

$$\begin{Bmatrix} \lambda & \alpha & \varepsilon_2 \\ \varepsilon_3 & \varepsilon_1 & \lambda' \end{Bmatrix}_{r_1r_2r_3r_4} \begin{Bmatrix} \lambda & \alpha & \varepsilon_2 \\ \varepsilon_3 & \varepsilon_1 & \varepsilon_4 \end{Bmatrix}_{r_1r_2r_3r_4} \begin{Bmatrix} \lambda & \varepsilon_5 & \varepsilon_2 \\ \varepsilon_3 & \varepsilon_1 & \varepsilon_4 \end{Bmatrix}_{r_1r_2r_3r_4} \begin{Bmatrix} \varepsilon_1 & \varepsilon_2 & \varepsilon_3 \\ \varepsilon_4 & \varepsilon_5 & \varepsilon_6 \end{Bmatrix}_{r_1r_2r_3r_4} \tag{5.4}$$

$$\begin{Bmatrix} \lambda & \alpha & \varepsilon_2 \\ \alpha' & \varepsilon_3 & \varepsilon_1 \end{Bmatrix}_{r_1r_2r_3r_4} \begin{Bmatrix} \lambda & \alpha & \varepsilon_2 \\ \varepsilon_3 & \lambda' & \varepsilon_1 \end{Bmatrix}_{r_1r_2r_3r_4} \begin{Bmatrix} \lambda & \varepsilon_4 & \varepsilon_2 \\ \alpha & \varepsilon_3 & \varepsilon_1 \end{Bmatrix}_{r_1r_2r_3r_4} \tag{5.5}$$

$$\begin{Bmatrix} \lambda & \alpha & \varepsilon_2 \\ \alpha' & \lambda' & \varepsilon_1 \end{Bmatrix}_{r_1r_2r_3r_4} \tag{5.6}$$

where $\lambda\alpha\varepsilon_2$ is the largest triad (so $\lambda \geqslant \alpha$, $\alpha \geqslant \lambda'$ and $\lambda \geqslant \alpha'$). The 6-*j* of (5.4) only occur for the groups where $\varepsilon\varepsilon\varepsilon$ exists. It is easy to show that none of the irreps λ, α and λ' can be of power greater than three in (5.5). We will define the 6-*j* in (5.4) and (5.5) to be part of the set of core 6-*j*.

For most groups (that is where the triad $\varepsilon\varepsilon\varepsilon$ does not exist) all basis 6-*j* belong to one of the forms of (5.1). However, to be consistent with the above classification the 6-*j* in (4.3) must be related by symmetry to a 6-*j* in the form

$$\begin{Bmatrix} \bar{\lambda} & \bar{\lambda}_b & 2 \\ \varepsilon_2 & \varepsilon_1 & \lambda' \end{Bmatrix}_{r_1r_2r_3r_4}$$

since $\bar{\lambda}\bar{\lambda}_b 2 r_4$ is the only non-primitive triad. For the few groups that contain $\varepsilon\varepsilon\varepsilon$, the basis 6-*j* in (4.2) belong to one of the forms of (5.1), whereas those in (4.4) belong to the form of (5.4).

We refer to the 6-*j* in (5.1), (5.4) and (5.5) as the core 6-*j*, and emphasise that our set of basis 6-*j* is a subset of the set of core 6-*j*. In the remainder of this section we shall give a recursive method of solving all non-core 6-*j*.

Any 6-*j* in the form of (5.3) may be related to 6-*j* in the other primitive forms by applying the Racah backcoupling relation (Butler 1975, equation (9.10)), together with the symmetry relations. The first 6-*j* that occurs is in the form of one in (5.1), and the second 6-*j* is of the form of one in (5.2). After application of the symmetries, we have

$$\begin{Bmatrix} \lambda & \alpha & \beta \\ \varepsilon_1 & \beta' & \alpha' \end{Bmatrix}_{r_1r_2r_3r} = \sum_{\substack{\rho=\lambda-1 \\ s_1s_2}}^{\lambda+1} \# \begin{Bmatrix} \lambda & \alpha & \beta \\ \beta'^* & \varepsilon_1^* & \rho \end{Bmatrix}_{s_1s_2r_3r} \begin{Bmatrix} \rho^* & \alpha & \beta' \\ \alpha'^* & \lambda & \varepsilon_1^* \end{Bmatrix}_{s_1r_2r_1s_2} \tag{5.7}$$

where $\lambda \pm 1$ denotes all irreps of power $p(\lambda) \pm 1$. Since we are only interested in the form of the equations for the 6-*j*, we have put all phase and dimension factors, in this equation and those that follow, into the symbol $\#$.

The Biedenharn-Elliott equation, when applied to a 6-*j* from (5.2), gives

$$\sum_r \begin{Bmatrix} \lambda & \alpha & \beta \\ \alpha' & \lambda' & \varepsilon_1 \end{Bmatrix}_{r_1r_2r_3r} \begin{Bmatrix} \lambda & \alpha & \beta \\ \bar{\beta} & \varepsilon_2 & \nu \end{Bmatrix}^*_{s_1s_2s_3r}$$
$$= \sum_{\substack{\rho=\lambda'-1 \\ t_1t_2t_3}}^{\lambda'+1} \# \begin{Bmatrix} \lambda'^* & \rho & \varepsilon_2 \\ \nu & \lambda^* & \varepsilon_1 \end{Bmatrix}_{r_2t_1s_1t_2} \begin{Bmatrix} \nu^* & \alpha & \bar{\beta} \\ \alpha' & \rho & \varepsilon_1 \end{Bmatrix}_{t_1r_2t_3s_2} \begin{Bmatrix} \lambda'^* & \alpha' & \beta^* \\ \bar{\beta}^* & \varepsilon_2^* & \rho \end{Bmatrix}_{t_2t_3s_3r_3} \tag{5.8}$$

where the symmetries have again been used to rearrange the forms. The coefficient 6-*j* (second from the left) is in the form of the basis 6-*j* (and is basis when ν is a minimum), and we have shown in our paper on non-primitive coupling coefficients (Searle and Butler 1988) that the Biedenharn-Elliott equation will allow us to completely solve the set of unknowns when all ν are considered. The first 6-*j* on the right-hand side has only primitive triads and is in one of (5.4), (5.5) or (5.6). The second 6-*j* is the same form as the unknown but β has been reduced to $\bar{\beta}$. Thus the largest non-primitive triad has been reduced (often further gains are made because $\nu = \bar{\lambda}$ as well). The third 6-*j* is of the form (5.1), and is to be solved by other means.

The 6-*j* of (5.6), where λ', λ, α' and α are all non-primitive, may be related to 6-*j* that belong to those in (5.1) or (5.4) by use of the Racah backcoupling equation, where the maximum power of ρ is two:

$$\begin{Bmatrix} \lambda & \alpha & \varepsilon_2 \\ \alpha' & \lambda' & \varepsilon_1 \end{Bmatrix}_{r_1r_2r_3r_4} = \sum_{\substack{\rho=0 \\ s_1s_2}}^{2} \# \begin{Bmatrix} \lambda'^* & \alpha^* & \rho^* \\ \varepsilon_2^* & \varepsilon_1^* & \lambda \end{Bmatrix}_{r_1r_4s_1s_2} \begin{Bmatrix} \lambda' & \alpha & \rho \\ \varepsilon_1^* & \varepsilon_2^* & \alpha'^* \end{Bmatrix}_{r_3r_2s_1s_2}. \tag{5.9}$$

This means that we have solved all primitive 6-*j* in terms of the core 6-*j*.

6. The core 6-*j*

A difficulty with finding a proof of completeness for our algorithm for the core 6-*j* is due to the fact that no single relation (orthonormality, Racah backcoupling or Biedenharn-Elliott sum rule) will always give sufficient linearly independent equations to solve for all unknowns. The set of core 6-*j* has the basis 6-*j* as a subset. The phase (and sometimes the multiplicity separation) of a basis 6-*j* is free so it can only be possible to find the magnitude of the unknown via equations which are quadratic. As a consequence we know that any complete set of suitable equations cannot be linear, so theorems for the completeness of linear equations are of little use.

When a free triad $\lambda\alpha\beta r$ exists for $r > 1$ we get one basis 6-j for each value of r and need to resolve the multiplicity of these couplings subject to the group selection rules. When the triads have different symmetry types for some of the values of r, the equations that depend on the symmetry give extra information. When different values of r have the same symmetry, symmetry will only partially solve the problem of separating the multiplicities and additional choices are required.

A second difficulty occurs if a 6-j chosen to be a basis 6-j turns out to be zero, because no phase is fixed for such a zero value. A 6-j is chosen to be the basis 6-j for a triad $\lambda\alpha\beta r$ depending on the value of β' and λ' (see § 4). If such a choice leads to a zero then the choice of λ' or β' must be revised, and we must solve for the magnitude of the revised choice of basis 6-j so as to fix the associated K matrix. The occurrence of zero values is normal for a triad $\lambda\alpha\beta r$ with multiplicity when there is insufficient symmetry information to completely separate the multiplicity. In this case we must choose the separation, and a zero for the value of r is the easiest choice to make, although this choice results in the phase of the corresponding triad remaining free until a revised value of β' and λ' is used for the given value of r.

The consequence of these problems is that it is difficult to enunciate a complete algorithm for the core 6-j, preventing us from proving that our algorithm is complete. However we have always been able to find sufficient equations to solve for any group we have so far attempted and we can prove completeness for SO_3.

SO_3 is the unique compact Lie group with one irrep of each power and it is multiplicity free. We use the example of SO_3 first to illustrate the kind of procedure to follow for typical groups and second to prove completeness in this special case. As with all groups that we have applied this algorithm to, we find that the orthonormality relation is sufficient to solve for almost all (but not all) of the core 6-j.

In SO_3 all primitive triads are stretched and there is only one primitive triad for each irrep so there are no basis 6-j for the case $\beta = \varepsilon$. Since there is only one irrep of each power the choice of β' and λ' in (4.2) is unique. We find that the 6-j in (5.4) do not occur and the set of 6-j in (5.5) reduce to

$$\begin{Bmatrix} \frac{3}{2} & 1 & \frac{1}{2} \\ \frac{1}{2} & 1 & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} 1 & \frac{1}{2} & \frac{1}{2} \\ 1 & \frac{1}{2} & \frac{1}{2} \end{Bmatrix}$$

whilst the 6-j with one non-primitive triad in (5.1) become, for all $\alpha \geqslant 1$,

$$\begin{Bmatrix} \alpha+1 & \alpha & 1 \\ \frac{1}{2} & \frac{1}{2} & \alpha+\frac{1}{2} \end{Bmatrix} \begin{Bmatrix} \alpha & \alpha & 1 \\ \frac{1}{2} & \frac{1}{2} & \alpha+\frac{1}{2} \end{Bmatrix} \begin{Bmatrix} \alpha & \alpha & 1 \\ \frac{1}{2} & \frac{1}{2} & \alpha-\frac{1}{2} \end{Bmatrix}.$$

We choose the first and last as basis 6-j for all triads $\alpha+1\alpha 1$ and $\alpha\alpha 1$ respectively.

The orthonormality equations give these basis 6-j immediately using the following equations (the summation is over the irreps of SO_3, not the powers):

$$\sum_{\rho=1 \text{ only}} \# \left| \begin{Bmatrix} \alpha+1 & \alpha & \rho \\ \frac{1}{2} & \frac{1}{2} & \alpha+\frac{1}{2} \end{Bmatrix} \right|^2 = 1$$

$$\sum_{\rho=0}^{1} \# \left| \begin{Bmatrix} \alpha & \alpha & \rho \\ \frac{1}{2} & \frac{1}{2} & \alpha-\frac{1}{2} \end{Bmatrix} \right|^2 = 1$$

where we recall that 6-j with the identity irrep are always known. We can solve for the above non-basis 6-j by using the following equations. The equations relate the unknowns to trivial 6-j and to the basis 6-j for the non-primitive triads that occur:

$$\sum_{\rho=0}^{1} \# \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & 1 \\ \frac{1}{2} & \frac{1}{2} & \rho \end{Bmatrix} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & \rho \end{Bmatrix}^* = 0$$

$$\begin{Bmatrix} \frac{1}{2} & 1 & \frac{3}{2} \\ \frac{1}{2} & 1 & \frac{1}{2} \end{Bmatrix} = \sum_{\rho=0}^{1} \# \begin{Bmatrix} 1 & \frac{1}{2} & \frac{3}{2} \\ \frac{1}{2} & 1 & \rho \end{Bmatrix} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & \rho \\ 1 & 1 & \frac{1}{2} \end{Bmatrix}$$

$$\sum_{\rho=0}^{1} \# \begin{Bmatrix} \alpha & \alpha & \rho \\ \frac{1}{2} & \frac{1}{2} & \alpha+\frac{1}{2} \end{Bmatrix} \begin{Bmatrix} \alpha & \alpha & \rho \\ \frac{1}{2} & \frac{1}{2} & \alpha-\frac{1}{2} \end{Bmatrix}^* = 0.$$

The remaining 6-j in (5.1) with two non-primitive triads have three possible forms:

$$\begin{Bmatrix} \lambda & \alpha & \beta \\ \beta-\frac{1}{2} & \frac{1}{2} & \lambda-\frac{1}{2} \end{Bmatrix} \begin{Bmatrix} \lambda & \alpha & \beta \\ \beta-\frac{1}{2} & \frac{1}{2} & \lambda+\frac{1}{2} \end{Bmatrix} \begin{Bmatrix} \lambda & \alpha & \beta \\ \beta+\frac{1}{2} & \frac{1}{2} & \lambda-\frac{1}{2} \end{Bmatrix}$$

where the first of these is chosen as the basis 6-j for $\lambda\alpha\beta$, and where $\beta > 1$ (as well as $\beta = 1$ for the third case). We may use the orthonormality equations to solve for these 6-j. The first two equations below relate the core 6-j to the basis 6-j, and the last is the normality relation required to find the magnitude of the basis 6-j (and is recursive in that it requires knowledge of smaller core 6-j),

$$\sum_{\beta'} \# \begin{Bmatrix} \lambda & \alpha & \beta' \\ \beta-\frac{1}{2} & \frac{1}{2} & \lambda+\frac{1}{2} \end{Bmatrix} \begin{Bmatrix} \lambda & \alpha & \beta' \\ \beta-\frac{1}{2} & \frac{1}{2} & \lambda-\frac{1}{2} \end{Bmatrix}^* = 0$$

$$\sum_{\lambda'} \# \begin{Bmatrix} \lambda' & \alpha & \beta \\ \beta+\frac{1}{2} & \frac{1}{2} & \lambda-\frac{1}{2} \end{Bmatrix} \begin{Bmatrix} \lambda' & \alpha & \beta \\ \beta-\frac{1}{2} & \frac{1}{2} & \lambda-\frac{1}{2} \end{Bmatrix}^* = 0$$

$$\sum_{\beta'} \# \left| \begin{Bmatrix} \lambda & \alpha & \beta' \\ \beta-\frac{1}{2} & \frac{1}{2} & \lambda-\frac{1}{2} \end{Bmatrix} \right|^2 = 1$$

where in each case the sum contains two terms.

In the above calculation for SO_3, we note that orthonormality is only once insufficient for a complete solution. For all groups that we have considered it is the core 6-j of low power that has caused us the most problems. SO_3 gives an example of this since it is a small core 6-j that cannot be solved by orthonormality.

7. Conclusion

We have significantly improved the algorithm for the calculation of primitive 6-j. By defining a subclass of primitive 6-j known as the core 6-j we have been able to give a complete method for calculating all non-core primitive 6-j. These core 6-j form a minority of the primitive 6-j, for example in the octahedral group (see the table on p 439 in Butler (1981)) there are 100 primitive 6-j, 45 of which are core (20 of these core 6-j are basis). A significant number of these core 6-j involve irreps of low power and seem to be the hardest to resolve.

We have been unable to give a complete algorithm to solve for the core 6-j for a compact group with faithful irreps, although we have been able to do so for SO_3 and have been able to resolve the problem for all groups we have so far considered.

References

Bickerstaff R P 1981 *PhD thesis* University of Canterbury, New Zealand
—— 1984 *J. Math. Phys.* **25** 2808–14
Bickerstaff R P, Butler P H, Butts M B, Haase R W and Reid M F 1982 *J. Phys. A: Math. Gen.* **15** 1087–117
Bickerstaff R P and Damhus T 1985 *Int. J. Quantum Chem.* **27** 381–91
Butler P H 1975 *Phil. Trans. R. Soc.* A **277** 545–85
—— 1976 *Int. J. Quantum Chem.* **10** 599–613
—— 1981 *Point Group Symmetry Applications: Methods and Tables* (New York: Plenum)
Chen J-Q, Gao M-J and Ma G-Q 1985 *Rev. Mod. Phys.* **57** 211–78
Derome J R 1966 *J. Math. Phys.* **7** 612–5
Derome J R and Sharp W T 1965 *J. Math. Phys.* **6** 1584–90
Haase R W and Dirl R 1986 *J. Math. Phys.* **27** 900–13
Hamer C J, Irving A C and Preece T E 1986 *Nucl. Phys.* B **270** 553–74
Judd B R 1986 *J. Math. Phys.* **27** 2616–22
—— 1987 *J. Phys. A: Math. Gen.* **20** L343–7
Judd B R, Lister G M S and O'Brien M C M 1986 *J. Phys. A: Math. Gen.* **19** 2473–86
Pluhar Z, Weigert L J and Holan P 1986 *J. Phys. A: Math. Gen.* **19** 29–34
Raynal J and Conte R 1985 *J. Math. Phys.* **26** 2413–40
—— 1985 *J. Math. Phys.* **26** 2441–56
Reid M F and Butler P H 1980 *J. Phys. A: Math. Gen.* **13** 2889–901
—— 1982 *J. Phys. A: Math. Gen.* **15** 2327–35
Searle B G and Butler P H 1988 *J. Phys. A: Math. Gen.* **21** 1977–81
Zeng G J 1987 *J. Phys. A: Math. Gen.* **20** 1961–71