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# Accurate computation of individual and tables of 3-j and 6-j symbols

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## Abstract

By rewriting the formulas for 3-j and 6-j symbols in terms of several possible alternating binomial sums, it is possible to calculate these quantities quickly and accurately, often exactly, using floating point operations. The binomial sums can be calculated by direct summation or by recursion. A simple method for uniquely parameterizing the well-known Regge symmetries of the 3-j and 6-j symbols makes it possible to systematize the choice of the smallest magnitude binomial sum (which enhances the accuracy of floating point calculations and speeds up exact calculations using large integer routines). Formulas for special cases of the 3-j symbols enable the construction of recursion sequences which are often substantially faster than direct summation, especially for very large angular momentum arguments. For both 3-j and 6-j symbols, recursion offers several advantages over direct summation in exact calculations and for calculating tables. © 1998 Published by Elsevier Science B.V.

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## 1. Introduction

Angular momentum plays a central role in quantum mechanics, and Wigner 3-j and 6-j symbols (or Clebsch–Gordan and Racah coefficients) are used to describe the coupling between two or more angular momenta. It is important for practical reasons to be able to quickly and accurately calculate 3-j and 6-j symbols for scattering [1], spectroscopy [2,3], and many other applications [4]. In some areas of research, such as the incidence of nontrivial zeroes [5–8], the calculations must be exact. Exact results are also used to test approximate methods for calculating 3-j and 6-j symbols, such as those used in the high quantum number (classical) limit [9–11].

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Because the formulas for both 3-j and 6-j symbols include an alternating sum, obtaining exact or even acceptably accurate values can sometimes be challenging, especially when the angular momentum arguments are large. The literature on the computation of 3-j and 6-j symbols is extensive [12–25]. A subroutine recently published by Lai and Chiu [22] is based on the clever recasting of the formulas for 3-j and 6-j symbols in terms of alternating binomial sums; their 3-j formula is similar to a binomial expression by Shimpuku [23] for Clebsch–Gordan coefficients. Roothaan [14] has obtained similar results. A binomial sum, of course, is an integer, and even for quite large angular momenta can be represented exactly as a floating point number, depending on hardware limitations, or as a prime-factored integer. This allows for accurate, often exact, computation of 3-j and 6-j symbols, since the pre-factors in front of the binomial sums can be evaluated without roundoff error.

Formulas for both the 3-j and 6-j symbols can be rewritten in terms of binomial sums in several ways. In this paper we show how to choose which formulas to use in order to obtain the fastest and most accurate calculations. The binomial sums can be calculated by direct summation or by several possible recursion sequences. A simple method for parameterizing the well-known Regge symmetries [26] of the 3-j and 6-j symbols enables a straightforward choice of the most optimal recursion sequence.

### 2. 3-j symbols

One common expression for the 3-j symbol is [18,19]

$$\begin{aligned} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} &= (-1)^{j_1-j_2-m_3} \left[ \frac{\prod_i (j_i + m_i)! (j_i - m_i)! (J - 2j_i)!}{(J + 1)!} \right]^{1/2} \\ &\times \sum_k (-1)^k / \left[ \prod_i (k - \alpha_i)! (\beta_i - k)! \right], \end{aligned} \tag{1}$$

where

$$J = j_1 + j_2 + j_3, \tag{2}$$

$$\alpha_1 = j_2 - j_3 - m_1, \quad \alpha_2 = 0, \quad \alpha_3 = j_1 - j_3 + m_2,$$

$$\beta_1 = j_2 + m_2, \quad \beta_2 = j_1 + j_2 - j_3, \quad \beta_3 = j_1 - m_1, \tag{3}$$

and

$$\max(\alpha_1, \alpha_2, \alpha_3) \leq \max(\beta_1, \beta_2, \beta_3).$$

This formula is valid only if  $j_i$  and  $m_i$  are both integer or both half-integer for  $i = 1, 2, 3$  and if  $j_1 + j_2 + j_3$  is an integer. The 3-j symbol is nonzero only if the three  $m$ 's sum to zero, the three  $j$ 's satisfy the triangle conditions, and  $|m_i| \leq j_i$  for  $i = 1, 2, 3$ .

In 1958, Regge [26] showed that the 3-j symbol has 72 symmetries; each 3-j symbol can be conveniently represented by the array

$$R = \left\| \begin{array}{ccc} -j_1 + j_2 + j_3 & j_1 - j_2 + j_3 & j_1 + j_2 - j_3 \\ j_1 - m_1 & j_2 - m_2 & j_3 - m_3 \\ j_1 + m_1 & j_2 + m_2 & j_3 + m_3 \end{array} \right\|, \tag{4}$$

which is a magic square (all row and column sums equal) of rank  $J = j_1 + j_2 + j_3$ . The 72 symmetries correspond to row or column interchanges or transposition of the matrix. For odd row or column permutations of the Regge matrix, the 3-j symbol is multiplied by  $(-1)^J$ ; otherwise, the value remains unchanged. For

example, exchanging the second and third rows corresponds to the well-known reflection symmetry of the 3-j symbol. By the triangle and other conditions given above, each entry in the Regge matrix is a nonnegative integer. For any  $i, j$ ,  $\beta_i - \alpha_j$  is one of the Regge matrix elements. It should be noted that the definition of a magic square sometimes includes the requirement that one or both diagonals, as well as the rows and columns, have the same sum. However, in this paper, as in other angular momentum literature, no conditions are placed on the diagonal sums.

It shall prove convenient to parameterize each set of 3-j symbols related by Regge symmetry by a unique set of  $j$ 's and  $m$ 's denoted  $j'_i$  and  $m'_i$ . This is done by rearranging the Regge matrix into a new matrix  $R'$  in a unique manner. It can easily be shown that in a 3 by 3 magic square, the largest and smallest elements fall either in the same row or in the same column. Assuming that they do not, then the Regge matrix may be arranged so that the smallest element,  $S$ , and the largest element,  $L$ , are on the diagonal. Then the row containing  $S$  and the column containing  $L$  have a common element  $C$ . Since  $J = L + C + (S + a) = (L - b) + C + S$ , where  $a$  and  $b$  are greater than zero, this leads to the contradiction  $a + b = 0$ , and so the largest and smallest elements must fall in the same row or column. We then rearrange the Regge matrix so that the smallest and largest elements are  $R'_{11}$  and  $R'_{12}$ . This fixes the first row and the column positions. It remains to specify the arrangement of the second and third rows. We require either that  $R'_{22} < R'_{32}$  or, if  $R'_{22} = R'_{32}$ , that  $R'_{23} \leq R'_{33}$ . This leads to the arrangement

$$R' = \begin{pmatrix} S & L & X + B - T \\ X & B & S + L - T \\ L + B - T & S + X - T & T \end{pmatrix}, \tag{5}$$

where  $S \leq B$ . Since  $S$  is the smallest element, we have  $S \leq (S + X - T)$ ; since  $L$  is the largest, we have  $(L + B - T) \leq L$ . These conditions yield, respectively,  $X \geq T$  and  $T \geq B$ . Therefore,  $S \leq B \leq T \leq X \leq L$ .

We now define the  $j'_i$  and  $m'_i$  to correspond to the transformed Regge matrix  $R'$ ,

$$R' = \begin{pmatrix} -j'_1 + j'_2 + j'_3 & j'_1 - j'_2 + j'_3 & j'_1 + j'_2 - j'_3 \\ j'_1 - m'_1 & j'_2 - m'_2 & j'_3 - m'_3 \\ j'_1 + m'_1 & j'_2 + m'_2 & j'_3 + m'_3 \end{pmatrix} = \begin{pmatrix} \beta'_1 - \alpha'_3 & \beta'_3 - \alpha'_1 & \beta'_2 - \alpha'_2 \\ \beta'_3 - \alpha'_2 & \beta'_2 - \alpha'_3 & \beta'_1 - \alpha'_1 \\ \beta'_2 - \alpha'_1 & \beta'_1 - \alpha'_2 & \beta'_3 - \alpha'_3 \end{pmatrix}, \tag{6}$$

and, by analogy to Eq. (1), sets of  $\alpha'_i$  and  $\beta'_i$ . From Eq. (6) and the fact that  $S$  and  $L$  are the smallest and largest elements, we have  $j'_1 \geq j'_3 \geq j'_2$ . In addition, by design,  $m'_2 \geq 0$  and if  $m'_2 = 0$  then  $m'_3 \geq 0$ . From Eqs. (5) and (6),  $S \leq B \leq T$  yields  $\beta'_1 \leq \beta'_2 \leq \beta'_3$  and  $T \leq X \leq L$  yields  $\alpha'_1 \leq \alpha'_2 \leq \alpha'_3$ . The condition  $m'_2 \geq 0$  yields  $\beta'_2 - \beta'_1 \leq \alpha'_3 - \alpha'_2$ . The condition  $m'_3 \geq 0$  if  $m'_2 = 0$  yields  $\alpha'_3 - \alpha'_1 \leq \beta'_3 - \beta'_1$  if  $\beta'_2 - \beta'_1 = \alpha'_3 - \alpha'_2$ .

It is important to note that the  $\alpha$ 's and  $\beta$ 's for the untransformed 3-j symbol are not necessarily the same as those for the transformed 3-j symbol. For example, for

$$\begin{pmatrix} 15 & 15 & 16 \\ 9 & -8 & -1 \end{pmatrix} = \begin{pmatrix} 20 & 11 & 15 \\ -3 & 4 & -1 \end{pmatrix}$$

the  $\alpha$ 's for the untransformed 3-j symbol (left-hand side) are  $-10, 0$ , and  $-9$  and the  $\beta$ 's are  $7, 14$ , and  $6$ . For the transformed 3-j symbol (right-hand side) the  $\alpha$ 's are  $-1, 0$ , and  $9$  and the  $\beta$ 's are  $15, 16$ , and  $23$ . Both 3-j symbols yield the same Regge matrix to within several symmetry transformations.

### Calculation of individual 3-j symbols

In a general 3-j subroutine, it is useful to check for special cases. One special case which will prove especially useful is  $m_1 = m_2 = m_3 = 0$  [11],

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 0 & 0 \end{pmatrix} = (-1)^{J/2} \left[ \frac{\prod_i (J - 2j_i)!}{(J + 1)!} \right]^{1/2} \frac{(J/2)!}{\prod_i (J/2 - j_i)!}, \tag{7}$$

if  $J$  is even and zero if  $J$  is odd. Of course, the magnitude of this expression should be less than or equal to 1. However, for large angular momenta the factorials can overflow. To combat this problem we rewrite the formula in terms of quantities which do not overflow. Let  $j'_1, j'_2,$  and  $j'_3$  be the minimum, middle, and maximum values of  $j_1, j_2,$  and  $j_3,$  and define

$$A = -j'_1 + j'_2 + j'_3, \quad B = j'_1 - j'_2 + j'_3, \quad C = j'_1 + j'_2 - j'_3. \tag{8}$$

Then noting that  $A \geq B \geq C$  and using

$$J! = (A + B + C)! = A!(A + 1)_B(A + B + 1)_C \tag{9}$$

and

$$(J/2)! = (A/2)!(A/2 + 1)_{B/2}(A/2 + B/2 + 1)_{C/2}, \tag{10}$$

where  $(a)_n$  refers to the Pochhammer symbol [27],

$$(a)_n = \Gamma(a + n)/\Gamma(a) = a(a + 1)(a + 2) \cdots (a + n - 1), \tag{11}$$

we can eliminate factors of  $A!$  and  $(A/2)!$  to obtain

$$\begin{aligned} \begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 0 & 0 \end{pmatrix} &= \frac{(-1)^{J/2}}{(J + 1)^{1/2}} \left[ \frac{(B/2 + 1)_{B/2}(A/2 + 1)_{B/2}^2}{(A + 1)_{B/2}(A + B/2 + 1)_{B/2}(B/2)!} \right]^{1/2} \\ &\times \left[ \frac{(C/2 + 1)_{C/2}(A/2 + B/2 + 1)_{C/2}^2}{(A + B + 1)_{C/2}(A + B + C/2 + 1)_{C/2}(C/2)!} \right]^{1/2} \end{aligned} \tag{12}$$

for even  $J,$  which can be rewritten as

$$\begin{aligned} \begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 0 & 0 \end{pmatrix} &= \frac{(-1)^{J/2}}{(J + 1)^{1/2}} \left[ \prod_{i=1}^{B/2} \frac{(B/2 + i)(A/2 + i)^2}{(A + i)(A + B/2 + i)i} \right]^{1/2} \\ &\times \left[ \prod_{i=1}^{C/2} \frac{(A/2 + i)(A/2 + B/2 + i)^2}{(A + B + i)(A + B + C/2 + i)i} \right]^{1/2}, \end{aligned} \tag{13}$$

a form in which each product term can be evaluated without concern for underflow. There are several equivalent expressions in which  $B!$  or  $C!$  may be eliminated instead of  $A!$ . However, since  $A$  is largest, eliminating  $A!$  minimizes the number of floating point operations in Eqs. (12) and (13). This strategy will be followed elsewhere in this paper.

The well-known permutation symmetry is related by Regge symmetry,

$$\begin{pmatrix} j_1 & j_1 & j_3 \\ m_1 & m_1 & m_3 \end{pmatrix} = \begin{pmatrix} j_1 - m_1 & j_1 + m_1 & j_3 \\ 0 & 0 & 0 \end{pmatrix}, \tag{14}$$

as are slightly more complicated conditions. If a 3- $j$  symbol is related by any Regge symmetry to this case, then for the transformed Regge matrix, we have  $m'_1 = m'_2 = m'_3 = 0$ . To prove this, we note that if all  $m$ 's are zero, then the bottom two rows of the Regge matrix are identical. Thus, the Regge matrix for any 3- $j$  symbol related

by Regge symmetry has two identical rows or columns, which we denote  $(A, B, C)$ , where without loss of generality  $A \geq B \geq C$ . Then the other row or column is  $(-A + B + C, A - B + C, A + B - C)$ . It is immediately apparent that the largest element is  $A + B - C \geq A$  and that the smallest element is  $-A + B + C \leq C$ . Since the top row of the transformed Regge matrix contains the largest and smallest elements, the second and third rows must contain  $(A, B, C)$ . Therefore, we have  $m_1 = m_2 = m_3 = 0$ . This makes it possible to test for this special case without directly testing for reflection symmetry in addition to permutation symmetry and other conditions.

As Shimpuku [23] and, later, Lai and Chiu [22] have noted, the expression for a Clebsch–Gordan coefficient or 3-j symbol can be rewritten in terms of an alternating binomial sum by multiplying and dividing by some appropriate set of factorials. The next step is to realize, as Roothaan [14] previously observed, that there are six ways to do this. For our purposes, we use a different notation, according to whether the arguments of the factorials are row entries,

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1 - j_2 - m_3} \left[ \frac{\prod_{j \neq i} R_{j1}! R_{j2}! R_{j3}!}{R_{i1}! R_{i2}! R_{i3}! (J + 1)!} \right]^{1/2} I_{Ri}(j_1, j_2, j_3, m_1, m_2, m_3), \tag{15}$$

or column entries,

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1 - j_2 - m_3} \left[ \frac{\prod_{j \neq i} R_{1j}! R_{2j}! R_{3j}!}{R_{1i}! R_{2i}! R_{3i}! (J + 1)!} \right]^{1/2} I_{Ci}(j_1, j_2, j_3, m_1, m_2, m_3), \tag{16}$$

of the Regge matrix. The binomial sum portions of the above formulas are

$$I_{R1}(j_1, j_2, j_3, m_1, m_2, m_3) = \sum_k (-1)^k \binom{-j_1 + j_2 + j_3}{j_2 + m_2 - k} \binom{j_1 - j_2 + j_3}{j_1 - m_1 - k} \binom{j_1 + j_2 - j_3}{k}, \tag{17}$$

$$I_{R2}(j_1, j_2, j_3, m_1, m_2, m_3) = \sum_k (-1)^k \binom{j_1 - m_1}{k} \binom{j_2 - m_2}{j_1 + j_2 - j_3 - k} \binom{j_3 - m_3}{j_2 + m_2 - k}, \tag{18}$$

$$I_{R3}(j_1, j_2, j_3, m_1, m_2, m_3) = \sum_k (-1)^k \binom{j_1 + m_1}{j_1 + j_2 - j_3 - k} \binom{j_2 + m_2}{k} \binom{j_3 + m_3}{j_1 - m_1 - k}, \tag{19}$$

$$I_{C1}(j_1, j_2, j_3, m_1, m_2, m_3) = \sum_k (-1)^k \binom{-j_1 + j_2 + j_3}{j_2 + m_2 - k} \binom{j_1 - m_1}{k} \binom{j_1 + m_1}{j_1 + j_2 - j_3 - k}, \tag{20}$$

$$I_{C2}(j_1, j_2, j_3, m_1, m_2, m_3) = \sum_k (-1)^k \binom{j_1 - j_2 + j_3}{j_1 - m_1 - k} \binom{j_2 - m_2}{j_1 + j_2 - j_3 - k} \binom{j_2 + m_2}{k}, \tag{21}$$

$$I_{C3}(j_1, j_2, j_3, m_1, m_2, m_3) = \sum_k (-1)^k \binom{j_1 + j_2 - j_3}{k} \binom{j_3 - m_3}{j_2 + m_2 - k} \binom{j_3 + m_3}{j_1 - m_1 - k}. \tag{22}$$

If two 3-j symbols are related by Regge symmetry, then the pre-factors in front of the summation in Eq. (1) are the same to within a sign since they involve  $J$  and the set of all nine entries of the Regge matrix, each of which is invariant under any Regge symmetry transformation. Therefore, the sums are also equal to within a sign. It follows that the optimal calculation sequence depends only on which set of factorials is introduced into the sum and not on the arrangement of the Regge matrix. Two methods for evaluating the binomial sums and from there calculating the 3-j symbol are direct summation and recursion, as shown in detail below.

**Method I – Direct summation**

The binomial sum can be performed exactly by large integer routines or much more quickly and often exactly by floating point operations. In any floating point calculation, there is some largest integer which can be represented exactly. It is important to know this limit because if the summation terms and any intermediates fall below it, the results will be exact. Otherwise, there may be some cancellation error, up to a maximum dictated by the ratio of the entire sum to its largest term.

In general, the most accurate floating point results (or the fastest large integer arithmetic results) are obtained from the binomial sum with the smallest magnitude. To compute the sum it is not necessary to reorder the Regge matrix as we describe. Instead, we may simply reorder the  $\alpha$ 's and  $\beta$ 's. Let  $A_1, A_2,$  and  $A_3$  be the minimum, middle, and maximum values of the  $\alpha$ 's and  $B_1, B_2,$  and  $B_3$  be the minimum, middle, and maximum values of the  $\beta$ 's. From Eq. (1) and the definition of the  $\alpha$ 's and  $\beta$ 's, it is fairly straightforward to see that the top indices in the binomial coefficients will be  $(B_1 - A_i), (B_2 - A_j),$  and  $(B_3 - A_n)$  for some permutation  $(i, j, n)$  of  $(1, 2, 3)$ . By using the fact that  $C!D! \geq E!F!$  when  $\max(C, D) \geq \max(E, F)$  and  $C + D = E + F$ , it is easy to prove that the smallest product of factorials, and therefore the smallest magnitude sum, is obtained by  $(i, j, n) = (1, 2, 3)$ . This strategy can be used to compare permutations with a common factor (for example, 123 and 132). To compare permutations with no common factor, two steps are necessary. For example, the 123 permutation has a smaller factorial product than the 213 permutation, which in turn has a smaller product than the 312 permutation. It now remains to simplify the pre-factor. Using

$$\frac{(B_2 - A_1)!}{(B_2 - A_2)!} = (B_2 - A_2 + 1)_{A_2 - A_1}, \tag{23}$$

$$\frac{(B_3 - A_2)!}{(B_3 - A_3)!} = (B_3 - A_3 + 1)_{A_3 - A_2}, \tag{24}$$

$$\frac{(B_1 - A_3)!}{(B_1 - A_1)!} = \frac{1}{(B_1 - A_3 + 1)_{A_3 - A_2} (B_1 - A_2 + 1)_{A_2 - A_1}}, \tag{25}$$

$$\frac{(B_3 - A_1)!(B_2 - A_3)!(B_1 - A_2)!}{J!} = \frac{(B_1 - A_3)!(B_1 - A_2)!}{(B_3 - A_1 + 1)_{B_2 - A_3} (B_2 + B_3 - A_1 - A_3 + 1)_{B_1 - A_2}}, \tag{26}$$

$$\frac{(B_2 - A_3)!}{(B_3 - A_1 + 1)_{B_2 - A_3}} = \frac{(B_1 - A_3)!(B_1 - A_3 + 1)_{B_2 - B_1}}{(B_3 - A_1 + 1)_{B_1 - A_3} (B_1 + B_3 - A_1 - A_3 + 1)_{B_2 - B_1}}, \tag{27}$$

and

$$\frac{(B_1 - A_2)!}{(B_2 + B_3 - A_1 - A_3 + 1)_{B_1 - A_2}} = \frac{(B_1 - A_3)!(B_1 - A_3 + 1)_{A_3 - A_2}}{(B_2 + B_3 - A_1 - A_3 + 1)_{A_3 - A_2} (B_2 + B_3 - A_1 - A_2 + 1)_{B_1 - A_3}}, \tag{28}$$

we obtain

$$\begin{aligned} \binom{j_1 \quad j_2 \quad j_3}{m_1 \quad m_2 \quad m_3} &= (-1)^{j_1 - j_2 - m_3} (B_1 - A_3)! \left[ \frac{(B_3 - A_3 + 1)_{A_3 - A_2}}{(B_2 + B_3 - A_1 - A_3 + 1)_{A_3 - A_2}} \right. \\ &\quad \times \frac{(B_1 - A_1 + 1)_{B_2 - B_1} (B_1 - A_3 + 1)_{B_2 - B_1}}{(B_1 - A_2 + 1)_{B_2 - B_1} (B_1 + B_3 - A_1 - A_3 + 1)_{B_2 - B_1}} \\ &\quad \times \left. \frac{1}{(B_3 - A_1 + 1)_{B_1 - A_3} (B_2 + B_3 - A_1 - A_2 + 1)_{B_1 - A_3}} \right]^{1/2} \\ &\quad \times \sum_k (-1)^k \binom{B_1 - A_1}{B_1 - k} \binom{B_2 - A_2}{B_2 - k} \binom{B_3 - A_3}{B_3 - k}. \end{aligned} \tag{29}$$

To minimize the computational effort, care was taken to eliminate the largest factorial in the pre-factor, namely  $(B_3 - A_1)!$ . The bracketed expressions can be written as products of terms each less than 1 in a manner similar to that shown in Eqs. (12) and (13). In a floating point 3-j calculation, it is possible for the prefactor to underflow if the angular momenta are extremely large. In such a case, calculating the 3-j symbol is best accomplished by large integer routines and prime factorization methods. The first term in the binomial sum is

$$t_{A_3} = \binom{B_1 - A_1}{B_1 - A_3} \binom{B_2 - A_2}{B_2 - A_3}. \quad (30)$$

Successive terms may be calculated from

$$t_k = -t_{k-1} \times \frac{B_1 + 1 - k}{k - A_1} \times \frac{B_2 + 1 - k}{k - A_2} \times \frac{B_3 + 1 - k}{k - A_3}. \quad (31)$$

The successive fractions on the right-hand side of Eq. (31) are factors for changing the bottom arguments of the binomial coefficients in Eq. (29) by one. Therefore, each multiplication must be performed before the corresponding division in order to assure that every intermediate is an integer.

## Method II – Center recursion

Recursion is often used to calculate 3-j symbols, especially tables of 3-j symbols. For every 3-j recursion relation, there are many possible binomial recursion relations. It is often possible to calculate the binomial sum faster by recursion than by direct summation. This is especially important for large angular momentum arguments. To illustrate this, we show in Fig. 1 a diagram of possible  $m_1$  and  $m_2$  values for  $j_1 = 12, j_2 = 8, j_3 = 14$ ; similar diagrams are shown in standard quantum mechanics textbooks such as Baym's [28]. The top right and bottom left corners are truncated because the absolute value of  $m_3$  must not exceed  $j_3$ . For 3-j symbols on the very outermost contour, the corresponding binomial sums have only one term; binomial sums for 3-j symbols on the second outermost contour have two terms; and so on. For every 3-j symbol on or inside the innermost contour, there are seven terms in each sum. For the 3-j symbol at the center of the diagram, all three  $m$ 's are zero; exact formulas for this 3-j symbol, and from there the binomial sum, are readily available. Exact formulas for adjacent 3-j symbols (for example,  $m_1 = -m_2 = 1, m_3 = 0$ ), are also available. The next outlying 3-j symbols or their binomial sums (for example,  $m_1 = -m_2 = 2, m_3 = 0$ ) can be calculated by recursion from the previous two, whereas direct summation would require one application of Eq. (30) and six of Eq. (31). This scheme and others in this section will be denoted center recursion because they start at or near the center of diagrams like the one shown in Fig. 1.

A number of 3-j recursion relations are available for which the  $j$ 's do not change and the  $m$ 's change by 0 or  $\pm 1$ . These include the fundamental recursion relations

$$\begin{aligned} & [(j_3 + m_3 + 1)(j_3 - m_3)]^{1/2} \binom{j_1 \quad j_2 \quad j_3}{m_1 \quad m_2 \quad m_3} \\ & + [(j_2 - m_2 + 1)(j_2 + m_2)]^{1/2} \binom{j_1 \quad j_2 \quad j_3}{m_1 \quad m_2 - 1 \quad m_3 + 1} \\ & + [(j_1 - m_1 + 1)(j_1 + m_1)]^{1/2} \binom{j_1 \quad j_2 \quad j_3}{m_1 - 1 \quad m_2 \quad m_3 + 1} = 0, \end{aligned} \quad (32)$$

and

$$[(j_3 - m_3 + 1)(j_3 + m_3)]^{1/2} \binom{j_1 \quad j_2 \quad j_3}{m_1 \quad m_2 \quad m_3}$$

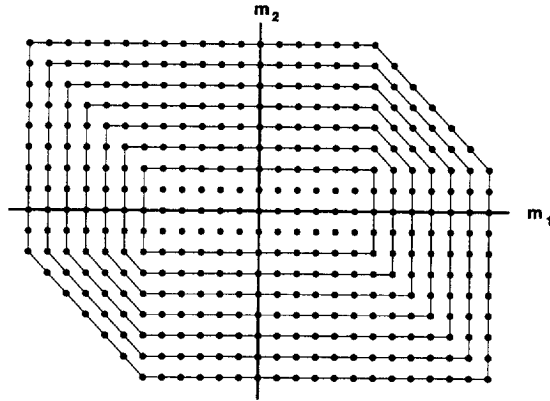


Fig. 1. Possible  $m_1, m_2$  values for 3-j symbols with  $j_1 = 12, j_2 = 8, j_3 = 14$ . The contours correspond to the number of terms in the binomial sum, with the outermost contours having the fewest terms.

$$\begin{aligned}
 &+[(j_2 + m_2 + 1)(j_2 - m_2)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 + 1 & m_3 - 1 \end{pmatrix} \\
 &+[(j_1 + m_1 + 1)(j_1 - m_1)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 + 1 & m_2 & m_3 - 1 \end{pmatrix} = 0, \tag{33}
 \end{aligned}$$

and a result by Schulten and Gordon,

$$\begin{aligned}
 &[(j_2 + m_2 + 1)(j_2 - m_2)(j_3 - m_3 + 1)(j_3 + m_3)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 + 1 & m_3 - 1 \end{pmatrix} \\
 &+[-(j_1 - m_1 + 1)(j_1 + m_1) + (j_2 - m_2)(j_2 + m_2 + 1) \\
 &+(j_3 - m_3)(j_3 + m_3 + 1)] \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \\
 &+[(j_2 + m_2)(j_2 - m_2 + 1)(j_3 - m_3)(j_3 + m_3 + 1)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 - 1 & m_3 + 1 \end{pmatrix} = 0. \tag{34}
 \end{aligned}$$

Eq. (34) (and any binomial sum equivalents) can be used to step along a constant  $m_1$ . By invoking permutation symmetry, recursion relations for constant  $m_2$  and  $m_3$  may be easily obtained. The fundamental recursion relations and others derived from them can be used to “turn the corner” from one line to another. The most obvious recursion sequence for calculating a 3-j symbol from  $m_i = 0$ , including initial points, would have  $\max(|m_1|, |m_2|, |m_3|) + 1$  steps. However, this is not necessarily the optimum recursion sequence. For example, the binomial sum for the 3-j symbol

$$\begin{pmatrix} 49 & 39 & 50 \\ -17 & 5 & 12 \end{pmatrix} = \begin{pmatrix} 53 & 36 & 49 \\ 9 & 2 & -11 \end{pmatrix} \tag{35}$$

has 33 terms. From the left-hand side of Eq. (35) it is readily apparent that one possible recursion sequence would have on the order of 18 steps – far fewer than direct summation. However, from the right-hand side we obtain an even shorter recursion sequence (12 steps).

In the above recursion relations, the top row of the Regge matrix remains unchanged, and at the starting points of the recursion sequences for Eq. (35), namely  $m_i = 0$ , the second and third rows of the Regge matrix are equal. (Later we shall discuss recursion sequences for which  $m_i = 0$  or  $\pm 1/2$  at the first starting point, i.e., the elements of the second and third rows of the Regge matrix differ by 0 or 1). However, it should be noted that by transforming the 3-j symbols in Eqs. (32)–(34) using Regge symmetry, it is possible to obtain

recursion relations and sequences for which any desired row or column remains unchanged. Therefore, the shortest recursion sequence may be obtained from the two rows or two columns of the Regge matrix which are most nearly equal, i.e., which have the smallest maximum difference between their respective elements.

When using recursion, it will prove most convenient to first calculate the transformed 3-j symbol and change the sign if necessary to obtain the untransformed 3-j symbol,

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{J\sigma} \begin{pmatrix} j'_1 & j'_2 & j'_3 \\ m'_1 & m'_2 & m'_3 \end{pmatrix}, \quad (36)$$

where the sign factor  $\sigma$  is 0 or 1. How to calculate this sign factor will be discussed later.

For the transformed Regge matrix, the second and third columns are most nearly equal. After some algebra, the maximum difference between the second and third rows can be seen to be

$$\max(|(L - T) - (X - B)|, (X - B) - (T - S), |(L - T) - (T - S)|).$$

By using the fact that  $|a - b| \leq \max(a, b)$  for nonnegative  $a$  and  $b$ , we find that this quantity cannot exceed  $\max(L - T, T - S)$ . The maximum difference between the first and second rows is

$$\max(X - S, L - B, |(X - S) - (L - B)|) = \max(X - S, L - B) \geq \max(T - S, L - T),$$

which equals or exceeds the maximum difference for the second and third rows. Comparisons with other row or column differences may be performed in a similar manner.

From Eq. (29) and the definition of the  $A$ 's and  $B$ 's, the number of terms in the sum is  $-j'_1 + j'_2 + j'_3 + 1$ . The number of steps in the shortest recursion sequence is

$$\max(|m'_1|, |m'_2|, |m'_3|) + n,$$

where  $[a]$  denotes the integer part of  $a$  and  $n$  is 1 or 2 depending on details of the recursion sequence to be discussed later. By comparing these results, it can be decided whether recursion or direct summation will take fewer steps.

As stated previously, it is most advantageous to calculate the smallest magnitude binomial sum. For a transformed Regge matrix,  $I_{C3}$  has the smallest magnitude; this can be proven by noting that  $(\beta'_1 - \alpha'_1)!(\beta'_2 - \alpha'_2)!(\beta'_3 - \alpha'_3)!$  is the smallest of the six possible products of factorials using the same methods as in the previous section. The question remains which binomial sums have the smallest magnitude for the other 3-j symbols in the recursion sequence. Going back to Eqs. (5) and (6), from the fact that  $S \leq M \leq L$  we obtain  $j'_1 \leq j'_3 \leq j'_2$ . From  $B \leq S + X - T$  we obtain  $m'_2 \geq 0$ . From  $S \leq S + X - T$  we obtain  $j'_1 - j'_3 \geq m'_2$ . From  $L \geq X$  and  $L \geq L + B - T$  we obtain  $j'_3 - j'_2 \geq |m'_1|$ . Comparisons between other matrix elements yield less restrictive conditions. Thus, given a set of  $j'_i$  for which  $j'_1 \geq j'_3 \geq j'_2$ , there is a region in  $(m'_1, m'_2)$  space in which every 3-j symbol corresponds directly to a transformed Regge matrix and  $I_{C3}$  is the smallest magnitude binomial sum. If  $j'_2$  is half-integer then this region is rectangular. If  $j'_2$  is integer, then for  $m'_2 = 0$ ,  $m'_3$  must be nonnegative, and so  $m'_1 \leq 0$ . Thus, in this case, the recursion envelope is a slightly truncated rectangle. The recursion envelope is illustrated for four possible cases ( $j'_1$  and  $j'_2$  integer or half-integer) in Fig. 2. Examples of these cases include, respectively, (a)  $j'_1 = 61, j'_2 = 54, j'_3 = 57$ , (b)  $j'_1 = 61.5, j'_2 = 54, j'_3 = 58.5$ , (c)  $j'_1 = 61, j'_2 = 53.5, j'_3 = 57.5$ , (d)  $j'_1 = 61.5, j'_2 = 53.5, j'_3 = 58$ . Since the recursion sequences to be discussed here start at or near the origin and proceed outward until the desired 3-j symbol is reached,  $I_{C3}$  is the smallest magnitude binomial sum throughout.

### Starting points

Since every known 3-j recursion relation relates at least three 3-j symbols, it is required to have at least two starting points in a recursion sequence. Several formulas have been derived for 3-j symbols at or near  $m_i = 0$

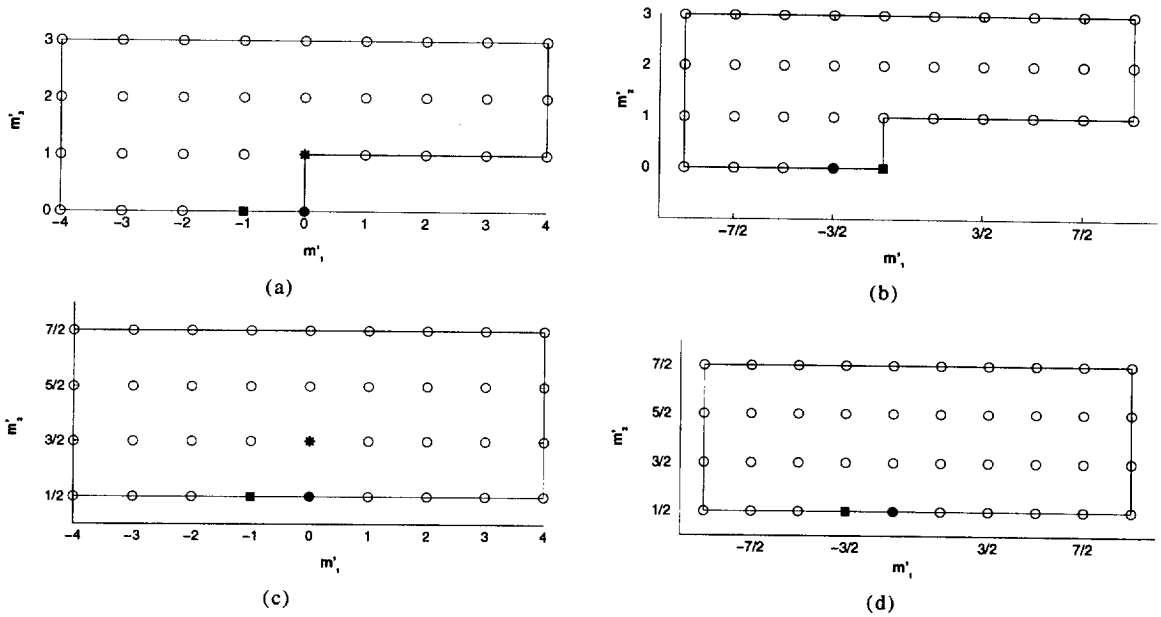


Fig. 2. Starting points for 3-j binomial sum recursion sequences: (a) integer  $j'_1$  and  $j'_2$ :  $\bullet$ , Eq. (37) or (38);  $\blacksquare$ , Eq. (39) or (40);  $*$ , Eq. (41) or (42); (b) half-integer  $j'_1$ , integer  $j'_2$ :  $\bullet$ , Eq. (43) or (44);  $\blacksquare$ , Eq. (45); (c) integer  $j'_1$ , half-integer  $j'_2$ :  $\bullet$ , Eq. (46) or (47);  $\blacksquare$ , Eq. (48);  $*$ , Eq. (49); (d) half-integer  $j'_1$  and  $j'_2$ :  $\bullet$ , Eq. (50) or (51);  $\blacksquare$ , Eq. (52).

or  $\pm 1/2$  (at or near the origin of the envelope in Fig. 2). Formulas for the  $I_{C3}$  binomial sums are presented here and are fully derived in Appendix A.

**Case I:  $j'_1$  and  $j'_2$  both integer**

The first starting point corresponds to all  $m$ 's equal to zero. If  $J$  is odd, the binomial sum is zero since the 3-j symbol is zero. Otherwise, by defining  $A = J/2 - j'_1$ ,  $B = J/2 - j'_2$ , and  $C = J/2 - j'_3$ , it is possible to write the binomial sum as

$$I_{C3}(j'_1, j'_2, j'_3, 0, 0, 0) = (-1)^C \frac{(B+1)_A (B+C+1)_A (C+A+1)_{C-A}}{A!^2 (A+1)_{C-A}} \tag{37}$$

for  $A \leq C$  and

$$I_{C3}(j'_1, j'_2, j'_3, 0, 0, 0) = (-1)^C \frac{(B+1)_A (B+C+1)_A (C+1)_{A-C}}{A!^2 (2C+1)_{A-C}} \tag{38}$$

otherwise. Since  $j'_1 \geq j'_3 \geq j'_2$  for the transformed 3-j symbol, it follows that  $A \leq C \leq B$ , in which case Eq. (37) should be used. However, several upcoming formulas involve intermediate binomial sums for which the  $j$ 's are not necessarily in this order; in these cases, Eq. (38) should be used. It should be noted that although the entire right-hand sides of Eqs. (37) and (38) are integer, the second fractions are not. Therefore, the first fraction should be evaluated first and the result multiplied by the second fraction in such a manner as to make each intermediate an integer. If  $m'_1 \neq 0$ , then the second starting point is

$$I_{C3}(j'_1, j'_2, j'_3, -1, 0, 1) = \frac{j'_1(j'_1+1) - j'_2(j'_2+1) + j'_3(j'_3+1)}{2(j'_1+1)j'_3} I_{C3}(j'_1, j'_2, j'_3, 0, 0, 0) \tag{39}$$

for even  $J$  and

$$I_{C3}(j'_1, j'_2, j'_3, -1, 0, 1) = -\frac{(J - 2j'_1 + 1)(J - 2j'_2 + 1)(J - 2j'_3)}{2(j'_1 + 1)j'_3(j'_3 + 1)} I_{C3}(j'_1, j'_2, j'_3 + 1, 0, 0, 0) \quad (40)$$

for odd  $J$ . If  $m'_1 = 0$ , then the second starting point is

$$I_{C3}(j'_1, j'_2, j'_3, 0, 1, -1) = \frac{-j'_1(j'_1 + 1) + j'_2(j'_2 + 1) + j'_3(j'_3 + 1)}{2(j'_1 + 1)j'_3} I_{C3}(j'_1, j'_2, j'_3, 0, 0, 0) \quad (41)$$

for even  $J$  and

$$I_{C3}(j'_1, j'_2, j'_3, 0, 1, -1) = -\frac{(J - 2j'_1 + 1)(J - 2j'_2 + 1)(J - 2j'_3)}{2(j'_2 + 1)j'_3(j'_3 + 1)} I_{C3}(j'_1, j'_2, j'_3 + 1, 0, 0, 0) \quad (42)$$

for odd  $J$ .

### Case II: $j'_1$ half-integer, $j'_2$ integer

The first starting point is

$$I_{C3}(j'_1, j'_2, j'_3, -1/2, 0, 1/2) = -\frac{(-j'_1 + j'_2 + j'_3 + 1)(j'_1 - j'_2 + j'_3)}{2(j'_1 + 1/2)(j'_3 + 1/2)} I_{C3}(j'_1 - 1/2, j'_2, j'_3 + 1/2, 0, 0, 0) \quad (43)$$

for even  $J$  and

$$I_{C3}(j'_1, j'_2, j'_3, -1/2, 0, 1/2) = \frac{(j'_1 - j'_2 + j'_3 + 1)}{2(j'_3 + 1/2)} I_{C3}(j'_1 + 1/2, j'_2, j'_3 + 1/2, 0, 0, 0) \quad (44)$$

for odd  $J$ . The second starting point is

$$I_{C3}(j'_1, j'_2, j'_3, -3/2, 0, 3/2) = I_{C3}(j'_1, j'_2, j'_3, -1/2, 0, 1/2) \times -\frac{(j'_1 + 1/2)^2 + (j'_3 + 1/2)^2 - j'_2(j'_2 + 1) - 1 + (-1)^J(j'_1 + 1/2)(j'_3 + 1/2)}{(j'_1 + 3/2)(j'_3 - 1/2)} \quad (45)$$

for even or odd  $J$ .

### Case III: $j'_1$ integer, $j'_2$ half-integer

The first starting point is

$$I_{C3}(j'_1, j'_2, j'_3, 0, 1/2, -1/2) = \frac{1}{2} I_{C3}(j'_1, j'_2 + 1/2, j'_3 - 1/2, 0, 0, 0) \quad (46)$$

for even  $J$  and

$$I_{C3}(j'_1, j'_2, j'_3, 0, 1/2, -1/2) = \frac{(-j'_1 + j'_2 + j'_3 + 1)}{2(j'_3 + 1/2)} I_{C3}(j'_1, j'_2 + 1/2, j'_3 + 1/2, 0, 0, 0) \quad (47)$$

for odd  $J$ . If  $m'_1 > 0$ , then the second starting point is

$$I_{C3}(j'_1, j'_2, j'_3, -1, 1/2, 1/2) = \frac{(j'_3 + 1/2) + (-1)^J(j'_2 + 1/2)}{(j'_1 + 1)} I_{C3}(j'_1, j'_2, j'_3, 0, 1/2, -1/2) \quad (48)$$

for even or odd  $J$ . If  $m'_1 = 0$ , then the second starting point is

$$I_{C3}(j'_1, j'_2, j'_3, 0, 3/2, -3/2) = I_{C3}(j'_1, j'_2, j'_3, 0, 1/2, -1/2) \times \frac{(j'_2 + 1/2)^2 + (j_3 + 1/2)^2 - j'_1(j'_1 + 1) - 1 + (-1)^J(j'_2 + 1/2)(j'_3 + 1/2)}{(j'_2 + 3/2)(j'_3 - 1/2)} \quad (49)$$

for even or odd  $J$ .

**Case IV:  $j'_1$  and  $j'_2$  both half-integer**

The first starting point is

$$I_{C3}(j'_1, j'_2, j'_3, -1/2, 1/2, 0) = \frac{(-j'_1 + j'_2 + j'_3 + 1)}{2(j'_1 + 1/2)} I_{C3}(j'_1 - 1/2, j'_2 + 1/2, j'_3, 0, 0, 0) \quad (50)$$

for even  $J$  and

$$I_{C3}(j'_1, j'_2, j'_3, -1/2, 1/2, 0) = \frac{1}{2} I_{C3}(j'_1 + 1/2, j'_2 + 1/2, j'_3, 0, 0, 0) \quad (51)$$

for odd  $J$ . The second starting point is

$$I_{C3}(j'_1, j'_2, j'_3, -3/2, 1/2, 1) = I_{C3}(j'_1, j'_2, j'_3, -1/2, 1/2, 0) \times \frac{j'_3(j'_3 + 1) - (j'_2 + 1/2)[(j'_1 + 1/2)(-1)^J + (j'_2 + 1/2)]}{(j'_1 + 3/2)j'_3} \quad (52)$$

for even or odd  $J$ .

*Recursion relations and recursion sequences*

In the following discussion,  $n_1$ ,  $n_2$ , and  $n_3$  will refer to the bottom arguments of the 3-j symbols used during recursion. Schulten's result can be used to derive binomial recursion relations which can be used to move in straight lines (one constant  $m$ ),

$$I_{C3}(j'_1, j'_2, j'_3, n_1 - 1, n_2 + 1, n_3) = [(j'_1 - n_1 + 1)(j'_2 + n_2 + 1)]^{-1} \times \{ [(j'_3 + n_3)(j'_3 - n_3 + 1) - (j'_1 - n_1)(j'_1 + n_1 + 1) - (j'_2 - n_2)(j'_2 + n_2 + 1)] \times I_{C3}(j'_1, j'_2, j'_3, n_1, n_2, n_3) - (j'_1 + n_1 + 1)(j'_2 - n_2 + 1) I_{C3}(j'_1, j'_2, j'_3, n_1 + 1, n_2 - 1, n_3) \}, \quad (53)$$

to move diagonally (up and to the left),

$$I_{C3}(j'_1, j'_2, j'_3, n_1, n_2 + 1, n_3 - 1) = [(j'_2 + n_2 + 1)(j'_3 + n_3)]^{-1} \times \{ [-(j'_1 + n_1)(j'_1 - n_1 + 1) + (j'_2 - n_2)(j'_2 + n_2 + 1) + (j'_3 - n_3)(j'_3 + n_3 + 1)] \times I_{C3}(j'_1, j'_2, j'_3, n_1, n_2, n_3) - (j'_2 - n_2 + 1)(j'_3 - n_3) I_{C3}(j'_1, j'_2, j'_3, n_1, n_2 - 1, n_3 + 1) \}, \quad (54)$$

to move up,

$$I_{C3}(j'_1, j'_2, j'_3, n_1 - 1, n_2, n_3 + 1) = [(j'_1 - n_1 + 1)(j'_3 - n_3)]^{-1} \times \{ [-(j'_2 + n_2)(j'_2 - n_2 + 1) + (j'_1 - n_1)(j'_1 + n_1 + 1) + (j'_3 - n_3)(j'_3 + n_3 + 1)] \times I_{C3}(j'_1, j'_2, j'_3, n_1, n_2, n_3) - (j'_1 + n_1 + 1)(j'_3 - n_3 + 1) I_{C3}(j'_1, j'_2, j'_3, n_1 + 1, n_2, n_3 - 1) \}, \quad (55)$$

to move left, or

$$\begin{aligned}
I_{C3}(j'_1, j'_2, j'_3, n_1 + 1, n_2, n_3 - 1) &= [(j'_1 + n_1 + 1)(j'_3 + n_3)]^{-1} \\
&\times \{[-(j'_2 + n_2)(j'_2 - n_2 + 1) + (j'_1 - n_1)(j'_1 + n_1 + 1) + (j'_3 - n_3)(j'_3 + n_3 + 1)] \\
&\times I_{C3}(j'_1, j'_2, j'_3, n_1, n_2, n_3) - (j'_1 - n_1 + 1)(j'_3 - n_3)I_{C3}(j'_1, j'_2, j'_3, n_1 - 1, n_2, n_3 + 1)\}, \quad (56)
\end{aligned}$$

to move right in the  $(n_1, n_2)$  recursion plane. In order to be able to reach the entire recursion plane, the following relations may be used to “turn the corner” from one line to another:

$$\begin{aligned}
I_{C3}(j'_1, j'_2, j'_3, n_1, n_2, n_3) &= [(j'_2 + n_2)(j'_3 + n_3)]^{-1} \\
&\times \{[(j'_2 + n_2)(j'_2 - n_2 + 1) - (j'_1 + n_1)(j'_1 - n_1 + 1)]I_{C3}(j'_1, j'_2, j'_3, n_1, n_2 - 1, n_3 + 1) \\
&+ (j'_1 - n_1 + 1)(j'_3 - n_3 + 1)I_{C3}(j'_1, j'_2, j'_3, n_1 - 1, n_2 - 1, n_3 + 2)\}, \quad (57)
\end{aligned}$$

to switch from recursion on constant  $n_2$  to constant  $n_1$ ,

$$\begin{aligned}
I_{C3}(j'_1, j'_2, j'_3, n_1, n_2 + 1, n_3 - 1) &= (j'_2 + n_2 + 1)^{-1} \{(j'_3 + n_3 + 1)I_{C3}(j'_1, j'_2, j'_3, n_1, n_2, n_3) \\
&- (j'_1 + n_1 + 1)I_{C3}(j'_1, j'_2, j'_3, n_1 + 1, n_2, n_3 - 1)\}, \quad (58)
\end{aligned}$$

to switch from constant  $n_2$  to constant  $n_3$ ,

$$\begin{aligned}
I_{C3}(j'_1, j'_2, j'_3, n_1 - 1, n_2 + 1, n_3) &= [(j'_1 - n_1 + 1)(j'_3 - n_3 + 1)]^{-1} \\
&\times \{[(j'_3 + n_3)(j'_3 - n_3 + 1) - (j'_2 + n_2 + 1)(j'_2 - n_2)]I_{C3}(j'_1, j'_2, j'_3, n_1, n_2 + 1, n_3 - 1) \\
&+ (j'_1 + n_1 + 1)(j'_2 - n_2)I_{C3}(j'_1, j'_2, j'_3, n_1 + 1, n_2, n_3 - 1)\}, \quad (59)
\end{aligned}$$

to switch from constant  $n_3$  to constant  $n_2$ ,

$$\begin{aligned}
I_{C3}(j'_1, j'_2, j'_3, n_1 - 1, n_2 + 1, n_3) &= [(j'_2 + n_2 + 1)(j'_3 + n_3 + 1)]^{-1} \\
&\times \{[(j'_3 + n_3 + 1)(j'_3 - n_3) - (j'_1 + n_1)(j'_1 - n_1 + 1)]I_{C3}(j'_1, j'_2, j'_3, n_1 - 1, n_2, n_3 + 1) \\
&+ (j'_1 + n_1)(j'_2 - n_2 + 1)I_{C3}(j'_1, j'_2, j'_3, n_1, n_2 - 1, n_3 + 1)\}, \quad (60)
\end{aligned}$$

to switch from constant  $n_3$  to constant  $n_1$ , and

$$\begin{aligned}
I_{C3}(j'_1, j'_2, j'_3, n_1, n_2, n_3) &= [(j'_1 + n_1)(j'_3 + n_3 + 1)]^{-1} \\
&\times \{[(j'_1 + n_1)(j'_1 - n_1 + 1) - (j'_2 + n_2)(j'_2 - n_2 + 1)]I_{C3}(j'_1, j'_2, j'_3, n_1 - 1, n_2, n_3 + 1) \\
&+ (j'_2 - n_2 + 1)(j'_3 - n_3 + 1)I_{C3}(j'_1, j'_2, j'_3, n_1 - 1, n_2 - 1, n_3 + 2)\}, \quad (61)
\end{aligned}$$

to switch from constant  $n_1$  to constant  $n_2$ .

We now turn to the discussion of recursion sequences. The above initial conditions and recursion relations can be used to reach anywhere in the recursion plane. Given a 3-j symbol, one of the following four sequences can be used to calculate the binomial sum. For each of these sequences, a sample 3-j symbol is given for which the binomial sum recursion sequence is shown in detail in Table 1 and illustrated in Fig. 3. In the following discussion,  $(n_1, n_2, n_3)$  will refer to intermediate  $m$  quantum numbers used during recursion.

#### Sequence I: $m'_1 = 0$

- (1) Calculate the  $(0, 0, 0)$  binomial sum from Eq. (37) or (38) or the  $(0, 1/2, -1/2)$  binomial sum from Eq. (46) or (47). If  $m'_2 = 0$  or  $1/2$ , recursion is complete.
- (2) Calculate the  $(0, 1, -1)$  binomial sum from Eq. (41) or (42) or the  $(0, 3/2, -3/2)$  binomial sum from Eq. (49). If  $m'_2 = 1$  or  $3/2$ , recursion is complete.

(3) Calculate the  $(0, n_2 + 1, -n_2 - 1)$  binomial sums for  $n_2$  from 1 or  $3/2$  to  $(m'_2 - 1)$  from Eq. (54). Recursion is now complete.

This sequence has  $[m'_2 + 1]$  steps and is shown in Fig. 3a and Table 1a for the 3-j symbol  $j_1 = 65/2, j_2 = 35, j_3 = 75/2, m_1 = 15/2, m_2 = -10, m_3 = 5/2$  ( $j'_1 = 40, j'_2 = 30, j'_3 = 35, m'_1 = 0, m'_2 = 5, m'_3 = -5$ ). The binomial sum requires 6 steps for recursion (including initial conditions) and 26 terms for direct summation.

**Sequence II:  $m'_1 > 0$**

- (1) Calculate one of the following binomial sums, depending on whether  $j'_1$  and  $j'_2$  are integer or half-integer:
  - (a) the  $(0, 0, 0)$  binomial sum from Eq. (37) or (38),
  - (b) the  $(-1/2, 0, 1/2)$  binomial sum from Eq. (43) or (44),
  - (c) the  $(0, 1/2, -1/2)$  binomial sum from Eq. (46) or (47), or
  - (d) the  $(-1/2, 1/2, 0)$  binomial sum from Eq. (50) or (51).
 Exit if recursion is complete.

- (2) Calculate one of the following binomial sums, depending on whether  $j'_1$  and  $j'_2$  are integer or half-integer:
  - (a) the  $(-1, 0, 1)$  binomial sum from Eq. (39) or (40),
  - (b) the  $(-3/2, 0, 3/2)$  binomial sum from Eq. (45),
  - (c) the  $(-1, 1/2, 1/2)$  binomial sum from Eq. (48), or
  - (d) the  $(-3/2, 1/2, 1)$  binomial sum from Eq. (52).
 Exit if recursion is complete.

If  $m'_2 = 0$  or  $1/2$ , then skip to step (6).

- (3) Calculate one of the following binomial sums from Eq. (57), depending on whether  $j'_1$  and  $j'_2$  are integer or half-integer:  $(0, 1, -1)$ ;  $(-1/2, 1, -1/2)$ ;  $(0, 3/2, -3/2)$ ; or  $(-1/2, 3/2, -1)$ .
- (4) Calculate the  $(0, n_2 + 1, -n_2 - 1)$  or  $(-1/2, n_2 - 1, -n_2 + 3/2)$  binomial sums for  $n_2$  from 1 or  $3/2$  to  $(m'_2 - 1)$  from Eq. (54).
- (5) Calculate the  $(1, m'_2, -m'_2 - 1)$  or  $(1/2, m'_2, -m'_2 - 1/2)$  binomial sum from Eq. (61). This turns the corner from constant  $n_1$  to constant  $n_2$ . If  $m'_1 = 1/2$  or 1, then recursion is complete.
- (6) Calculate the  $(n_1, m'_2, -n_1 - m'_2)$  binomial sums from Eq. (56) for  $n_1$  from  $3/2$  or 2 to  $m'_1$ . Recursion is now complete.

This sequence has  $[|m'_3| + 2]$  steps and is shown in Fig. 3b and Table 1b for the 3-j symbol  $j_1 = 30, j_2 = 39, j_3 = 37, m_1 = -5, m_2 = -3, m_3 = 8$  ( $j'_1 = 81/2, j'_2 = 30, j'_3 = 71/2, m'_1 = 9/2, m'_2 = 2, m'_3 = -13/2$ ). The binomial sum requires 9 steps for recursion (including initial conditions) and 26 terms for direct summation.

The other two recursion sequences can be divided into a diagonal portion (which is identical for both) and a straight line portion.

**Diagonal portion, Sequences III and IV:  $m'_1 < 0$**

- (1) Same as for Sequence II.
- (2) Same as for Sequence II.

If  $m'_2 = 0$  or  $1/2$ , skip to step (2) of the straight line portion of Sequence IV.

- (3) Calculate one of the following binomial sums from Eq. (58), depending on whether  $j'_1$  and  $j'_2$  are integer or half-integer:  $(-1, 1, 0)$ ;  $(-3/2, 1, -1/2)$ ;  $(0, 3/2, -3/2)$ ; or  $(-1/2, 3/2, -1)$ .
- (4) Calculate the  $(n_1, -n_1 - n_3, n_3)$  binomial sums for  $n_1$  from  $-2$  or  $-5/2$  to the smaller of  $-m'_2$  and  $m'_1$  from Eq. (53). If  $m'_1 = n_1$  and  $m'_3 = n_3$ , then recursion is complete.

**Straight line portion, Sequence III:  $m'_3 \leq 0$**

- (1) Calculate the  $(m'_1, -m'_1 - n_3 + 1, n_3 - 1)$  binomial sum from Eq. (60). This turns the corner from constant  $n_3$  to constant  $n_1$ . If  $m'_3 = n_3 - 1$ , then recursion is complete.
- (2) Calculate the  $(m'_1, n_2, -m'_1 - n_2)$  binomial sums from Eq. (54) for  $n_2$  from  $-m'_1 - n_3 + 2$  to  $m'_2$ . Recursion is now complete.

This sequence has  $[m'_2 + 2]$  steps and is shown in Fig. 3c and Table 1c for the 3-j symbol  $j_1 = 39, j_2 = 35, j_3 =$

35,  $m_1 = -1, m_2 = -11, m_3 = 12$  ( $j'_1 = 43, j'_2 = 31, j'_3 = 35, m'_1 = -3, m_2 = 7, m_3 = -4$ ). The binomial sum requires 9 steps for recursion (including initial conditions) and 32 terms for direct summation.

**Straight line portion, Sequence IV:  $m'_3 > 0$**

- (1) Calculate the  $(-m'_2 - n_3 - 1, m'_2, n_3 + 1)$  binomial sum from Eq. (59). This turns the corner from constant  $n_3$  to constant  $n_1$ . If  $m'_1 = n_1 - 1$ , then recursion is complete.
- (2) Calculate the  $(n_1, m'_2, -m'_2 - n_1)$  binomial sums from Eq. (55) for  $n_1$  from  $-m'_2 - n_3 - 2$  to  $m'_1$ . Recursion is now complete.

This sequence has  $[|m'_1| + 2]$  steps and is shown in Fig. 3d and Table 1d for the 3-j symbol  $j_1 = 37, j_2 = 41, j_3 = 37, m_1 = -15, m_2 = 13, m_3 = 2$  ( $j'_1 = 93/2, j'_2 = 63/2, j'_3 = 38, m'_1 = -15/2, m_2 = 7/2, m_3 = 4$ ). The binomial sum requires 9 steps for recursion (including initial conditions) and 24 terms for direct summation.

**Method III - Edge recursion**

One advantage of recursion over direct summation is that the intermediate binomial sums are often much smaller in magnitude than the largest term in the direct summation. In floating point calculations this can make recursion more accurate than direct summation. In exact calculations using large integer routines, this can yield a significant speed advantage since less work would be required for large integer operations. A recursion sequence which has the same number of steps as direct summation would therefore be useful.

In the recursion relations discussed in the previous section, the entries of the second and third rows of the Regge matrix change by 0 or  $\pm 1$ . In order to produce a recursion sequence with the number of steps being the same as the number of terms in the direct summation, the number of terms in the successive 3-j binomial sums should change by 1. For the transformed Regge matrix, the number of terms in the binomial sum is  $R'_{11} + 1$ . For the Regge matrix

$$R'' = \begin{vmatrix} R'_{11} - k & R'_{12} + k & R'_{13} \\ R'_{21} + k & R'_{22} - k & R'_{23} \\ R'_{31} & R'_{32} & R'_{33} \end{vmatrix}, \tag{62}$$

where  $R'_{ij}$  are elements of the transformed Regge matrix and  $k$  is a nonnegative integer no larger than  $R'_{11}$ , the number of terms in the sum is  $R'_{11} - k + 1$ . In addition, since it has the same properties as the transformed Regge matrix (for example, the order of the  $j$ 's), it follows that  $I_{C3}$  is its smallest magnitude binomial sum. We denote this scheme edge recursion because each successive 3-j symbol in the sequence lies on successive inner contours in diagrams like the one shown in Fig. 1.

A recursion relation among three of the consecutive 3-j symbols, namely

$$\begin{pmatrix} j'_1 + \frac{k}{2} & j'_2 - \frac{k}{2} & j'_3 \\ m'_1 - \frac{k}{2} & m'_2 + \frac{k}{2} & m'_3 \end{pmatrix}, \tag{63}$$

is derived in Appendix A. The corresponding binomial sum recursion relation is

$$\begin{aligned} &I_{C3} \left( j'_1 + \frac{k-1}{2}, j'_2 - \frac{k-1}{2}, j'_3, m'_1 - \frac{k-1}{2}, m'_2 + \frac{k-1}{2}, m'_3 \right) \\ &= [(-j'_1 + j'_2 + j'_3 - k + 1)(j'_2 - m'_2 - k + 1)]^{-1} \left\{ [-(j'_1 + j'_2 - j'_3)(j'_3 - m'_3 + 1) \right. \\ &\quad \left. + (j'_2 - m'_2 + k)(j'_1 - j'_2 + j'_3 + k + 1) + (j'_1 - m'_1 + k)(-j'_1 + j'_2 + j'_3 + k + 1)] \right\} \end{aligned}$$

Table 1  
Recursion sequences for several 3-j symbols

$n_1$	$n_2$	$n_3$	Eq.	Remarks
(a) $j_1 = 65/2, j_2 = 35, j_3 = 75/2, m_1 = 15/2, m_2 = -10, m_3 = 5/2$ ( $j'_1 = 40, j'_2 = 30, j'_3 = 35, m'_1 = 0, m_2 = 5, m_3 = -5$ )				
0	0	0	-	Zero because $J$ is odd.
0	1	-1	(37)	
0	2	-2	(54)	
0	3	-3	(54)	
0	4	-4	(54)	
0	5	-5	(54)	
(b) $j_1 = 30, j_2 = 39, j_3 = 37, m_1 = -5, m_2 = -3, m_3 = 8$ ( $j'_1 = 81/2, j'_2 = 30, j'_3 = 71/2, m'_1 = 9/2, m_2 = 2, m_3 = -13/2$ )				
-1/2	0	1/2	(43)	
-3/2	0	3/2	(45)	
-1/2	1	-1/2	(57)	Turn the corner to constant $n_1$ .
-1/2	2	-3/2	(54)	
1/2	2	-5/2	(61)	Turn the corner to constant $n_2$ .
3/2	2	-7/2	(56)	
5/2	2	-9/2	(56)	
7/2	2	-11/2	(56)	
9/2	2	-13/2	(56)	
(c) $j_1 = 39, j_2 = 35, j_3 = 35, m_1 = -1, m_2 = -11, m_3 = 12$ ( $j'_1 = 43, j'_2 = 31, j'_3 = 35, m'_1 = -3, m_2 = 7, m_3 = -4$ ).				
0	0	0	-	Zero because $J$ is odd.
-1	0	1	(40)	
-1	1	0	(58)	Turn the corner to constant $n_3$ .
-2	2	0	(53)	
-3	3	0	(53)	
-3	4	-1	(60)	Turn the corner to constant $n_1$ .
-3	5	-2	(54)	
-3	6	-3	(54)	
-3	7	-4	(54)	
(d) $j_1 = 37, j_2 = 41, j_3 = 37, m_1 = -15, m_2 = 13, m_3 = 2$ ( $j'_1 = 93/2, j'_2 = 63/2, j'_3 = 38, m'_1 = -15/2, m_2 = 7/2, m_3 = 4$ ).				
-1/2	1/2	0	(50)	
-3/2	1/2	1	(52)	
-3/2	3/2	0	(58)	Turn the corner to constant $n_3$ .
-5/2	5/2	0	(53)	
-7/2	7/2	0	(53)	
-9/2	7/2	1	(59)	Turn the corner to constant $n_2$ .
-11/2	7/2	2	(55)	
-13/2	7/2	3	(55)	
-15/2	7/2	4	(55)	

$$\begin{aligned}
 & \times I_{C3} \left( j'_1 + \frac{k}{2}, j'_2 - \frac{k}{2}, j'_3, m'_1 - \frac{k}{2}, m'_2 + \frac{k}{2}, m'_3 \right) \\
 & - (j'_1 - m'_1 + k + 1)(j'_1 - j'_2 + j'_3 + k + 1) \\
 & \times I_{C3} \left( j'_1 + \frac{k+1}{2}, j'_2 - \frac{k+1}{2}, j'_3, m'_1 - \frac{k+1}{2}, m'_2 + \frac{k+1}{2}, m'_3 \right) \Big\}. \tag{64}
 \end{aligned}$$

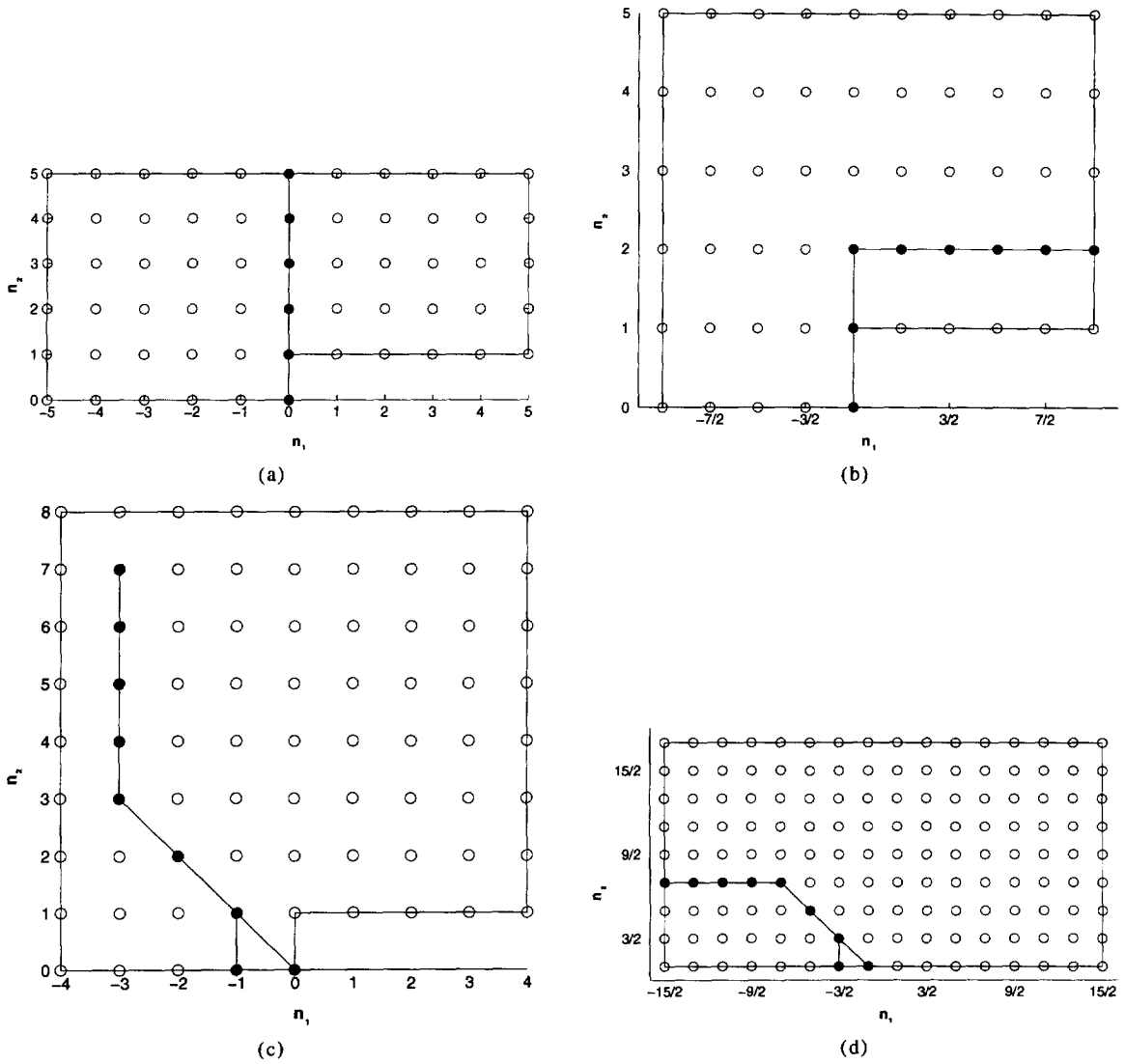


Fig. 3. Schematic of binomial sum recursion sequences for 3-j symbols in (a) Table 1a, (b) Table 1b, (c) Table 1c, and (d) Table 1d.

As in the previous section, the recursion sequence shown here requires two starting points. The first starting point is  $k = R'_{11}$ , for which there is only one term in the binomial sum. Substituting this  $k$  into Eq. (63) and the resulting  $j$ 's and  $m$ 's into Eq. (22) yields

$$I_{C3} \left( \frac{J}{2}, \frac{J}{2} - j'_3, j'_3, j'_1 + m'_1 - \frac{J}{2}, \frac{J}{2} - j'_1 + m'_2, m'_3 \right) = (-1)^{j'_2 + m'_2} \binom{J - 2j'_3}{j'_2 + m'_2}. \tag{65}$$

The second starting point is  $k = R'_{11} - 1$ , for which the binomial sum has two terms. From Eq. (63) and (22) and some manipulations of the form

$$\binom{n}{m} = \frac{n + m - 1}{m} \binom{n}{m - 1}, \tag{66}$$

we obtain

$$\begin{aligned}
 & I_{C3} \left( \frac{J-1}{2}, \frac{J+1}{2} - j'_3, j'_3, j'_1 + m'_1 - \frac{J-1}{2}, \frac{J-1}{2} - j'_1 + m'_2, m'_3 \right) \\
 &= I_{C3} \left( \frac{J}{2}, \frac{J}{2} - j'_3, j'_3, j'_1 + m'_1 - \frac{J}{2}, \frac{J}{2} - j'_1 + m'_2, m'_3 \right) \\
 &\quad \times \frac{(j'_3 + m'_3)(j'_1 - j'_3 - m'_2 + 1) - (j'_2 + m'_2)(j'_3 - m'_3)}{(j'_1 - j'_3 - m'_2 + 1)}. \tag{67}
 \end{aligned}$$

Applying Eq. (64) successively from  $k = R'_{11} - 1$  down to  $k = 1$  yields the transformed binomial sum.

This completes the calculation of the binomial sum for the transformed 3-j symbol. The rest of the transformed 3-j symbol may be calculated as shown in Eq. (29). Only one task remains: to calculate the sign factor  $\sigma$  in Eq. (36) to obtain the untransformed 3-j symbol. If  $J$  is even, of course, this is unnecessary since no sign changes occur under any symmetry transformations. If  $J$  is odd, sign changes occur under odd row or column permutations of the Regge matrix but not under transposition. Thus, the sign factor depends directly on the parity of the row or column transformations required to obtain the untransformed Regge matrix. For example, for the 3-j symbol

$$\begin{pmatrix} 8 & 12 & 15 \\ -2 & 1 & 1 \end{pmatrix},$$

the untransformed Regge matrix is

$$R = \left\| \begin{array}{ccc} 19 & 11 & 5 \\ 10 & 11 & 14 \\ 6 & 13 & 16 \end{array} \right\|. \tag{68}$$

To obtain the transformed Regge matrix

$$R = \left\| \begin{array}{ccc} 5 & 19 & 11 \\ 16 & 6 & 13 \\ 14 & 10 & 11 \end{array} \right\| \tag{69}$$

requires a (132) row permutation, which is odd and causes a sign change, and a (231) column permutation, which is even and causes no sign change. Thus, the total sign change is negative.

The parity (even or odd) of a permutation can be calculated very simply. Let  $(ijk)$  be some permutation of (123). Then the quantity  $(k-i+3) \bmod 3$  is 2 if the permutation is even and 1 if it is odd. Once this is calculated for the row and column permutations then the total sign factor can be obtained from  $\sigma = (\sigma_{\text{row}} + \sigma_{\text{column}}) \bmod 2$ .

### Calculation of tables of 3-j symbols

So far, this paper has described how to compute individual 3-j symbols. In many calculations, however, sequences of 3-j symbols are required. Schulten and Gordon and other workers have noted that recursion is an efficient method for accomplishing this. Any 3-j recursion scheme can be adapted into a binomial scheme. This can prove useful if exact results are absolutely essential. For example, the straight line recursion relations, Eqs. (53)–(56), which follow directly from Schulten and Gordon's results, can be used to calculate lines of 3-j symbols with a constant  $m$ . One calculation scheme of theirs which has so far not been treated is the set of all possible 3-j symbols for which only one top argument, say  $j_1$ , may change. To calculate the 3-j symbols, they use

$$j_1 A(j_1 + 1) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} + B(j_1) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} + (j_1 + 1) A(j_1) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = 0, \quad (70)$$

where

$$A(j_1) = [(j_1 - j_2 + j_3)(j_1 + j_2 - j_3)(-j_1 + j_2 + j_3 + 1)(j_1 + j_2 + j_3 + 1)(j_1 - m_1)(j_1 + m_1)]^{1/2}, \quad (71)$$

$$B(j_1) = -(2j_1 + 1)[j_2(j_2 + 1)m_1 - j_3(j_3 + 1)m_1 - j_1(j_1 + 1)(m_3 - m_2)]. \quad (72)$$

This leads directly to the binomial sum relation

$$j_1(j_1 - j_2 + j_3 + 1)(j_1 + m_1)(j_1 - m_1)I_{C3}(j_1 + 1, j_2, j_3, m_1, m_2, m_3) - B(j_1)I_{C3}(j_1, j_2, j_3, m_1, m_2, m_3) + (j_1 + 1)(-j_1 + j_2 + j_3 + 1)(j_1 + j_2 - j_3)(j_1 + j_2 + j_3 + 1)I_{C3}(j_1 - 1, j_2, j_3, m_1, m_2, m_3) = 0. \quad (73)$$

Calculation of the prefactors can be economized by first calculating a table of square roots and storing them for later use. The prefactors involve square roots of factorials whose arguments change by one as the recursion progresses. Thus, successive prefactors can be obtained from previous ones by a few multiplications and divisions. This method can be used for any recursion scheme in order to save calculation time.

It should be noted that for individual 3-j symbols, the recursion schemes were carefully chosen to make  $I_{C3}$  the smallest magnitude binomial sum throughout. In general,  $I_{C3}$  will not always have the smallest magnitude. All of the recursion relations reported here can be rewritten in terms of other binomial sums. If the arguments of the 3-j symbols have special values, it may prove useful to investigate the possibility that binomial sums other than  $I_{C3}$  have the smallest magnitude. However, in a completely general calculation,  $I_{C3}$  will very probably work as well as any other sum.

When inspecting the properties of a set of 3-j symbols, it may be useful to first know how much computational effort will be required, which roughly matches the number of 3-j symbols. In order to calculate this number, it is useful to remember that each set of 3-j symbols related by Regge symmetry is characterized by a set of five nonnegative integers  $S \leq B \leq T \leq X \leq L$ . A more convenient set of parameters for counting purposes is the five nonnegative integers  $c_1 = S$  and

$$c_2 = B - S, \quad (74)$$

$$c_3 = T - B, \quad (75)$$

$$c_4 = X - T, \quad (76)$$

$$c_5 = L - X. \quad (77)$$

In terms of the  $c$ 's, the design of the transformed Regge matrix yields  $c_4 \geq c_2$  and, if  $c_4 = c_2$ , then  $c_5 \geq c_3$ . In addition, the transformed Regge matrix can be written

$$R' = \begin{vmatrix} c_1 & c_1 + c_2 + c_3 + c_4 + c_5 & c_1 + c_2 + c_4 \\ c_1 + c_2 + c_3 + c_4 & c_1 + c_2 & c_1 + c_4 + c_5 \\ c_1 + c_2 + c_4 + c_5 & c_1 + c_4 & c_1 + c_2 + c_3 \end{vmatrix}, \quad (78)$$

which has a rank of  $J = 3c_1 + 2c_2 + c_3 + 2c_4 + c_5$ . The size of a fully symmetry reduced table of 3-j symbols for which  $j_1 + j_2 + j_3$  is equal to some  $J$  is the number of nonnegative integer solutions of  $3c_1 + 2c_2 + c_3 + 2c_4 + c_5 = J$ , subject to the above conditions on the  $c$ 's. Writing  $J = 12n + i$ , where  $0 \leq i \leq 11$ , we obtain

$$N_{R3}(12n + i) = \sum_{j=0}^4 d_{ij} \binom{n + 4 - j}{4}, \quad (79)$$

Table 2  
Size of Regge symmetry reduced tables of 3-j symbols:  $d_{ij}$  for Eq. (79)

$i$	$d_{i0}$	$d_{i1}$	$d_{i2}$	$d_{i3}$	$d_{i4}$
0	1	123	512	283	5
1	1	155	518	187	3
2	3	187	518	155	1
3	5	223	512	123	1
4	9	260	497	98	0
5	13	302	473	76	0
6	21	338	449	56	0
7	29	380	413	42	0
8	42	413	380	29	0
9	56	449	338	21	0
10	76	473	302	13	0
11	98	497	260	9	0

where the  $d_{ij}$  are listed in Table 2 and the formula is derived in Appendix B.

### 3. 6-j symbols

One common expression for the 6-j symbol is [5]

$$\left\{ \begin{matrix} a & b & c \\ d & e & f \end{matrix} \right\} = \Delta(abc)\Delta(cde)\Delta(aef)\Delta(bdf) \sum_n \frac{(-1)^n(n+1)!}{\prod_i(\alpha_i - n)! \prod_j(n - \beta_j)!}, \tag{80}$$

where each triplet satisfies the triangle conditions and

$$\Delta(abc) = \left[ \frac{(a+b-c)!(a-b+c)!(-a+b+c)!}{(a+b+c+1)!} \right]^{1/2}, \tag{81}$$

$$\alpha_1 = a + b + d + e, \quad \alpha_2 = a + c + d + f, \quad \alpha_3 = b + c + e + f, \tag{82}$$

$$\beta_1 = a + b + c, \quad \beta_2 = a + e + f, \quad \beta_3 = b + d + f, \quad \beta_4 = c + d + e,$$

and the sum is over all nonnegative integer  $n$  for which every factorial has a nonnegative argument. If the triangle conditions are not satisfied, the 6-j symbol vanishes. The 6-j symbols are often represented in the form of a 3 by 4 array called the R-symbol [29],

$$R = \left\| \begin{matrix} -c + d + e & b + d - f & a + e - f & a + b - c \\ -b + d + f & c + d - e & a - b + c & a - e + f \\ -a + e + f & -a + b + c & c - d + e & b - d + f \end{matrix} \right\|. \tag{83}$$

From the triangle conditions and from

$$R_{ij} = \alpha_i - \beta_j, \tag{84}$$

it is readily apparent that each  $\alpha$  and  $\beta$  is a nonnegative integer and that  $\alpha_i \geq \beta_j$  for all  $i$  and  $j$ . The elements of the R-symbol also satisfy

$$R_{ij} + R_{kl} = R_{il} + R_{kj} \tag{85}$$

and

$$J = \sum_{i,j} R_{ij} = 2(a + b + c + d + e + f). \tag{86}$$

The 6-j symbol has 24 symmetries that are described as classical: it is invariant with respect to any column permutation and with respect to the interchange of upper and lower arguments of any two columns. Regge [26] discovered several additional symmetries such as

$$\left\{ \begin{matrix} a & b & c \\ d & e & f \end{matrix} \right\} = \left\{ \begin{matrix} a & \frac{c-b+e+f}{2} & \frac{b-c+e+f}{2} \\ d & \frac{b+c-e+f}{2} & \frac{b+c+e-f}{2} \end{matrix} \right\}, \tag{87}$$

which yield a total of 144 symmetries. Shelepin [29] later showed that these 144 symmetries are isomorphic with the set of all row and column permutations of  $R$ . Unlike the case for 3-j symbols, if two 6-j symbols are related by Regge symmetry, whether the  $j$ 's are integer or half-integer, then they have the same  $\alpha$ 's and  $\beta$ 's. This can be verified by inspection of the  $R$  matrix under (12) and (13) row permutations and (12), (13), and (14) column permutations since the entire set of Regge symmetries can be obtained from products of these operations.

From these results we now construct a convenient parameterization of each set of 6-j symbols related by classical or other Regge symmetries. Let us define  $A_1, A_2,$  and  $A_3$  to be the smallest, middle, and largest values of  $\alpha_1, \alpha_2,$  and  $\alpha_3$  and  $B_1, B_2, B_3,$  and  $B_4$  to be the smallest, second smallest, second largest, and largest values of  $\beta_1, \beta_2, \beta_3,$  and  $\beta_4$ . In a manner similar to the 3-j symbols, the row- and column-permuted R-symbol  $R'$  for which  $R'_{ij} = A_i - B_j$  is unique to each set of 6-j symbols related by Regge symmetry. The 6-j symbol which directly corresponds to the transformed R-symbol will be denoted

$$\left\{ \begin{matrix} A & B & C \\ D & E & F \end{matrix} \right\} = \left\{ \begin{matrix} \frac{R'_{13}+R'_{24}}{2} & \frac{R'_{14}+R'_{32}}{2} & \frac{R'_{22}+R'_{33}}{2} \\ \frac{R'_{11}+R'_{22}}{2} & \frac{R'_{11}+R'_{33}}{2} & \frac{R'_{21}+R'_{34}}{2} \end{matrix} \right\} \tag{88}$$

and will prove especially useful when discussing binomial sum recursion. From Eq. (80) and the definition of the  $A$ 's and  $B$ 's, the number of terms in the binomial sum is  $A_1 - B_4 + 1$ . The elements of the transformed R-symbol satisfy the inequality  $R'_{ij} \leq R'_{k\ell}$  if  $i \leq k$  and  $j \geq \ell$ . From  $R'_{14} \leq R'_{23} \leq R'_{32}$  we obtain  $A \leq B \leq C$ . Similar comparisons yield  $A \leq D, A \leq E, A \leq F,$  and  $B \leq F$ .

*Calculation of individual 6-j symbols*

Several special cases of the 6-j symbol have simple formulas which take far less effort to calculate than the general formula. By examining the  $A$ 's and  $B$ 's, it is possible to detect these special cases – and all their Regge symmetry transformations – with far less effort than by directly testing the 6-j arguments. For example, if  $B_4 = A_1$  then the summation has only one term. Some algebra similar in spirit to Eqs. (23)–(28) yields

$$6j(B_4 = A_1) = (-1)^{B_4} \left[ \prod_{i=1}^{B_4-B_3} \frac{(B_3 + 1 + i)(A_3 - A_1 + i)}{(A_3 - B_1 + i)(A_2 - B_2 + i)} \right]^{1/2} \times \left[ \frac{1}{(B_1 + 1)(B_2 + 1)} \prod_{i=1}^{A_2-A_1} \frac{(A_1 - B_1 + i)(B_4 - B_2 + i)(B_4 - B_3 + i)}{(A_1 + B_1 - A_2 + i)(A_1 + B_2 - A_2 + i)i} \right]^{1/2}, \tag{89}$$

where each product is considered to be 1 if its upper index is 0. This formula includes (among many others) the cases [10]

$$\left\{ \begin{matrix} 0 & b & c \\ d & e & f \end{matrix} \right\} = \frac{(-1)^{b+d+e} \delta_{bc} \delta_{ef}}{[(2b+1)(2e+1)]^{1/2}} \tag{90}$$

and

$$\left\{ \begin{matrix} a & b & a+b \\ a & b & f \end{matrix} \right\} = (-1)^{2(a+b)} \frac{(2a)!(2b)!}{(a+b-f)!(a+b+f+1)!}, \tag{91}$$

where  $\delta_{ij}$  refers to the Kronecker delta, which is 1 if  $i = j$  and zero otherwise.

It is also easy to check for trivially zero 6-j symbols. For example, for the 6-j symbol

$$\left\{ \begin{matrix} 1 & 0 & 1 \\ 0 & 0 & 0 \end{matrix} \right\}$$

we have  $A_1 - B_4 = -1$ , which indicates that at least one triplet violates the triangle conditions.

As Lai and Chiu have noted, the expression for a 6-j symbol can be rewritten in terms of an alternating binomial sum in a manner similar to the 3-j symbol. There are 24 ways to do this,

$$\left\{ \begin{matrix} a & b & c \\ d & e & f \end{matrix} \right\} = \left\{ \begin{matrix} A & B & C \\ D & E & F \end{matrix} \right\} = \left[ \frac{R'_{1j}! R'_{1k}! R'_{1\ell}! R'_{2i}! R'_{2k}! R'_{2\ell}! R'_{3i}! R'_{3j}! R'_{3\ell}! (B_\ell + 1)!}{R'_{1i}! R'_{2j}! R'_{3j}! (B_i + 1)! (B_j + 1)! (B_k + 1)!} \right]^{1/2} \times I_{ijk\ell}(A, B, B, D, E, F), \tag{92}$$

where  $ijk\ell$  is a permutation of 1234,  $R'_{ij}$  are elements of the transformed R-symbol, and  $I_{ijk\ell}$  is the binomial sum

$$I_{ijk\ell} = \sum_n (-1)^n \binom{n+1}{B_\ell + 1} \binom{A_1 - B_i}{A_1 - n} \binom{A_2 - B_j}{A_2 - n} \binom{A_3 - B_k}{A_3 - n}. \tag{93}$$

If two 6-j symbols are related by Regge symmetry, then the pre-factors in front of the summation in Eq. (80) are equal since they involve the set of  $B$ 's and the set of all twelve entries of the R-symbol, each of which is invariant under any Regge symmetry transformation. Therefore, the sums are also equal. It follows that the optimal calculation sequence depends only on which set of factorials is introduced into the sum and not on the arrangement of the R-symbol. Two methods for evaluating the binomial sums and from there calculating the 6-j symbol are direct summation and recursion, as we now show.

**Method I – Direct summation**

The same issues involving accuracy and efficiency of the calculation of 3-j symbols apply to the calculation of 6-j symbols. Essentially the same process, namely systematically choosing the smallest magnitude binomial sum, will be followed here. It should be noted that for the 3-j symbols, it was required to introduce factorials into the sum in order to obtain an integer. However, the summation terms in Racah's expression for the 6-j symbol, Eq. (80), are already integer. To see this, we note that since

$$J = \sum_i A_i = \sum_j B_j \tag{94}$$

and the sum of all factorial arguments in the denominator is  $n$ , then each term is  $n + 1$  times a multinomial coefficient and is therefore integer. Despite this, it still makes sense to construct a binomial sum because the factor introduced into the sum, namely

$$f_{ijk\ell} = \frac{(A_1 - B_i)!(A_2 - B_j)!(A_3 - B_k)!}{(B_\ell + 1)!} = \left[ (B_\ell + 1) \binom{B_\ell}{A_1 - B_i} \binom{A_2 + A_3 - B_j - B_k}{A_2 - B_j} \right]^{-1} \tag{95}$$

is clearly less than 1. For a given  $\ell$ , by using the method for finding the smallest product of factorials shown in the 3-j section, we find that  $i < j < k$  yields the smallest factor. This eliminates all but four permutations (1234, 1243, 1342, and 2341). Permutations containing two common factors (e.g., 1234 and 1243) can be compared by noting that  $A_p \leq B_r + B_s$  for any  $(p, r, s)$ , which can be proven from Eq. (82), and that  $(D - E)!/(F + 1)! \leq (D - F)!/(E + 1)!$  if  $E \leq F$  and  $D \leq E + F$ . Successive comparisons of this type yield  $f_{1234} \leq f_{1243} \leq f_{1342} \leq f_{2341}$  and therefore that  $I_{1234}$  is the smallest magnitude sum. After substituting

$$\frac{(A_1 - B_4)!(A_2 - B_3)!(A_3 - B_1)!}{B_2!} = \frac{(A_1 - B_4)!(A_2 - B_3)!}{(A_3 - B_1 + 1)_{A_1 - B_4} (A_1 + A_3 - B_1 - B_4 + 1)_{A_2 - B_3}}, \tag{96}$$

$$\frac{(A_3 - B_2)!(A_2 - B_4)!(A_1 - B_3)!}{B_1!} = \frac{(A_2 - B_4)!(A_1 - B_3)!}{(A_3 - B_2 + 1)_{A_2 - B_4} (A_2 + A_3 - B_2 - B_4 + 1)_{A_1 - B_3}}, \tag{97}$$

$$\frac{(B_4 + 1)!(A_3 - B_4)!}{(B_3 + 1)!(A_3 - B_3)!} = \frac{(B_3 + 2)_{B_4 - B_3}}{(A_3 - B_4 + 1)_{B_4 - B_3}}, \tag{98}$$

$$\frac{(A_1 - B_2)!(A_2 - B_1)!}{(A_2 - B_2)!(A_1 - B_1)!} = \frac{(A_1 - B_1 + 1)_{A_2 - A_1}}{(A_1 - B_2 + 1)_{A_2 - A_1}}, \tag{99}$$

and

$$\begin{aligned} \frac{(A_2 - B_3)!}{(A_1 + A_3 - B_1 - B_4 + 1)_{A_2 - B_3}} &= \frac{(A_1 - B_4)!}{(A_2 + A_3 - B_1 - B_3 + 1)_{A_1 - B_4}} \\ &\times \frac{(A_1 - B_4 + 1)_{B_4 - B_3} (A_1 - B_3 + 1)_{A_2 - A_1}}{(A_1 + A_3 - B_1 - B_4 + 1)_{B_4 - B_3} (A_1 + A_3 - B_1 - B_3 + 1)_{A_2 - A_1}} \end{aligned} \tag{100}$$

and several more similar results, we obtain

$$\begin{aligned} \left\{ \begin{matrix} a & b & c \\ d & e & f \end{matrix} \right\} &= (A_1 - B_4)!^2 (A_1 - B_4 + 1)_{B_4 - B_3} \left[ \frac{1}{(B_1 + 1)(B_2 + 1)} \right. \\ &\times \frac{(B_3 + 2)_{B_4 - B_3}}{(A_3 - B_4 + 1)_{B_4 - B_3} (A_1 + A_3 - B_1 - B_4 + 1)_{B_4 - B_3}} \\ &\times \frac{1}{(A_2 + A_3 - B_2 - B_4 + 1)_{B_4 - B_3}} \frac{1}{(A_3 - B_1 + 1)_{A_1 - B_4} (A_3 - B_2 + 1)_{A_1 - B_4}} \\ &\times \left. \frac{1}{(A_2 + A_3 - B_2 - B_4 + 1)_{A_1 - B_4} (A_2 + A_3 - B_2 - B_3 + 1)_{A_1 - B_4}} \right]^{1/2} \\ &\times \sum_{n=B_4}^{A_1} (-1)^n \binom{n+1}{n-B_4} \binom{A_1 - B_1}{A_1 - n} \binom{A_2 - B_2}{A_2 - n} \binom{A_3 - B_3}{A_3 - n}, \end{aligned} \tag{101}$$

a form in which the prefactor may be evaluated without concern for overflow. The first term in the binomial sum is

$$t_{B_4} = (-1)^{B_4} \binom{A_1 - B_1}{A_1 - B_4} \binom{A_2 - B_2}{A_2 - B_4} \binom{A_3 - B_3}{A_3 - B_4}. \tag{102}$$

Successive terms may be calculated from

$$t_n = -t_{n-1} \frac{n+1}{n-B_4} \times \frac{A_1 - n + 1}{n - B_1} \times \frac{A_2 - n + 1}{n - B_2} \times \frac{A_3 - n + 1}{n - B_3}. \tag{103}$$

Each successive fraction on the right-hand side of Eq. (103) is the factor for changing the bottom arguments of the binomial coefficients in Eq. (101) by one. Therefore, each multiplication must be performed before the corresponding division in order to assure that every intermediate is an integer.

**Method II – Recursion**

Essentially the same considerations that apply to 3-j binomial recursion schemes apply to 6-j calculations as well. A 6-j binomial sum recursion scheme with as many steps as the number of terms in the direct summation can be constructed in a manner similar to that for the 3-j symbols. From the formula for the transformed R-symbol, the number of terms in the binomial sum is  $R'_{14} + 1$ . We seek a series of 6-j symbols for which the number of terms in the sum changes incrementally by 1. One such set of 6-j symbols is

$$\left\{ \begin{matrix} A - k & B & C \\ D & E & F \end{matrix} \right\}, \tag{104}$$

where  $A$  through  $F$  are from Eq. (88). Here, the number of terms is  $R'_{14} - k + 1$ , where  $k$  is a nonnegative integer no larger than  $R'_{14}$ . The corresponding R-symbol is

$$R'' = \left\| \begin{matrix} R'_{11} & R'_{12} & R'_{13} - k & R'_{14} - k \\ R'_{21} & R'_{22} & R'_{23} - k & R'_{24} - k \\ R'_{31} + k & R'_{32} + k & R'_{33} & R'_{34} \end{matrix} \right\|. \tag{105}$$

Since this new R-symbol has the same properties as the original transformed R-symbol (for example, the previously reported inequalities), it follows that  $I_{1234}$  is the smallest magnitude binomial sum for the entire series of 6-j symbols. A recursion relation reported by Schulten and Gordon,

$$aE(a + 1) \left\{ \begin{matrix} a + 1 & b & c \\ d & e & f \end{matrix} \right\} + F(a) \left\{ \begin{matrix} a & b & c \\ d & e & f \end{matrix} \right\} + (a + 1)E(a) \left\{ \begin{matrix} a + 1 & b & c \\ d & e & f \end{matrix} \right\} = 0, \tag{106}$$

where

$$E(a) = [(a - b + c)(a + b - c)(-a + b + c + 1)(a + b + c + 1)(a - e + f) \times (a + e - f)(-a + e + f + 1)(a + e + f + 1)]^{1/2}, \tag{107}$$

$$F(a) = (2a + 1)\{a(a + 1)[-a(a + 1) + b(b + 1) + c(c + 1)] + e(e + 1)[a(a + 1) + b(b + 1) - c(c + 1)] + f(f + 1)[a(a + 1) - b(b + 1) + c(c + 1)] - 2a(a + 1)d(d + 1)\}, \tag{108}$$

can be used to step along 6-j symbols of the form shown in Eq. (104). Substituting  $a = A - k, b = B, c = C, d = D, e = E$ , and  $f = F$  into this result and some tedious manipulations yield the binomial recursion relation

$$I_{1234}(A - k + 1, B, C, D, E, F) = -[4(A - k)(A + E - F - k + 1)(A + B - C - k + 1) \times (A - B + C - k + 1)(A - E + F - k + 1)]^{-1}\{4F(A - k)I_{1234}(A - k, B, C, D, E, F) + 4(A - k + 1)(-A + E + F + k + 1)(-A + B + C + k + 1) \times (A + B + C - k + 1)(A + E + F - k + 1)I_{1234}(A - k - 1, B, C, D, E, F)\}. \tag{109}$$

The extra factors of 4 are inserted to ensure that the coefficients are integer. By going through all the possible cases of  $A, B$ , etc. being integer or half-integer, it can be determined that  $F(a)$  is sometimes quarter-integer.

The first starting point is  $k = R'_{14} = A + B - C$ , for which the binomial sum has only one term. Substituting this  $k$  into Eq. (104) and the resulting angular momentum arguments into Eq. (93) yields

$$I_{1234}(C - B, B, C, D, E, F) = (-1)^{C+D+E} \binom{C + D - E}{B + D - F} \binom{C - D + E}{B - D + F}. \quad (110)$$

The second starting point is  $k = R'_{14} - 1$ , for which there are two terms in the binomial sum. Similar manipulations and the use of Eq. (66) yields

$$\begin{aligned} I_{1234}(C - B + 1, B, C, D, E, F) &= I_{1234}(C - B, B, C, D, E, F) \\ &\quad \times [(-C + D + E)(B + D - F)(-B + C + E - F + 1) \\ &\quad - (C + D + E + 2)(-B + C - E + F + 1)(B - D + F)] \\ &\quad / [(-B + C - E + F + 1)(-B + C + E - F + 1)]. \end{aligned} \quad (111)$$

Applying Eq. (109) successively from  $k = R'_{14} - 1$  down to  $k = 1$  yields the transformed binomial sum. From there it is straightforward to calculate the 6-j symbol, as shown in Eq. (101).

#### Calculation of tables of 6-j symbols

In a manner similar to the 3-j symbol, any 6-j recursion relation can be rewritten as binomial sum relation. The issues concerning the calculation of tables of 6-j symbols by binomial recursion are similar to those for 3-j symbols and will not be repeated here.

Once again, for counting purposes we seek a convenient set of nonnegative parameters which are unique to every set of 6-j symbols related by Regge symmetry. To begin with, we define the following nonnegative integers  $d_o$  through  $d_6$ :

$$\begin{aligned} d_o &= B_1, & d_1 &= B_2 - B_1, & d_2 &= B_3 - B_2, & d_3 &= B_4 - B_3, \\ d_4 &= A_1 - B_4, & d_5 &= A_2 - A_1, & d_6 &= A_3 - A_2. \end{aligned} \quad (112)$$

The  $d$ 's are not independent. From this result and Eq. (94), we obtain

$$d_o = d_2 + 2d_3 + 3d_4 + 2d_5 + d_6, \quad (113)$$

and from there

$$\begin{aligned} B_1 &= d_2 + 2d_3 + 3d_4 + 2d_5 + d_6, \\ B_2 &= d_1 + d_2 + 2d_3 + 3d_4 + 2d_5 + d_6, \\ B_3 &= d_1 + 2d_2 + 2d_3 + 3d_4 + 2d_5 + d_6, \\ B_4 &= d_1 + 2d_2 + 3d_3 + 3d_4 + 2d_5 + d_6, \\ A_1 &= d_1 + 2d_2 + 3d_3 + 4d_4 + 2d_5 + d_6, \\ A_2 &= d_1 + 2d_2 + 3d_3 + 4d_4 + 3d_5 + d_6, \\ A_3 &= d_1 + 2d_2 + 3d_3 + 4d_4 + 3d_5 + 2d_6, \end{aligned} \quad (114)$$

and finally

$$J = 3d_1 + 6d_2 + 9d_3 + 12d_4 + 8d_5 + 4d_6. \quad (115)$$

The six nonnegative integers  $d_1$  through  $d_6$  are independent and comprise the Regge symmetry parameterization of the 6-j symbol. Unlike the Regge parameters for the 3-j symbol, the  $d$ 's are unrestricted with respect to each other. From Eqs. (93), (112), and (114), the number of terms in the binomial sum is  $d_4 + 1$ .

Giovannini and Smith [30] have noted that it is not possible to choose any set of arguments of the 6-j symbol for which  $J = 1, 2, \text{ or } 5$  and for which all triangle conditions are satisfied. This immediately follows from Eq. (115).

When studying the properties of 6-j symbols, in order to estimate the required computational effort required, it is useful to know the number of 6-j symbols that need to be calculated. The size of a fully symmetry reduced table of 6-j symbols for which  $2(a + b + c + d + e + f)$  is equal to some  $J$  is the number of nonnegative integer solutions of  $3d_1 + 6d_2 + 9d_3 + 12d_4 + 8d_5 + 4d_6 = J$ . Writing  $J = 72n + i$ , where  $0 \leq i \leq 71$ , we obtain

$$N_{R6}(72n + i) = \sum_{j=0}^5 d_{ij} \binom{n + 5 - j}{5}, \quad (116)$$

where the  $d_{ij}$  are listed in Table 3. This formula is derived in Appendix B.

#### 4. Results and discussion

As Lai and Chiu have noted, rewriting the formulas for 3-j symbols in terms of integer (binomial) sums enables accurate, often exact, floating point computation of these quantities. Although the sum in Racah's formula for the 6-j symbol is already integer, it is possible to rewrite this formula in terms of a binomial sum which is even smaller in magnitude. Below some limiting magnitude, depending on hardware considerations, integers can be represented exactly in floating point. If the summation terms and intermediates fall below this limit, then the sum will be exact and the 3-j or 6-j symbol accurate to machine precision since the prefactor in front of the sum introduces no rounding error. If the floating point limit is exceeded then some rounding may occur.

For both 3-j and 6-j symbols, there are several possible formulas involving binomial sums. One essential result of this work is that by choosing the smallest magnitude binomial sum, the accuracy of floating point calculations (or speed of calculations using large integer routines) can be maximized. This choice can be made systematic with the help of new Regge symmetry parameterizations for both the 3-j and 6-j symbols. Essentially, given a 3-j or 6-j symbol, the Regge matrix or R-symbol is transformed in a special manner to give a unique transformed 3-j or 6-j symbol. By using this strategy it is also possible to speedily detect special cases for which the formulas are particularly simple.

These advantages can be extended to recursion schemes. For any 3-j or 6-j recursion relation, there are many possible corresponding binomial sum results. The 3-j and 6-j Regge symmetry parameterizations enable the construction of recursion schemes with as many steps as direct summation. In addition, for the 3-j symbols, special formulas at or near  $m_i = 0$  (several of which appear not to be listed elsewhere in the literature) serve as initial points for recursion sequences which are often much shorter than direct summation. All of these schemes are carefully constructed so that the smallest magnitude intermediate binomial sums are chosen at each step.

One issue it is necessary to carefully explore is whether calculation of the binomial sum ever produces a floating point overflow (which would require passing the limits of about  $10^{38}$  and  $10^{307}$  in single and double precision, respectively). This would most likely occur while calculating the largest term in direct summation calculations. To answer this question, special routines for calculating just the binomial sum portions of the 3-j and 6-j symbols were constructed. For each  $J$ , 3-j or 6-j binomial sums for every possible set of Regge parameters  $\{c_i\}$  or  $\{d_i\}$  were tested. In single precision, no overflows occurred up to  $J = 137$  for 3-j symbols and  $J = 318$  for 6-j symbols. In double precision,  $J$ 's up to 300 for 3-j symbols and 600 for 6-j symbols were fully tested. No double precision overflows ever occurred.

Table 3  
Size of Regge symmetry reduced tables of 6-j symbols:  $d_{ij}$  for Eq. (116)

$i$	$d_{i0}$	$d_{i1}$	$d_{i2}$	$d_{i3}$	$d_{i4}$	$d_{i5}$	$i$	$d_{i0}$	$d_{i1}$	$d_{i2}$	$d_{i3}$	$d_{i4}$	$d_{i5}$
0	1	960	10781	15779	3534	49	36	89	4339	16365	9625	686	0
1	0	914	11015	15867	3277	31	37	72	4357	16701	9399	575	0
2	0	987	11225	15663	3195	34	38	83	4545	16719	9187	570	0
3	1	1086	11390	15464	3129	34	39	104	4744	16680	9016	560	0
4	1	1107	11589	15425	2958	24	40	105	4843	16845	8817	494	0
5	0	1129	11821	15327	2807	20	41	102	4967	16995	8589	451	0
6	2	1290	11965	14989	2829	29	42	139	5249	16791	8435	490	0
7	1	1251	12210	15038	2589	15	43	123	5284	17106	8196	395	0
8	2	1350	12375	14839	2523	15	44	144	5483	17067	8025	385	0
9	3	1460	12541	14607	2476	17	45	167	5701	16995	7855	386	0
10	2	1482	12773	14509	2325	13	46	164	5825	17145	7627	343	0
11	2	1521	12984	14398	2190	9	47	168	5960	17256	7416	304	0
12	7	1716	13049	14099	2220	13	48	224	6235	16995	7321	329	0
13	3	1675	13347	14067	2006	6	49	197	6311	17289	7045	262	0
14	4	1785	13513	13835	1959	8	50	220	6529	17217	6875	263	0
15	8	1920	13624	13624	1920	8	51	259	6740	17106	6740	259	0
16	8	1959	13835	13513	1785	4	52	263	6875	17217	6529	220	0
17	6	2006	14067	13347	1675	3	53	262	7045	17289	6311	197	0
18	13	2220	14099	13049	1716	7	54	329	7321	16995	6235	224	0
19	9	2190	14398	12984	1521	2	55	304	7416	17256	5960	168	0
20	13	2325	14509	12773	1482	2	56	343	7627	17145	5825	164	0
21	17	2476	14607	12541	1460	3	57	386	7855	16995	5701	167	0
22	15	2523	14839	12375	1350	2	58	385	8025	17067	5483	144	0
23	15	2589	15038	12210	1251	1	59	395	8196	17106	5284	123	0
24	29	2829	14989	11965	1290	2	60	490	8435	16791	5249	139	0
25	20	2807	15327	11821	1129	0	61	451	8589	16995	4967	102	0
26	24	2958	15425	11589	1107	1	62	494	8817	16845	4843	105	0
27	34	3129	15464	11390	1086	1	63	560	9016	16680	4744	104	0
28	34	3195	15663	11225	987	0	64	570	9187	16719	4545	83	0
29	31	3277	15867	11015	914	0	65	575	9399	16701	4357	72	0
30	49	3534	15779	10781	960	1	66	686	9625	16365	4339	89	0
31	40	3528	16104	10616	816	0	67	651	9796	16530	4068	59	0
32	50	3699	16143	10417	795	0	68	717	9995	16365	3969	58	0
33	61	3887	16161	10205	790	0	69	790	10205	16161	3887	61	0
34	58	3969	16365	9995	717	0	70	795	10417	16143	3699	50	0
35	59	4068	16530	9796	651	0	71	816	10616	16104	3528	40	0

All of the 3-j formulas presented here were tested on an IBM RS6000 workstation in IEEE single and double precision (about 7 and 15 significant figures, respectively) and compared to quadruple precision (about 31 significant figures) direct summation results. Every 3-j symbol with integer arguments up to  $J = 150$  (507251436 3-j symbols, with up to 51 terms in the binomial sum) was calculated by binomial direct summation, center recursion, and edge recursion in single and double precision. If a 3-j symbol was related by Regge symmetry to the  $m_i = 0$  case, then the closed form expression was used. For single precision, 3-j symbols up to  $J = 137$  were calculated. This large number of 3-j symbols was chosen in order to ensure that every 3-j formula was thoroughly tested. For each calculation method and precision and for each  $J$ , careful track was kept of the maximum absolute error.

Fig. 4 shows the results as log error plots. If for a given  $J$  the maximum error was zero (complete agreement with quadruple precision direct summation results), the point was omitted from the plot. Separate plots are shown for direct summation (Fig. 4a), center recursion (Fig. 4b), and edge recursion (Fig. 4c). In each case,

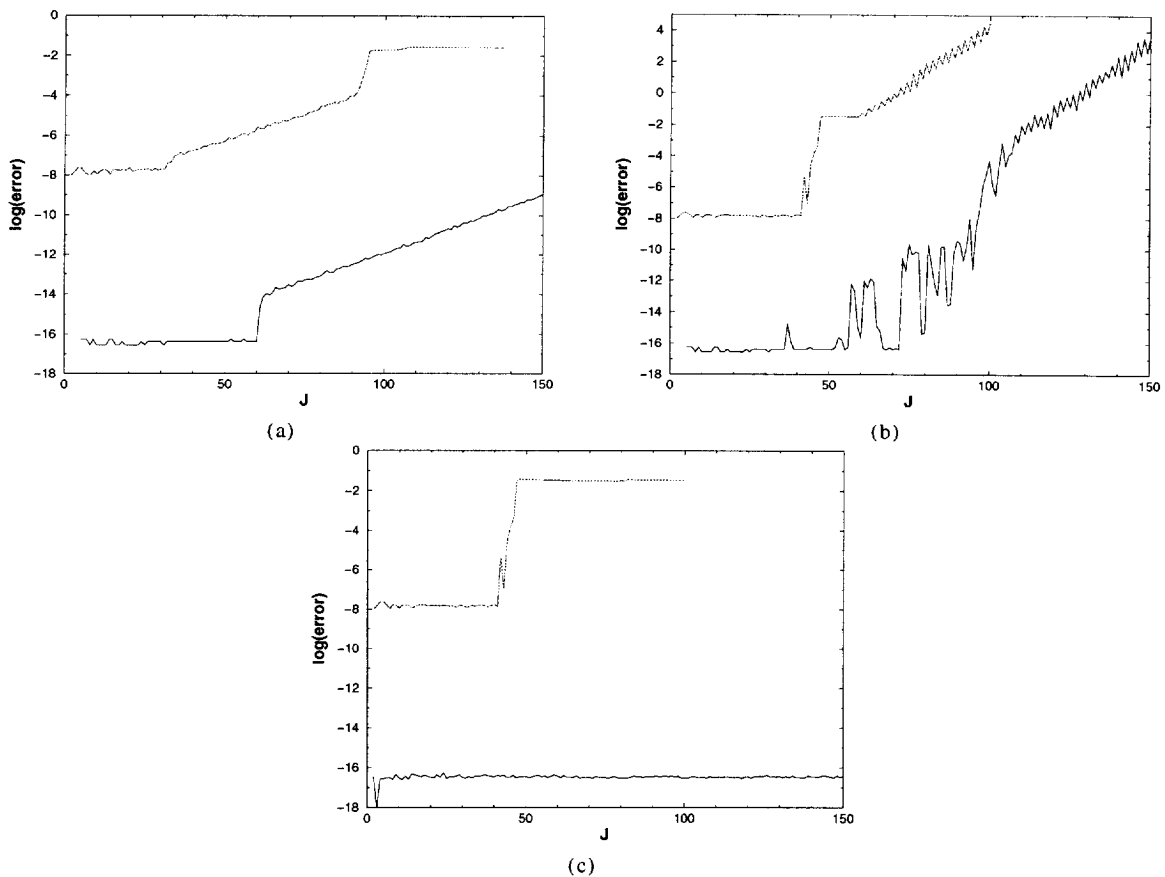


Fig. 4. Accuracy of single and double precision 3-j binomial formulas: (a) direct summation, (b) center recursion, and (c) edge recursion.

the plots show several regions: a low  $J$  region in which the error is essentially constant and is due to truncation (no cancellation occurs in the binomial sum), and intermediate or large  $J$  regions in which the maximum error rises at different rates.

For direct summation, the maximum error increases fairly smoothly after about  $J = 63$  for double precision. The single precision maximum error rises at a similar logarithmic rate but for smaller  $J$  until about  $J = 90$ , when it suddenly shoots up to about  $10^{-2}$  and remains essentially constant. It would be reasonable to expect similar behavior for the double precision results somewhere beyond  $J = 150$ .

For center recursion, the maximum error does not increase as smoothly. Above about  $J = 60$  and  $J = 105$  for single and double precision, respectively, the maximum error shows a zigzag behavior in which the maximum error for an odd  $J$  is lower than that for the adjacent even  $J$ 's. For edge recursion, the error shows sudden jumps rather than a smooth logarithmic rise. For single precision, this jump occurs at about  $J = 50$  (from about  $10^{-8}$  to about  $10^{-2}$ ). For double precision, no jumps occur up to  $J = 150$ . Presumably such a jump would occur at some higher  $J$ . The difference in the accuracy of the two recursion schemes may stem from the fact that the beginning steps of edge recursion have fairly small binomial sums. In fact, the boundary point binomial sum, Eq. (65), is a single binomial coefficient. Thus, errors would tend not to build until the later steps of the recursion sequence. For center recursion, however, the binomial sums start out large, and so errors can begin to propagate at the third or fourth step (the first two or three binomial sums are calculated exactly).

In addition to carefully tracking maximum absolute errors, 3-j symbols for which the error by either recursion

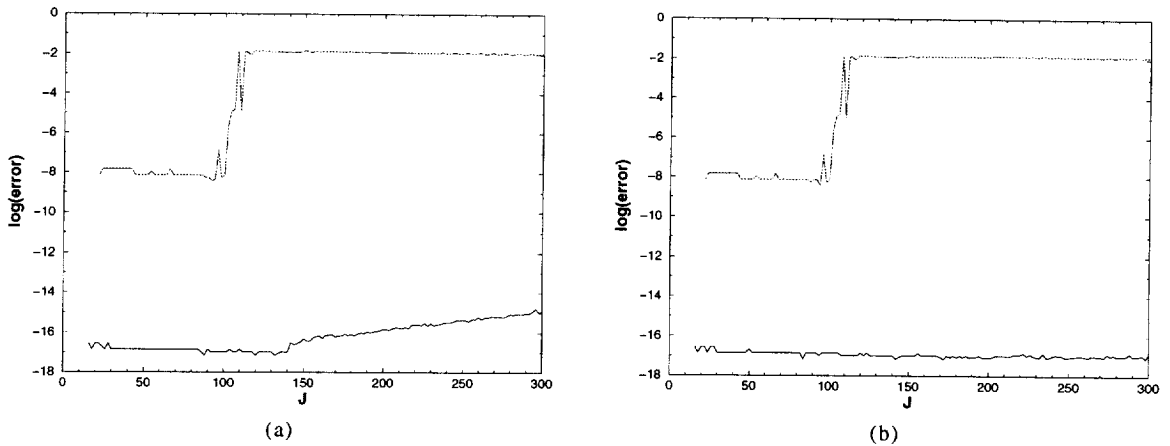


Fig. 5. Accuracy of single and double precision 6-j binomial formulas: (a) direct summation and (b) recursion.

scheme was above a cutoff of  $10^{-8}$  were tabulated. In many cases, including some with the worst errors, center recursion had fewer steps than direct summation. In other words, a 3-j subroutine which chose the faster of center recursion or direct summation would not necessarily be more accurate than a binomial center recursion 3-j subroutine.

One important consideration in scattering and other calculations in which many 3-j or 6-j symbols are calculated is the safe range of angular momentum arguments for each method for calculating binomial sums. For double precision results, the most commonly used working precision, the maximum error is below  $10^{-10}$  at or below  $J = 132, 74$ , and at least 150 for direct summation, center recursion, and edge recursion, respectively. These are conservative safety limits because only a small fraction of 3-j symbols for a given  $J$  have an absolute error above the cutoff.

To detect possible rounding error, the largest magnitude binomial sum term or intermediate can be tested against the floating point limit. If this limit is not exceeded, then no rounding occurs. If the limit is exceeded, then some rounding error may occur. For direct summation, the maximum possible roundoff error is dictated by the ratio of the sum to the largest term (unless the sum is zero). For either recursion scheme, rounding error may accumulate as the calculation proceeds. No rigorous error bound formulas are now known for either recursion scheme or have been found in this work.

Similar tests as above were performed for 6-j symbols. Every 6-j symbol with integer arguments up to  $J = 300$  (538,724,429 6-j symbols, with up to 26 terms in the binomial sum) was calculated by direct summation and by recursion in single and double precision. As with the 3-j symbols, these results were compared with quadruple precision direct summation. The results are shown in Fig. 5 for (a) direct summation and (b) recursion. For both single precision direct summation and single precision recursion, between  $J = 100$  and  $J = 110$ , the maximum error jumps from about  $10^{-8}$  to about  $10^{-1}$  and remains essentially constant thereafter. In double precision, the direct summation maximum error rises very slowly from about  $10^{-16}$  at  $J = 140$  to about  $10^{-14}$  at  $J = 300$ . The recursion maximum error remains essentially constant at around  $10^{-16}$  throughout.

All of the above discussion pertains to floating point subroutines, which are used when speed is the priority. When absolute accuracy is essential, the binomial sums can be calculated in large integer subroutines. In this case, for both 3-j and 6-j symbols, recursion has several advantages over direct summation. The chief advantage is the smaller intermediates and therefore greater speed: the largest term in the direct summation can be much larger than the intermediate recursion binomial sums. Another advantage is that recursion is much more well-suited for prime factorization techniques. At each recursion step, it is easy to keep track of the common prime factors among adjacent binomial sum terms and prime factorization makes it possible to reduce the size of large

integers that are to be manipulated and therefore speed up the calculation. Direct summation is less convenient because the partial sums can be much larger in magnitude than recursion intermediates and because their prime factorization properties are unknown. If, for example, the partial sums contained very large prime factors, then the advantages of prime factorization would be lost.

The methods described here have been optimized for the computation of individual 3-j and 6-j symbols. In calculations requiring many 3-j or 6-j symbols, depending on the problem, it may be possible to achieve further speedups. One fairly obvious strategy is to precalculate a table of binomial coefficients. This would eliminate, for example, a multiplication and several divisions in Eqs. (31) and (103) where individual summation terms are calculated from previous terms. However, this and other optimizations introduce the possibility of programming errors involving interactions with the calling program. When developing the calling program, it should be verified that test cases using optimized and unoptimized 3-j and 6-j routines give identical results.

Table 4 shows timing comparisons for the methods described here and several others in the literature (from the CPC library and modified as little as possible). All results are averages of 10 identical timing runs. In the 3-j timing runs, every 3-j symbol with integer arguments and with  $J = 90$  was calculated (2238751 3-j symbols, with up to 31 summation terms). In the DS/ER timing runs, for each 3-j symbol, the number of direct summation terms was compared to the number of steps required for edge recursion. Whichever method had the smaller number of steps was used to calculate the 3-j symbol. A similar comment applies to CR/ER (center recursion/edge recursion). In the 6-j timing runs, every possible 6-j symbol with integer arguments and  $J = 240$  was calculated (4348212 6-j symbols, with up to 21 summation terms). All of these runs were performed on an IBM RS/6000 Model 580 in double precision. Timing runs with and without precalculated tables of binomial coefficients are reported ( $t_{\text{bin}}$  and  $t_{\text{nobin}}$ , respectively).

In the 3-j calculations, precalculating binomial tables saves about 41% for direct summation and 8.3% for edge recursion. Direct summation would be expected to have a larger speedup factor because binomial coefficients are used in calculating every summation term, whereas in edge recursion binomial coefficients are used only in the first two recursion steps (similar considerations apply for the 6-j results). As implemented here, binomial coefficients are not used in edge recursion. However, far greater savings are obtained by choosing the shorter of center recursion and direct summation or edge recursion. Timing results are also shown for Schulten and Gordon's method. Although theirs is the fastest of all the methods shown, we emphasize that all the other timing runs are for the calculation of individual 3-j symbols from scratch. If, for example, the edge recursion scheme were adapted to the calculation of tables of 3-j symbols, the times would likely be comparable or slightly smaller than those of Schulten and Gordon.

Finally, we note that since the required sequences of angular momentum coefficients depend on the type of calculation, these timing results should be regarded as ballpark estimates of what can be expected in different applications. In particular, the savings resulting from optimizations such as precalculation of binomial tables may vary considerably.

## 5. Conclusions

In this paper, the previous work of Lai and Chiu on binomial sum 3-j and 6-j methods is improved in accuracy and extended to recursion schemes. This is made possible by observing that there are several possible binomial sum formulas for both the 3-j and 6-j symbols. By using new Regge symmetry parameterizations it is simple to choose the most optimal sum. In addition, it is possible to speedily detect special cases for which the formulas are particularly simple. For the 3-j symbols, a new type of recursion scheme, center recursion, is described which is often far faster than direct summation.

By combining the Regge symmetry parameterizations with generating function techniques, it is possible to determine the size of Regge symmetry reduced 3-j or 6-j tables. Similar methods can be used to determine the number of 3-j or 6-j symbols belonging to almost any conceivable class.

Table 4

CPU times for the calculation of sets of 3-j and 6-j symbols with integer arguments and with  $J = 90$  and  $J = 240$ , respectively; see text for further information

Method	$t_{\text{nobin}}, \text{s}^a$	$t_{\text{bin}}, \text{s}^b$	Remarks
<i>3-j symbols</i>			
DS	58.8	34.8	Direct summation
CR	69.0	–	Center recursion
ER	45.7	41.9	Edge recursion
DS/CR	8.81	8.78	Shorter of DS and CR
ER/CR	8.83	8.81	Shorter of ER and CR
VR	6.53	–	Venkatesh and Rao (Clebsch–Gordan coefficients)
SG	5.86	–	Schulten and Gordon
<i>6-j symbols</i>			
DS	98.8	56.4	Direct summation
Rec	295.6	282.8	Recursion
VR1	94.5	–	VR Set I formulas (Racah coefficients)
VR2	91.5	–	VR Set II formulas (Racah coefficients)

<sup>a</sup> Table of binomial coefficients not precalculated.

<sup>b</sup> Table of binomial coefficients precalculated.

When 3-j and 6-j formulas are rewritten in terms of binomial sums, the square roots must cancel and each binomial sum must have a rational coefficient. This can be used to check each step of the derivation.

In floating point calculations of 3-j and 6-j symbols, especially those with large angular momentum arguments, binomial recursion and direct summation schemes show distinctly different behavior. In direct summation, the minimum accuracy tends to rise smoothly with  $J$ . For all of the recursion schemes treated here, the minimum accuracy can exhibit sudden jumps. For  $J$ 's up to 150, edge recursion is the most accurate method for calculating 3-j symbols with integer arguments (the most commonly computed). For  $J$ 's up to 300, recursion is more accurate for 6-j symbols than direct summation, especially at the higher  $J$ 's.

For exact calculations using large integer routines, recursion is recommended. In addition to the obvious speed advantages for calculating tables, recursion is faster than direct summation for calculating individual 3-j and 6-j symbols because the recursion intermediates are smaller than the largest direct summation terms. In addition, in exact calculations using large integer routines, prime factorization techniques lend themselves far better to recursion than direct summation because the partial sums may not factorize conveniently.

Standard Fortran 77 subroutines for 3-j and 6-j symbols using floating point binomial sum direct summation or recursion are available from the authors.

Many of the issues for 3-j and 6-j symbols discussed here also apply to 9-j and higher 3n-j symbols. Work on 9-j symbols is in progress.

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**Appendix A. Derivation of 3-j binomial sum formulas**

Every 3-j binomial sum initial condition and recursion relation can be derived from the corresponding 3-j symbol formula by using Eqs. (16) and (22). Derivations for the starting points shall be presented first, then recursion formulas.

Most of the first starting points contain, as an intermediate, the 3-j symbol with  $m_i = 0$ , as shown in Eq. (7). From the definitions  $A = J/2 - j_1$ ,  $B = J/2 - j_2$ , and  $C = J/2 - j_3$  and such identities as  $j_1 = B + C$ , Eqs. (37) and (38) directly follow.

If  $J$  is even, then substituting  $m_i = 0$  into Eq. (34) yields

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ -1 & 0 & 1 \end{pmatrix} = \frac{j_1(j_1 + 1) - j_2(j_2 + 1) - j_3(j_3 + 1)}{2[j_1(j_1 + 1)j_3(j_3 + 1)]^{1/2}} \begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 0 & 0 \end{pmatrix}, \tag{A.1}$$

a result which appears in slightly modified form in Brink and Satchler. From this result, Eqs. (39) and (41) directly follow. If  $J$  is odd, then substituting  $m_i = 0$  into a slightly modified result from Edmonds,

$$\begin{aligned} & [(J + 2)(J - 2j_1 + 1)(J - 2j_2 + 1)(J - 2j_3 + 1)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 + 1 \\ m_1 & m_2 & m_3 \end{pmatrix} \\ & + [(j_2 - m_2)(j_2 + m_2 + 1)(j_3 + m_3)(j_3 + m_3 + 1)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 + 1 & m_3 - 1 \end{pmatrix} \\ & + 2m_2[(j_3 + m_3)(j_3 - m_3)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \\ & + [(j_2 + m_2)(j_2 - m_2 + 1)(j_3 - m_3)(j_3 - m_3 + 1)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 - 1 & m_3 + 1 \end{pmatrix} = 0, \end{aligned} \tag{A.2}$$

and invoking permutation and reflection symmetry yields

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ -1 & 0 & 1 \end{pmatrix} = -\frac{1}{2} \left[ \frac{(J + 2)(J - 2j_1 + 1)(J - 2j_2 + 1)(J - 2j_3)}{j_1(j_1 + 1)j_3(j_3 + 1)} \right]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 + 1 \\ 0 & 0 & 0 \end{pmatrix}, \tag{A.3}$$

and from there Eqs. (40) and (42).

As stated previously, the 3-j symbol is invariant under transposition of the Regge matrix,

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{pmatrix} j_1 & \frac{j_2 + j_3 + m_1}{2} & \frac{j_2 + j_3 - m_1}{2} \\ j_2 - j_3 & \frac{j_3 - m_3 - j_2 + m_2}{2} & \frac{j_3 + m_3 - j_2 - m_2}{2} \end{pmatrix}. \tag{A.4}$$

Performing this transformation on one of the fundamental recursion relations, Eq. (32), and some tedious manipulations yield

$$\begin{aligned} & [(j_3 + m_3 + 1)(j_2 + m_2)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \\ & + [(j_2 - m_2 + 1)(j_3 - m_3)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 - 1 & m_3 + 1 \end{pmatrix} \\ & + [(j_1 - j_2 + j_3 + 1)(j_1 + j_2 - j_3)]^{1/2} \begin{pmatrix} j_1 & j_2 - 1/2 & j_3 + 1/2 \\ m_1 & m_2 - 1/2 & m_3 + 1/2 \end{pmatrix} = 0. \end{aligned} \tag{A.5}$$

Substituting  $m_2 = -m_3 = 1/2$  into this result and invoking reflection symmetry yields

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 1/2 & -1/2 \end{pmatrix} = -\frac{1}{2} \left[ \frac{(j_1 - j_2 + j_3 + 1)(j_1 + j_2 - j_3)}{(j_2 + 1/2)(j_3 + 1/2)} \right]^{1/2} \begin{pmatrix} j_1 & j_2 - 1/2 & j_3 + 1/2 \\ 0 & 0 & 0 \end{pmatrix} \tag{A.6}$$

for even  $J$ , which appears in modified form in Brink and Satchler. Column permutations of this result and some simple algebra yield Eqs. (43), (46), and (50).

For odd  $J$ , substituting  $m_i = 0$  into a slightly modified result from Edmonds,

$$\begin{aligned} & [(J + 2)(J - 2j_1 + 1)]^{1/2} \begin{pmatrix} j_1 & j_2 + 1/2 & j_3 - 1/2 \\ m_1 & m_2 & m_3 \end{pmatrix} \\ & - [(j_2 + m_2 + 1/2)(j_3 - m_3 + 1/2)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 - 1/2 & m_3 + 1/2 \end{pmatrix} \\ & + [(j_2 - m_2 + 1/2)(j_3 + m_3 + 1/2)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 + 1/2 & m_3 - 1/2 \end{pmatrix} = 0, \end{aligned} \tag{A.7}$$

and invoking permutation and reflection symmetry yields

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ 1/2 & 0 & -1/2 \end{pmatrix} = \frac{1}{2} \left[ \frac{(j_1 + j_2 + j_3 + 2)(j_1 - j_2 + j_3 + 1)}{(j_1 + 1/2)(j_3 + 1/2)} \right]^{1/2} \begin{pmatrix} j_1 + 1/2 & j_2 & j_3 + 1/2 \\ 0 & 0 & 0 \end{pmatrix}, \tag{A.8}$$

which appears in modified form in Brink and Satchler. Column permutations and some simple algebra yield Eqs. (44), (47), and (51).

Substituting  $m_2 = -m_3 = 1/2$  into Eq. (34) and performing some column permutations and  $m$  sign changes (inversions) yields

$$\begin{aligned} & \begin{pmatrix} j_1 & j_2 & j_3 \\ 3/2 & 0 & -3/2 \end{pmatrix} = \begin{pmatrix} j_1 & j_2 & j_3 \\ 1/2 & 0 & -1/2 \end{pmatrix} \\ & \times \frac{(j_1 + 1/2)^2 + (j_3 + 1/2)^2 - j_2(j_2 + 1) - 1 + (-1)^J(j_1 + 1/2)(j_3 + 1/2)}{[(j_1 - 1/2)(j_1 + 3/2)(j_3 - 1/2)(j_3 + 1/2)]^{1/2}} \end{aligned} \tag{A.9}$$

for even or odd  $J$ . After permuting columns 1 and 2, Eq. (49) immediately follows.

Substituting  $m_1 = m_2 = 1/2$  into Eq. (32) and performing some simple manipulations yields

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ 1/2 & 1/2 & -1 \end{pmatrix} = \frac{(j_1 + 1/2) + (-1)^J(j_2 + 1/2)}{[j_3(j_3 + 1)]^{1/2}} \begin{pmatrix} j_1 & j_2 & j_3 \\ -1/2 & 1/2 & 0 \end{pmatrix} \tag{A.10}$$

for even or odd  $J$ . From this point it is simple to obtain Eq. (48).

The 3- $j$  symbol analogue of Eq. (52) is derived in two steps. First, by substituting  $m_2 = -m_3 = 1/2$  into one of the fundamental recursion relations, Eq. (32), we obtain

$$\begin{aligned} & [(j_3 - 1/2)(j_3 + 1/2)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ 1 & 1/2 & -3/2 \end{pmatrix} \\ & = -(j_2 + 1/2) \begin{pmatrix} j_1 & j_2 & j_3 \\ 1 & -1/2 & -1/2 \end{pmatrix} - [j_1(j_1 + 1)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 1/2 & -1/2 \end{pmatrix}. \end{aligned} \tag{A.11}$$

Permuting columns 1 and 3 of Eq. (A.9), invoking reflection symmetry, and substituting into Eq. (A.10) yields

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ 1 & 1/2 & -3/2 \end{pmatrix} = \begin{pmatrix} j_1 & j_2 & j_3 \\ 1 & 1/2 & -3/2 \end{pmatrix} \frac{(j_2 + 1/2)[(j_3 + 1/2)(-1)^J + (j_2 + 1/2)] - j_1(j_1 + 1)}{[j_1(j_1 + 1)(j_3 - 1/2)(j_3 + 3/2)]^{1/2}}, \tag{A.12}$$

which yields Eq. (52).

We now turn to recursion relations. Schulten and Gordon's result, Eq. (34), and column permutations yield Eqs. (53)–(56).

Shifting  $m_1, m_2,$  and  $m_3$  in Eq. (33) by  $-1, -1,$  and  $2$  and combining with Eq. (32) to eliminate the 3-j symbol with bottom arguments  $(m_1 - 1, m_2, m_3 + 1)$  yields

$$\begin{aligned} & [(j_2 - m_2 + 1)(j_2 + m_2)(j_3 + m_3 + 1)(j_3 - m_3)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \\ & + [(j_1 + m_1)(j_1 - m_1 + 1) - (j_2 + m_2)(j_2 - m_2 + 1)] \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 - 1 & m_3 + 1 \end{pmatrix} \\ & + [(j_1 + m_1)(j_1 - m_1 + 1)(j_3 - m_3 - 1)(j_3 + m_3 + 2)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 - 1 & m_2 - 1 & m_3 + 2 \end{pmatrix} = 0, \end{aligned} \tag{A.13}$$

and from there Eq. (57). From one of the fundamental recursion relations, Eq. (32), we obtain Eq. (58).

Shifting the  $m$ 's in Eq. (32) by  $0, 1,$  and  $-1$  and combining with Eq. (33) to eliminate the 3-j symbol with bottom arguments  $(m_1, m_2, m_3)$  yields

$$\begin{aligned} & [(j_2 + m_2 + 1)(j_2 - m_2) - (j_3 - m_3 + 1)(j_3 + m_3)] \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 + 1 & m_3 - 1 \end{pmatrix} \\ & + [(j_1 + m_1 - 1)(j_1 - m_1)(j_2 - m_2)(j_2 + m_2 + 1)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 + 1 & m_2 & m_3 - 1 \end{pmatrix} \\ & - [(j_1 + m_1)(j_1 - m_1 + 1)(j_3 + m_3)(j_3 - m_3 + 1)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 - 1 & m_2 + 1 & m_3 \end{pmatrix} = 0, \end{aligned} \tag{A.14}$$

from which Eq. (59) immediately follows. Shifting the  $m$ 's in Eq. (33) by  $1, 0,$  and  $-1$  and combining with Eq. (32) to eliminate the 3-j symbol with bottom arguments  $(m_1, m_2, m_3)$  yields

$$\begin{aligned} & [(j_1 - m_1 + 1)(j_1 + m_1) - (j_3 - m_3)(j_3 + m_3 + 1)] \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 - 1 & m_2 & m_3 + 1 \end{pmatrix} \\ & + [(j_1 - m_1 + 1)(j_1 + m_1)(j_2 + m_2)(j_2 - m_2 + 1)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 - 1 & m_3 + 1 \end{pmatrix} \\ & + [(j_1 - m_1 + 1)(j_1 + m_1)(j_2 - m_2)(j_2 + m_2 + 1)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 - 1 & m_2 + 1 & m_3 \end{pmatrix} = 0, \end{aligned} \tag{A.15}$$

and from there Eq. (60). Shifting the  $m$ 's in Eq. (33) by  $-1, -1,$  and  $2$  and combining with Eq. (32) to eliminate the 3-j symbol with bottom arguments  $(m_1, m_2 - 1, m_3 + 1)$  yields

$$\begin{aligned} & [(j_1 - m_1 + 1)(j_1 + m_1) - (j_2 - m_2 + 1)(j_2 + m_2)] \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 - 1 & m_2 & m_3 + 1 \end{pmatrix} \\ & + [(j_1 - m_1 + 1)(j_1 + m_1)(j_3 - m_3)(j_3 + m_3 + 1)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \\ & - [(j_2 + m_2)(j_2 - m_2 + 1)(j_3 - m_3 - 1)(j_3 + m_3 + 2)]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 - 1 & m_2 - 1 & m_3 + 2 \end{pmatrix} = 0, \end{aligned} \tag{A.16}$$

and from there Eq. (61).

Finally, we note, as stated previously, that the 3-j symbol may change sign under permutation of the first and third rows of the Regge matrix,

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^J \begin{pmatrix} \frac{j_2 + j_3 - m_1}{2} & \frac{j_1 + j_3 - m_2}{2} & \frac{j_1 + j_2 - m_3}{2} \\ \frac{j_2 + j_3 + m_1}{2} - j_1 & \frac{j_1 + j_3 + m_2}{2} - j_2 & \frac{j_1 + j_2 + m_3}{2} - j_3 \end{pmatrix}. \tag{A.17}$$

Applying this transformation to each 3-j symbol in Eq. (34), permuting columns 1 and 3, and performing some tedious manipulations yields

$$\begin{aligned}
 & [(j_2 - m_2)(j_1 - j_2 + j_3 + 1)(j_1 - m_1 + 1)(-j_1 + j_2 + j_3)]^{1/2} \begin{pmatrix} j_1 + 1/2 & j_2 - 1/2 & j_3 \\ m_1 - 1/2 & m_2 + 1/2 & m_3 \end{pmatrix} \\
 & + [-(j_1 + j_2 - j_3)(j_3 - m_3 + 1) + (j_2 + m_2)(j_1 - j_2 + j_3 + 1) \\
 & + (j_1 - m_1)(-j_1 + j_2 + j_3 + 1)] \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \\
 & + [(j_1 - j_2 + j_3)(j_2 - m_2 + 1)(j_1 - m_1)(-j_1 + j_2 + j_3 + 1)]^{1/2} \begin{pmatrix} j_1 - 1/2 & j_2 + 1/2 & j_3 \\ m_1 + 1/2 & m_2 - 1/2 & m_3 \end{pmatrix} = 0,
 \end{aligned}
 \tag{A.18}$$

which leads to the binomial sum recursion relation

$$\begin{aligned}
 & -(j_1 - j_2 + j_3 + 1)(j_1 - m_1 + 1)I_{C3}(j_1 + 1/2, j_2 - 1/2, j_3, m_1 - 1/2, m_2 + 1/2, m_3) \\
 & + [-(j_1 + j_2 - j_3)(j_3 - m_3 + 1) + (j_2 + m_2)(j_1 - j_2 + j_3 + 1) \\
 & + (j_1 - m_1)(-j_1 + j_2 + j_3 + 1)]I_{C3}(j_1, j_2, j_3, m_1, m_2, m_3) \\
 & - (j_2 - m_2 + 1)(-j_1 + j_2 + j_3 + 1)I_{C3}(j_1 - 1/2, j_2 + 1/2, j_3, m_1 + 1/2, m_2 - 1/2, m_3) = 0.
 \end{aligned}
 \tag{A.19}$$

Substituting  $j_1 = j'_1 + k/2, j_2 = j'_2 - k/2, j_3 = j'_3, m_1 = m'_1 - k/2, m_2 = m'_2 + k/2,$  and  $m_3 = m'_3$  into this result yields Eq. (64).

**Appendix B. Size of symmetry reduced tables of 3-j and 6-j symbols**

In order to derive Eq. (79), it is convenient to define  $c'_4$  according to  $c_4 = c_2 + c'_4$  and  $c_5$  according to  $c_5 = c_3 + c'_5$ . The number of sets of 3-j symbols unrelated by Regge symmetry for which  $c_2 < c_4$  is the number of nonnegative integer solutions of  $3c_1 + 4c_2 + c_3 + 2c'_4 + c_5 = J,$  which is the coefficient of  $x^J$  in the generating function [31,32]

$$P_1(x) = (1 + x^3 + x^6 + \dots)(1 + x^4 + x^8 + \dots)(x^2 + x^4 + x^6 + \dots)(1 + x + x^2 + \dots).
 \tag{B.1}$$

Similarly, the number of 3-j symbols unrelated by Regge symmetry for which  $c_2 = c_4$  and  $c_3 \leq c_5$  is the number of nonnegative integer solutions of  $3c_1 + 4c_2 + 2c_3 + c'_5 = J,$  which is the coefficient of  $x^J$  in the generating function

$$P_2(x) = (1 + x^3 + x^6 + \dots)(1 + x^4 + x^8 + \dots)(1 + x^2 + x^4 + \dots)(1 + x + x^2 + \dots).
 \tag{B.2}$$

Using

$$\frac{1}{1 - x} = 1 + x + x^2 + \dots
 \tag{B.3}$$

and some simple algebra, we obtain the total generating function

$$P(x) = P_1(x) + P_2(x) = \frac{(1 + x)(1 + x^3)^2(1 + x^6)(1 + x^2)^3(1 + x^4 + x^8)^4}{(1 - x^{12})^5}.
 \tag{B.4}$$

Finally, expanding the numerator with the help of the symbolic algebra package MAPLE [33] and using [31]

$$\frac{1}{(1-x)^s} = \sum_{k=0}^{\infty} \binom{s+k-1}{s-1} x^k, \tag{B.5}$$

we obtain

$$P(x) = Q(x) \sum_{k=0}^{\infty} \binom{k+4}{4} x^{12k}, \tag{B.6}$$

where

$$\begin{aligned} Q(x) = & 1 + x + 3x^2 + 5x^3 + 9x^4 + 13x^5 + 21x^6 + 29x^7 + 42x^8 + 56x^9 + 76x^{10} + 98x^{11} + 123x^{12} \\ & + 155x^{13} + 187x^{14} + 223x^{15} + 260x^{16} + 302x^{17} + 338x^{18} + 380x^{19} + 413x^{20} + 449x^{21} + 473x^{22} \\ & + 497x^{23} + 512x^{24} + 518x^{25} + 518x^{26} + 512x^{27} + 497x^{28} + 473x^{29} + 449x^{30} + 413x^{31} + 380x^{32} \\ & + 338x^{33} + 302x^{34} + 260x^{35} + 283x^{36} + 187x^{37} + 155x^{38} + 23x^{39} + 98x^{40} + 76x^{41} + 56x^{42} \\ & + 42x^{43} + 29x^{44} + 21x^{45} + 13x^{46} + 9x^{47} + 5x^{48} + 3x^{49} + x^{50} + x^{51}. \end{aligned} \tag{B.7}$$

The coefficient of  $x^r$  in the product of two polynomials  $g(x) = \sum_n c_n x^n$  and  $h(x) = \sum_n d_n x^n$  is  $\sum_{m+n=r} c_m d_n$ . Thus, in order to find the coefficient of  $x^J$  in  $P(x)$ , since the infinite sum in Eq. (B.6) has only powers of  $x^{12}$ , it is convenient to write  $J = 12n + i$ . Eq. (79) and Table 2 immediately follow.

The size of a fully Regge symmetry reduced table of 6-j symbols is found in a similar manner. However, in this case, the generating function is

$$\frac{1}{1-x^3} \frac{1}{1-x^6} \frac{1}{1-x^9} \frac{1}{1-x^{12}} \frac{1}{1-x^8} \frac{1}{1-x^4}, \tag{B.8}$$

which follows directly from Eq. (115). This can be rewritten as

$$P(x) = \frac{Q(x)}{(1-x^{72})^6}, \tag{B.9}$$

where

$$Q(x) = (1+x^3)(1+x^6)^2(1+x^9)(1+x^{18})(1+x^{36})^5(1+x^8+x^{16})(1+x^{12}+x^{24})^4(1+x^{24}+x^{48}). \tag{B.10}$$

Expanding  $Q(x)$  and using Eqs. (B.5), (B.9), and (B.10) yields Eq. (116) and Table 3.

### References

- [1] R.B. Bernstein, *Atom-Molecule Collision Theory* (Plenum, New York, 1976); many articles in this book describe the use of angular momentum coefficients.
- [2] J.M. Blatt, V.F. Weisskopf, *Theoretical Nuclear Physics* (Wiley, New York, 1952).
- [3] I.I. Sobel'man, *An Introduction to the Theory of Atomic Spectra* (Academic Press, New York, 1975).
- [4] R.N. Zare, *Angular Momentum* (Wiley, New York, 1988).
- [5] L.C. Biedenharn, J.C. Louck, *The Racah-Wigner Algebra in Quantum Theory* (Addison-Wesley, Reading, MA, 1981).
- [6] K.S. Rao, C.B. Chiu, *J. Phys. A.* 22 (1989) 3779.
- [7] R.E. Tuzun, Regge symmetry reduced tables of 3-j symbols: non-trivial zeros up to  $J = 300$ , ORNL Report TM/13195, to be submitted.

- [8] R.E. Tuzun, Regge symmetry reduced tables of 6-j symbols: non-trivial zeros up to  $J = 600$ , ORNL Report TM/13196, to be submitted.
- [9] K. Schulten, R.G. Gordon, *Comput. Phys. Commun.* 11 (1976) 269.
- [10] D.A. Varshalovich, A.N. Moskalev, V.K. Khersonskii, *Quantum Theory of Angular Momentum* (World Scientific, Singapore, 1988).
- [11] A.R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton Univ. Press, Princeton, 1957).
- [12] V. Rajeswari, K.S. Rao, *J. Phys. A* 22 (1989) 4113.
- [13] K.S. Rao, K. Venkatesh, *Comput. Phys. Commun.* 15 (1978) 227.
- [14] C.C.J. Roothaan, *Int. J. Quantum Chem. Symp.* 27 (1993) 13.
- [15] C.C.J. Roothaan, S.-T. Lai, *Int. J. Quantum Chem.* 63 (1997) 57.
- [16] K. Schulten, R.G. Gordon, *J. Chem. Phys.* 64 (1976) 2918.
- [17] S.D. Majumdar, *Prog. Theor. Phys.* 20 (1958) 798.
- [18] G. Racah, *Phys. Rev.* 62 (1942) 438.
- [19] K.S. Rao, *Comput. Phys. Commun.* 22 (1981) 297.
- [20] K. Schulten, R.G. Gordon, *J. Math. Phys.* 16 (1975) 1971.
- [21] E.U. Condon, G.H. Shortley, *The Theory of Atomic Spectra* (Cambridge Univ. Press, Cambridge, 1935).
- [22] S.-T. Lai, Y.-N. Chiu, *Comput. Phys. Commun.* 61 (1990) 350.
- [23] T. Shimpuku, *Prog. Theor. Phys. Suppl.* (1960) 1–136.
- [24] M.E. Rose, *Elementary Theory of Angular Momentum* (Wiley, New York, 1957).
- [25] D.M. Brink, G.R. Satchler, *Angular Momentum* (Clarendon Press, Oxford, 1968).
- [26] T. Regge, *Nuovo Cimento* 10 (1958) 544.
- [27] I.S. Gradshteyn, I.M. Ryzhik, *Table of Integrals, Series, and Products* (Academic Press, New York, 1980).
- [28] G. Baym, *Lectures on Quantum Mechanics* (Benjamin/Cummings, Reading, MA, 1969).
- [29] L.A. Shelepin, *JETP* 46 (1964) 1033.
- [30] A. Giovannini, D.A. Smith, On algebraic structures associated with the 3-j and 6-j symbols, in: *Spectroscopic and Group Theoretical Methods in Physics* (Wiley, New York, 1968).
- [31] R.A. Brualdi, *Introductory Combinatorics* (North-Holland, New York, 1992).
- [32] J. Riordan, *An Introduction to Combinatorial Analysis* (Wiley, New York, 1958).
- [33] B.W. Char, K.O. Geddes, G.H. Gonnet, B.L. Leong, M.B. Monagan, S.M. Watt, *MAPLE V Language Reference Manual* (Springer, New York, 1991).