# A NOTE ON RECURSIVE CALCULATIONS OF PARTICULAR 9*j* COEFFICIENTS

# J.-C. Pain

Commissariat à l'énergie atomique et aux énergies alternatives, DAM, DIF, F-91297 Arpajon, France E-mail: jean-christophe.pain@cea.fr

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The calculation of angular-momentum coupling transformation matrices can be very time consuming and alternative methods, even if they apply only in special cases, are helpful. We present a recursion relation for the calculation of particular 9jsymbols used in the quantum theory of angular momentum.

Keywords: angular momentum, 9j coefficient, recursion relation

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The coupling of N angular momenta is related to the definition of a 3(N-1)j symbol. The 9j symbols, characterizing the coupling of four angular momenta, are involved for instance in the computation of the matrix elements of the products of tensor operators, and in the transformation from LS to jj coupling [1, 2]. The triple sum series of Jucys and Bandzaitis [3] is the simplest known algebraic form for the 9j coefficient. Fourty years ago, Ališauskas and Jucys [4-8] derived an algebraic expression, in which 9j symbols are written as the threefold summation of multiplications and divisions of factorials. More recently, Wei [9, 10] proposed to express 9j symbols as a summation of the products of binomial coefficients and devised an algorithm to calculate the binomial coefficients recursively. Although some relationships between particular 9j symbols have been obtained in special cases [11], it is quite difficult to find recursion formulas for the 9j symbol itself, due to the fact that it contains nine arguments.

The general recursion relations for arbitrary 9j symbols were introduced in [12], [3] (with incorrect phase factors), and in [13] (in corrected form). However, as a rule in these relations, several angular momentum parameters are changing. It seems that relations with changing single momentum parameter are possible only if some other parameters of the 9j accept extreme or

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fixed small values. For instance, the following 9j symbol:

$$\begin{cases} \ell_1 \ \ell_2 \ L \\ j_1 \ j_2 \ L \\ \frac{1}{2 \sqrt{2} \sqrt{2}} 1 \end{cases}$$
 (1)

is often encountered in atomic physics and plays a major role in nuclear physics, especially for the study of  $\beta$ -decay [14, 15]. It can be evaluated in terms of 3j symbols [13]:

$$\begin{cases} \ell_1 \ \ell_2 \ L\\ j_1 \ j_2 \ L\\ 1/2 \ 1/2 \ 1 \end{cases} = \frac{1}{\sqrt{6(2L+1)(2j_1+1)(2j_2+1)}} \\ \times \frac{\left( \ell_1 \ \ell_2 \ L\\ 1/2 \ 1/2 \ -1 \right)}{\left( L \ j_1 \ j_2 \\ 0 \ 0 \ 0 \right)},$$
(2)

but the latter relation is verified only if  $j_1$ ,  $j_2$ , and L are integers so that  $j_1 + j_2 + L$  is even [13, 16]. More generally, algebraic expressions for 9j symbols

$$\begin{cases} \ell_1 \ \ell_2 \ L \\ j_1 \ j_2 \ L' \\ \frac{1}{2} \frac{1}{2} 1 2 \ 1 \end{cases}$$
(3)

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are tabulated as twelve entries of table 10.3 of Ref. [13], for

$$\left\{ \begin{array}{c} a + \lambda \, b + \mu \, c + \nu \\ a & b & c \\ \frac{1}{2} & \frac{1}{2} & 1 \end{array} \right\} \,. \tag{4}$$

Moreover, in Appendix 5 of Ref. [3], only two entries for

$$X(b,d,f) = \begin{cases} b+p\,d+q\,f+r\\ b & d & f\\ \beta & \delta & \phi \end{cases}$$
(5)

with  $\beta = \delta = \frac{1}{2}$ ,  $\phi = 1$ ,  $p = q = \frac{1}{2}$  and, respectively, r = 0 or r = 1 are included, when the remaining ten entries of table 10.3 of Ref. [13] with  $p = \pm 1/2, q = \pm 1/2, r = 0, \pm 1$  can be generated using some compositions of the "mirror reflection" substitutions  $b \to \overline{b} = -b - 1, d \to \overline{d} = -d - 1, f \to \overline{f} =$ -f - 1 (see Eqs. (II.5.2) to (II.5.8) in Appendix 5 of Ref. [3]).

Special 9j coefficients under consideration include three or four stretched triplets of angular momentum parameters [17]. In particular, eight entries of table 10.3 of Ref. [13] with  $L' = L \pm 1$  are expressed without sum by means of the following expression [3, 13]:

$$\begin{cases} a \ b & a + b \\ d \ e & f \\ g \ h \ a + b + f \end{cases} = \\ (-1)^{a+d-g} \frac{\Delta(a+b+f \ g \ h)}{\Delta(adg)\Delta(beh)\Delta(def)} \\ \times \left[ \frac{(2a)!(2b)!(2f)!}{(2a+2b+1)(2a+2b+2f+1)!} \right]^{1/2} \\ \times \frac{(a+b+g+h+f+1)!(g-a+d)!}{(g+h-a-b-f)!(a+g+d+1)!} \\ \times \frac{(e-b+h)!(d+e-f)!}{(b+e+h+1)!(d+e+f+1)!}, \tag{6}$$

where

$$\Delta(abc) = \left[\frac{(a+b-c)!(a-b+c)!(-a+b+c)!}{(a+b+c+1)!}\right]^{1/2},$$
(7)

together with different symmetry properties of 9j symbols. The following useful relation was mentioned by Jang [18]:

$$A_{j_1,j_2}(L) \left\{ \begin{array}{cc} \ell_1 & \ell_2 & L \\ j_1 & j_2 & L+1 \\ \frac{1}{2} & \frac{1}{2} & 1 \end{array} \right\} =$$

$$B_{\ell_1,\ell_2,j_1,j_2}(L) \begin{cases} \ell_1 \ \ell_2 \ L\\ j_1 \ j_2 \ L\\ 1/2 \ 1/2 \ 1 \end{cases} + C_{j_1,j_2}(L) \begin{cases} \ell_1 \ \ell_2 \ L\\ j_1 \ j_2 \ L - 1\\ 1/2 \ 1/2 \ 1 \end{cases} , \qquad (8)$$

with  $S = j_1 + j_2 + L$ , and where

$$A_{j_1,j_2}(L) = [L(2L+3)(S+2)(S-2j_1+1)]^{1/2}$$
$$\times [(S-2j_2+1)(S-2L)]^{1/2}, \qquad (9)$$

$$B_{\ell_1,\ell_2,j_1,j_2}(L) = (2L+1) \left[ \bar{j}_1 - \bar{j}_2 - \bar{L} + \frac{2\bar{L}(\bar{j}_2 + 3/4 - \bar{\ell}_2)}{\bar{\ell}_1 + \bar{j}_2 - \bar{j}_1 - \bar{\ell}_2} \right], \quad (10)$$

and

$$C_{j_1,j_2}(L) = \left[ (L+1)(2L-1)(S+1)(S-2j_1) \right]^{1/2} \times \left[ (S-2j_2)(S-2L+1) \right]^{1/2}.$$
 (11)

We follow the convention of Biedenharn et al. [19],  $\bar{x} = x(x+1)$ . Formula (8) is a particular case of the general recursion relations for 9j symbols [3, 12, 13]. Each 9j symbol depends on L via two of its arguments.

Defining for instance  $u_L = \begin{cases} \ell_1 \ \ell_2 \ L \\ j_1 \ j_2 \ L + 1 \\ 1/2 \ 1/2 \ 1 \end{cases}$ , we have  $u_{L-1} = \begin{cases} \ell_1 \ \ell_2 \ L - 1 \\ j_1 \ j_2 \ L \\ 1/2 \ 1/2 \ 1 \end{cases}$ , which does not appear in Eq. (8) except if (i - 1) = 1 (2 - 1)

Eq. (8), except if  $(j_1, j_2)$  and  $(\ell_1, \ell_2)$  are interchanged. However, one has

$$\begin{cases} \ell_1 \ \ell_2 \ L \\ j_1 \ j_2 \ L+1 \\ 1/2 \ 1/2 \ 1 \end{cases} = \\ \begin{bmatrix} \frac{2L+1}{L + (\ell_1 - j_1)(2\ell_1 + 1) + (\ell_2 - j_2)(2\ell_2 + 1)} - 1 \end{bmatrix} \\ \times \left[ \frac{L(2L-1)(S-2L)}{(L+1)(2L+3)(S-2L+1)} \right]^{1/2} \\ \times \left[ \frac{(S-2j_1 + 1)(S-2j_2 + 1)(S+2)}{(S-2j_1)(S-2j_2)(S+1)} \right]^{1/2} \times \end{cases}$$

$$\times \left\{ \begin{array}{l} \ell_1 \ \ell_2 \ L\\ j_1 \ j_2 \ L - 1\\ \frac{1}{2} \ \frac{1}{2} \ 1 \end{array} \right\} , \tag{12}$$

which can be combined to Eq. (8) to obtain a relation between the coefficients  $\begin{cases} \ell_1 & \ell_2 & L \\ j_1 & j_2 & L + 1 \\ 1/2 & 1/2 & 1 \end{cases}$  and  $\begin{cases} \ell_1 & \ell_2 & L \\ j_1 & j_2 & L \\ 1/2 & 1/2 & 1 \end{cases}$ .

Using the Regge symmetry of Wigner 3j symbols [20], for  $\ell_1 - j_1 = \ell_2 - j_2 = \pm 1/2$  (separately for both + and - signs) [3, 13], one finds, concerning the two other 9j symbols involved in Eq. (8), that in some particular cases, as for the 9j symbol of Eq. (1), explicit formulas in terms of 3j symbols do exist [16, 21]:

$$\begin{cases} \ell_1 \ \ell_2 \ L \\ j_1 \ j_2 \ L - 1 \\ \frac{1}{2^{1/2} \ 1^2} \end{cases} = \\ \frac{(j_1 - \ell_1)(2\ell_1 + 1) + (j_2 - \ell_2)(2\ell_2 + 1) - L}{\sqrt{6L(2L - 1)(2L + 1)(2j_1 + 1)(2j_2 + 1)}} \\ \times (-1)^{\ell_2 + j_2 + 1/2} \frac{\begin{pmatrix} \ell_1 \ \ell_2 \ L \\ \frac{1}{2^{-1/2} \ 0} \end{pmatrix}}{\begin{pmatrix} L - 1 \ j_1 \ j_2 \\ 0 \ 0 \ 0 \end{pmatrix}}$$
(13)

and

$$\begin{cases} \ell_1 \ \ell_2 \ L \\ j_1 \ j_2 \ L+1 \\ 1/2 \ 1/2 \ 1 \end{cases} = \\ \frac{(j_1 - \ell_1)(2\ell_1 + 1) + (j_2 - \ell_2)(2\ell_2 + 1) + L + 1}{\sqrt{6(L+1)(2L+1)(2L+3)(2j_1 + 1)(2j_2 + 1)}} \\ \times (-1)^{\ell_2 + j_2 + 1/2} \frac{\begin{pmatrix} \ell_1 \ \ell_2 \ L \\ 1/2 - 1/2 \ 0 \end{pmatrix}}{\begin{pmatrix} L + 1 \ j_1 \ j_2 \\ 0 \ 0 \ 0 \end{pmatrix}},$$
(14)

but in that case  $j_1 + j_2 + L$  must be odd. In this way, six entries from above mentioned twelve entries of table 10.3 of Ref. [13] are covered with three expressions. Although different approaches are needed for the remaining six entries of Table 10.3 of Ref. [13] with  $\ell_1 - j_1 = j_2 - \ell_2$ , which corresponds to the odd linear combinations of  $j_1 + j_2 + L'$ , all twelve tabulated expressions are ratios of the factorized elementary linear functions under the square root. Therefore, it is possible to write the binary recursion relations, for example, which allow to express

$$\begin{cases} \ell_1 \ \ell_2 \ L+1 \\ j_1 \ j_2 \ L'+1 \\ \frac{1}{2} \frac{1}{2} \frac{1}{2} \end{cases}$$
 (15)

in terms of

$$\begin{cases} \ell_1 \ \ell_2 \ L \\ j_1 \ j_2 \ L' \\ \frac{1}{2} \frac{1}{2} 1 2 \ 1 \end{cases}$$
 (16)

separately for  $L' - L = 0, \pm 1$ . In order to investigate recursion relations for these 9j symbols taken independently, let us start from the following identity [13, 15, 18]:

$$\begin{cases} \ell_1 \ \ell_2 \ L\\ j_1 \ j_2 \ L\\ 1/2 \ 1/2 \ 1 \end{cases} = \frac{\bar{\ell_1} + \bar{j_2} - \bar{j_1} - \bar{\ell_2}}{\sqrt{3\bar{L}}} \begin{cases} \ell_1 \ \ell_2 \ L\\ j_1 \ j_2 \ L\\ 1/2 \ 1/2 \ 0 \end{cases},$$
(17)

which, as mentioned in Ref. [18], was quoted incorrectly in Refs. [14, 22]. Using the expression of the 9j symbol in terms of a 6j symbol [22]:

$$\begin{cases} \ell_1 \ \ell_2 \ L\\ j_1 \ j_2 \ L\\ \frac{1}{2} \frac{1}{2} \frac{1}{2} 0 \end{cases} = \frac{(-1)^{j_1 + \ell_2 + L + \frac{1}{2}}}{\sqrt{2(2L+1)}} \begin{cases} \ell_1 \ \ell_2 \ L\\ j_2 \ j_1 \ \frac{1}{2} 2 \end{cases} ,$$
(18)

we obtain [13]:

.

$$\begin{cases} \ell_1 \ \ell_2 \ L\\ j_1 \ j_2 \ L\\ 1/2 \ 1/2 \ 1 \end{cases} = \frac{(-1)^{j_1 + \ell_2 + L + 1/2}}{\sqrt{6\bar{L}(2L+1)}} \\ \times \left(\bar{\ell}_1 + \bar{j}_2 - \bar{j}_1 - \bar{\ell}_2\right) \left\{ \ell_1 \ \ell_2 \ L\\ j_2 \ j_1 \ 1/2 \right\} .$$
(19)

Defining the reduced coefficient

$$Q_L = \sqrt{2L+1} \left\{ \begin{array}{c} \ell_1 & \ell_2 & L\\ j_1 & j_2 & L\\ 1/2 & 1/2 & 1 \end{array} \right\}$$
(20)

and using the recursion relation for 6j symbols described in Ref. [23], we find

$$D_{\ell_1,\ell_2,j_1,j_2}(L+1) Q_{L+1} - E_{\ell_1,\ell_2,j_1,j_2}(L) Q_L$$
$$+ D_{\ell_1,\ell_2,j_1,j_2}(L) Q_{L-1} = 0, \qquad (21)$$

where

$$\begin{split} D_{\ell_1,\ell_2,j_1,j_2}(L) &= \\ & \left\{ (L^2 - 1) \left[ L^2 - (\ell_1 - \ell_2)^2 \right] \left[ (\ell_1 + \ell_2 + 1)^2 - L^2 \right] \right\}^{1/2} \times \end{split}$$

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$$\times \left\{ \left[ L^2 - (j_2 - j_1)^2 \right] \left[ (j_2 + j_1 + 1)^2 - L^2 \right] \right\}^{1/2}$$
 (22)

and

$$E_{\ell_1,\ell_2,j_1,j_2}(L) =$$

$$(2L+1)\{\bar{L}[-\bar{L}+\ell_1(\ell_1+1)+\ell_2(\ell_2+1)]$$

$$+j_2(j_2+1)[\bar{L}+\ell_1(\ell_1+1)-\ell_2(\ell_2+1)]$$

$$+j_1(j_1+1)[\bar{L}-\ell_1(\ell_1+1)+\ell_2(\ell_2+1)]$$

$$-3\bar{L}/2\}.$$
(23)

It can be better, in the case of large arguments in the 9j symbols, to work with the ratio of consecutive elements [24]

$$R_L = \frac{Q_L}{Q_{L-1}}, \qquad (24)$$

which obeys the following recursion relation:

$$R_{L+1} = F_{\ell_1, \ell_2, j_1, j_2}(L) R_L + G_{\ell_1, \ell_2, j_1, j_2}(L), \quad (25)$$

with

$$F_{\ell_1,\ell_2,j_1,j_2}(L) = \frac{E_{\ell_1,\ell_2,j_1,j_2}(L)}{D_{\ell_1,\ell_2,j_1,j_2}(L+1)}$$
(26)

and

$$G_{\ell_1,\ell_2,j_1,j_2}(L) = -\frac{D_{\ell_1,\ell_2,j_1,j_2}(L)}{D_{\ell_1,\ell_2,j_1,j_2}(L+1)}.$$
 (27)

The 9j symbol of Eq. (13) can be formulated in terms of two 6j symbols [13]:

$$\begin{cases} \ell_1 \ \ell_2 \ L \\ j_1 \ j_2 \ L-1 \\ 1/2 \ 1/2 \ 1 \end{cases} (-1)^{j_1 + \ell_2 + L - 1/2} \sqrt{6L(4L^2 - 1)} = \\ \sqrt{(L^2 - (j_1 - j_2)^2)[(j_1 + j_2 + 1)^2 - L^2]} \begin{cases} \ell_1 \ \ell_2 \ L \\ j_2 \ j_1 \ 1/2 \end{cases} \\ + \sqrt{(L^2 - (\ell_1 - \ell_2)^2)[(\ell_1 + \ell_2 + 1)^2 - L^2]} \begin{cases} \ell_1 \ \ell_2 \ L - 1 \\ j_2 \ j_1 \ 1/2 \end{cases} \end{cases}.$$
(28)

Each of the two 6j symbols involved in the latter identity can be evaluated by recurrence, but we did not find any recursion relation for the 9j symbol itself.

We proposed a recursive calculation for special cases of 9j symbols, encountered, for instance, in the transformation matrices from LS to jj coupling schemes, or in the evaluation of matrix elements of tensor operators. We hope that the recursion relation will be useful for the enumeration and algebraic manipulation of 9j symbols.

### References

- Z.B. Rudzikas, *Theoretical Atomic Spectroscopy* (Cambridge University Press, Cambridge, 1997), http://dx.doi.org/10.2277/052144425X
- [2] B.R. Judd, *Operator Techniques in Atomic Spectroscopy* (McGraw-Hill, New York, 1963)
- [3] A.P. Jucys and A.A. Bandzaitis, *Teoriya Momenta Kolichestva Dvizheniya v Kvantovoi Mekhanike (Angular Momentum Theory in Quantum Mechanics)* [in Russian] (1st ed.: Mintis, Vilnius, 1965, 2nd ed.: Mokslas, Vilnius, 1977)
- [4] S.J. Ališauskas and A. Jucys, J. Math. Phys. 12, 594–605 (1971), http://dx.doi.org/10.1063/1.1665626
  Erratum: J. Math. Phys. 13, 575 (1972), http://dx.doi.org/10.1063/1.1666016
- [5] A.C.T. Wu, J. Math. Phys. 14, 1222–1223 (1973), http://dx.doi.org/10.1063/1.1666469
- [6] L.C. Biedenharn and J.D. Louck, *Angular Momentum in Quantum Physics* (Addison-Wesley, Reading, MA, 1981)
- [7] D. Zhao and R.N. Zare, Mol. Phys. 65, 1263–1268 (1988), http://dx.doi.org/10.1080/00268978800101761
- [8] K.S. Rao, V. Rajeshwari, and C.B. Chiu, Comput. Phys. Commun. 56, 231–248 (1989), http://dx.doi.org/10.1016/0010-4655(89)90021-0
- [9] L. Wei, Comput. Phys. 12, 632–634 (1998), http://dx.doi.org/10.1063/1.168745
- [10] L. Wei, Comput. Phys. Commun. **120**, 222–230 (1999), http://dx.doi.org/10.1016/S0010-4655(99)00232-5
- [11] G. Gaigalas, T. Žalandauskas, and Z. Rudzikas, Lith. J. Phys. 41, 226–231 (2001)
- [12] A.V. Karosienė, S.J. Ališauskas, and A.A. Bandzaitis, Lietuvos Fiz. Rinkinys 5, 13–21 (1965) [in Russian]
- [13] D.A. Varshalovich, A.N. Moskalev, and V.K. Khersonskii, *Quantum Theory of Angular Momentum* (World Scientific, Singapore, 1988)
- [14] A. de-Shalit and I. Talmi, *Nuclear Shell Theory* (Academic, New York, 1963)
- [15] L. Szybisz and V. Seshagiri Rao, Lett. Nuovo Cimento 14, 237–240 (1975)
- [16] D.M. Brink and G.R. Satchler, *Angular Momentum* (Clarendon Press, Oxford, 1968)
- [17] R.T. Sharp, Nucl. Phys. A 95, 222–228 (1967), http://dx.doi.org/10.1016/0375-9474(67)90163-7
- [18] S. Jang, J. Math. Phys. **9**, 397–402 (1968), http://dx.doi.org/10.1063/1.1664592
- [19] L.C. Biedenharn, J.M. Blatt, and M.E. Rose, Rev. Mod. Phys. 24, 249–257 (1952), http://dx.doi.org/10.1103/RevModPhys.24.249
- [20] T. Regge, Nuovo Cimento 10, 544–545 (1958), http://dx.doi.org/10.1007/BF02859841
- [21] M. Nomura, J. Phys. Soc. Jpn. 58, 2677–2686 (1989), http://dx.doi.org/10.1143/JPSJ.58.2677

- [22] M. Rotenberg, R. Bivins, N. Metropolis, and J.K. Wooten, *The 3-j and 6-j symbols* (The Technology Press, M. I. T., Cambridge, MA, 1959)
- [23] K. Schulten and R.G. Gordon, J. Math. Phys. 16, 1961– 1970 (1975),

http://dx.doi.org/10.1063/1.522426

 [24] J.H. Luscombe and M. Luban, Phys. Rev. E 57, 7274– 7277 (1998), http://dx.doi.org/10.1103/PhysRevE.57.7274

## DĖL KAI KURIŲ 9j KOEFICIENTŲ REKURENTINIO SKAIČIAVIMO

## J.-C. Pain

Atominės energijos ir alternatyviųjų energijų komisariatas, Arpajon, Prancūzija

### Santrauka

Judėjimo kiekio momentų perrišimo matricų skaičiavimas gali būti labai ilgas ir čia naudingi alternatyvūs metodai, netgi jei jie tinka tik ypatingais atvejais. Pateikiamas rekurentinis sąryšis skaičiuoti tam tikrus 9j koeficientus, naudojamus judėjimo kiekio momento kvantinėje teorijoje.