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Stretched 9-j coefficients and summation theorems

K Srinivasa Rao† and J Van der Jeugt‡

Department of Applied Mathematics and Computer Science, University of Gent, Krijgslaan 281-S9, B-9000 Gent, Belgium*

Abstract. It is well known that the 9-j coefficient has 72 symmetries and that its simplest known form is the triple-sum series which exhibits none of these symmetries. A study of the expressions for the stretched 9-j coefficients (stretched in the sense that that one or more of its six triangle inequality components are stretched) via the triple-sum series shows the existence of the ${}_2F_1(1)$, ${}_3F_2(1)$ and the ${}_4F_3(1)$ summation theorems and reveals some new summation theorems as well.

The 9-j coefficient, or the ls–jj transformation coefficient which plays a crucial role in the evaluation of two-body matrix elements, arising in atomic, molecular and nuclear physics studies, exhibits 72 symmetries through its representation as a sum over the projection quantum numbers of a product of six 3-j coefficients (see, for instance, Biedenharn and Louck 1981, Wigner 1940). The simplest known form for this recoupling coefficient is the triple-sum series of Jucys and Bandzaitis (1977) which, however, does not exhibit any of these 72 symmetries. It has been pointed out that as a consequence of this lack of symmetry, a given 9-j coefficient, for large angular momenta, which has one term, could have several tens of thousands of terms when the triple-sum representation for its symmetries is examined. This inherent disadvantage was converted into an advantage by the numerical computation of the 9-j coefficient (Srinivasa Rao *et al* 1989).

Almost three decades ago, Bandzaitis, Karosienne and Jucys (1964) derived formulae for the stretched 9-j coefficients, in which one or more of the angular momenta belonging to any of the six triads (a, b, c, say) correspond to the limits of the triangular inequality $|a-b| \leqslant c \leqslant a+b$. Sharp (1967) showed that there are, in all, five distinctly different doubly stretched cases and two triply stretched ones, while any singly stretched 9-j coefficient can be brought to one standard form through the symmetries of the coefficient.

The inherent lack of symmetry in the Jucys–Bandzaitis triple-sum series for the 9-j coefficient and the observation that a given 9-j coefficient may have one or more terms has led us to search for the stretched 9-j coefficient formulae and the triple-sum series for summation theorems. Here we show that the Vandermonde theorem (the terminating version of the famous Gauss theorem) for the ${}_2F_1(1)$, the ${}_3F_2(1)$ summation theorem of Pfaff–Saalschütz and the more recent Karlsson (1971)–Minton (1970) summation theorem for the ${}_4F_3(1)$, all occur naturally in our study. What is interesting is that, besides these well known theorems, the study opens up the scope for finding genuinely new summation theorems. After presenting the relevant details regarding the triple-sum series and stretched 9-j coefficients, we show their interconnection which reveals summation theorems.

† Permanent address: The Institute of Mathematical Sciences, Madras-600 113, India.

‡ Senior Research Associate of NFWO (National Fund for Scientific Research of Belgium).

* e-mail: rao@imsc.ernet.in and Joris.VanderJeugt@rug.ac.be

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The triple-sum series of Jucys–Bandzaitis (1977) is the simplest known form for the 9-j coefficient and it is given by

$$\begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix} = K \sum_{x,y,z} \frac{1}{x!y!z!} \frac{(x1-x)!(x2+x)!(x3+x)!}{(x4-x)!(x5-x)!} \frac{(y1+y)!(y2+y)!}{(y3+y)!(y4-y)!(y5-y)!}$$
$$\times \frac{(z1-z)!(z2+z)!}{(z3-z)!(z4-z)!(z5-z)!} \frac{(p1-y-z)!}{(p2+x+y)!(p3+x+z)!} \tag{1}$$

where

$$K = (-1)^{x5} \frac{(d,a,g)(b,e,h)(i,g,h)}{(d,e,f)(b,a,c)(i,c,f)}$$
$$\begin{aligned} &0 \leqslant x \leqslant \min(x4, x5) = XF \\ &0 \leqslant y \leqslant \min(y4, y5) = YF \\ &0 \leqslant z \leqslant \min(z4, z5) = ZF \end{aligned} \tag{2}$$

$$\begin{array}{lll} x1 = 2f & y1 = -b+e+h & z1 = 2a \\ x2 = d+e-f & y2 = g+h-i & z2 = -a+b+c \\ x3 = c-f+i & y3 = 2h+1 & z3 = a+d+g+1 \\ x4 = -d+e+f & y4 = b+e-h & z4 = a+d-g \\ x5 = c+f-i & y5 = g-h+i & z5 = a-b+c \\ p1 = a+d-h+i & p2 = -b+d-f+h & p3 = -a+b-f+i \end{array} \tag{3}$$

$$(a,b,c) = \left[\frac{(a-b+c)!(a+b-c)!(a+b+c+1)!}{(-a+b+c)!} \right]^{1/2}. \tag{4}$$

Note that the 18 parameters $x1, x2, \ldots, p3$ given in (3) are different for different symmetries of the 9-j coefficient since they are dependent on the positions of $a, b, \ldots, i$ in the 3×3 array. They are also not independent since there are nine relations between them, e.g. $x2 + x4 = y1 + y4$, $x3 + x5 = z2 + z5$, etc.

The lack of symmetry is best illustrated through the example

$$\begin{Bmatrix} 30 & 20 & 10 \\ 30 & 10 & 20 \\ 60 & 30 & 30 \end{Bmatrix} = 0.000\,268\,45 \tag{5}$$

which has $XF = 0$, $YF = 0$ and $ZF = 0$, so that it is a single term. But its symmetry (a cyclic column permutation and an odd row permutation of the 9-j treated as a 3×3 array)

$$\begin{Bmatrix} 20 & 10 & 30 \\ 30 & 30 & 60 \\ 10 & 20 & 30 \end{Bmatrix} = 0.000\,268\,45 \tag{6}$$

has $XF = 60$, $YF = 20$, $ZF = 40$ and an actual number of 33 761 terms. This number is determined by taking into account the constraints on the ranges of x, y, z, placed by $p1, p2, p3$, i.e.

$$y + z \leqslant p1 \qquad \text{and if } p2, p3 < 0 \text{ then} \qquad x + y \geqslant |p2|, x + z \geqslant |p3|. \tag{7}$$

If we were to use the expression due to Wigner (1940) for the 9-j coefficient, where it is written as a single sum over a product of three 6-j coefficients (the 6-j coefficient itself being given by the single-sum expression due to Racah (1942)), then the 9-j coefficient in (5) would require 40 terms or 120 references to the 6-j coefficients, while that in (6) would require one term or three references to the 6-j coefficient. From this, it can be argued that the triple-sum series (1) requires less time for its computation than the conventional single sum over a product of 6-j coefficients, especially for large angular momenta.

Sharp (1967) has classified the doubly stretched 9-j coefficients into five distinct types: (I)–(V). These are:

$$\text{(I)}\quad \begin{Bmatrix} a & b & c \\ d & e & f \\ a+d & b+e & i \end{Bmatrix} \text{ corresponding to } y4=0 \text{ and } z4=0 \tag{8}$$

$$\text{(II)}\quad \begin{Bmatrix} a & b & c \\ d & d+f & f \\ a+d & h & i \end{Bmatrix} \text{ corresponding to } e=d+f \text{ and } z4=0 \tag{9}$$

$$\text{(III)}\quad \begin{Bmatrix} a & b & c \\ d & e & f \\ a+d & a+d+i & i \end{Bmatrix} \text{ corresponding to } y5=0 \text{ and } z4=0 \tag{10}$$

$$\text{(IV)}\quad \begin{Bmatrix} a & b & c \\ d & b+h & f \\ a+d & h & i \end{Bmatrix} \text{ corresponding to } e=b+h \text{ and } z4=0 \tag{11}$$

$$\text{(V)}\quad \begin{Bmatrix} a & b & c \\ d & e & f \\ a+d=h+i & h & i \end{Bmatrix} \text{ corresponding to } g=h+i=a+d \tag{12}$$

(where, in (V), $g=a+d \Leftrightarrow z4=0$).

Any doubly stretched 9-j coefficient can be classified into one of these types using the well known symmetries (column, row permutations and transposition about the leading diagonal) of this coefficient. Explicit formulae for these five types have been derived by Sharp (1967) from the expression for the singly stretched 9-j coefficient

$$\begin{Bmatrix} a & b & c \\ d & e & f \\ a+d & h & i \end{Bmatrix} \text{ corresponding to } z4=0 \text{ (or } g=a+d). \tag{13}$$

The formulae from Sharp (1967) are single-sum series, except for type (III) which is a single term. From the fact that $z4=0$ for all five types and, in addition, $y4=0$ for type (I) and $y5=0$ for type (III), it follows that the triple-sum series reduces to a double-sum series for types (II), (IV) and (V) and to a single-sum series for (I) and (III). However, this is not the complete picture! In this paper, we analyse the type (III) doubly stretched 9-j coefficient through its triple-sum series representation and the consequences of some of the symmetries on it.

Case (i). When we set $y5=0$ and $z4=0$ in the triple-sum series we get, for the type (III) doubly stretched 9-j coefficient, the expression

$$\begin{Bmatrix} a & b & c \\ d & e & f \\ a+d & a+d+i & i \end{Bmatrix} = (-1)^{x5}\frac{(d,a,a+d)(b,e,a+d+i)}{(d,e,f)(b,a,c)}\frac{(i,a+d,a+d+i)}{(i,c,f)}$$
$$\times\frac{y1!y2!}{y3!y4!}\frac{z1!z2!}{z3!z5!}\sum_x\frac{(-1)^x}{x!}\frac{(x1-x)!(x2+x)!(x3+x)!}{(x4-x)!(x5-x)!(p2+x)!(p3+x)!}. \tag{14}$$

Interestingly, the triple-sum series for a symmetry of these 9-j coefficients (see below) appears to be a double sum since it has $z5 = 0$ and hence $z = 0$. However, if the additional constraints on the summation indices (7) are taken into account, then, since $x \leqslant x5(= c - f + i)$ and $y \leqslant y5(= d - e + f)$, $x + y \geqslant -p2(= c + d - e + i)$, the apparent double sum reduces to a single term and we have the result

$$\begin{Bmatrix} a+d & a+d+i & i \\ a & b & c \\ d & e & f \end{Bmatrix} = (-1)^{d-e+f} \frac{(a+d+i, b, e)}{(a, b, c)(d, e, f)(i, c, f)} \times \left[\frac{(2a)!(2d)!(2i)!}{(2a+2d+1)(2a+2d+2i+1)!} \right]^{1/2}. \tag{15}$$

This result has been derived by Sharp (1967) from the formula for the singly stretched 9-j coefficient in terms of a double sum given by Sharp and von Baeyer (1966).

When the single-sum series part of (14) is rearranged into a generalized hypergeometric function, we have

$$S_x = \frac{x1!x2!x3!}{x4!x5!p2!p3!} {}_4F_3 \begin{pmatrix} 1+x2, 1+x3, -x4, -x5; 1 \\ -x1, 1+p2, 1+p3 \end{pmatrix} \tag{16}$$

where the ${}_4F_3(1)$ is not a Saalschützian and therefore cannot be a Racah or 6-j coefficient (Srinivasa Rao and Rajeswari 1993). However, it is a zero-balanced ${}_{p+1}F_p(1)$, i.e. its numerator- and denominator-parameter sums are equal: $x1 + x2 + x3 = p2 + p3 + x4 + x5$.

A comparison of these results for the two symmetries of the doubly stretched 9-j coefficient (14) and (15) gives, after simplification, for the summation part, the result

$$S_x = (-1)^{x1-x4-x5} \tag{17}$$

which when expressed in terms of the ${}_4F_3(1)$ yields

$${}_4F_3 \begin{pmatrix} 1+x2, 1+x3, -x4, -x5; 1 \\ -x1, 1+p2, 1+p3 \end{pmatrix} = (-1)^{x1-x4-x5} \frac{\Gamma(1+x4, 1+x5, 1+p2, 1+p3)}{\Gamma(1+x1, 1+x2, 1+x3)}. \tag{18}$$

where we have used the notation

$$\Gamma(a, b, \ldots) = \Gamma(a)\Gamma(b) \ldots .$$

If we now make the identifications

$$\begin{aligned} -x1 &= b1 & -x4 &= b1 + m1 & (m1 &= x1 - x4) \\ 1 + p2 &= b2 & 1 + x2 &= b2 + m2 & (m2 &= x2 - p2) \\ 1 + p3 &= b3 & 1 + x3 &= b3 + m3 & (m3 &= x3 - p3) \end{aligned} \tag{19}$$

and rewrite our result, we have

$${}_4F_3 \begin{pmatrix} -(m1+m2+m3), b1+m1, b2+m2, b3+m3; 1 \\ b1, b2, b3 \end{pmatrix} = (-1)^{m1+m2+m3} \frac{(m1+m2+m3)!}{(b1)_{m1}(b2)_{m2}(b3)_{m3}} \tag{20}$$

where $(b)_m = \Gamma(b+m)/\Gamma(b)$ is the Pochhammer symbol. This is the Karlsson–Minton summation theorem for terminating zero-balanced ${}_{p+1}F_p(1)$ series corresponding to $p = 3$ (cf (1.9.3) of Gasper and Rahman (1991)).

Case (ii). For another symmetry of the 9-j coefficient considered in case (i), the triple-sum series yields the result

$$\begin{Bmatrix} c & b & a \\ f & e & d \\ i & a+d+i & a+d \end{Bmatrix} = \frac{(f,c,i)(b,e,a+d+i)(a+d,i,a+d+i)}{(f,e,d)(b,c,a)(a+d,a,d)} \times \frac{(x1)!(x2)!(x3)!}{(x4)!}\frac{(y1)!(y2)!}{(y3)!(y4)!}\frac{(z1)!}{(z3)!(z5)!(p2)!}{}_2F_1\left(\begin{matrix}-z3,-z4;1\\-z1\end{matrix}\right) \tag{21}$$

where

$$\begin{aligned} &x1 = 2d && y1 = a-b+d+e+i && z1 = 2c \\ &x2 = -d+e+f && y2 = 2i && z2 = a+b-c \\ &x3 = 2a && y3 = 2(a+d+i)+1 && z3 = c+f+i+1 \\ &x4 = d+e-f && y4 = -a+b-d+e-i && z4 = c+f-i \\ &x5 = 0 && y5 = 0 && z5 = a-b+c \\ &p1 = c+f-i && p2 = a-b+f+i && p3 = a+b-c. \end{aligned} \tag{22}$$

Comparison with the column-permutated result in (15) yields immediately, after simplification, using the symmetry property of the 9-j coefficient, the result

$$\begin{aligned} {}_2F_1\left(\begin{matrix}-z3,-z5;1\\-z1\end{matrix}\right) &= (-1)^{-a+b-c}\frac{(-a+b+c)!(a-b+f+i)!}{(-c+f-i)!(2c)!} \\ &= \frac{(-z1+z3)_{z5}}{(-z1)_{z5}} \end{aligned} \tag{23}$$

which is clearly a manifestation of the Vandermonde summation theorem

$${}_2F_1\left(\begin{matrix}a,-n;1\\c\end{matrix}\right) = \frac{(c-a)_n}{(c)_n}. \tag{24}$$

Case (iii). We consider another symmetry of the 9-j coefficient for which the triple-sum series again reduces to a single-sum series

$$\begin{aligned} \begin{Bmatrix} b & c & a \\ a+d+i & i & a+d \\ e & f & d \end{Bmatrix} &= (-1)^{x5+z5}\frac{(a+d+i,b,e)}{(a+d+i,i,a+d)}\frac{(c,i,f)(d,e,f)}{(c,b,a)(d,a,a+d)} \\ &\times \frac{x1!x2!x3!}{x4!x5!}\frac{(z1-z5)!(z2+z5)!}{z5!(z3-z5)!(z4-z5)!(p3+z5)!} \\ &\times \sum_y \frac{(-1)^y}{y!}\frac{(y2+y)!(p1-z5-y)!}{(y3+y)!(y4-y)!(y5-y)!}. \end{aligned} \tag{25}$$

Comparison with a symmetry (cyclic-column permutation with an odd-row permutation) of (15), yields, on simplification, the result

$$\begin{aligned} &{}_3F_2\left(\begin{matrix}1+y2,-y4,-y5;1\\1+y3,-p1+z5\end{matrix}\right) \\ &\quad = \frac{\Gamma(y3-y2+y5,1+y3+y4+y5,1+y3,-y2+y3+y4)}{\Gamma(y3-y2,1+y3+y4,1+y3+y5,-y2+y3+y4+y5)} \end{aligned} \tag{26}$$

using the Saalschütz property satisfied by the parameters of the ${}_3F_2(1)$, i.e. $1+y2-y4-y5 = y3+z5-p1$. This formula (26) can be shown to be the Pfaff–Saalschütz summation theorem (cf Gasper and Rahman 1991):

$$ {}_3F_2\left(\begin{matrix} a, b, -n; 1 \\ c, 1+a+b-c-n \end{matrix}\right) = \frac{(c-a)_n(c-b)_n}{(c)_n(c-a-b)_n}. \tag{27} $$

Case (iv) . Next, we consider a symmetry of the type (III) 9-j coefficient for which the triple-sum series reduces to a double-sum series

$$ \begin{Bmatrix} f & i & c \\ e & a+d+i & b \\ d & a+d & a \end{Bmatrix} = \frac{(e,d,f)(i,a+d+i,a+d)(a,d,a+d)}{(e,a+d+i,b)(i,f,c)(a,c,b)} \\ \times \frac{y1!y2!}{y3!y4!y5!} \sum_{x,z} \frac{(-1)^{x+z}}{x!z!} \frac{(x1-x)!(x2+x)!(x3+x)!}{(x4-x)!(x5-x)!} \\ \times \frac{(z1-z)!(z2+z)!}{(z3-z)!(z5-z)!(p3+z)!(p2+x+z)!}. \tag{28} $$

Comparison of this result with a symmetry (an odd-column permutation, a cyclic-row permutation and a reflection about the diagonal) of the single-term expression (15), after simplification, yields the result for the double sum

$$ \sum_{x,z} \frac{(-1)^{x+z}}{x!z!} \frac{(x1-x)!(x2+x)!(x3+x)!}{(x4-x)!(x5-x)!(p2+z)!} \frac{(z1-z)!(z2+z)!}{(z3-z)!(z5-z)!(p3+x+z)!} \\ = \frac{(-1)^{z2+z5}(x1+x2+1)!x2!(z1+z2-z5)!}{(x2+x4+1)!(x2-p3+1)!(x2-p3-z1)!} \tag{29} $$

where

$$ \begin{aligned} x1 &= 2b & z1 &= 2f \\ x2 &= a-b+d+e+i & z2 &= c-f+i \\ x3 &= a-b+c & z3 &= d+e+f+1 \\ x4 &= a+b+d-e+i & z5 &= c+f-i \\ x5 &= -a+b+c & p3 &= a-b-f+i \\ p2 &= a-b+d+e-i. \end{aligned} \tag{30} $$

This sum depends on seven independent variables, e.g. $x1, x2, x4, z1, z2, z5$ and $p3$; the remaining variables are then given by $x3 = z5+p3$, $x5 = z2-p3$, $z5 = x2-p3+1$ and $p2 = x2-z1-z2+z5$. Furthermore, there are inequality conditions governed by the requirement that the factorials should be non-negative. The factor $(p3+x+z)!$ in this sum makes it a genuine double-sum series. Numerically, the validity of this summation theorem has been checked with MACSYMA (1985). In addition, the summation in x (or z separately) cannot be performed with the help of other summation theorems (like the Minton or Karlson–Minton summation theorems for the ${}_4F_3(1)$). If we consider the symmetry of the 9-j coefficient

$$ \begin{Bmatrix} b & c & a \\ d & e & f \\ a+d+i & i & a+d \end{Bmatrix} $$

for which the triple-sum series also reduces to a double sum, it can be summed using first the Minton theorem for a ${}_4F_3(1)$—though a numerator parameter contains the other summation index, the characteristic of the Minton theorem is the presence of a numerator and a denominator parameter which differ by 1—and the resulting series can be summed using the ${}_2F_1(1)$ summation theorem of Vandermonde.

Case (v). Here we consider a symmetry of the 9-j coefficient which does not reduce the triple-sum series

$$\begin{Bmatrix} d & e & f \\ a+d & a+d+i & i \\ a & b & c \end{Bmatrix} = (-1)^{x5} \frac{(a+d,d,a)(e,a+d+i,b)(c,a,b)}{(a+d,a+d+i,i)(e,d,f)(c,f,i)}$$
$$\times \sum_{x,y,z} \frac{(-1)^{x+y+z}}{x!y!z!} \frac{(x2+x)!(x3+x)!}{(x5-x)!} \frac{(y1+y)!(y2+y)!}{(y3+y)!(y4-y)!(y5-y)!}$$
$$\times \frac{(z2+z)!}{(z3-z)!(z5-z)!} \frac{(p1-y-z)!}{(p2+x+y)!(p3+x+z)!}. \tag{31}$$

On comparing this with an appropriate symmetry of the 9-j coefficient in (15), we get

$$\sum_{x,y,z} \frac{(-1)^{x+y+z}}{x!y!z!} \frac{(x2+x)!(x3+x)!}{(x5-x)!} \frac{(y1+y)!(y2+y)!}{(y3+y)!(y4-y)!(y5-y)!}$$
$$\times \frac{(z2+z)!}{(z3-z)!(z5-z)!} \frac{(p1-y-z)!}{(p2+x+y)!(p3+x+z)!}$$
$$= (-1)^{x5+z5} \frac{x3!y1!z2!}{x5!y5!z5!} \frac{1}{z3(y3+y5)!(-y1+y3-1)!} \tag{32}$$

where we choose $x3, x5, y1, y4, z5$ and $p2$ to be the independent variables and the dependent variables are then related to these through

$$\begin{aligned} x2 &= y4+p2 & y2 &= x5-z5+p2 \\ y5 &= x3+y1-y3-z5+1 & z2 &= x3+x5-z5 \\ z3 &= y4+p2+1 & p1 &= -x5+y4+z5 \\ p3 &= x3-z5. \end{aligned}$$

The numerical validity of this summation theorem has also been verified with the help of the computer program MACSYMA. This triple sum cannot be summed with the help of the Minton theorem.

Finally, we have shown that the comparison of a stretched 9-j coefficient formula with the Jucys–Bandzaitis triple-sum series, in conjunction with the symmetries of the 9-j coefficient, reveals the Vandermonde, Pfaff–Saalschütz and Karlsson–Minton summation theorems, respectively, for the ${}_2F_1(1)$, ${}_3F_2(1)$ and ${}_4F_3(1)$ series, as well as *new* summation theorems for double- and triple-sum series. This is a direct consequence of the highly asymmetric nature of the triple-sum series. A complete classification of the summation theorems from a study of all the 72 symmetries of the 9-j coefficient on the triple-sum series and their relation to the other stretched formulae will be reported elsewhere.

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