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On recurrence relations for the 3-j coefficient

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A four-term recurrence relation for the 3-j coefficient is derived from a four-term recurrence relation for the ${}_3F_2(1)$ hypergeometric function, which is intimately connected to the 3-j (or Clebsch-Gordan) coefficient. This new recurrence relation can also be derived from two known three-term recurrence relations for the ${}_3F_2(1)$. Application of the four-term recurrence relation to generate tables of the 3-j coefficients is discussed.

Keywords: Generalized hypergeometric series, Angular momentum coupling coefficient, Clebsch-Gordan coefficient, Recurrence relation.

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1 Introduction

The Gauss hypergeometric function of unit argument, ${}_2F_1(1)$, satisfies a three-term recurrence relation (c.f. Bailey, 1935; Slater, 1964). It is well-known that by suitably combining two three-term recurrence relations in a single variable, it is possible to derive a four-term recurrence relation for the given function. It is known that the ${}_3F_2(1)$ satisfies a four-term recurrence relation and it forms the basis for our new recurrence relation for the angular momentum coupling coefficient.

The intimate connection between the Clebsch-Gordan, or 3-j coefficient, and the generalized hypergeometric function of unit argument, ${}_3F_2(1)$, was established, independently, by Vander Waerden (1932), Wigner (1931), Racah (1942) and Majumdar (1958), using

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diverse methods (cf. Biedenharn and Louck, 1981); and also by Srinivasa Rao et.al. (1992).

The discovery of six new symmetries for the 3-j coefficient, by Regge (1959), along with its twelve 'classical' symmetries, resulted in a set of 72 symmetries for the 3-j coefficient. The group theoretical aspects of these symmetries was studied, in terms of a set of six ${}_3F_2(1)$s, by Srinivasa Rao et.al. (1978).

It is well-known, in literature, that every orthogonal polynomial satisfies a three-term recurrence relation. The $3-j$ coefficient has been shown by Karlin and McGregor (1961) to be related to the Hahn and the dual Hahn polynomials. This connection was exploited to establish two new three-term recurrence relations for the 3-j coefficient by Rajeswari and Srinivasa Rao (1989). These relations are different from the ones found earlier by Louck (1958).

The relationship between the Clebsch-Gordan, or the 3-j angular momentum coupling coefficient, and the set of six ${}_3F_2(1)$ hypergeometric functions (c.f. Srinivasa Rao and Rajeswari, 1993), of the Van der Waerden form, is:

$$\begin{aligned}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} &= \delta(m_1+m_2+m_3,0)\prod_{i,k=1}^{3}[R_{ik}!/(J+1)!]^{1/2} \\ &\quad \times(-1)^{\sigma(pqr)}\,[\Gamma(1-A,1-B,1-C,D,E)]^{-1} \\ &\quad \times {}_3F_2(A,B,C;D,E;1), \qquad (1.1)\end{aligned}$$

where

$$A=-R_{2p},\quad B=-R_{3q},\quad C=-R_{1r},\quad D=1+R_{3r}-R_{2p},\quad E=1+R_{2r}-R_{3q}$$

and

$$\Gamma(x,y,\cdots)=\Gamma(x)\Gamma(y)\cdots,$$

for all permutations of $(pqr)=(123)$, and

$$\sigma(pqr)=\begin{cases} R_{3p}-R_{2q} & \text{for even permutaions ,} \\ R_{3p}-R_{2q}+J & \text{for odd permutations,}\end{cases}$$

with $J=j_1+j_2+j_3$. The defining relations for the numerator and denominator parameters, R_{ik}'s, are the elements of the Regge (1959) 3×3 square symbol:

$$\|R_{ik}\| \;=\; \left\| \begin{array}{ccc} -j_1+j_2+j_3 & j_1-j_2+j_3 & j_1+j_2-j_3 \\ j_1-m_1 & j_2-m_2 & j_3-m_3 \\ j_1+m_1 & j_2+m_2 & j_3+m_3 \end{array} \right\|. \qquad (1.2)$$

In 1958, Regge made a discovery of six new symmetry properties for the 3-j coefficient. He arranged the nine non-negative integer parameters, listed by Racah (1942):

$$-j_1+j_2+j_3,\ j_1-j_2+j_3,\ j_1+j_2-j_3,$$

$$j_1-m_1,\ j_2-m_2,\ j_3-m_3,\ j_1+m_1,\ j_2+m_2,\ j_3+m_3,$$

into a 3×3 square symbol and identified the 3-j coefficient with that symbol:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \left\| \begin{array}{ccc} -j_1+j_2+j_3 & j_1-j_2+j_3 & j_1+j_2-j_3 \\ j_1-m_1 & j_2-m_2 & j_3-m_3 \\ j_1+m_1 & j_2+m_2 & j_3+m_3 \end{array} \right\| \equiv \|R_{ik}\|.$$

Note that all the sums of the columns and the rows of the symbol add to $J=j_1+j_2+j_3$, as in the case of a *magic* square. Regge asserted that the 3-j coefficient being invariant to 3! column permutations, 3! row permutations and to a reflection about the diagonal of the 3×3 square symbol, gives rise to 72 symmetries. Of these, the symmetries due to 3! column permutations and the interchange of rows 2 and 3 in (2), are called as 'classical' symmetries. In fact, in a short communication, Regge (1958) wrote down explicitly only these six new symmetries, dramatically discovered by him.

It is possible, to invert the relation (1.1), to express the ${}_3F_2(1)$ in terms of the 3-j coefficient (see Appendix for the details). After inversion, we get:

$$\begin{aligned} {}_3F_2(A,B,C;D,E;1) &= (-1)^{D-E}\frac{\Gamma(1-A,1-B,1-C,s-1)^{1/2}}{\Gamma(D-A,D-B,D-C,E-A,E-B,E-C)^{1/2}} \\ &\quad \times\Gamma(D,E)\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}, \end{aligned} \tag{1.3}$$

where

$$j_1=\frac{1}{2}(E-A-C-1),\quad j_2=\frac{1}{2}(D-B-C-1),\quad j_3=\frac{1}{2}(D+E-A-B-2),$$

$$m_1=\frac{1}{2}(E+A-C-1),\quad m_2=\frac{1}{2}(C-B-D+1),\quad m_3=\frac{1}{2}(D+B-E-A)$$

and $s=D+E-A-B-C$ is called the parameter excess.

2 Main Results

The Pochhammer symbol is defined as:

$$(x)_n=\frac{\Gamma(x+n)}{\Gamma(x)}=x(x+1)(x+2)\cdots(x+n-1),\quad (x)_0=1$$

and one of its properties is:

$$x(x+1)_n = (x+n)(x)_n.$$

Using this property, for the n-th term, one obtains the following four-term recurrence relation:

$$\begin{aligned}(2\,C-A-B)\ {}_3F_2(A,B,C;D,E)\ +\ A\ {}_3F_2(A+1,B,C;D,E)\\ +\,B\ {}_3F_2(A,B+1,C;D,E)\quad=\quad 2\,C\ {}_3F_2(A,B,C+1;D,E),\end{aligned}\qquad(2.1)$$

where, following standard conventions, the unit argument of the ${}_3F_2(1)$ has been suppressed.

The intimate relationship that exists between the ${}_3F_2(1)$ and the 3-j coefficient, given by (1.3), enables one to obtain the following four-term recurrence relation satisfied by the 3-j coefficient, as a direct consequence of the four-term recurrence relation for the ${}_3F_2(1)$ given in (2.1):

$$\begin{aligned}(2j_3-j_1-j_2-m_1+m_2)\sqrt{(J+1)}\begin{pmatrix} j_1 & j_2 & j_3\\ m_1 & m_2 & m_3\end{pmatrix}\\ =\ [(j_1-m_1)(j_3+m_3)(j_1-j_2+j_3)]^{\frac{1}{2}}\begin{pmatrix} j_1-\frac{1}{2} & j_2 & j_3-\frac{1}{2}\\ m_1+\frac{1}{2} & m_2 & m_3-\frac{1}{2}\end{pmatrix}\\ +[(j_2+m_2)(j_3-m_3)(-j_1+j_2+j_3)]^{\frac{1}{2}}\begin{pmatrix} j_1 & j_2-\frac{1}{2} & j_3-\frac{1}{2}\\ m_1 & m_2-\frac{1}{2} & m_3+\frac{1}{2}\end{pmatrix}\\ -2\,[(j_1+m_1)(j_2-m_2)(j_1+j_2-j_3)]^{\frac{1}{2}}\begin{pmatrix} j_1-\frac{1}{2} & j_2-\frac{1}{2} & j_3\\ m_1-\frac{1}{2} & m_2+\frac{1}{2} & m_3\end{pmatrix}.\end{aligned}\qquad(2.2)$$

A numerical verification of the four-term recurrence relation, for

$$j_1=2, j_2=2, j_3=1, m_1=1, m_2=-1, m_3=0,$$

using the tables of Rotenberg et.al. (1959), gave for the lhs and the rhs of (2.2) the value of $4/\sqrt{5}$.

The first entry, in page 47 of [7], is for the 3-j coefficient:

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0\\ \frac{1}{2} & -\frac{1}{2} & 0\end{pmatrix} = \underline{1} = \frac{1}{\sqrt{2}},$$

where the notation $\underline{1}$ for the number is that of Rotenberg et.al. [7] – who used the convention of underscoring negative exponents. The tables are for the squares of the

3-j coefficients (or, symbols), whose values are expressed in terms of products of prime factors (see p.33, [7]) and the value is preceded by an asterisk (*) for negative radicals.

When these j_i, m_i values are used in (2.2), we get the relation:

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} = \frac{1}{\sqrt{2}}, \qquad \text{since} \qquad \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = 1.$$

Repeated use of (2.2) guarantees the generation of the entire table of values. This is the best application possible of the four-term recurrence relation, (2.2), derived in this paper.

To be specific, from the numerical point of view, choose

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{pmatrix} 2 & 2 & 1 \\ 1 & -1 & 0 \end{pmatrix}.$$

Using these values of j_i and m_i for the 3-j coefficient in (2.2), we get, after simplifications:

$$-4\sqrt{6}\begin{pmatrix} 2 & 2 & 1 \\ 1 & -1 & 0 \end{pmatrix} = \begin{pmatrix} \frac{3}{2} & 2 & \frac{1}{2} \\ \frac{3}{2} & -1 & -\frac{1}{2} \end{pmatrix} + \begin{pmatrix} 2 & \frac{3}{2} & \frac{1}{2} \\ 1 & -\frac{3}{2} & \frac{1}{2} \end{pmatrix} - 6\sqrt{3}\begin{pmatrix} \frac{3}{2} & \frac{3}{2} & 1 \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}.$$

When we use for the LHS 3-j coefficient, in the four-term recurrence relation, (2.2), the three 3-j coefficients on the RHS of this equation, and simplify, we finally get:

$$\frac{4\sqrt{2}}{\sqrt{5}}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} = \frac{4\sqrt{2}}{\sqrt{5}} \times \frac{1}{\sqrt{2}} = \frac{4}{\sqrt{5}}.$$

Thus, there is a cascading effect produced by the four-term recurrence relation, so that ultimately the last step in the sequence will be the first entry of Rotenberg's Table.

It is note-worthy that (2.1) valid for unit argument is also valid for a ${}_3F_2(z)$, with arbitrary z as argument.

Further, (2.1) is a consequence of the following two known contiguous relations:

$$A * F(A+1) - C * F(C+1) = (A - C) * F, \tag{2.3}$$

$$B * F(B+1) - C * F(C+1) = (B - C) * F, \tag{2.4}$$

where we have used the obvious notation (see, for instance, Bailey, 1935; Slater, 1964) $F = {}_3F_2(A, B, C; D, E; z)$, denoting only the parameter that changes.

It is straight forward to derive, from the above three-term contiguous recurrence relations, the following two 3-term recurrence relations for the 3-j coefficient:

$$\begin{aligned}
&(j_2 - j_3 + m_1)\sqrt{(J+1)} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \\
&= -[(j_1 - m_1)(j_3 + m_3)(j_1 - j_2 + j_3)]^{\frac{1}{2}} \begin{pmatrix} j_1 - \frac{1}{2} & j_2 & j_3 - \frac{1}{2} \\ m_1 + \frac{1}{2} & m_2 & m_3 - \frac{1}{2} \end{pmatrix} \\
&+ [(j_1 + m_1)(j_2 - m_2)(j_1 + j_2 - j_3)]^{\frac{1}{2}} \begin{pmatrix} j_1 - \frac{1}{2} & j_2 - \frac{1}{2} & j_3 \\ m_1 - \frac{1}{2} & m_2 + \frac{1}{2} & m_3 \end{pmatrix},
\end{aligned} \tag{2.5}$$

$$\begin{aligned}
&(j_1 - j_3 - m_2)\sqrt{(J+1)} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \\
&= -[(j_2 + m_2)(j_3 - m_3)(-j_1 + j_2 + j_3)]^{\frac{1}{2}} \begin{pmatrix} j_1 & j_2 - \frac{1}{2} & j_3 - \frac{1}{2} \\ m_1 & m_2 - \frac{1}{2} & m_3 + \frac{1}{2} \end{pmatrix} \\
&+ [(j_1 + m_1)(j_2 - m_2)(j_1 + j_2 - j_3)]^{\frac{1}{2}} \begin{pmatrix} j_1 - \frac{1}{2} & j_2 - \frac{1}{2} & j_3 \\ m_1 - \frac{1}{2} & m_2 + \frac{1}{2} & m_3 \end{pmatrix}.
\end{aligned} \tag{2.6}$$

It is to be noted that these three-term recurrence relations are not given in literature [3, 7]. A combination of these two recurrence relations would imply (2.2). It relates a $3 - j$ coefficient with $J(= j_1 + j_2 + j_3)$ to a 3-j coefficient with $J - 1$. Needless to say, in principle, the relation can be used to generate all 3-j coefficients from those of a lower J.

3 Conclusion

To conclude, a four-term relation has been derived for the 3-j coefficient, from the corresponding relation for the ${}_3F_2(1)$ function. This is indeed a direct consequence of the definition of the 3-j coefficient in terms of the ${}_3F_2(1)$. Such relations for angular momentum coupling coefficients, from a theoretical point of view, are of relevance in the numerical computation of matrix elements of tensor operators, via the Wigner-Eckart theorem, in atomic, molecular and nuclear (structure / reaction) studies.

4 Appendix

In this appendix, we give the details on how to invert (1.1) to get (1.3). The values of the parameters $A, B, \cdots$ in (1.1) are

$$\begin{aligned}
&A = -R_{2p}, \qquad B = -R_{3q}, \qquad C = -R_{1r}, \\
&D = 1 + R_{3r} - R_{2p}, \qquad E = 1 + R_{2r} - R_{3q},
\end{aligned} \tag{4.1}$$

with $(pqr) = (123)$, cyclic. For $p = 1, q = 2, r = 3$, the above parameters become:

$$\begin{array}{lllll} \text{A} & = & -R_{21} & = & -j_1 + m_1, \\ \text{B} & = & -R_{32} & = & -j_2 - m_2, \\ \text{C} & = & -R_{13} & = & -j_1 - j_2 + j_3, \\ \text{D} & = & 1 + R_{33} - R_{21} & = & 1 - j_1 + j_3 - m_2, \\ \text{E} & = & 1 + R_{23} - R_{32} & = & 1 - j_2 + j_3 + m_1. \end{array} \qquad (4.2)$$

and these equations can be conveniently cast into the matrix form as:

$$\begin{pmatrix} \text{A} \\ \text{B} \\ \text{C+1} \\ \text{D} \\ \text{E} \end{pmatrix} = M \begin{pmatrix} j_1 \\ j_2 \\ j_3 + 1 \\ m_1 \\ m_2 \end{pmatrix} \qquad (4.3)$$

where M is the 5×5 matrix:

$$M = \begin{pmatrix} -1 & 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 & -1 \\ -1 & -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 & -1 \\ 0 & -1 & 1 & 1 & 0 \end{pmatrix}. \qquad (4.4)$$

The values of j_1, j_2, j_3, m_1 and m_2 are obtained by inverting (4.3), to get:

$$\begin{pmatrix} j_1 \\ j_2 \\ j_3 + 1 \\ m_1 \\ m_2 \end{pmatrix} = M^{-1} \begin{pmatrix} \text{A} \\ \text{B} \\ \text{C+1} \\ \text{D} \\ \text{E} \end{pmatrix}. \qquad (4.5)$$

with

$$M^{-1} = \frac{1}{2} \begin{pmatrix} -1 & 0 & -1 & 0 & 1 \\ 0 & -1 & -1 & 1 & 0 \\ -1 & -1 & 0 & 1 & 1 \\ 1 & 0 & -1 & 0 & 1 \\ 0 & -1 & 1 & -1 & 0 \end{pmatrix} \qquad (4.6)$$

Using M^{-1}, to write down, Eq. (4.5) explicitly, we get:

$$\begin{aligned} j_1 &= \tfrac{1}{2}(-A - C + E - 1) \\ j_2 &= \tfrac{1}{2}(-B - C + D - 1) \\ j_3 &= \tfrac{1}{2}(-A - B + D + E - 2) \\ m_1 &= \tfrac{1}{2}(A - C + E - 1) \\ m_2 &= \tfrac{1}{2}(-B + C - D + 1) \\ m_3 &= -m_1 - m_2 = \tfrac{1}{2}(-A + B + D - E). \end{aligned} \tag{4.7}$$

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