# TOPICS IN
# QUANTUM THEORY OF ANGULAR MOMENTUM

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CERTIFICATE

This is to ceritify that the Ph.D. thesis submitted by Miss.V.Rajeswari, to the University of Madras, entitled: TOPICS IN QUANTUM THEORY OF ANGULAR MOMENTUM, is a record of bonafide research work done by her, during 1983 - 1988, under my Supervision. The research work presented in this thesis has not formed the basis for the award to the candidate of any Degree, Diploma, Associateship, Fellowship or other similar title. It is further certified that the thesis represents independent work on the part of the candidate, and collaboration was necessitated by the nature and scope of the problems dealt with.

K. Srinivasa Rao

(K. SRINIVASA RAO)

Supervisor.

Contents

PREFACE

This thesis consists of the research work undertook by the author, on *Topics in Quantum Theory of Angular Momentum* under the guidance of Dr.K.Srinivasa Rao of the Institute of Mathematical Sciences, Madras during the period 1983-1988 with financial assistance from the Institute of Mathematical Sciences (Junior Research Fellowship) and the Council of Scientific and Industrial Research, Government of India (Senior Research Fellowship). Collaboration with my thesis Supervisor and others was necessitated by the nature and range of the problems dealt with and it is acknowledged explicitly at the appropriate places. Eight research papers were published in journals, three papers have been submitted for publication and one is under preparation. These are listed below:

1. *On the polynomial zeros of the Clebsch-Gordan and Racah Coefficients* - ( with K.Srinivasa Rao ) J. Phys. A: Math. Gen. **17** (1984) L243.
2. *Classification of the polynomial zeros of the 3-j and the 6-j coefficients* - ( with K.Srinivasa Rao ) Rev. Mex. de Fis. **31** (1985) 575.
3. *Saalschutzians and the Racah Coefficients* - ( with K.Srinivasa Rao ) Int. J. Theor. Phys. **24** (1985) 983.
4. *An algorithm to generate the polynomial zeros of degree one of the Racah Coefficients* - ( with K.Srinivasa Rao ) J.Phys.A : Math. Gen. **20** (1986) 507.
5. *Solutions of Diophantine equations and degree-one polynomial zeros of Racah Coefficients* - ( with K.Srinivasa Rao and

R.C.King) J. Phys. A: Math. Gen. **21** (1988) 1959.

6. *Polynomial zeros of the 9-j coefficient* -(with K.Srinivasa Rao) J. Phys. A: Math. Gen. **21** (1988) 4255.
7. *A note on the triple sum series for the 9-j coefficient* ( with K.Srinivasa Rao ) J. Math. Phys.(*to appear*).
8. Response in Am. Math. Soc. Notices - ( with K.Srinivasa Rao) **31** (1984) 165.
9. *A new FORTRAN program for the 9-j Angular Momentum Coefficient* - ( with K.Srinivasa Rao and Charles B.Chiu ) Comp. Phys. Commn. (Submitted).
10. *Multiplicative Diophantine Equations* - ( with K.Srinivasa Rao and T.S.Santhanam ) Jour. of Number Theory (submitted).
11. *The interrelationship between the four sets of* $_3F_2(1)$*s for the 3-j coefficient* - (with K.Srinivasa Rao ) Phys. Lett. A (submitted).
12. *Hahn Polynomials and recurrence relation for the 3-j coefficients (under preparation)*.

This research work is presented in seven chapters, the first of which provides the mathematical background required. There are four Appendices, at the end, which give some of the Fortran programs used to generate the results presented. The list of references is given after the Appendices. Finally, a list of mathematical symbols used is provided for ready reference.

V. Rajeswari
(V.RAJESWARI)

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## Introduction

Quantum theory of angular momentum provides an invaluable tool for the study of all quantum mechanical phenomena which occur in the fields of atomic, molecular and nuclear physics. Technically one could consider the two epoch making papers of Regge in 1958, '59 (Regge (1958), (1959)) to provide a dividing line between what could be called the *classical* work in this field and the more recent developments. Among the noteworthy contributors to the *classical* work are Wigner, Racah, Rose, Yang, Clebsch, Gordan, Fano, Howell, Biedenharn and others. The article by Smorodinskii and Shelepin (1972) entitled *Clebsch - Gordan coefficients viewed from different sides* refers to the new developments which have Regge's discovery of the new symmetries (Regge (1958), (1959)) as the starting point. These new developments pertain to generalisation of angular momentum coefficients to arbitrary complex arguments: to higher groups such as SO(4), SO(5); SU(3), SU(6), SU(1,1), $G_2$, $F_4$ etc. They are intertwined with aspects of: algebra, geometry (multidimensional and projective), topology, function theory (analytic, special), differential equations, combinatorial analysis, calculus of finite differences and number theory. In the words of Smorodinskii and Shelepin (1972), the theory of angular momentum as of today "takes a new form of calculas going beyond the scope of the *classical* theory". Most of these developments have been discussed extensively in the two volumes entitled *Angular Momentum in*

*Quantum Physics* and *The Racah-Wigner Algebra in Quantum Theory* by Biedenharn and Louck (1981a, 1981b).

This thesis presents the recent research work pertaining to the following topics: connection between the Clebsch-Gordan (or 3-j), the Racah (or 6-j), the $\ell s$ - jj (or 9-j) transformation coefficients and generalized hypergeometric functions of unit argument; the study of the *polynomial* (or *non-trivial*) zeros of these angular momentum coefficients along with algorithms to generate the *polynomial* zeros of degree (or weight) one of these coefficients. The proper perspective for this work is in the context of contemporary work done by Brudno, Bremner, Louck, Biedenharn, Van den Berghe, De Meyer, Van der Jeugt, Koozekanani, Varshalovich, Bowick, Wu, Alisauskas, Jucys, Bandzaitis, Labarthe and Lindner.

In Chapter 1 the basic definitions for the angular momentum coupling (Clebsch - Gordan or 3-j) coefficients, and the angular momentum recoupling (Racah or 6-j, $\ell s$-jj or 9-j) coefficients are provided. From this starting point the symmetries of these coefficients, viewed in terms of sets of hypergeometric functions of unit argument, and their *polynomial* or *non-trivial* zeros are studied. In this chapter a fundamental theorem which deals with the minimum number of parameters necessary and sufficient to obtain the complete set of solutions for multiplicative Diophantine equations of degree n is stated and proved. This theorem is a modification of the theorem due to E.T.Bell (1933) in his classic paper entitled *Reciprocal arrays and Diophantine analysis* . The homogeneous multiplicative Diophantine equation of degree n is given by:

$$x_1 x_2 \dots x_n = u_1 u_2 \dots u_n \ , \ (n > 1) \qquad (*)$$

where $x_i$, $u_i$ are independent variables. The statement of the theorem is:

*Theorem:* Every solution of the homogeneous multiplicative Diophantine equation given by (*) can be expressed in the form:

$$x_i = \prod_{j=1}^{n} \phi_{ij} \qquad \text{and} \qquad u_j = \prod_{i=1}^{n} \phi_{ij} \ ,$$

for all i, j = 1,2,...,n where all the $n^2$ independent parameters $\phi_{ij}$ can be arranged into a n x n square array with $\phi_{ij}$ being at the intersection of the ith row and jth column subject to the greatest common divisor (g.c.d.) conditions:

$$(x_i \ , u_i \ ) = \phi_{ii} \ .$$

The proof provided here is both simple and straightforward *without recourse to reciprocal arrays* used by E.T.Bell. This fundamental theorem is essential to obtain the complete solution to the problem of polynomial zeros of degree 1 of the 3-j, 6-j and the 9-j coefficients, dealt with in the subsequent chapters.

Chapter 2 deals with the interrelationship between the sets of hypergeometric functions of unit argument which were shown in Chapter 1 to be necessary and sufficient to account for the known symmetries of the 3-j and the 6-j coefficients. The mathemtical formulae required to establish this are: (a) the reversal of series property for the ${}_{p+1}F_p(1)$s; (b) the Erdelyi - Weber transformation. It is shown that starting with a member belonging to the van der Waerden set of six ${}_3F_2(1)$s for the 3-j coefficient and using the reversal of series property, the remaining five members of this set can be generated. In the case of the 6-j coefficient, in Chapter 1, two equivalent sets of ${}_4F_3(1)$s were introduced - a set I of three ${}_4F_3(1)$s and a set II of four ${}_4F_3(1)$s. These are shown here to be related to one-another through the reversal of series property. Further, just as there exist a set of six ${}_3F_2(1)$s of the van der Waerden form, it is shown that sets of six ${}_3F_2(1)$s can be obtained for the Majumdar, Racah and Wigner forms, from the van der Waerden set, by using the Erdelyi-Weber transformation. However, while the van der Waerden set of six ${}_3F_2(1)$s is necessary and sufficient to account for the 72 symmetries of the 3-j coefficient, each of the Majumdar, Racah and Wigner sets, due to the nature of its parameters, is found to account for only 12 of the 72 symmetries.

In Chapter 3, it is shown that the series part of the 3-j coefficient can be rearranged into a formal binomial expansion using the generalised power (or lowering factorial). A particular case of this result is the one obtained by Sato and Kaguei (1972). The fact that for n = 1 the generalised power (defined as a lowering factorial) is the same as the ordinary power reveals explicitly the *polynomial* zeros of degree 1 of this coefficient.

Thus the closed form expression:

$$(1 - \delta\ (n,1)\ \delta\ (x,y))\ ,$$

for the *polynomial* zeros of degree 1 is obtained. The expressions for x and y can be simply related to the numerator and denominator parameters respectively of the set of ${}_3F_2(1)$s. The complete set of *polynomial* zeros of degree 1 of the 3-j coefficient are then obtained from either the above closed form expression or the four-parameter solution to the homogeneous multiplicative Diophantine equation of degree 2. (This four-parameter solution was also obtained by Brudno (1985)). A procedure, similar to the one adopted by Bowick (1976), has been used to sieve out the *equivalent* zeros of degree 1 and retain only the *inequivalent* ones. Explicitly, to every *inequivalent polynomial* zero of degree 1 correspond 72 *equivalent* ones (including the *inequivalent* one) and they are generated by using the 72 symmetries of the 3-j coefficient. Of the 36 *inequivalent polynomial* zeros of the 3-j coefficient reproduced by Biedenharn and Louck (1981b) from the work of Bowick (1976), 21 are found to be *polynomial* zeros of degree 1 computed as above. The remaining 15 *polynomial* zeros are classified according to their degree (SrinivasaRao and Rajeswari, (1985a) - 13 are of degree 2 and 2 were found to be of degree 4. These are tabulated.

The main objective of Chapter 4 is to obtain the complete set of solutions for the *polynomial* zeros of degree 1 of the 6-j coefficient. Following the method detailed in Chapter 3, two formal binomial expansions can be obtained for the 6-j coefficient. One of these which utilises the raising factorial corresponds to the result of Sato (1955). The other, obtained by Srinivasa Rao and Venkatesh (1977), which utilises the lowering factorial is an exact binomial expansion for n = 1 and hence it reveals the closed form expression:

$$(1 - \delta(n,1)\,\delta(x,y)),$$

for the *polynomial* zeros of degree 1 (Srinivasa Rao and Rajeswari 1984) of the 6-j coefficient. The parameters x and y are related to the numerator and denominator parameters of the set of ${}_4F_3(1)$s respectively. The *polynomial* zeros of degree 1 of the 6-j coefficient are also shown to be related to the solutions of the homogeneous multiplicative Diophantine equation of degree 3. The fewer parameter solutions obtained by Brudno and Louck (1985), Bremner (1986), Bremner and Brudno (1986) are compared with those obtained from the solutions to the constrained multiplicative Diophantine equation of degree 3, *which alone generates the required complete set of polynomial zeros of degree one* (Srinivasa Rao, Rajeswari & King 1988). An alternative proof† is given for the theorem of E.T.bell stated in Chapter 1, using an induction hypothesis on N where N is given by:

$$x_1\, x_2 \ldots x_n = u_1\, u_2 \ldots u_n = N.$$

In passing, mention is made of the only possible physical

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explanations which exist for a few of the *polynomial* zeros of degree 1 of the 6-j coefficient. While Van den Berghe et al (1984), and Vander Jeugt et al (1983) interpreted nine of the *inequivalent polynomial* zeros as those which arise due to the imbedding of the exceptional Lie algebras in SO(3), it is pointed out that all except one of them are *polynomial* zeros of degree 1. Two algorithms are proposed to generate the *polynomial* zeros of degree 1 of the 6-j coefficient from the constraint equation:

$$ghi = a\,b\,c + d\,e\,f + a\,d\,g + b\,e\,h + c\,f\,i\ ,$$

which is satisfied by the nine parameters: $a$, $b$, $c$, $d$, $e$, $f$, $g$, $h$, and $i$, necessary and sufficient to solve the multiplicative Diophantine equation of degree 3, viz. $x_1\ x_2\ x_3\ =\ u_1\ u_2\ u_3$. In these algorithms, the constraint equation is reduced to either:

$$\alpha\, x\, y\ =\ \beta\, x + \gamma\, y + \delta \qquad \text{or} \qquad \alpha' x + \beta' y\ =\ \gamma' ,$$

and solutions for these are due to Brahmegupta (see Dickson, 1952) and Paoli (see Dickson, 1952).Either these solutions were used or the closed form expression was used to generate the complete set of *polynomial* zeros of degree one of the 6-j coefficient. Koozekanani and Biedenharn (1974) calculated the *polynomial* zeros of the 6-j coefficient for arguments $\leq$ 18.5, and using the symmetries of these coefficients ordered these in a speedometric fashion. They found the zeros of the 6-j coefficient with the help of a computer program which resorted to the use of numbers decomposed into powers of prime factors. Our method of computation stated above revealed that 1174 of the 1420 tabulated by

Koozekanani and Biedenharn (1974) are *polynomial* zeros of degree 1. The remaining 246 of the *polynomial* zeros were sorted out according to their degree (Srinivasa Rao and Rajeswari 1985a).

Hitherto the computation of the 9-j coefficient has been with the help of a single sum over a product of three 6-j coefficients due to Wigner (1940). As the 6-j coefficient is itself a set of ${}_4F_3(1)$s this method implies a sum over four indices. In literature, there exists a triple sum series due to Jucys and Bandzaitis (1977) for the 9-j coefficient, as well as a sum over six indices obtained by Wu (1972) using the Bargmann generating function method. It is reasonable to assume that the triple sum series of Jucys and Bandzaitis would be more economical and efficient compared to the conventional single sum over the product of three 6-j coefficients. In chapter 5, it is established that the numerical computation of the 9-j coefficient using this triple sum series is in general superior to the conventional method mentioned above. Starting with a suitable product of three ${}_4F_3(1)$ functions and making three judicious substitutions it has been shown that the triple sum series of Jucys and Bandzaitis (1977) is in fact a particular case of the most general triple hypergeometric series, evaluated at unit argument for all the three variables. This identification enables us to think of evaluating the triple sum series as a folded triple sum. One observation is that the 72 symmetries of the 9-j coefficient are not manifest in the triple sum series.

This results in the fact that the number of terms involved in the triple sum series is different for different symmetries of the same coefficient! For example, in the case of:

$$\begin{Bmatrix} 30 & 20 & 10 \\ 30 & 10 & 20 \\ 60 & 30 & 30 \end{Bmatrix} ,$$

the triple sum series can be shown to have only a single term. However its symmetries have several terms and the symmetry

$$\begin{Bmatrix} 20 & 10 & 30 \\ 30 & 30 & 60 \\ 10 & 20 & 30 \end{Bmatrix} ,$$

is computed as a sum of 33761 terms of the triple sum series! Having realised this, given a 9-j coefficient, it is necessary to find that symmetry for which the number of terms in the triple sum series will be a minimum and the 9-j coefficient should be computed only for that symmetry. This infact was the strategy that was adopted in the numerical evaluation of the triple sum series, using repeatedly the Horner's rule (Lee 1966) for polynomial evaluation. A new FORTRAN program based on this approach for computing the 9-j coefficient was found to be 2 to 4 times faster than the conventional single sum series, for smaller values of the angular momenta and even higher advantage factors have been found to be possible for larger values of angular momenta (Srinivasa Rao, Rajeswari and Chiu 1988), provided the number of terms to be summed does not exceed 200 (on an IBM PC - AT) or 600 (on a VAX - 11/780).

The identification of the triple sum series with a triple hypergeometric series in Chapter 5 enables *for the first time* the study of *polynomial* or *non-trivial* zeros for the 9-j coefficient (Srinivasa Rao and Rajeswari 1988b). It is to be noted that the conventional single sum over the product of three 6-j coefficients *will not reveal* these polynomial zeros. If XF, YF and ZF denote the upper limits of the summation indices in the triple sum series, then the *polynomial* zeros of degree 1 of the 9-j coefficient are given by the closed form expression:

$$1 - \delta^{\alpha 1, XF, YF, ZF}_{\beta 1,\ 1,\ 0,\ 0} - \delta^{\alpha 2, XF, YF, ZF}_{\beta 2,\ 0,\ 1,\ 0} - \delta^{\alpha 3, XF, YF, ZF}_{\beta 3,\ 0,\ 0,\ 1},$$

where the following notation has been introduced:

$$\delta^{a,b,c,d}_{p,q,r,s} = \delta(a,p)\ \delta(b,q)\ \delta(c,r)\ \delta(d,s)\ .$$

The $\alpha$'s and $\beta$'s are given by:

$$\alpha 1 = (x2 + 1).(x3 + 1).x4.x5\ ,\quad \beta 1 = x1.(p2 + 1).(p3 + 1)\ ,$$
$$\alpha 2 = (y1 + 1).(y2 + 1).y4.y5\ ,\quad \beta 2 = p1.(p2 + 1).(y3 + 1)\ ,$$
$$\alpha 3 = (z2 + 1).\ z3.\ z4.\ z5\ ,\quad \beta 3 = p1.z1.(p3 + 1).$$

Since the $\alpha$'s and $\beta$'s are themselves products of three factors with x4 or x5; y4 or y5; z4 or z5 being set equal to 1 (for they correspond to XF, YF or ZF respectively. Note. The xi's, yi's, zi's and pi's are defined in Chapter 1), we find that once again the homogeneous multiplicative Diophantine equation of degree 3, is encountered in the study of *polynomial* zeros of degree 1 of the 9-j coefficient. However, unlike the case of the 6-j coefficient which is a polynomial in a single variable, the 9-j coefficient being a polynomial in three variables, the study of its zeros of degree 1 involves the solutions of a set of 24 multiplicative

Diophantine equation of degree 3. A detailed study of these 24 cases revealed that 12 of these do not yield any degree 1 zeros which have been shown to be due to inherent inconsistencies related to the violation of triangular inequalities, etc. Of the remaining 12 multiplicative Diophantine equations of degree 3, four are found to be full nine parameter solutions and the other eight involve fewer than nine parameters in their solutions with one of the angular momenta itself being a free parameter. The *polynomial* zeros of degree 1 of the 9-j coefficient were generated using the closed form expression and also a set of solutions of the multiplicative Diophantine equations. It is clear that while the solutions of a single multiplicative Diophantine equation generate all the *polynomial* zeros of degree 1 of the 3-j and 6-j coefficient, all the *polynomial* zeros of degree 1 of the 9-j coefficient arise from the solutions to *a set of* multiplicative Diophantine equations, *for there exists no single solution which will generate them all.*

In Chapter 7, the connection between the 3-j coefficient and the discrete orthogonal Hahn polynomial is established. It is shown that Majumdar's form of ${}_3F_2(1)$ for this coefficient is readily identifiable with the Hahn polynomial which is described by Karlin and Mc Gregor (1961). The four recurrence relations obtained by them for the Hahn polynomial are used to derive recurrence relations for the 3-j coefficient, and two of these relations have been used by Schulten and Gordan (1975) in the exact recursive evaluation of the 3-j coefficient. Of the four recurrence relations for the 3-j coefficient, derived as a direct consequence of the three-term recurrence relations obtained by Karlin and Mc Gregor (1961) for the Hahn and dual Hahn polynomials, three are found to be independent and two of these three are recurrences in both j and m. These appear to be new as they are not available in literature (Biedenharn and Louck, 1981a, 1981b).

To summarise, in this thesis, the following results have been obtained:

(i) It is shown that the set of six ${}_3F_2(1)$s for the 3-j coefficient of the van der Waerden form can all be generated by starting with one of them and applying the reversal of a ${}_3F_2(1)$ repeatedly. This same reversal relation for a ${}_4F_3(1)$ is shown to connect the set I and set II of ${}_4F_3(1)$s for the 6-j coefficient. As in the case of van der Waerden form, a set of six ${}_3F_2(1)$s are derived for Wigner, Racah and Majumdar forms of the 3-j coefficient by applying one of the transformations given by Erdelyi and Weber (1952) for a ${}_3F_2(1)$, to the van der Waerden set. But, unlike the van der Waerden set which accounts for all the known 72 symmetries of the 3-j coefficient, it is found that the other three sets account only for 12 symmetries each.

(ii) The 3-j coefficient is rewritten as a formal binomial expansion and thereby a closed form expression is obtained for the *polynomil* zeros of degree one of this coefficient. Using Bell's theorem it is established that four integer parameters are necessary and sufficient to generate *all* the *polynomial* zeros of degree 1 of this coefficient. The closed form expression as well as the four-parameter formula have been used to generate these zeros.

(iii) By rewriting the 6-j coefficient as a formal binomial expansion a closed form expression is obtained for the *polynomial* zeros of degree 1 of this coefficient. Bell's theorem is again used to establish that eight integer parameters are necessary and sufficient to obtain the complete solution to this problem, of generating zeros of degree 1, and it is shown that the fewer parametric solutions given by other authors generate only a partial list of the complete set of zeros. Two algorithms are presented to solve the constraint equation :

$$z = x + y + u + v + w ,$$

where $(x.y.z = u.v.w)$ and these algorithms have been successfully tested on a computer to generate the complete list of degree 1 zeros of the 6-j coefficient.

(iv) A new FORTRAN program has been developed to compute the 9-j coefficient using the triple sum series due to Jucys and Bandzaitis (1977) and this new code is found to have an advantage factor of 2 to 4 (for the nine angular momenta a, b, c, d, e, f, g, h, i ≤ 10 and an even larger advantage factor for larger values of angular momenta) over the conventional program as long as the number of terms to be summed in the triple sum series does not exceed 200 on the PCs or 600 on the VAX - 11/780 computer.

(v) The triple sum series for the 9-j coefficient is identified with a triple hypergeometric series using which the *polynomial* zeros of the 9-j coefficient have been studied for the first time. As a direct consequence, a closed form expression for the zeros of degree 1 of the 9-j coefficient has been obtained and the zeros were generated using the closed form expression as well as a *set* of parametric formulae based on the solutions of 12 homogeneous multiplicative Diophantine equations of degree 3.

(vi) The 3-j coefficient is identified with a discrete orthogonal Hahn polynomial and the three term recurrence relations derived for the Hahn polynomial by Karlin and Mc Gregor have been used to derive three fundamental recurrence relations for the 3-j coefficient.

## Chapter 1

## Mathematical Formalism

In this chapter the basic definitions for the angular momentum coupling (Clebch-Gordan or 3-j) coefficients and the recoupling (Racah or 6-j and *ls-jj* or 9-j) coefficients, their series representations and symmetries are described. These series representations are used in the study of the polynomial or *non-trivial* zeros of these coefficients in the following chapters. A modified form of a fundamental theorem, originally due to E.T.Bell, is stated and proved. It deals with the minimum number of parameters necessary and sufficient to obtain the complete set of solutions for a homogeneous multiplicative Diophantine equation of degree n. This theorem is essential to obtain the complete solution to the problem of polynomial zeros of degree 1 of the 3-j, the 6-j and the 9-j coefficients.

### 1.1 The Clebsch-Gordan (or 3-j) coefficient and its symmetries

Consider the addition of two angular momenta (in units of $\hbar=1$) $j_1$ and $j_2$ to get a total angular momentum $j_3$ :

$$j_3 = j_1 + j_2 \ . \tag{1}$$

There exist two orthonormal bases : one in which the operators $j_1^2$, $j_2^2$, $j_3^2$ and $j_{3z}$ are diagonal, the eigen state corresponding to which is denoted by $|(j_1j_2)j_3m_3\rangle$ and another in which the operators $j_1^2, j_{1z}, j_2^2$ and $j_{2z}$ are diagonal whose eigen states are denoted by $|j_1m_1\rangle\ |j_2m_2\rangle$. These basis vectors - for the coupled state of the system viz. $|(j_1j_2)j_3m_3\rangle$ and the uncoupled state

$|j_1m_1\rangle\ |j_2m_2\rangle$ - are related by the orthogonal transformation :

$$|(j_1j_2)j_3m_3\rangle = \sum_{m_1,m_2} C(j_1j_2j_3;m_1m_2m_3)\ |j_1m_1\rangle\ |j_2m_2\rangle . \qquad (2)$$

In (2), $C(j_1j_2j_3;m_1m_2m_3)$ is the transformation coefficient known as the Clebsch - Gordan coefficient after the work of Clebsch (1872) and Gordan (1875) on the invariant theory of algebraic forms which is an equivalent formulation of the coupling problem of angular momentum. In Physics literature these are also synonymously referred to as the vector addition or vector coupling coefficients. Since the significance of these coefficients in relation to the quantum thoery of angular momentum and rotation matrices appeared first in Wigner's classic papers of 1927 (Wigner 1927a,1927b), Biedenharn and Louck in their treatise on *Angular Momentum in Quantum Physics - Theory and Applications* choose to designate them as Wigner coefficients. (For a list of the notation of Wigner and related coefficients refer to p.150 of Biedenharn and Louck (1981a)). It has a non-zero value only when the triad $(j_1j_2j_3)$ satisfies the triangular inequality:

$$|j_1 - j_2| \le j_3 \le j_1 + j_2 , \qquad (3)$$

and when the projection quantum numbers $m_1$ ,$m_2$ ,$m_3$ satisfy the relation :

$$m_3 = m_1 + m_2 . \qquad (4)$$

The inverse of (2) is :

$$|j_1m_1\rangle\ |j_2m_2\rangle = \sum_{j_3,m_3} C(j_1j_2j_3;m_1m_2m_3)\ |(j_1j_2)j_3m_3\rangle \qquad (2a)$$

which is obtained using the orthogonality properties of the Clebsch-Gordan coefficients:

$$\sum_{m_1, m_2} C(j_1 j_2 j_3; m_1 m_2 m_3)\ C(j_1 j_2 j_3'; m_1 m_2 m_3') = \delta(j_3, j_3')\delta(m_3, m_3'), \quad (2b)$$

and

$$\sum_{j_3, m_3} C(j_1 j_2 j_3; m_1 m_2 m_3)\ C(j_1 j_2 j_3; m_1' m_2' m_3) = \delta(m_1, m_1')\delta(m_2, m_2'), \quad (2c)$$

where $\delta(i,k)$ denotes the Kronecker delta function. Many approaches have been adopted in literature to derive the explicit expression for the Clebsch - Gordan coefficient, and the detailed expression depends on the method of derivation. In this respect there exist four fundamental forms for this coefficient viz. Wigner's, Racah's, van der Waerden's and Majumdar's forms. Wigner gave the following form (1940):

$$\begin{aligned} C(j_1 j_2 j_3; m_1 m_2 m_3) = {} & \delta(m_1+m_2, m_3)[j_3]\Delta(j_1 j_2 j_3)\{(j_3+m_3)!(j_3-m_3)!\}^{1/2} \\ & \times \{(j_1+m_1)!(j_1-m_1)!(j_2+m_2)!(j_2-m_2)!\}^{-1/2} \\ & \times \sum_S (-1)^{j_2+m_2+S} (j_2+j_3+m_1-s)!(j_1-m_1+s)! \\ & \times \{s!(j_3-j_1+j_2-s)!(j_3+m_3-s)!(j_1-j_2-m_3+s)!\}^{-1}, \quad (5) \end{aligned}$$

for this coefficient, while Racah (1942) arrived at the expression:

$$\begin{aligned} C(j_1 j_2 j_3; m_1 m_2 m_3) = {} & \delta(m_1+m_2, m_3)[j_3]\{(j_1+j_2-j_3)!(j_1-m_1)!(j_2-m_2)! \\ & \times (j_3-m_3)!(j_3+m_3)!\}^{1/2}\{(j_1+j_2+j_3+1)!(j_1-j_2+j_3)! \\ & \times (-j_1+j_2+j_3)!(j_1+m_1)!(j_2+m_2)!\}^{-1/2} \\ & \times \sum_t (-1)^{j_1-m_1+t} (j_1+m_1+t)!(j_3+j_2-m_1-t)! \\ & \times \{t!(j_3-m_3-t)!(j_1-m_1-t)!(j_2-j_3+m_1+t)!\}^{-1}. \quad (6) \end{aligned}$$

for the same coefficient. Racah ( 1942 ) has remarked that the expressions derived by him as well as by Wigner are "unsymmetrical and unpractical for the use", and making use of the identity:

$$\frac{a!}{b!c!} = \sum_s (a-b)!(a-c)!\{s!(a-b-s)!(a-c-s)!(b+c-a+s)!\}^{-1}, \tag{7}$$

Racah (1942) rewrote the summation part in (6) as :

$$\sum_t (-1)^{j_1-m_1+t} (j_1+m_1+t)!(j_3+j_2-m_1-t)!\{t!(j_3-m_3-t)!(j_1-m_1-t)!$$

$$\times(j_2-j_3+m_1+t)!\}^{-1} = \sum_{t,u}(-1)^{j_1-m_1+t} (j_1+m_1+t)!(j_2+m_2)!$$

$$\times (-j_1+j_2+j_3)!\{t!u!(j_2-j_3+m_1+t)!(j_2+m_2-u)!$$

$$\times(-j_1+j_2+j_3-u)!(j_1-j_2-m_3-t+u)!\}^{-1}. \tag{8}$$

In (8) making the change of variable from t to p :

$$p = j_1 - j_2 - m_3 + u - t \tag{9}$$

and by using the identity :

$$\sum_s(-1)^s (t-s)!\{s!(x-s)!(z-s)!\}^{-1} = (t-x)!(t-z)!\{x!z!(t-x-z)!\}^{-1}, \tag{10}$$

for $0 \leq x \leq t$ and $0 \leq z \leq t$, Racah (1942) obtained for the right hand side of (8):

$$\sum_u(-1)^{j_2+m_2-u} (j_1+m_1)!(j_1-j_2+j_3)!(j_2+m_2)!(-j_1+j_2+j_3)! \{u!(j_2+m_2-u)!$$

$$\times (j_3+j_2-j_1-u)!(j_3+m_3-u)!(j_1-j_2-m_3+u)!(j_1-j_3-m_2+u)!\}^{-1}. \tag{11}$$

In (11) making the transformation :

$$z = j_2 + m_2 - u \tag{12}$$

Racah (1942) arrived at the following symmetric form (also known as the van der Waerden's form (1932)):

$$C(j_1 j_2 j_3; m_1 m_2 m_3) = \delta(m_1+m_2, m_3)[j_3]\, \Delta(j_1 j_2 j_3) \prod_{i=1}^{3} \{(j_i+m_i)!(j_i-m_i)!\}^{1/2}$$

$$\times\sum_z (-1)^z\{z!(j_1+j_2-j_3-z)!(j_1-m_1-z)!(j_2+m_2-z)!$$

$$\times(-j_2+j_3+m_1+z)!(-j_1+j_3-m_2+z)!\}^{-1}. \tag{13}$$

The expression derived by Majumdar (1958) is given by:

$$C(j_1j_2j_3;m_1m_2m_3) = \delta(m_1+m_2,m_3)[j_3]\{(-j_1+j_2+j_3)!(j_1+m_1)!(j_1-m_1)!$$
$$\times (j_2-m_2)!(j_3+m_3)!\}^{1/2}\{(j_1-j_2+j_3)!(j_1+j_2-j_3)!$$
$$\times (j_1+j_2+j_3+1)!(j_2+m_2)!(j_3-m_3)!\}^{-1/2}$$
$$\times \sum_t (-1)^{j_2+m_2+t}(2j_3-t)!(j_1+j_2-j_3+t)!\{t!$$
$$\times(j_3+m_3-t)!(-j_1+j_2+j_3-t)!(j_1-j_3-m_2+t)!\}^{-1}. \quad (14)$$

In the above expressions $\Delta(j_1j_2j_3)$ and $[x]$ denote, respectively:

$$\Delta(j_1j_2j_3) = \{(-j_1+j_2+j_3)!(j_1-j_2+j_3)!(j_1+j_2-j_3)!/(j_1+j_2+j_3+1)!\}^{1/2},$$
$$[x]=(2x+1)^{1/2},$$

and the limits of the summation indices are such that the arguments of the factorials are always non-negative.Among the four forms mentioned above,the symmetric van der Waerden form -(13)- is the one that will be used the most often (for reasons based on the symmetries of this coefficient, to be discussed later), and it is rewritten as follows :

$$C(j_1j_2j_3;m_1m_2m_3)= \delta(m_1+m_2,m_3)[j_3]\Delta(j_1j_2j_3)\prod_{i=1}^{3}\{(j_i+m_i)!(j_i-m_i)!\}^{1/2}$$
$$\times \sum_z (-1)^z \{z!\prod_{k=1}^{2}(z-\alpha_k)!\prod_{l=1}^{3}(\beta_l-z)!\}^{-1}, \quad (15)$$

where

$$\alpha_1= j_1-j_3+m_2,\ \alpha_2= j_2-j_3-m_1, \quad (16)$$
$$\beta_1= j_1-m_1,\ \beta_2= j_2+m_2,\ \beta_3= j_1+j_2-j_3. \quad (17)$$

and
$$z_{min} \le z \le z_{max},$$
with
$$z_{min}= \max(0,\alpha_1,\alpha_2) \text{ and } z_{max}= \min(\beta_1,\beta_2,\beta_3). \quad (18)$$

In Chapter 2 the interrelationship between these four forms for the Clebsch - Gordan coefficient via ${}_3F_2(1)$s will be established and their relative merits discussed.

The symmetries of the Clebsch - Gordan coefficient are interpreted more easily in terms of the Wigner's 3-j symbol (Wigner 1940) :

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1-j_2-m_3} [j_3]^{-1} C(j_1 j_2 j_3; m_1, m_2, -m_3), \tag{19}$$

where the projection quantum numbers in the 3-j coefficient satisfy the condition:

$$m_1 + m_2 + m_3 = 0. \tag{20}$$

Wigner (1940) showed that the 3-j coefficient possesses the following symmetry properties:

(i) It is invariant under even permutation of its columns;

(ii) Under odd column permutations the 3-j coefficient gets multiplied by the phase factor $(-1)^{j_1+j_2+j_3}$;

(iii) When all the projection quantum numbers are reversed in their signs, viz. $m_i \rightarrow -m_i$, the 3-j coefficient acquires the same phase factor as in (ii).

The aforesaid 12 symmetries of the 3-j coefficient are referred to as the *classical* symmetries.

Regge (1958) pointed out that the previously known symmetries of the 3-j coefficient formed only part of a larger group of symmetries which had 72 elements. Regge represented the 3-j coefficient by the 3x3 array with nine non-negative integer elements :

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \left\| \begin{array}{ccc} -j_1+j_2+j_3 & j_1-j_2+j_3 & j_1+j_2-j_3 \\ j_1-m_1 & j_2-m_2 & j_3-m_3 \\ j_1+m_1 & j_2+m_2 & j_3+m_3 \end{array} \right\| . \tag{21}$$

He asserted that the 3x3 square symbol is invariant (up to the phase factor $(-1)^{j_1+j_2+j_3}$ ) under :

(i) permutations of its columns ($S_3$, 6 in number),

(ii) permutations of its rows ($S_3$, 6 in number), and

(iii) transposition about its leading diagonal ($S_2$, 2 in number).

For odd permutations of rows and columns the square symbol gets multiplied by the phase factor $(-1)^{j_1+j_2+j_3}$. Hence the symmetry group has 72 elements, being the product of the three permutation groups of three, three, and two objects, respectively: $S_3 \times S_3 \times S_2$. Among the above mentioned 72 symmetries, those due to the 3! column permutations and the exchange of the last two rows of the square symbol correspond to the *classical* symmetries. The square symbol introduced by Regge is a magic square in that each of the column and row sums equal : $J = j_1+j_2+j_3$. Though Regge gave six new symmetries for the 3-j coefficient, he did not write these explicitly in his paper (Regge 1958), and these can be found in the papers of Srinivasa Rao (1978) and Venkatesh (1978).

**1.2 Generalized hypergeometric functions**

Gauss (1866) defined the ordinary hypergeometric series as :

$$ {}_2F_1(a,b;c;z) = \sum_{n=0}^{\infty} \frac{(a,n)(b,n)}{(1,n)(c,n)} z^n, \tag{22}$$

where

$$(a,n) = \Gamma(a+n)\,\{\Gamma(a)\}^{-1} \equiv a(a+1)(a+2)\cdots(a+n-1) \tag{23}$$

and , in particular, $(a,0) \equiv 1$. The parameters a,b,c and z may be real or complex. If either of the numerator parameters a or b of the function ${}_2F_1(a,b;c;z)$ is a negative integer, the series has only a finite number of terms and in fact it reduces to a polynomial. However, if the denominator parameter c is zero or a negative integer, the function is not defined since all but a finite number of terms of the series become infinite. The series is convergent for all values of z, real or complex, such that : $|z|<1$. and divergent for all values of z, real or complex, such that : $|z|>1$. For z = 1, the series is convergent if $R\ell(c-a-b) > 0$ and divergent if $R\ell(c-a-b) < 0$. For z = -1, the series is convergent if $R\ell(c-a-b+1) > 0$ and divergent if $R\ell(c-a-b+1) < 0$.

The Gauss series satisfies the differential equation:

$$\{\theta\ (\theta + c - 1) - z\ (\ \theta + a)\ (\ \theta + b)\}\omega = 0 \tag{24}$$

where $\theta \equiv z\,\dfrac{d}{dz}$ and $\omega = {}_2F_1(a,b;c:z)$.

The generalized Gauss function, or generalized hypergeometric function or series, is defined as:

$${}_pF_q((\alpha_p);(\beta_q);z) \equiv \sum_{n=0}^{\infty} \frac{((\alpha_p),n)\ z^n}{(1,n)((\beta_q),n)}\ , \tag{25}$$

where the p numerator parameters $\alpha_1,\alpha_2,\cdots,\alpha_p$, and the q denominator parameters $\beta_1,\beta_2,\cdots,\beta_q$ are denoted by $(\alpha_p)$ and $(\beta_q)$, respectively. Any of these parameters and the variable z may be real or complex but the denominator parameters $(\beta_q)$ must not be negative integers, as in that case the series is not defined. If any of the numerator parameters $(\alpha_p)$ is a negative integer, the function reduces to a polynomial.

The series ${}_pF_q(z)$ converges for all values of z, real or complex when $p \leq q$. For $p > q+1$, the series converges only when

$z=0$. If $p = q+1$, the series is convergent only in the unit disc $|z| < 1$. The function corresponding to $p = q+1$ has been most widely studied and in this case the series is convergent

if $\qquad |z| < 1$ ,

or if $\qquad z = 1$ and $R\ell(\Sigma\, \beta_q - \Sigma\, \alpha_p) > 0$,

or if $\qquad z = -1$ and $R\ell(\Sigma\, \beta_q - \Sigma\, \alpha_p + 1) > 0$.

Whipple (1925) classified the general series $_{p+1}F_p(z)$ as well-poised, nearly-poised, Saalschutzian ,etc. depending upon the conditions satisfied by the parameters. In particular, the function $_{p+1}F_p(z)$ is called Saalschutzian if

$$1 + \sum_{k=1}^{p+1} \alpha_k = \sum_{k=1}^{p} \beta_k \; . \tag{26}$$

The relation between generalized hypergeometric functions of unit argument - viz. the $_3F_2(1)$ and the Saalschutzian $_4F_3(1)$ - and the 3-j and the 6-j coefficients will be discussed next.

**1.3 The 3-j coefficient and the set of six $_3F_2(1)$s**

Racah (1942) has shown that assuming the argument of one of the five factorials in (15) as the summation index instead of z, leads to some symmetry properties of the Clebsch - Gordan coefficient. Making such a substitution for each of the five factorials in (15) successively, Srinivasa Rao (1978) has arrived at five series representations for the Clebsch-Gordan coefficient. These five together with the one given in (15) constitute a set of six series representations for this coefficient. In terms of the elements of the square symbol, $\| R_{ik} \|$ , this set of six series representations is written in the following compact notation as :

$$\|R_{ik}\| = \delta\,(m_1+m_2+m_3,0)\,(-1)^{\Theta(pqr)} \prod_{i,k=1}^{3} \{R_{ik}!/(J+1)!\}^{1/2}$$
$$\times \sum_s (-1)^s \{s!(R_{2p}-s)!(R_{3q}-s)!(R_{1r}-s)!$$
$$\times (s+R_{3r}-R_{2p})!(s+R_{2r}-R_{3q})!\}^{-1}, \qquad (27)$$

for all six permutations of $(p\ q\ r) = (1\ 2\ 3)$ with

$$J = j_1+j_2+j_3$$

and

$$\Theta(pqr) = \begin{cases} R_{3p}-R_{2q} & \text{for even permutations,} \\ R_{3p}-R_{2q}+J & \text{for odd permutations.} \end{cases} \qquad (28)$$

The series given by (15) corresponds to $(p\ q\ r) = (1\ 2\ 3)$ in (27). It has been shown by Srinivasa Rao (1978) that the set of six series representations given by (27) can also be obtained by permuting the indices ( 1 2 3 ) in the expansion for the 3-j coefficient given by (15) and (19) and remembering that the series acquires an additional phase factor of $(-1)^J$ for odd permutations. In establishing the one-to-one correspondence between the series obtained by the substitution procedure and that obtained by permuting the indices in (15), use is made of the fact that $4j_i$ is an even integer so that $(-1)^{4j_i}$ is always positive.

Rose (1955) has pointed out that the Clebsch-Gordan coefficient can be expressed in terms of a ${}_3F_2(1)$ hypergeometric function. To arrive at this relationship, all the factorials in the series expansion for the 3-j coefficient are replaced by the $\Gamma$ functions, and use is made of the relation :

$$\Gamma(1-n-z) = (-1)^z\,\Gamma(n)\,\Gamma(1-n)\,\{\Gamma(n+z)\}^{-1} \qquad (29)$$
$$= (-1)^z\,\Gamma(1-n)\,\{(n,z)\}^{-1}, \qquad (30)$$

obtained from :

and $$\Gamma(n)\,\Gamma(1-n) = \Pi \,\mathrm{Cosec}(\Pi n) \tag{31}$$

$$\Gamma(n+z)\,\Gamma(1-n-z) = \Pi \,\mathrm{Cosec}\{\Pi(n+z)\} = (-1)^{z}\, \Pi \,\mathrm{Cosec}(\Pi n). \tag{32}$$

In (30) the Pocchammer symbol defined by (23) has been introduced. Using (30), those $\Gamma$ functions in the series representation whose arguments contain the summation index z with a negative sign are rewritten in terms of a $\Gamma$ function with a positive index of summation, and the resulting expression is then identifiable with a generalized hypergeometric function of unit argument. In this manner the series in (27) can be rewritten in terms of ${}_3F_2(1)$s given by (Srinivasa Rao and Venkatesh 1978 ; Venkatesh 1978) :

$$\|R_{ik}\| = \delta(m_1+m_2+m_3,0)\,(-1)^{\theta(pqr)} \prod_{i,k=1}^{3} \{R_{ik}!/(J+1)!\}^{1/2}$$
$$\times \{\Gamma(1-A,1-B,1-C,D,E)\}^{-1}\,{}_3F_2(A,B,C;D,E;1), \tag{33}$$

where

$$A = -R_{2p},\ B = -R_{3q},\ C = -R_{1r},\ D = R_{3r}-R_{2p}+1,\ E = R_{2r}-R_{3q}+1, \tag{34}$$

and $$\Gamma(X,Y,\cdots) = \Gamma(X)\,\Gamma(Y)\cdots, \tag{35}$$

for all permutations of $(p\ q\ r) = (1\ 2\ 3)$. Each of the six series is invariant under the seperate permutations of $(R_{2p}, R_{3q}, R_{1r})$ and $(R_{3r}-R_{2p},\ R_{2r}-R_{3q})$ and it thereby exhibi t s an $S_3 \times S_2$ symmetry. Thus, each series accounts for 12 distinct symmetries of the 3-j coefficient and the set of six series representations us therefore necessary and sufficient to account for all the 72 symmetries of this coefficient.

### 1.4 The Racah Coefficient and its symmetries

The Racah coefficient is the transformation coefficient which occurs in the recoupling of three angular momenta. Consider the coupling of three angular momenta :

$$j_1 + j_2 + j_3 = J \tag{36}$$

In terms of the coupling of two angular momenta, any two of the three angular momenta could be coupled to form an intermediate angular momentum, which can then be coupled to the third one to yield the final $J$. Two of the coupling schemes are :

$$j_1 + j_2 = j_{12} \qquad \text{and} \qquad j_{12} + j_3 = J, \tag{37}$$

$$j_2 + j_3 = j_{23} \qquad \text{and} \qquad j_1 + j_{23} = J, \tag{38}$$

where $j_{12}$ and $j_{23}$ are the intermediate angular momenta. The orthonormal basis vectors corresponding to these coupling schemes can be written as :

$$|(j_1 j_2)j_{12} j_3 J\ M> \qquad \text{and} \qquad |j_1(j_2 j_3)j_{23} J\ M>, \tag{39}$$

and these two set of states are related through the transformation :

$$|(j_1 j_2)j_{12} j_3 J\ M> = \sum_{j_{23}} U(j_1 j_2 J\ j_3;\ j_{12} j_{23})\ |j_1(j_2 j_3)j_{23} J\ M>. \tag{40}$$

Here $U(j_1 j_2 J\ j_3;\ j_{12} j_{23})$ is called the recoupling coefficient. It is straightforward to obtain an explicit expression for the U coefficient in terms of the Clebch-Gordan coefficients since, by decoupling the state $|(j_1 j_2)j_{12} j_3 J\ M>$ into $|j_1 m_1>|j_2 m_2>|j_3 m_3>$ and by recoupling them suitably using (2a), (2b) and (2c) one can get the state $|j_1(j_2 j_3)j_{23} J\ M>$. This expression for the U coefficient as the product of four Clebsch-Gorden coefficients summed over all the projection quantum numbers is :

$$U(j_1 j_2 J\ j_3; j_{12} j_{23}) = \sum_{\text{all } m's} C(j_1 j_2 j_{12};\ m_1 m_2 m_{12})\ C(j_{12} j_3 J\ ;\ m_{12} m_3 M)$$
$$\times\ C(j_2 j_3 j_{23};\ m_2 m_3 m_{23})\ C(j_1 j_{23} J\ ;\ m_1 m_{23} M). \quad (41)$$

In fact, it can be verified that out of the six projection quantum numbers only two are independent (say, $m_1$ and $m_2$) due to the additive property of the projections (20).

The Racah coefficient $W(j_1 j_2 J\ j_3;\ j_{12} j_{23})$ is defined by :

$$W(j_1 j_2 J\ j_3;\ j_{12} j_{23}) = \{[j_{12}]\ [j_{23}]\}^{-1}\ U(j_1 j_2 J\ j_3;\ j_{12} j_{23}). \quad (42)$$

Racah (1942) showed that the U coefficient can be reduced to a single sum series which is independent of the projection quantum numbers. This remarkably simple expression derived by Racah (1942) is given by :

$$W(abcd;ef) = \Delta(abe)\ \Delta(cde)\ \Delta(acf)\ \Delta(bdf)\ w(abcd;ef), \quad (43)$$

where

$$w(abcd;ef) = \sum_z (-1)^z\ (a+b+c+d+1-z)!\{z!(a+b-e-z)!(c+d-e-z)!$$
$$\times\ (a+c-f-z)!(b+d-f-z)!(e+f-a-d+z)!$$
$$\times\ (e+f-b-c+z)!\}^{-1}. \quad (44)$$

The symmetries of the Racah coefficient are interpreted more easily in terms of the Wigner's (1940) 6-j symbol :

$$\left\{ \begin{matrix} a & b & e \\ d & c & f \end{matrix} \right\} = (-1)^{a+b+c+d}\ W(abcd;ef), \quad (45)$$

and these have been discussed by Racah (1942) as well as by Wigner (1940). Racah (1942) derived the symmetry properties of the W coefficient from its expansion given by (43), while Wigner (1940) arrived at the symmetries of the 6-j symbol (45) from its expansion in terms of the Clebsch-Gordan coefficients. These symmetries are referred to as the *Classical* symmetries and they are as follows. The 6-j symbol is invariant under :

(i) the 3! column permutations;

(ii) the interchanges of any two elements in its first row with the corresponding elements in its second row.

These 24 (3!x4) symmetries are also called the tetrahedral symmetries due to their correspondence with those of a regular tetrahedron, as pointed out by Wigner (1940).

Regge (1959) discovered six new symmetries of the Racah coefficient, which increased the total number of symmetries to 144. It is in Regge's paper that one finds the symmetric form for the Racah coefficient :

$$W(abcd;ef) = N \sum_p (-1)^p (p+1)! \{ \prod_{i=1}^{4} (p-\alpha_i)! \prod_{j=1}^{3} (\beta_j - p)! \}^{-1}, \quad (46)$$

with

$$N = (-1)^{a+b+c+d} \Delta(abe)\, \Delta(cde)\, \Delta(acf)\, \Delta(bdf), \quad (47)$$

and

$$\alpha_1 = a+b+e,\ \alpha_2 = c+d+e,\ \alpha_3 = a+c+f,\ \alpha_4 = b+d+f,$$

$$\beta_1 = a+b+c+d,\ \beta_2 = a+d+e+f,\ \beta_3 = b+c+e+f. \quad (48)$$

The $\alpha$'s and $\beta$'s are positive integers and the limits of p are given by :

$$p_{min} \le p \le p_{max},$$

with

$$p_{min} = \max(\alpha_1, \alpha_2, \alpha_3, \alpha_4) \quad \text{and} \quad p_{max} = \min(\beta_1, \beta_2, \beta_3) \quad (49)$$

Based on the series representation given by (46), Regge (1959) makes the significant and obvious observation that the Racah coefficient exhibits invariance to a 144-element symmetry group which is " isomorphic to the direct product of the permutation groups of 3 and 4 objects " - viz. the three $\beta$'s and the four $\alpha$'s. It is interesting to note that the simple change of variable :

$$p = a + b + c + d - z = \beta_1 - z \ , \qquad (50)$$

in (44) leads to the elegant form (46). However, it is only (44) which is widely quoted in early books on angular momentum (Rose 1955).

### 1.5 The Racah coefficient and sets of ${}_4F_3(1)$s

Many authors have pointed out the relationship between Racah coefficients and ${}_4F_3(1)$ hypergeometric function ( e.g. Biedenharn (1953), Rose (1955), Jahn and Howell (1959)). Using the method described earlier to relate the 3-j coefficient to the set of ${}_3F_2(1)$s, the series expansion for the Racah coefficient can be recast into a ${}_4F_3(1)$ hypergeometric series. The ${}_4F_3(1)$ given by Rose (1955) and Biedenharn (1953) is obtained by rewriting Racah's original expression (44). It should be noted that Racah's expression correspond to making the substitution for z, given by (50), viz.

$$z = \beta_1 - p \qquad (51)$$

in (46).

Srinivasa Rao et.al. (Srinivasa Rao, Santhanam, and Venkatesh (1975) made the observation that by making the substitutions :

$$z = \beta_2 - p \qquad (52)$$

and

$$z = \beta_3 - p \qquad (53)$$

in (46) successively, one can obtain two more series representations for the Racah coefficient similar to (44) which again can be rearranged into ${}_4F_3(1)$ hypergeometric series. This set of three ${}_4F_3(1)$s are given by ( Srinivasa Rao, Santhanam, and

Venkatesh (1975), Srinivasa Rao and Chiu (1988)) :

$$W(abcd;ef) = (-1)^{E+1}\, N\, \Gamma(1-E)\, \{\Gamma(1-A,1-B,1-C,1-D,F,G)\}^{-1}$$
$$\times\ {}_4F_3(A,B,C,D;E,F,G;1), \qquad (54)$$

where

$$A = -R_{1p},\ B = -R_{2p},\ C = -R_{3p},\ D = -R_{4p},\ E = -R_{1p}-R_{2p}-R_{3q}-R_{4r}-1,$$
$$F = R_{3q}-R_{3p}+1,\ G = R_{4r}-R_{4p}+1, \qquad (54a)$$

for $(p\ q\ r) = (1\ \ 2\ \ 3)$ cyclically. In (54a) $R_{jk}$'s denote the elements of the Bargmann (1962) - Shelepin (1964) $4 \times 3$ array for the 6-j coefficient:

$$\begin{Bmatrix} a & b & e \\ d & c & f \end{Bmatrix} = \begin{Vmatrix} \beta_1-\alpha_1 & \beta_2-\alpha_1 & \beta_3-\alpha_1 \\ \beta_1-\alpha_2 & \beta_2-\alpha_2 & \beta_3-\alpha_2 \\ \beta_1-\alpha_3 & \beta_2-\alpha_3 & \beta_3-\alpha_3 \\ \beta_1-\alpha_4 & \beta_2-\alpha_4 & \beta_3-\alpha_4 \end{Vmatrix}, \qquad (55)$$

here the $\alpha$'s and $\beta$'s are as in (48). The 6-j coefficient is invariant under the 3! column permutations and the 4! row permutations of this array.

For all the physical values of a,b,c,d,e and f all the numerator parameters A,B,C and D are nonpositive and the denominator parameter E, being also negative, satisfies the condition (A,B,C or D) > E, by virtue of the triangular conditions as implied by $\Delta(XYZ)$ viz.:

$$(-X + Y + Z) \geq 0,$$
$$(\ X - Y + Z) \geq 0, \qquad (56)$$
$$(\ X + Y - Z) \geq 0.$$

For the ${}_4F_3(1)$ series to be convergent (Rose (1955)), there must be a numerator parameter such that

$$(A,B,C,D) \geq (F,G). \tag{57}$$

However, comparison of the denominator parameters with the numerator parameters, along with the triangular conditions, yields the condition :

$$(F,G) > (A,B,C,D), \tag{58}$$

for all the three series of set I. From (57) and (58) it follows that both F and G must be greater than zero for the ${}_4F_3(1)$ series to be convergent. It has been found that ( Srinivasa Rao, Santhanam, and Venkatesh (1975)) the 4! permutations of A,B,C and D and the 2! permutations of F and G leads to 48 (4! x 2!) distinct symmetries of the Racah coefficient. The permutation of a positive parameter with a negative parameter leads at best to a $j \rightarrow -j-1$ substitution - which is a valid mathematical symmetry in angular momentum theory - or a symmetry like the one obtained by Minton (1970) which violates triangular inequ alities ( Yakimiw (1971), Vinaya Joshi (1971)). Since each ${}_4F_3(1)$ series exhibits 48 of the 144 symmetries, it follows that the set I of three ${}_4F_3(1)$s is necessary and sufficient to account for the symmetries of the Racah coefficient.

By making the substitutions :

$$z = p - \alpha_i \ , \quad i = 1,2,3,4, \tag{59}$$

successively in (46), Srinivasa Rao and Venkatesh (1977) arrived at another set of four Saalschutzian ${}_4F_3(1)$s for the Racah coefficient ( Srinivasa Rao and Venkatesh (1977), Srinivasa Rao and Chiu (1988)) :

$$W(abcd:ef) = (-1)^{A'-2}\, N\, \Gamma(A')\, \{\Gamma(1-B', 1-C', 1-D', E', F', G')\}^{-1}$$
$$\times\ {}_4F_3(A', B', C', D'; E', F', G'; 1) \ , \tag{60}$$

where

$$A' = R_{q2}+R_{r1}+R_{s3}+2, \quad B' = -R_{p1}, \quad C' = -R_{p2}, \quad D' = -R_{p3},$$
$$E' = R_{q1}-R_{p1}+1, \ F' = R_{r1}-R_{p1}+1, \ G' = R_{s1}-R_{p1}+1, \tag{61}$$

for (p q r s) = (1 2 3 4) cyclically and $R_{jk}$'s are again the elements of the Bargmann - Shelepin array (55). In (54) and (60), the parameters of the ${}_4F_3(1)$s satisfy the Saalschutzian condition (26). In each ${}_4F_3(1)$ of this set, three of the numerator parameters, viz. $B'$, $C'$ and $D'$ are non-positive and the denominator parameters , viz. $E'$, $F'$ and $G'$ are required to be positive. Hence, each series exhibits 36 (3! × 3!) distinct symmetries of the Racah coefficient, so that the set II of four ${}_4F_3(1)$s is necessary and sufficient to account for all the 144 symmetries.

Thus, the 144 symmetries of the Racah coefficient are exhibited by the single series expansion (46), or by the set I of three ${}_4F_3(1)$s, or, equivalently, by the set II of four ${}_4F_3(1)$s. In Chapter 2 we establish that these two sets of ${}_4F_3(1)$s are related to each other by the property of reversal of the terminating Saalschutzian hypergeometric series.

**1.6 The coupling of four angular momenta and the 9-j coefficient**

The two-electron system is one of the instances where the coupling of four angular momenta arises. Since each electron has an orbital angular momentum and a spin angular momentum (denoted by $\ell_1, s_1$ and $\ell_2, s_2$ respectively), a state of total angular momentum

J and projection $J_z$ is constructed either by adding $\ell_1$ and $s_1$ (to $j_1$) and adding $\ell_2$ and $s_2$ (to $j_2$) and then adding the total angular momenta of the individual particles viz. $j_1$ and $j_2$ to give J -referred to as the j-j coupling scheme -, or by adding $\ell_1$ and $\ell_2$ to L, $s_1$ and $s_2$ to S and finally couple L and S to give the total angular momentum J - referred to as the L-S coupling scheme. The basis vectors in these two coupling schemes are denoted by :

$$|(\ell_1 s_1)j_1(\ell_2 s_2)j_2 J\ M> \quad \text{and} \quad |(\ell_1\ell_2)L\ (s_1 s_2)S\ J\ M> \quad (62)$$

respectively, and the two sets of states are related through the unitary transformation :

$$|(\ell_1 s_1)j_1(\ell_2 s_2)j_2 J\ M> = \sum_{L,S} \begin{Bmatrix} \ell_1 & s_1 & j_1 \\ \ell_2 & s_2 & j_2 \\ L & S & J \end{Bmatrix} |(\ell_1\ell_2)L\ (s_1 s_2)S\ J\ M>, \quad (63)$$

where the transformation coefficient is known as the LS-jj transformation coefficient. Eqn (63) represents a special case of the problem of adding four angular momenta to a total angular momentum J :

$$j_1 + j_2 + j_3 + j_4 = J \quad (64)$$

Choosing two of the ways to recouple the four angular momenta (63) can be written as :

$$|(j_1 j_2)j_{12}(j_3 j_4)j_{34}JM> = \sum_{j_{13},j_{24}} \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & J \end{Bmatrix} |(j_1 j_3)j_{13}(j_2 j_4)j_{24}JM>. \quad (63a)$$

The unitary property of the recoupling transformation on four angular momenta implies the following orthogonality relation for these coefficients :

$$\sum_{j_{12},j_{34}} \begin{bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & J \end{bmatrix} \begin{bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j'_{13} & j'_{24} & J \end{bmatrix} = \delta(j_{13}, j'_{13})\ \delta(j_{24}, j'_{24}). \tag{65}$$

Wigner (1940) introduced the 9-j symbol which is related to the *ls-jj* transformation coefficient by the relation :

$$\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & J \end{Bmatrix} = \{[j_{12}][j_{34}][j_{13}][j_{24}]\}^{-1} \begin{bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & J \end{bmatrix}. \tag{66}$$

The *ls-jj* transformation coefficient can be expressed in terms of the Clebsch - Gordan coefficients by decoupling the state $|(j_1j_2)j_{12}(j_3j_4)j_{34}J\ M>$ in the defining relation (63a) into $|j_1m_1>|j_2m_2>|j_3m_3>|j_4m_4>$ and recoupling them suitably to form the state $|(j_1j_3)j_{13}(j_2j_4)j_{24}J\ M>$. This expresses the 9-j symbol as a product of six 3-j symbols summed over all the projection quantum numbers (Wigner (1940), Edmonds (1957)) :

$$\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & J \end{Bmatrix} = \sum_{\substack{\text{all} \\ m's}} \begin{pmatrix} j_1 & j_2 & j_{12} \\ m_1 & m_2 & m_{12} \end{pmatrix} \begin{pmatrix} j_3 & j_4 & j_{34} \\ m_3 & m_4 & m_{34} \end{pmatrix} \begin{pmatrix} j_{12} & j_{34} & J \\ m_{12} & m_{34} & M \end{pmatrix} \times$$

$$\times \begin{pmatrix} j_1 & j_3 & j_{13} \\ m_1 & m_3 & m_{13} \end{pmatrix} \begin{pmatrix} j_2 & j_4 & j_{24} \\ m_2 & m_4 & m_{24} \end{pmatrix} \begin{pmatrix} j_{13} & j_{24} & J \\ m_{13} & m_{24} & M \end{pmatrix}. \tag{67}$$

From (67) it is obvious that the nine angular momenta in the 9-j symbol satisfy the triangular inequalities implied by the six triads :

$\Delta(j_1j_2j_{12}), \Delta(j_3j_4j_{34}), \Delta(j_{12}j_{34}J), \Delta(j_1j_3j_{13}), \Delta(j_2j_4j_{24}), \Delta(j_{13}j_{24}J)$.

Further, of the nine projection quantum numbers only three are independent due to the relation (20) which exists among them.

Wigner (1940) (see also Edmonds (1957)) has shown that the

9-j symbol can also be expressed as a product of three 6-j symbols summed over a single index and this reads as :

$$\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & J \end{Bmatrix} = \sum_x (-1)^{2x}(2x+1)\begin{Bmatrix} j_1 & j_3 & j_{13} \\ j_{24} & J & x \end{Bmatrix} \begin{Bmatrix} j_2 & j_4 & j_{24} \\ j_3 & x & j_{34} \end{Bmatrix} \begin{Bmatrix} j_{12} & j_{34} & J \\ x & j_1 & j_2 \end{Bmatrix} \tag{68}$$

with
$$X_{min} \le x \le X_{max} ,$$
and
$$X_{min} = \max\ (|j_1-J|, |j_3-j_{24}|, |j_2-j_{34}|),$$
$$X_{max} = \min\ ( j_1+J\ ,\ j_3+j_{24}\ ,\ j_2+j_{34}\ ).$$

Relation (68) also follows from the fundamental theorem of recoupling theory ( Biedenharn and Louck (1981a)) according to which every recoupling coefficient ( 3n-j coefficient, n = 3,4,$\cdots$) is expressible as a summation over products of Racah coefficients. ( see also Biedenharn (1953)).

The symmetry properties of the 9-j symbol were discussed in detail by Jahn and Hope (1954). Wigner (1940) has indicated that the symmetries of the 9-j symbol can be obtained either from (68) or more easily from the symmetries of the 3-j symbols in (67). The symmetries of the 9-j coefficient are:

(i) An odd permutation of the columns of the 9-j symbol results in an odd column permutation of three of 3-j symbols, and hence the 9-j symbol acquires a phase factor of $(-1)^{\sigma}$, where $\sigma = j_1+j_2+j_3+j_4 +j_{12}+j_{34}+j_{13}+j_{24}+J$. An even permutation of the columns leaves the 9-j symbol invariant.

(ii) Due to similar reasons as in (i) above, the 9-j symbol is invariant under even permutations of the rows and acquires a phase factor of $(-1)^{\sigma}$ for odd row permutations.

(iii) A transposition of the 9-j symbol about its leading diagonal leaves it invariant.

Thus, the symmetry group of the 9-j coefficient has 72 elements, it being the product of the three permutation groups of three, three and two objects, viz. $S_3 \times S_3 \times S_2$ , respectively.

Eq.(68) for the 9-j symbol is independent of the projection quantum numbers but it represents a four-fold summation since each of the 6-j symbols is itself a single sum expansion. In literature there exists two other expansions for the 9-j symbol, each derived by different methods. One of them is a six-fold summation obtained by Wu (1972) on the basis of Bargmann's generating function approach. This is not of interest here. Another expression for the 9-j symbol is due to Jucys and Bandzaitis (1977) and who express the 9-j symbol as a triple sum series. This is the simplest known form for the 9- coefficient and it is:

$$\begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix} = (-1)^{x5} \frac{(d\ a\ g)\ (b\ e\ h)\ (i\ g\ h)}{(d\ e\ f)\ (b\ a\ c)\ (i\ c\ f)} \sum_{x,y,z} \frac{(-1)^{x+y+z}}{x!\ y!\ z!}$$

$$\times \frac{(x1 - x)!(x2 + x)!(x3 + x)!}{(x4 - x)!\ (x5 - x)!} \frac{(y1 + y)!\ (y2 + y)!}{(y3 + y)!(y4 - y)!(y5 - y)!}$$

$$\times \frac{(z1 - z)!\ (z2 + z)!}{(z3 - z)!(z4 - z)!(z5 - z)!} \frac{(P1 - y - z)!}{(P2 + x + y)!(P3 + x + z)!} \tag{69}$$

where

$$\begin{aligned} 0 \le x \le \min(-d + e + f\ ,\ c + f - i) = XF\ , \\ 0 \le y \le \min(g - h + i\ ,\ b + e - h) = YF\ , \\ 0 \le z \le \min(a - b + c\ ,\ a + d - g) = ZF\ , \end{aligned} \tag{70}$$

$$x1 = 2f,\ x2 = d+e-f,\ x3 = c-f+i,\ x4 = -d+e+f,\ x5 = c+f-i,$$
$$y1 = -b+e+h,\ y2 = g+h-i,\ y3 = 2h+1,\ y4 = b+e-h,\ y5 = g-h+i, \tag{71}$$
$$z1 = 2a,\ z2 = -a+b+c,\ z3 = a+d+g+1,\ z4 = a+d-g,\ z5 = a-b+c,$$
$$P1 = a+d-h+i,\ P2 = -b+d-f+h,\ P3 = -a+b-f+i,$$

and

$$(a\ b\ c) = \frac{(a + b + c + 1)!\ \Delta(a\ b\ c)}{(-a + b + c)!}. \tag{72}$$

It is pointed out that although (69) is the simplest known algebraic form for the 9-j symbol, *it does not show* any of the known symmetries of this coefficient. In Chapter 5, it will be established that the 9-j symbol can be computed more efficiently using this series representation and in Chapter 6, this triple series is used in the study of the polynomial zeros of the 9-j coefficient.

## 1.7 Multiplicative Diophantine Equations

Bell(1933) in his classic paper on *Reciprocal Arrays and Diophantine Analysis* categorised multiplicative Diophantine equations into seven types and obtained the solutions for them in terms of the minimum number of necessary and sufficient parameters. Of these the one which is of interest here is the homogeneous multiplicative Diophantine equation of degree n. A modified version of Bell's theorem which gives the complete solution to the problem of multiplicative Diophantine equations of degree n is stated below and a proof of this theorem which is simpler and straightforward than that due to Bell is provided.

Theorem 1 : Every solution of the homogeneous multiplicative Diophantine equation:

$$x_1 x_2 \cdots x_n = u_1 u_2 \cdots u_n, \quad (n > 1) \tag{73}$$

can be expressed in the form :

$$x_i = \prod_{j=1}^{n} \phi_{ij} \qquad \text{and} \qquad u_j = \prod_{i=1}^{n} \phi_{ij} \tag{74}$$

for all $i,j = 1,2,\cdots,n$, where the $n^2$ independent parameters $\phi_{ij}$ $(i,j = 1,2,\cdots,n)$ are positive integers which can be arranged as a $n \times n$ square array $A(\phi)$ with $\phi_{ij}$ being at the intersection of the i-th row and the j-th column, subject to the greatest common divisor (g.c.d.) conditions:

$$(x_i \, ,u_i \,) = \phi_{ii} \tag{75}$$

applying to only the diagonal elements of the array.

It is to be noted that this statement of the theorem differs from that of Bell in that the two arrays $A(\phi)$ and its reciprocal $A^R(\phi)$ of Bell (1933) have been replaced by the array $A(\phi)$ and its transpose. Hence the proof that is provided here *dispenses with the use of reciprocal arrays* in obtaining the required solutions. (Note: Given $A(\phi)$, its reciprocal $A^R(\phi)$ is obtained by arranging the diagonals of $A(\phi)$ as the rows of $A^R(\phi)$ - for details refer Bell (1933)).

To prove Theorem 1, it is first shown that it holds independently for n = 2 and 3 and then we complete the proof by induction. First consider the case n = 2. As usual, given any non-negative integers x and y, the g.c.d. of x and y is denoted by $(x,y)$; x divides y is denoted by $x|y$ in the sense that $y/x$ is an integer. For n = 2, (73) becomes:

$$x_1 \, x_2 = u_1 \, u_2 \, , \tag{76}$$

and to find its solutions, let $(x_1 \, ,u_1 \,) = z_1$, then $x_1 = z_1 z_2$

and $u_1 = z_1 z_3$ with

$$(z_2, z_3) = 1. \tag{77}$$

Substituting for $x_1$ and $u_1$ in (76) and cancelling $z_1$ gives:

$$x_2 z_2 = u_2 z_3 . \tag{78}$$

By virtue of (77) it follows that $z_2 | u_2$ and $z_3 | x_2$ so that $x_2 = z_3 z_4$ and $u_2 = z_2 z_5$. Now substituting for $x_2$ and $u_2$ in (78) and cancelling $z_2 z_3$ then gives $z_4 = z_5$. Noting (77) once again, comparison of $x_2$ and $u_2$ indicates that $(x_2, u_2) = z_4$. Summarizing, we have :

$$x_1 = z_1 z_2 , \quad x_2 = z_3 z_4 , \quad u_1 = z_1 z_3 , \quad u_2 = z_2 z_4 , \tag{79}$$

with the g.c.d.conditions :

$$(x_1, u_1) = z_1 \quad \text{and} \quad (x_2, u_2) = z_4 . \tag{80}$$

Thus the general solution of (76) is given by (79) and necessarily involves four parameters subject to the g.c.d. conditions (80). This solution may conveniently be displayed in the form of an array:

$$\begin{array}{c|cc} & u_1 & u_2 \\ \hline x_1 & z_1 & z_2 \\ x_2 & z_3 & z_4 \end{array} \quad = \quad \begin{array}{c|cc} & u_1 & u_2 \\ \hline x_1 & \phi_{11} & \phi_{12} \\ x_2 & \phi_{21} & \phi_{22} \end{array} \tag{81}$$

where we have relabeled $z_1$, $z_2$, $z_3$ and $z_4$ as $\phi_{11}$, $\phi_{12}$, $\phi_{21}$ and $\phi_{22}$, respectively and the products of the elements in the rows are $x_1$ and $x_2$ while the products of the elements in the columns are $u_1$ and $u_2$.

Following the above proof for $n = 2$, we give the proof for $n = 3$ when (73) becomes :

$$x_1 x_2 x_3 = u_1 u_2 u_3. \tag{82}$$

If $(x_1, u_1) = \alpha$ and $(x_2, u_2) = e$, then

$$x_1 = \alpha z_1 , \quad u_1 = \alpha z_2 \quad \text{with} \quad (z_1, z_2) = 1, \tag{83a}$$

and $$x_2 = e z_3 , \quad u_2 = e z_4 \quad \text{with} \quad (z_3, z_4) = 1. \tag{83b}$$

Substituting for $x_1$, $x_2$, $u_1$ and $u_2$ in (82) and cancelling $ae$, we have

$$z_1 \; z_3 \; x_3 \; = \; z_2 \; z_4 \; u_3 \; . \tag{84}$$

By virtue of (83) it follows that $z_1 | z_4 u_3$ and $z_2 | z_3 x_3$ so that:

$$z_4 \; u_3 \; = \; z_5 \; z_1 \quad \text{and} \quad z_3 \; x_3 \; = \; z_6 \; z_2 \; . \tag{85}$$

Substituting (85) in (84) yields : $z_5 = z_6$ . To solve the two Diophantine equations in (85), let:

$$(z_1 \; , z_4) = b \qquad \text{and} \qquad (z_2 \; , z_3) = d,$$

then $\quad z_1 = b\,c, \quad z_4 = b\,h \;$ and $\; z_2 = d\,g, \quad z_3 = d\,f$ , (86)

with $\quad (c \; , h) = 1 \;$ and $\; (f \; , g) = 1.$ (87)

Substituting (86) in (85), we get:

$$h \; u_3 = z_5 \; c \qquad \text{and} \qquad f \; x_3 = z_5 \; g \; . \tag{88}$$

Due to the relative prime conditions (87) , (88) imply:

$$h | z_5 \; , \quad c | u_3 \; , \qquad \text{and} \qquad f | z_5 \; , \quad g | x_3 \tag{89}$$

so that

$$z_5 = h \; \xi \; , \quad u_3 = c \; \xi' \quad \text{and} \quad z_5 = f \; \eta \; , \quad x_3 = g \; \eta' . \tag{90}$$

Substituting (90) in (88) we get $\xi = \xi'$ and $\eta = \eta'$. Use of the solutions for $z_1$, $z_2$, $z_3$, $z_4$ given by (86) in the relative prime conditions (83) satisfied by them gives :

$$(b\,c, \; d\,g) = 1 \quad \text{and} \quad (d\,f, \; b\,h) = 1.$$

Or, explicitly, we have :

$$(b \; , d) = (b \; , g) = (c \; , d) = (c \; , g) = 1,$$

and

$$(b \; , f) = (d \; , h) = (f \; , h) = 1. \tag{91}$$

Finally, from (91) since $z_5 = h\,\xi$ and $z_5 = f\,\eta$ , we have to solve the Diophantine equation :

$$h \; \xi = f \; \eta \quad \text{with} \quad (f \; , h) = 1. \tag{92}$$

Eq.(92) implies $h|\eta$ and $f|\xi$, or $\eta = h\,i$ and $\xi = f\,i'$, which on substituting into (92) yields $i = i'$. Therefore,

$$\eta = h\,i \qquad \text{and} \qquad \xi = f\,i \tag{93}$$

From (83), (86), (90) and (93), we have the solution to (82) as :

$$\begin{aligned} x_1 &= a\,b\,c\,, & u_1 &= a\,d\,g\,, \\ x_2 &= d\,e\,f\,, & u_2 &= b\,e\,h\,, \\ x_3 &= g\,h\,i\,, & u_3 &= c\,f\,i\,, \end{aligned} \tag{94}$$

with the three g.c.d. conditions :

$$(x_1, u_1) = a, \quad (x_2, u_2) = e \quad \text{and} \quad (x_3, u_3) = i. \tag{95}$$

The last of the g.c.d. conditions is a consequence of $(gh, cf) = 1$ obtained from (87) and (91), which on multiplying by $i$ yields, from (94) : $(x_3, u_3) = i$. These three g.c.d. conditions imply the nine relative prime conditions given in (87) and (91).

Renaming $a, b, c, \cdots, i$ as $\phi_{11}, \phi_{12}, \cdots, \phi_{33}$, the solution for n = 3 is given by the $3 \times 3$ array :

$$\begin{array}{c|ccc} & u_1 & u_2 & u_3 \\ \hline x_1 & \phi_{11} & \phi_{12} & \phi_{13} \\ x_2 & \phi_{21} & \phi_{22} & \phi_{23} \\ x_3 & \phi_{31} & \phi_{32} & \phi_{33} \end{array} \; . \tag{96}$$

Eq.(94) now read as

$$x_i = \prod_{j=1}^{3} \phi_{ij} \qquad \text{and} \qquad u_j = \prod_{i=1}^{3} \phi_{ij} \tag{97}$$

and (95) becomes :

$$(x_i, u_i) = \phi_{ii} \quad , \quad \text{for } i = 1,2,3. \tag{98}$$

Following Bell (1933), we call (73) as the Type I multiplicative Diophantine equation of degree n. Setting $u_3 = 1$ in (82) leads us to the lowest non-trivial inhomogeneous multiplicative Diophantine equation, called Type II by Bell, viz.:

$$x_1 \; x_2 \; x_3 \; = \; u_1 \; u_2 \; . \tag{99}$$

The solution for this equation can be simply obtained from that of the homogeneous equation (82) by setting $u_3 = 1$ in (96) which implies $\phi_{13} = \phi_{23} = \phi_{33} = 1$. Thus the solution to (99) is :

$$\begin{array}{c|cc} & u_1 & u_2 \\ \hline x_1 & \phi_{11} & \phi_{12} \\ x_2 & \phi_{21} & \phi_{22} \\ x_3 & \phi_{31} & \phi_{32} \end{array} \tag{100}$$

with the g.c.d. conditions given by :

$$(x_i \; , u_i \; ) = \phi_{ii} \; , \qquad \text{for} \quad i = 1,2. \tag{101}$$

Having derived the result for $n = 2$ and 3 for Type I and for $n = 3$, $m = 2$ for Type II multiplicative Diophantine equations, the Theorem 1 can be proved by induction from $n$ to $n+1$. To do so, assume (73) - (75) to hold for not only $n = 2,3$ but also for all values upto and including $n$, we shall prove that these hold for $n+1$ variables. Applying the theorem for $n = 2$ to :

$$(x_1 \; x_2 \; \cdots \; x_n \; ) \; x_{n+1} \quad = \quad (u_1 \; u_2 \; \cdots \; u_n \; ) \; u_{n+1}, \tag{102}$$

and let

$$(x_{n+1} \; , u_{n+1} \; ) = \lambda \tag{103}$$

be the g.c.d. condition. Then

$$x_{n+1} \; = \lambda \; x'_{n+1} \qquad \text{and} \quad u_{n+1} \; = \lambda \; u'_{n+1} \; ,$$

with

$$(x'_{n+1} \; , u'_{n+1}) = 1 \; . \tag{104}$$

Substituting $x_{n+1}$ and $u_{n+1}$ in (102) and cancelling $\lambda$ gives:

$$(x_1 \; x_2 \; \cdots \; x_n \; ) \; x'_{n+1} \quad = \quad (u_1 \; u_2 \; \cdots \; u_n \; ) \; u'_{n+1}. \tag{105}$$

By virtue of (104) it follows that $x'_{n+1} | (u_1 \; u_2 \; \cdots \; u_n \; )$ and $u'_{n+1} | (x_1 \; x_2 \; \cdots \; x_n)$ so that

$$u_1\ u_2\ \cdots\ u_n = \mu\ x'_{n+1} \qquad \text{and} \qquad x_1\ x_2\ \cdots\ x_n = \mu'\ u'_{n+1} . \quad (106)$$

Substituting (106) in (105) yields : $\mu = \mu'$. Hence, the two inhomogeneous equations to be solved are :

$$u_1\ u_2\ \cdots\ u_n = \mu\ x'_{n+1} \qquad \text{and} \qquad x_1\ x_2\ \cdots\ x_n = \mu\ u'_{n+1} \quad (107)$$

implying $(u_1\ u_2\ \cdots\ u_n\ ,\ x_1\ x_2\ \cdots\ x_n\ ) = \mu\ (x'_{n+1}\ ,u'_{n+1}\ ) = \mu$ .

The solutions of these equations are obtained from the corresponding homogeneous equation by setting the required u's (or x's) equal to one in (73) to (75). Omitting the degenerations of the form $(x,1) = 1$, the solutions for the inhomogeneous equations in (107) are given by :

$$\begin{array}{c|cc} & \mu & x'_{n+1} \\ \hline u_1 & \xi_{11} & \xi_{12} \\ u_2 & \xi_{21} & \xi_{22} \\ \vdots & \vdots & \vdots \\ u_n & \xi_{n1} & \xi_{n2} \end{array} \qquad \text{with} \qquad \begin{array}{l} (u_1\ ,\mu\ ) = \xi_{11}\ , \\ (u_2\ ,x'_{n+1}) = \xi_{22} . \end{array} \quad (108)$$

and

$$\begin{array}{c|cc} & \mu & u'_{n+1} \\ \hline x_1 & \nu_{11} & \nu_{12} \\ x_2 & \nu_{21} & \nu_{22} \\ \vdots & \vdots & \vdots \\ x_n & \nu_{n1} & \nu_{n2} \end{array} \qquad \text{with} \qquad \begin{array}{l} (x_1\ ,\mu\ ) = \nu_{11}\ , \\ (x_2\ ,u'_{n+1}\ ) = \nu_{22} . \end{array} \quad (109)$$

From (108) and (109) we have :

$$\mu = \xi_{11}\ \xi_{21}\ \cdots\ \xi_{n1} = \nu_{11}\ \nu_{21}\ \cdots\ \nu_{n1} . \quad (110)$$

Eq.(110) is a homogeneous multiplicative Diophantine equation of degree n whose solution is known to be :

$$
\begin{array}{c|cccc}
 & \xi_{11} & \xi_{21} & \cdots & \xi_{n1} \\
\hline
\nu_{11} & \phi_{11} & \phi_{12} & \cdots & \phi_{1n} \\
\nu_{21} & \phi_{21} & \phi_{22} & \cdots & \phi_{2n} \\
\vdots & \vdots & \vdots & \cdots & \vdots \\
\nu_{n1} & \phi_{n1} & \phi_{n2} & \cdots & \phi_{nn}
\end{array}
\quad \text{with } (\xi_{i1}, \nu_{i1}) = \phi_{ii}. \qquad (111)
$$

Therefore, the solution of (102) is given by :

$$
\begin{array}{c|ccccc}
 & u_1 & u_2 & & u_n & u_{n+1} \\
\hline
x_1 & \phi_{11} & \phi_{12} & \cdots & \phi_{1n} & \nu_{12} \\
x_2 & \phi_{21} & \phi_{22} & \cdots & \phi_{2n} & \nu_{22} \\
\vdots & \vdots & \vdots & \cdots & \vdots & \vdots \\
x_n & \phi_{n1} & \phi_{n2} & \cdots & \phi_{nn} & \nu_{n2} \\
x_{n+1} & \xi_{12} & \xi_{22} & \cdots & \xi_{n2} & \lambda
\end{array}
\quad \text{with } \begin{array}{l} (x_i, u_i) = \phi_{ii}, \\ (x_{n+1}, u_{n+1}) = \lambda. \end{array} \qquad (112)
$$

Relabelling the (2n+1) parameters $\nu_{12}, \nu_{22}, \cdots, \nu_{n2}$ ; $\lambda$ ; $\xi_{12}$, $\xi_{22}$, $\cdots$ ,$\xi_{n2}$ as $\phi_{1,n+1}$, $\phi_{2,n+1}$, $\cdots$, $\phi_{n,n+1}$; $\phi_{n+1,n+1}$ ; $\phi_{n+1,1}$, $\phi_{n+1,2}$, $\cdots$ ,$\phi_{n+1,n}$ ,respectively, we can write the solution for the homogeneous Type I multiplicative Diophantine equation of degree n+1 by simply replacing the index n by n+1 in (73) - (75). This completes the proof of the Theorem 1 by induction.

The other types of multi plicative Diophantine equations have been dealt with in Srinivasa Rao, Santhanam and Rajeswari (1987) and they are not dealt with in this Thesis since they are not directly relevant to its contents. The above proved Theorem 1 is used in the study of the polynomial zeros of degree 1 of the 3-j, 6-j and 9-j coefficients in the following chapters.

## Chapter 2

## Interrelationships between the sets of ${}_pF_q(1)$s for the 3-j and the 6-j coefficients.

### 2.1 Introduction

In the previous Chapter the four fundamental forms - viz. the Wigner, Racah, van der Waerden and Majumdar forms - known in literature for the 3-j coefficient were given. It was shown that there exist a set of six series representations for the 3-j coefficient corresponding to the van der Waerden's form. In the case of the 6-j coefficient two sets of series representations were also written down.

In this Chapter the two transformation formulae for terminating hypergeometric series of unit argument required for use later on are recalled. One of them pertains to the reversal of a terminating hypergeometric series of unit argument of the type ${}_{p+1}F_p$ and the other is a transformation between two terminating ${}_3F_2(1)$s due to Erdelyi and Weber (1952). It is shown that the set of six ${}_3F_2(1)$s for the 3-j coefficient can all be generated by starting with one of them and using repeatedly the reversal relation for a ${}_3F_2(1)$. This same reversal relation is shown to connect the set I and set II of ${}_4F_3(1)$s for the 6-j coefficient.Using the Erdelyi-Weber transformation for a ${}_3F_2(1)$ the Wigner, Racah and Majumdar forms of the 3-j coefficient are derived from the vander Waerden's form. The asymmetric nature of these three forms in comparison to the van der Waerden's form is discussed.

## 2.2 Mathematical Formulae

### (a) Reversal of a terminating hypergeometric series

As stated earlier in Chapter 1, when one of the numerator parameters in a hypergeometric series is negative, say $-n$, the series terminates with $(n+1)$ terms. When more than one numerator parameter is negative, the one whose magnitude is the smallest determines the number of terms. In such cases the series can be summed in reverse order and the result identified with a different hypergeometric series. The property of reversal of series of a terminating ${}_{p+1}F_p(1)$ can be obtained as follows:

Let $${}_{p+1}F_p((a_p),-n;(b_p);1) = \sum_{r=0}^{n} \frac{((a_p),r)(-n,r)}{(1,r)((b_p),r)}, \tag{1}$$

where one of the numerator parameters is a negative integer. When the series is summed in reverse order, the last term becomes the first term and so on. Hence the series can also be written as:

$${}_{p+1}F_p((a_p),-n;(b_p);1) = \sum_{r=0}^{n} \frac{((a_p),n-r)(-n,n-r)}{(1,n-r)((b_p),n-r)}. \tag{2}$$

Using the identities (Slater (1965)) satisfied by the Pochammer symbols :

$$(a,n-r) = (-1)^r(a,n)/(1-a-n,r), \tag{3}$$

$$1/(n-r)! = (-1)^r(-n,r)/n!, \tag{4}$$

$$(-a,n) = (-1)^n a!/(a-n)!, \tag{5}$$

the right hand side of (2) can be rewritten as:

$$(-1)^n\frac{((a_p),n)}{((b_p),n)} \sum_{r=0}^{n} \frac{((1-(b_p)-n),r)\ (-n,r)}{(1,r)\ (1-(a_p)-n),r)}. \tag{6}$$

Hence we get the reversal of series property as:

$$ {}_{p+1}F_p((a_p),-n;(b_p);1) = (-1)^n \frac{((a_p),n)}{((b_p),n)} \; {}_{p+1}F_p\left[\begin{matrix} 1-(b_p)-n\ ,-n \\ 1-(a_p)-n \end{matrix};1\right] \tag{7} $$

In (7) it is straightforward to verify that if the hypergeometric series on the left hand side is a Saalschutzian then the one that is obtained on reversal is also Saalschutzian.

**(b) The Erdelyi-Weber (or E-W) (1952) transformation**

In this section a transformation formula between two terminating ${}_3F_2(1)$s is recalled. This is one of a large group of known transformations (cf. Bailey(1935)) and the proof given by Erdelyi and Weber runs along the following lines: Let

$$ {}_3F_2(-n,\alpha,\beta;\gamma,\delta;1) = \frac{\Gamma(\delta)}{\Gamma(\beta,\delta-\beta)} \int_0^1 {}_2F_1(-n,\alpha;\gamma;t)\ t^{\beta-1}(1-t)^{\delta-\beta-1}\ dt \tag{8} $$

which can be checked easily by expanding both sides in power series. The well-known identity:

$$ {}_2F_1(-n,\alpha;\gamma;t) = \frac{\Gamma(\gamma,\gamma+n-\alpha)}{\Gamma(\gamma+n,\gamma-\alpha)}\ {}_2F_1(-n,\alpha;\alpha-n-\gamma+1;1-t), \tag{9} $$

is used for the ${}_2F_1$ in (8), and the right hand side of (8) becomes:

$$ {}_3F_2(-n,\alpha,\beta;\gamma,\delta;1) = \frac{\Gamma(\delta,\gamma,\gamma+n-\alpha)}{\Gamma(\beta,\delta-\beta,\gamma+n,\gamma-\alpha)} \int_0^1 {}_2F_1(-n,\alpha;\alpha-n-\gamma+1;1-t) \times t^{\beta-1}(1-t)^{\delta-\beta-1}dt. \tag{10} $$

Changing the variable of integration to :

$$ t' = (1-t)\ , \tag{11} $$

eqn.(10) can be rewritten as:

$$ {}_3F_2(-n,\alpha,\beta;\gamma,\delta;1) = \frac{\Gamma(\delta,\gamma,\gamma+n-\alpha)}{\Gamma(\beta,\delta-\beta,\gamma+n,\gamma-\alpha)} \int_0^1 {}_2F_1(-n,\alpha;\alpha-n-\gamma+1;t) \times (1-t')^{\beta-1}(t')^{\delta-\beta-1}\ dt'. \tag{12} $$

Now using (8) once again to identify the integral with a ${}_3F_2(1)$ the following transformation formula is obtained:

$$ {}_3F_2(-n,\alpha,\beta;\gamma,\delta;1) = \frac{\Gamma(\gamma,\gamma+n-\alpha)}{\Gamma(\gamma+n,\gamma-\alpha)}\ {}_3F_2(-n,\alpha,\delta-\beta;1+\alpha-\gamma-n,\delta;1). \quad (13) $$

The above transformation can, infact, be derived from the Tables II A and II B in Bailey (1935) which summarize and group the equivalent numerator and denominator parameters of ${}_3F_2(1)$s obtained by Thomae in the notation introduced by Whipple in 1923. Explicitly, in this notation, (13) corresponds to :

$$ F_p(0;4,5) = (-1)^m \frac{\Gamma(\alpha_{124},\alpha_{024},\alpha_{014})}{\Gamma(\alpha_{123},\alpha_{124},\alpha_{125})} F_n(4;01). $$

**2.3 Reversal of series applied to the sets of hypergeometric series for the 3-j and the 6-j coefficients**

It can now be established that the set of six ${}_3F_2(1)$s for the 3-j coefficient given in chapter-1, can also be generated by starting with one of them and applying the reversal relation (7) repeatedly. Further the set I and set II of ${}_4F_3(1)$s for the 6-j coefficient can be shown to be related by this same relation (7).

(a) The 3-j coefficient was expressed in terms of a set of six ${}_3F_2(1)$s (Srinivasa Rao 1978) in chapter 1 as :

$$ \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \delta(m_1+m_2+m_3,0)(-1)^{\theta(pqr)} \prod_{i,k=1}^{3} \{R_{ik}!/(J+1)!\}^{1/2} $$

$$ \times\ \{\Gamma(1-A,1-B,1-C,D,E)\}^{-1}\ {}_3F_2(A,B,C;D,E;1), \quad (14) $$

where

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

for all permutations of $(p\ q\ r) = (1\ 2\ 3)$,

$$ \theta(pqr) = \begin{cases} R_{3p}-R_{2q} & \text{for even permutations,} \\ R_{3p}-R_{2q}+J & \text{for odd permutations.} \end{cases} \quad (15) $$

and $$\Gamma(X,Y,\cdots) = \Gamma(X)\,\Gamma(Y)\cdots.$$

The $R_{jk}$'s are the elements of the Regge (1958) array :

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \left\| \begin{array}{ccc} -j_1+j_2+j_3 & j_1-j_2+j_3 & j_1+j_2-j_3 \\ j_1-m_1 & j_2-m_2 & j_3-m_3 \\ j_1+m_1 & j_2+m_2 & j_3+m_3 \end{array} \right\| . \tag{16}$$

The reversal relation (7) (corresponding to p = 2) is applied to the ${}_3F_2(1)$ in the series representation (14) for (p q r) = (1 2 3). Since all the numerator parameters in the ${}_3F_2(1)$ are negative integers (we exclude the possibility of one or more of the numerator parameters being zero since in that case the ${}_3F_2(1)$ reduces to unity), $-n$ in (7) could be identified as $(-j_1+m_1)$ or $(-j_1-j_2+j_3)$ or $(-j_2-m_2)$, depending upon whether $(j_1-m_1)$ or $(j_1+j_2-j_3)$ or $(j_2+m_2)$ determines the number of terms in the ${}_3F_2(1)$. For example setting:

$$n = (j_1 - m_1)$$

the transformation (7) looks as follows:

$$\begin{aligned} &{}_3F_2(-j_1+m_1,-j_2-m_2,-j_1-j_2+j_3;1-j_1+j_3-m_2,1-j_2+j_3+m_1;1) \\ &\quad = (-1)^{j_1-m_1}\,\Gamma(1+j_2+m_2,1+j_1+j_2-j_3,1-j_1+j_3-m_2,1-j_2+j_3+m_1) \\ &\qquad \times \{\Gamma(1+j_2-j_1-m_3,1+j_2-j_3+m_1,1+j_3+m_3,1+j_1-j_2+j_3)\}^{-1} \\ &\qquad \times {}_3F_2(-j_1+m_1,-j_3-m_3,-j_1+j_2-j_3;1-j_1+j_2-m_3,1+j_2-j_3+m_1;1). \end{aligned} \tag{17}$$

In writing (17) use has been made of relation (5), whenever a Pochammer symbol involves a negative integer in its argument. Substituting (17) for the ${}_3F_2(1)$ in (14) corresponding to (p q r)= (1 2 3) it is straightforward to see that this yields the series representation for the 3-j coefficient for (p q r) = (1 3 2).

Similarly the identifications:

$$n = (j_2 + m_2) \quad\text{and}\quad n = (j_1 + j_2 - j_3) ,$$

in the ${}_3F_2(1)$ for (p q r) = (1 2 3) lead respectively to the series representations corresponding to (p q r) = (3 2 1) and (p q r) = (2 3 1). It is to be noted that each one of the three ${}_3F_2(1)$s obtained in the above manner has two more negative integers in their numerator parameter set and hence the transformation (7) could be applied in those cases also. In all these cases we are led to the series representations corresponding to (p q r) = (3 1 2) and (p q r) = (2 1 3). Hence starting from one of the series representations and applying (7) repeatedly we generate the set of six series representations of the 3-j coefficient.

(b) In the case of the 6-j coefficient, the set I of three series representations given in Chapter 1 when written explicitly are:

$$W(abcd;ef) = (-1)^{E+1}\, N\, \Gamma(1-E)\, \{\Gamma(1-A,1-B,1-C,1-D,F,G)\}^{-1} \times {}_4F_3(A,B,C,D;E,F,G;1), \tag{18}$$

where A, B, C, D, E, F & G for the three cases are:

(i) $A = e-a-b,\ B = e-c-d,\ C = f-a-c,\ D = f-b-d,$
$E = -a-b-c-d-1,\ F = e+f-a-d+1,\ G = e+f-b-c+1.$ (19)

(ii) $A = b-a-e,\ B = c-d-e,\ C = c-a-f,\ D = b-d-f,$
$E = -a-d-e-f-1,\ F = b+c-e-f+1,\ G = b+c-a-d+1.$ (20)

(iii) $A = a-b-e,\ B = d-c-e,\ C = a-c-f,\ D = d-b-f,$
$E = -b-c-e-f-1,\ F = a+d-e-f+1,\ G = a+d-b-c+1.$ (21)

The set II of four series representations are:

$$W(abcd;ef) = (-1)^{A'-2}\, N\, \Gamma(A')\, \{\Gamma(1-B',1-C',1-D',E',F',G')\}^{-1} \times {}_4F_3(A',B',C',D';E',F',G';1)\ , \tag{22}$$

with the parameters A', B', C', D', E', F' & G' for the four series being given by:

(i) $A' = a+b+e+2,\ B' = a-c-f,\ C' = b-d-f,\ D' = e-c-d,$

$$E' = a+b-c-d+1,\ F' = a+e-d-f+1,\ G' = b+e-c-f+1. \tag{23}$$

(ii) $A' = c+d+e+2,\ B' = c-a-f,\ C' = d-b-f,\ D' = e-a-b,$

$$E' = c+d-a-b+1,\ F' = c+e-b-f+1,\ G' = d+e-a-f+1. \tag{24}$$

(iii) $A' = a+c+f+2,\ B' = c-d-e,\ C' = a-b-e,\ D' = f-b-d,$

$$E' = a+c-b-d+1,\ F' = a+f-d-e+1,\ G' = c+f-b-e+1. \tag{25}$$

(iv) $A' = b+d+f+2,\ B' = b-a-e,\ C' = d-c-e,\ D' = f-a-c,$

$$E' = b+d-a-c+1,\ F' = b+f-c-e+1,\ G' = d+f-a-e+1. \tag{26}$$

The transformation (7) (for p=3) is now applied to the ${}_4F_3(1)$ in the set I of series representations - say eqn.(18) - with the parameters given by (19). Since all the numerator parameters in the ${}_4F_3(1)$ are negative integers, the one whose magnitude is the minimum determines the number of terms. Assuming:

$$n = c + d - e \tag{27}$$

in (7) the transformation reads as:

$${}_4F_3\left[\begin{matrix}e-a-b,\ e-c-d,\ f-a-c,\ f-b-d\ ;\ 1\\ -a-b-c-d-1, e+f-a-d+1, e+f-b-c+1\end{matrix}\right] =$$

$$= (-1)^{c+d-e}\ \Gamma(1+a+b-e, 1+a+c-f, 1+b+d-f, a+b+e+2, e+f-a-d+1,$$

$$e+f-b-c+1)\ \{\Gamma(1+a+b-c-d, 1+a+e-d-f, 1+b+e-c-f, a+b+c+d+2,$$

$$1+c+f-a, 1+d+f-b)\}^{-1}\ {}_4F_3\left[\begin{matrix}a+b+e+2, a-c-f, b-d-f, e-c-d;\ 1\\ a+b-c-d+1, a+e-d-f+1, b+e-c-f+1\end{matrix}\right]. \tag{28}$$

In writing (28), relation (5) has been used wherever necessary. Substituting (28) in (18) automatically leads to one of the series representations belonging to set II viz. that given by eqn.(22) with the parameters given by (23). The identification in (27) corresponds to assuming that B determines the number of terms in the ${}_4F_3(1)$ given by (19). Instead, one could consider the cases when A, C or D determines the number of terms. In each case application of the transformation (7) leads to one of the series representations belonging to set II.

A similar result holds for the ${}_4F_3(1)$s given by (20) and (21) also. In Table 1 the actual correspondence between the set I and set II of series representations on reversal, is given.

Similarly, starting with one of the series representations of set II and applying (7) to the ${}_4F_3(1)$ leads to one of the series belonging to set I. In this case each ${}_4F_3(1)$ has three of its numerator parameters -viz. B′, C′ & D′ - negative and hence each one of them could be assumed to determine the number of terms in ${}_4F_3(1)$. The results in this case are given in Table 2.

Therefore, the set I and set II of series representations for the 6-j coefficient are not independent and are simply related by the reversal of series of the terminating ${}_4F_3(1)$.

**2.4 The interrelationship between the four fundamental forms of the 3-j coefficient**

In Chapter 1 four different forms for the 3-j coefficient which exist in literature - viz. the ones given by Racah (1942), Wigner (1940), van der Waerden (1932) and Majumdar (1958), were given. The van der Waerden's form was dealt with in detail in that chapter. The other three forms when rewritten in terms of a ${}_3F_2(1)$, using the methods described in the previous chapter are as follows. The Racah's form is given by:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \delta(m_1+m_2+m_3,0)\,(-1)^{2j_1-j_2+m_2} \prod_{i,k=1}^{3} \{R_{ik}!/(J+1)!\}^{1/2}$$
$$\times\,\Gamma(1+j_2+j_3-m_1)\,\{\Gamma(1+j_2-j_3+m_1,1-j_1+j_2+j_3,$$
$$1+j_1-j_2+j_3,1+j_1-m_1,1+j_2+m_2,1+j_3+m_3)\}^{-1}$$
$$\times\,{}_3F_2(1+j_1+m_1,-j_3-m_3,-j_1+m_1;-j_2-j_3+m_1,1+j_2-j_3+m_1;1). \tag{29}$$

The Wigner's form becomes:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \delta(m_1+m_2+m_3,0)\,(-1)^{2j_2-j_1-m_1} \prod_{i,k=1}^{3} \{R_{ik}!/(J+1)!\}^{1/2}$$

$$\times\, \Gamma(1+j_2+j_3+m_1)\,\{\Gamma(1+j_1-j_2+m_3,\, 1-j_1+j_2+j_3,$$

$$1+j_3-m_3,\, 1+j_2-m_2,\, 1+j_2+m_2,\, 1+j_1+m_1)\}^{-1}$$

$$\times\, {}_3F_2(1+j_1-m_1, -j_3+m_3, j_1-j_2-j_3; -j_2-j_3-m_1, 1+j_1-j_2+m_3; 1) \tag{30}$$

and the Majumdar's form is rewritten as:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \delta(m_1+m_2+m_3,0)\,(-1)^{2j_2-j_1-m_1} \prod_{i,k=1}^{3} \{R_{ik}!/(J+1)!\}^{1/2}$$

$$\times\, \Gamma(2j_3+1)\,\{\Gamma(1+j_1-j_3-m_2,\, 1-j_1+j_2+j_3,$$

$$1+j_1-j_2+j_3,\, 1+j_3-m_3,\, 1+j_2+m_2,\, 1+j_3+m_3)\}^{-1}$$

$$\times\, {}_3F_2(1+j_1+j_2-j_3, -j_3+m_3, j_1-j_2-j_3; -2j_3, 1+j_1-j_3-m_2; 1). \tag{31}$$

In literature, these ${}_3F_2(1)$s have been referred to by Smorodinskii and Shelepin (1972). It will be shown that the Racah, Wigner and Majumdar forms given by eqns.(29), (30) and (31) can be obtained from the van der Waerden's form by using the Erdelyi-Weber transformation eqn.(13) for the ${}_3F_2(1)$ and that each one of these series is in fact one member of a set of six such series representations.

Identifying the numerator and denominator parameters of the $F(1)$ in the van der Waerden's form as:

$$\alpha = A,\ \beta = B,\ n = -C,\ \gamma = D \text{ and } \delta = E\ , \tag{32}$$

and applying the E-W transformation leads to:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \delta(m_1+m_2+m_3,0)\,(-1)^{\theta(pqr)} \prod_{i,k=1}^{3} \{R_{ik}!/(J+1)!\}^{1/2}$$

$$\times\, \Gamma(1-D')\{\Gamma(1-A', 1+B'-E', 1-C', E', 1+A'-D', 1+C'-D')\}^{-1}$$

$$\times\, {}_3F_2(A', B', C'; D', E'; 1), \tag{33}$$

where

$A' = -R_{2p}$, $B' = 1+R_{2r}$, $C' = -R_{1r}$, $D' = -R_{1r}-R_{3r}$, $E' = R_{2r}-R_{3q}+1$ . (34)

This set of ${}_3F_2(1)$s will be called as the Wigner set of ${}_3F_2(1)$s, since, in (34), setting (p q r) = (3 2 1) results in the Wigner form of the 3-j coefficient given by (30).

Alternatively, identifyng the parameters in (14) as:

$$\alpha = A,\ \beta = C,\ n = -B,\ \gamma = D \text{ and } \delta = E\ , \tag{35}$$

and using the E-W transformation (13) yields for the 3-j coefficient, the form (33), but the numerator and denominator parameters of the ${}_3F_2(1)$ will now be:

$A' = -R_{2p}$, $B' = 1+R_{3p}$, $C' = -R_{3q}$, $D' = -R_{3q} - R_{3r}$, $E' = 1+R_{2r} - R_{3q}$. (36)

This set will be called the Racah set of ${}_3F_2(1)$s, since in identifying (p q r) = (1 3 2), the Racah form of the 3-j coefficient, viz, (29) can be obtained. Biedenharn and Louck (1981a) in their treatise point out that Racah's form may be obtained from Wigner's form by using the two transformations that arise due to interchanging the second and third rows of (15) followed by the interchange of the first and second rows of (15).

Finally, a third identification for the parameters in (14) as:

$$\alpha = A,\ \beta = B,\ n = -C,\ \gamma = E \text{ and } \delta = D\ , \tag{37}$$

and use of (13) will yield for the 3-j coefficient the form (33) with the numerator and denominator parameters given by:

$A' = -R_{2p}$, $B' = 1+R_{1p}$, $C' = -R_{1r}$, $D' = -R_{2p}-R_{3p}$, $E' = 1 + R_{3r}-R_{2p}$. (38)

This set of ${}_3F_2(1)$s will be called the Majumdar set, since for (p q r) = ( 3 2 1) the Majumdar form of the 3-j coefficient given by (31) is obtained.

Thus, it is found that starting with the highly symmetric van der Waerden set of ${}_3F_2(1)$s, three sets of ${}_3F_2(1)$s corresponding to Wigner, Racah and Majumdar forms can be obtained by simply using the Erdelyi-Weber transformation in three different ways. Conversely, the same E-W transformation can be used to get the van der Waerden set from the Wigner, Racah or Majumdar sets, by virtue of the fact that the matrix relating the numerator and denominator parameters in (13) acts like a projection operator.

In fact, in (14), three more identifications can be made for the parameters as:

$$\alpha = B,\ \beta = A,\ n = -C,\ \gamma = E \text{ and } \delta = D, \tag{39}$$

or

$$\alpha = B,\ \beta = C,\ n = -B,\ \gamma = E \text{ and } \delta = D\ , \tag{40}$$

or

$$\alpha = B,\ \beta = A,\ n = -C,\ \gamma = D \text{ and } \delta = E\ . \tag{41}$$

The numerator and denominator parameters of the resulting ${}_3F_2(1)$ in these three cases viz. (39), (40) and (41) are given by:

$$A' = -R_{3q},\ B' = 1+R_{3r},\ C' = -R_{1r},\ D' = -R_{1r}-R_{2r},\ E' = 1+R_{3r}-R_{2p}\ , \tag{42}$$

$$A' = -R_{2p},\ B' = 1+R_{2q},\ C' = -R_{3q},\ D' = -R_{2p}-R_{2r},\ E' = 1+R_{3r}-R_{2p}\ , \tag{43}$$

and

$$A' = -R_{3q},\ B' = 1+R_{1q},\ C' = -R_{1r},\ D' = -R_{2q}-R_{3q},\ E' = 1+R_{2r}-R_{3q}\ . \tag{44}$$

Hence eqns. (42), (43) and (44) would once again generate the Wigner, Racah and Majumdar sets of series representations on which is superposed the $m_i \to -m_i$ tramsformation. Raynal (1978) has shown that, starting with a given ${}_3F_2(1)$ belonging to the van der

Waerden set and resorting to the work of Whipple (1925) on the symmetries of the ${}_3F_2(1)$ functions, the Racah, Wigner and Majumdar forms can be obtained.

It should be pointed out that,

$$(p\ q\ r) = (1\ 3\ 2) \text{ in } (34),$$
$$(p\ q\ r) = (1\ 3\ 2) \text{ in } (36), \quad (45)$$
and
$$(p\ q\ r) = (3\ 2\ 1) \text{ in } (44),$$
correspond to eqns. (28) , (29) and (30) of Raynal (1978) respectively.

It is to be noted that in the van der Waerden set of ${}_3F_2(1)$s all the three numerator parameters are negative integers and both the denominator parameters are positive integers. Hence in this case the 3! permutations of the numerator parameters are all allowed and lead to meaningful symmetries of the 3-j coefficient so that the van der Waerden set accounts for all the known 72 symmetries of this coefficient. But in the case of the Wigner, Racah and Majumdar sets of ${}_3F_2(1)$s two of the numerator parameters (A′ and C′) are negative integers and the other (B′) is a positive integer. Among the denominator parameters one (D′) is a negative integer and the other (E′) is a positive integer. In these cases the only permutation which leads to a meaningful symmetry is that of the two numerator parameters which are negative integers. Permutation of a positive parameter with a negative parameter does not lead to any known symmetry of the 3-j coefficient. For example, in the Wigner ${}_3F_2(1)$, (34), corresponding to (p q r) = ( 1 3 2), interchange of B′ and C′ results in the 3-j coefficient being related to:

$$\begin{bmatrix} (j_1-j_3+m_2-1)/2 & j_2 & (-j_1+j_3+m_2-1)/2 \\ m_1+(-j_1-j_3+m_2-1)/2 & j_1+j_3+1 & m_3+(-j_1-j_3+m_2-1)/2 \end{bmatrix}, \quad (46)$$

which though appears like a Regge symmetry, can be shown to violate the triangular inequality. Thus, the only allowed symmetries in the Wigner, Racah and Majumdar sets of ${}_3F_2(1)$s are those due to the interchange of A′ and C′, as is manifestly evident in (33) and hence these sets account only for 12 of the 72 symmetries of the 3-j coefficient. The asymmetric nature of these forms has been realised by Racah (1942) himself which is reflected in his statement that his formula "is similar to Wigner's formula and is, also, unsymmetrical and unpractical for the use".

## 2.5 Conclusion

To conclude, the results obtained in this chapter are the following:

(i) The van der Waerden set of ${}_3F_2(1)$s for the 3-j coefficient has been shown to be generated by starting with one of them and applying the reversal of a terminating hypergeometric series repeatedly.

(ii) The same reversal relation has been shown to relate the set-I and set-II of ${}_4F_3(1)$s for the 6-j coefficient. (Srinivasa Rao and Rajeswari (1985b)).

(iii) It has been shown that the Wigner, Racah and Majumdar sets of ${}_3F_2(1)$s for the 3-j coefficient can be obtained from the symmetric van der Waerden form by the use of the Erdelyi-Weber transformation for a terminating ${}_3F_2(1)$. (Srinivasa Rao and Rajeswari (1989)).

**Table 1**

The correspondence between set I and set II of ${}_4F_3(1)$s under reversal.

| Eq. no. of series belonging to set I | No. of terms determined by | Eq. no. of series belonging to set II |
|---|---|---|
| (19) | A | (24) |
| | B | (23) |
| | C | (26) |
| | D | (25) |
| (20) | A | (26) |
| | B | (25) |
| | C | (24) |
| | D | (23) |
| (21) | A | (25) |
| | B | (26) |
| | C | (23) |
| | D | (24) |

**Table 2**

The correspondence between set I and set II of ${}_4F_3(1)$s under reversal.

| Eq. no. of series belonging to set II | No. of terms determined by | Eq. no. of series belonging to set I |
|---|---|---|
| (23) | B′ | (21) |
| | C′ | (20) |
| | D′ | (19) |
| (24) | B′ | (20) |
| | C′ | (21) |
| | D′ | (19) |
| (25) | B′ | (20) |
| | C′ | (21) |
| | D′ | (19) |
| (26) | B′ | (20) |
| | C′ | (21) |
| | D′ | (19) |

Chapter 3

# Polynomial zeros of the 3-j coefficient

## 3.1 Introduction

The 3-j coefficients play an important role in the study of all quantum mechanical phenomena. The vanishing of these coefficients have physical significance in that they imply selection rules for certain transitions. In this chapter after mentioning what the *polynomial* (or,*non-trivial*) zeros of the 3-j coefficient are, the canonical parameters for this coefficient given by Bryant and Jahn (1960), as quoted by Bowick (1976), are discussed. The 3-j coefficient is rewritten into a formal binomial expansion and using it a closed form expression is written down for the polynomial zeros of degree one of this coefficient. The parametric formula derived by Brudno (1985) for these zeros in terms of four integral parameters is disucssed and using Bell's theorem it is established that this four parameter formula gives the complete solution to the polynomial zeros of degree one of the 3-j coefficient.

## 3.2 Polynomial zeros of the 3-j coefficient

It was mentioned in chapter 1 that the 3-j coefficient vanishes if the angular momenta $(j_1, j_2, j_3)$ do not satisfy the triangular inequality; or, if the projection quantum numbers $m_1, m_2, m_3$ do not add to zero. The zeros which arise in these cases are called trivial zeros. On the other hand, there exist zeros of this coefficient for allowed values of the angular momenta and projection quantum numbers too. These are termed as the *polynomial* (or,*non-trivial*) zeros which were tabulated for the first time by

Varshalovich, Moskalaev and Kersonskii (1975) for $(j_1+ j_2+ j_3) = J \leq 27$. Bowick (1976) reduced this list by eliminating the *classical* as well as Regge symmetries (Regge 1958) of this coefficient. The method adopted by Bowick (1976) to distinguish the *equivalent* 3-j coefficient from the *inequivalent* ones is described below.

**3.3 Canonical parameters for the 3-j coefficient**

Since the 3-j coefficient possesses 72 symmetries it is clear that it belongs to a set of 72 each of which has the same numerical value (differing at most by a phase factor). The elements of this set are called *equivalent* 3-j coefficients, though the ones that are related by Regge symmetries may have all the arguments to be different unlike those elements which are related by the *classical* symmetries. Hence to distinguish between the *equivalent* and *inequivalent* ones, it is necessary to have a set of parameters which would be the same for all the *equivalent* ones and different for the *inequivalent* ones. For this purpose Bowick (1976) used the integral parametrisation developed by Bryant and Jahn (1960). These integral parameters are obtained as follows:

Given a 3-j coefficient :

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \quad \text{with} \quad J = j_1+j_2+j_3 \ ,$$

one forms the symbol :

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}_r \ ,$$

with $r = J - 2j_3 = j_1+j_2-j_3$, $a + r = j_1-m_1$, $b + r = j_2+m_2$,

$$c + r = j_1+m_1, \quad d + r = j_2-m_2 \ , \tag{1}$$

and using known symmetry properties of this symbol orders it in such a way that :

$$a \geq b \geq 0, \quad c \geq d \geq 0, \tag{2}$$

$$(a + b) \geq (c + d), \tag{3}$$

and
$$(a - b) \geq (c - d) \text{ if } (a + b) = (c + d). \tag{4}$$

With the symbol brought into this final standard form, the required parameters are:

$$(p_1, p_2, p_3, n_1, n_2) = (a + r, b + r, r, c, d),$$

with
$$p_1 + p_2 + p_3 + n_1 + n_2 = J \,.. \tag{5}$$

Further it has been established (Bryant and Jahn 1960) that the number of distinct 3-j coefficients with a given value of J is equal to the number of distinct partitions $(q_1, q_2, n_1, n_2, 3p_3)$ of J:

$$J = q_1 + q_2 + n_1 + n_2 + 3\, p_3 \text{ and } p_3 = 0, 1, 2, \ldots, [J/3],$$

$$q_1 \geq q_2 \geq 0, \; n_1 \geq n_2 \geq 0, \; (q_1 + q_2) \geq (n_1 + n_2),$$

$$\text{and if } (q_1 + q_2) = (n_1 + n_2) \text{ then } (q_1 - q_2) = (n_1 - n_2), \tag{6}$$

where [J/3] stands for the largest integer less than J/3. Hence it is clear that $(p_1, p_2, p_3, n_1, n_2)$ along with J uniquely characterise a 3-j coefficient.

It is to be noted that in terms of the elements of the 3 x 3 Regge (1958) array :

viz.
$$\| R_{ik} \| = \left\| \begin{matrix} -j_1+j_2+j_3 & j_1-j_2+j_3 & j_1+j_2-j_3 \\ j_1-m_1 & j_2-m_2 & j_3-m_3 \\ j_1+m_1 & j_2+m_2 & j_3+m_3 \end{matrix} \right\| \tag{7}$$

we have,

$$(a + r, b + r, r, c, d) = (R_{21}, R_{32}, R_{13}, R_{31}-R_{13}, R_{22}-R_{13}). \tag{8}$$

The elements of the 3x3 Regge array satisfy the nine relations :

$$R_{\ell p} + R_{mp} = R_{nq} + R_{nr}, \tag{9}$$

for cyclic permutations of both $(\ell\ m\ n)$ = (1 2 3) and (p q r) =

(1 2 3). Using (9), relation (8) can be rewritten as:

$$(a + r,\ b + r,\ r,\ c,\ d) = (R_{21},\ R_{32},\ R_{13},\ R_{23} - R_{32},\ R_{33} - R_{21})$$
$$= (-A,\ -B,\ -C,\ E-1,\ D-1)\ , \qquad (10)$$

where A, B, C, D, E are the parameters of the ${}_3F_2(1)$ for the 3-j coefficient given in Chapter 1, corresponding to (p q r)= (1 2 3).

Lockwood (1976) introduced five new parameters for the 3-j coefficient which he called as *canonical* parameters. These are defined in terms of the $\alpha$'s and $\beta$'s that occur in the series representation for the 3-j coefficient (viz.(16),(17) of Chapter 1) as follows. The parameters $\beta_1$, $\beta_2$ and $\beta_3$ are ordered as $p \le q \le r$ and $\alpha_1, \alpha_2$, 0 as $f \le g \le h$. The new parameters are defined as:

$$n = p-h,\ a = h-g,\ b = h-f,\ c = q-p \text{ and } d = r-p\ . \qquad (11)$$

In terms of these new parameters, eliminating all but h, and substituting (s + h) for the summation index in the series representation, Lockwood rewrote the 3-j coefficient as the product of a phase factor P, a numerical factor R, and the series:

$$T = \sum_s (-1)^s \{s!(s+a)!(s+b)!(n-s)!(n+c-s)!(n+d-s)!\}^{-1}. \qquad (12)$$

Lockwood observed that P,R and T are invariant under the interchange of $a$ and $b$ or of $c$ and $d$ and concluded that there exists a four-element symmetry group. It was pointed out by Srinivasa Rao (1980) that P,R and T are infact invariant under the interchange of $a$ and $b$, and of n, (n + $c$) and (n + $d$) and hence the series (12) exhibits twelve symmetries. He also observed that n,(n + $c$) and (n + $d$) can be identified with the Regge array elements $R_{2p}$, $R_{3q}$ and $R_{1r}$ while $a$ and $b$ can be identified with $(R_{3r} - R_{2p})$ and $(R_{2r} - R_{3q})$, for $(p\ q\ r) = (1\ 2\ 3)$.

Hence the parameters introduced by Bowick (1976) as well as the (correctly interpreted) parameters of Lockwood correspond to the numerator and denominator parameters of one of the set of six ${}_3F_2(1)$s for the 3-j coefficient given by Srinivasa Rao (1978).

**3.4 The 3-j coefficient as a symbolic binomial expansion**

Symbolic methods for generating the 3-j coefficient have been noted by several authors, Ansary (1968), Sato and Kaguei (1972), Gelfand, Minlos and Shapiro (1963). Following the procedure given by Sato (1955) and using the definition of the lowering factorial:

$$p^{(x)} = \frac{p!}{(p-x)!}\ , \tag{13}$$

in the expression for the 3-j coefficient (viz.(27) of Chapter 1):

$$\begin{aligned}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} &= \delta\ (m_1 + m_2 + m_3, 0)\ (-1)^{\theta(pqr)} \prod_{i,k=1}^{3} \{R_{ik}!/(J+1)!\}^{1/2} \\ &\times \sum_{s} (-1)^{s} \{s!(R_{2p} - s)!(R_{3q} - s)!(R_{1r} - s)! \\ &\times (s + R_{3r} - R_{2p})!(s + R_{2r} - R_{3q})!\}^{-1},\end{aligned} \tag{14}$$

the formal binomial expansion for the 3-j coefficient can be written as :

$$\begin{aligned}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} &= \delta(m_1 + m_2 + m_3, 0)(-1)^{\theta(pqr)} \prod_{i,k=1}^{3} \{R_{ik}!/(J+1)!\}^{1/2} \\ &\times \{\Gamma(n+1,\ C_u+1,\ C_v+1,\ B_{rp}+n+1,\ B_{rq}+n+1\}^{-1} \\ &\times \{(B_{rp} + n)(B_{rq} + n) - C_u C_v)\}^{(n)}.\end{aligned} \tag{15}$$

where $n = \min\ (R_{2p}, R_{3q}, R_{1r})$, $C_u$, $C_v$ represent the Rik's in the triple $(R_{2p}, R_{3q}, R_{1r})$ other than n, $B_{rp} = R_{3r} - R_{2p}$ and $B_{rq} = R_{2r} - R_{3q}$. This result (15) is general when compared with that obtained by

Sato and Kaguei (1972). Their particular result can be derived by putting (p q r) = ( 2 3 1) in (15), while (15) itself holds for all the six permutations of (p q r) = ( 1 2 3).

Equation (15) is symbolic for $n > 2$, since it uses the generalised power (Ansary 1968 ), but exact for $n = 1$, since $p^{(1)} = p$ . Hence the binomial form for the 3-j coefficient explicitly reveals a subset of the non-trivial zeros, since when $n = 1$,

$$(B_{rp} + n)\ (B_{rq} + n) \quad = \quad C_u\ C_v \ , \tag{16}$$

implies a zero. These zeros which correspond to $n = 1$ can be represented by the simple multiplicative factor:

$$(\ 1 - \delta(n,1)\ \delta(X,Y))\ , \tag{17}$$

multiplying the standard expression (14) for the 3-j coefficient where n is the index that decides the number of terms in the binomial expansion, and it being (say), $R_{\ell q}$, X and Y are given by:

$$X = R_{mr} . R_{kp} \qquad \text{and} \qquad Y = R_{mp} . R_{kr}\ . \tag{18}$$

for cyclic permutations of both (p q r) = (1 2 3) and ($\ell$ m k) = (1 2 3).It can be seen that the conditions given by Lindner (1985) are the same as those given by (17) and (18).

The condition for the degree 1 zeros given above can also be simply interpreted via the set of ${}_3F_2(1)$s, eqn.(14) for the 3-j coefficient, and in this case the expansion ends after the second term (n + 1 gives the number of terms in the series),

i.e.
$$1 + \frac{A\ B\ C}{D\ E} = 0\ , \tag{19}$$

or
$$A\ B\ C = -D\ E\ , \tag{20}$$

with A, B, or C being -1. Based on the criteria given in (17) and (18) along with the parametrisation of Bryant and Jahn (1960) discussed previously a FORTRAN program has been developed to generate the *equivalent* and *inequivalent* zeros of degree 1 of the 3-j coefficient. The listing of the code is given in Appendix-A. The *equivalent* zeros of degree 1 were generated up to $j_1 \leq 13.0$ and the ordering prescription given by Rotenberg et.al.(1959) has been adopted. In Table 1 is listed the *equivalent* zeros of degree 1 for $j_1 \leq 8.0$. The *inequivalent* ones were seperated out of the list containing the *equivalent* ones and these are listed in Table 2 for $J$ (= $p_1 + p_2 + p_3 + n_1 + n_2$) $\leq$ 38. This reveals that up to J = 27 there are 25 zeros of degree 1 and these form a majority of the zeros listed by Bowick† (1976) in the same range. In Table 3 the zeros of higher degree upto J =27 as contained in the table of Bowick (1976) are listed. In the following we discuss the parametrisation for the degree-1 zeros of the 3-j coefficient.

**3.5. Parametrisation of the polynomial zeros of degree 1 of the 3-j coefficient**

Brudno (1985) has given parametric formulae for the degree-1 zeros (or linear or weight 1 zeros as they are synonymously

† In the Table of Bowick (1976) the entries corresponding to J = 17 (8,2,1,3,3) and J = 23 (10,3,1,5,4) are missing. Also the entry given for J = 23 (14,1,1,6,1) is not a zero and those with J = 24 (16,1,1,3,3) and J = 27 (12,3,1,8,3) are wrong entries and these are corrected in our Table.

referred to) of the 3-j coefficient. Two one-parameter formulae have been given by him ,viz.

$$\begin{pmatrix} 3n & 2n+1 & n+1 \\ 3n-1 & -2n & 1-n \end{pmatrix} , \tag{21}$$

and

$$\begin{pmatrix} 2n+1 & 2n & 2 \\ n+1 & -n & -1 \end{pmatrix} . \tag{22}$$

where n = 1, 2, ...

Apart from these a four-parameter formula has also been derived by Brudno (1985) in the following manner:

The condition for the zeros -viz.(20)- in terms of the parameters of the ${}_3F_2(1)$ in (14) when written explicitly (for (p q r) = (1 2 3)) reads as:

$$\begin{aligned} F &= (j_1 + j_2 - j_3)\,(j_1 - m_1)\,(j_2 + m_2) \\ &= (j_3 - j_2 + m_1 + 1)\,(\,j_3 - j_1 - m_2 + 1\,). \end{aligned} \tag{23}$$

In (23) any one of the three quantities: $(j_1+j_2-j_3)$, $(j_1-m_1)$ or $(j_2+m_2)$ could be equal to unity and we can assume without loss of generality that :

$$j_1 + j_2 - j_3 = 1 , \tag{24a}$$

and F which is now a product of two integers is decomposed into four integers:

$$F = a\,b\,c\,d . \tag{25}$$

Considering one particular partition of F viz. $(ab)$ $(cd)$, we have:

$$j_1 - m_1 = a\,b , \tag{24b}$$

$$j_2 + m_2 = c\,d , \tag{24c}$$

$$j_3 - j_2 + m_1 + 1 = a\,c , \tag{24d}$$

$$j_3 - j_1 - m_2 + 1 = b\,d . \tag{24e}$$

The five equations (24a) - (24e) yield the solution for the 3-j coefficient as:

$$\begin{bmatrix} a(b+c)/2 & d(b+c)/2 & ((b+c)(a+d)-2)/2 \\ a(c-b)/2 & d(c-b)/2 & (b-c)(a+d)/2 \end{bmatrix} . \qquad (26)$$

where the parameters $a,b,c,d$ can take on any integer value from 1 to $\infty$. Brudno's(1985) conclusions are however imprecise and we wish to make the following observations:

(i) Of the 24 possible ways of partitioning $abcd$ to identify the X and Y parts in (18) of the 3-j coefficient, which yield the condition for polynomial zeros of degree 1, in addition to (26) only two other independent forms result. These are:

$$\begin{bmatrix} a(b+d)/2 & c(b+d)/2 & ((b+d)(a+c)-2)/2 \\ a(d-b)/2 & c(d-b)/2 & (b-d)(a+c)/2 \end{bmatrix} , \qquad (27)$$

$$\begin{bmatrix} a(c+d)/2 & b(c+d)/2 & ((a+b)(c+d)-2)/2 \\ a(d-c)/2 & b(d-c)/2 & (c-d)(a+b)/2 \end{bmatrix} . \qquad (28)$$

All others are related by the tetrahedral symmetries - viz. column permutations and / or $m_i \to -m_i$; or Regge symmetries.

(ii) The three forms (26), (27) and (28) yield different (Regge inequivalent) *polynomial* zeros of degree one, if and only if $a \neq b \neq c \neq d$. For, when $b = c$ or $b = d$ or $c = d$ one of the three forms becomes a parity 3-j coefficient (i.e. $m_1 = m_2 = 0$ and $(j_1 + j_2 + j_3)$ odd) and the other two forms merge. Further, when $a = b$ or $a = c$ or $a = d$, two of the three forms can be related to each other by a Regge symmetry.

In fact (23) can be written as:

$$F = u\,y = x\,v , \qquad (29)$$

where x, y, u and v are positive integers. It should be noted that this equation is a homogeneous multiplicative Diophantine equation of degree 2, and the solution was given in terms of four integer parameters $a$, $b$, $c$, $d$ by Brudno (1985). That this four-parameter solution infact gives the complete solution to the problem was established by Brudno and Louck (1985). They rewrite (29), which gives the condition for the zeros of degree 1 as:

$$(x + u)\ (y - v) = (x - u)\ (y + v)\ , \tag{30}$$

and prove that the complete solution to this equation is given by:

$$x = \alpha\beta, \quad y = \beta\delta, \quad u = \alpha\gamma, \quad v = \gamma\delta\ , \tag{31}$$

where $\alpha$, $\beta$, $\gamma$, $\delta$ take on all positive integral values. They also show that the same conclusion can be arrived at using a result of Pasternak ( cf. Dickson (1952) p 252). To this end, (30) is transformed using the identity:

$$4\ A\ B = (A + B)^2 - (A - B)^2, \tag{32}$$

and rewritten in the form :

$$X^2 + Y^2 = U^2 + V^2\ , \tag{33}$$

where

$$\begin{aligned} X &= x + y + u - v\ , \qquad & Y &= x - y - u - v\ , \\ U &= x + y - u + v\ , \qquad & V &= x - y + u + v\ . \end{aligned} \tag{34}$$

Pasternak, in 1906, had proved that all the solutions of the Diophantine equation (33) are given by:

$$\begin{aligned} X &= k\ r + \ell\ s\ , \qquad & Y &= \ell\ r - k\ s\ , \\ U &= k\ r - \ell\ s\ , \qquad & V &= \ell\ r + k\ s\ , \end{aligned} \tag{35}$$

where $k$, $r$, $\ell$, $s$ are integers. Brudno and Louck (1985) establish that this implies the result given by (31).

It is to be noted that considering (29) as it is, without any transformations, one can establish the above result by resorting to Bell 's theorem (Bell 1933) stated and proved in Chapter 1. The *polynomial* zeros of degree one were generated for the 3-j coefficient by using the four-parameter solution, the details of which are given in Appendix A.

### 3.6 Conclusions

In conclusion, the results obtained in this chapter are:

(i) By rewriting the 3-j coefficient as a formal binomial expansion, a closed form expression has been obtained for the polynomial zeros of degree one of this coefficient.

(ii) Using Bell's theorem, it is established that the four-parameter solution given by Brudno generates the complete list of polynomial zeros of degree one of the 3-j coefficient.

(iii) The *equivalent* as well as the *inequivalent* polynomial zeros of degree one of the 3-j coefficient have been generated using Fortran programs based on the closed form expression or the four-parameter solution to the multiplicative Diophantine equation of degree 2.

Table 1.
The *equivalent* zeros of degree 1 of the 3-j coefficient.

| $j_1$ | $j_2$ | $j_3$ | $m_1$ | $m_2$ | $m_3$ |
|---|---|---|---|---|---|
| 3.0 | 3.0 | 2.0 | 2.0 | -2.0 | 0.0 |
| 3.5 | 3.0 | 1.5 | 1.5 | -1.0 | -0.5 |
| 4.5 | 4.0 | 2.5 | 3.5 | -3.0 | -0.5 |
| 5.0 | 4.0 | 2.0 | 3.0 | -2.0 | -1.0 |
| 5.0 | 4.5 | 1.5 | 2.0 | -1.5 | -0.5 |
| 5.0 | 5.0 | 4.0 | 3.0 | -4.0 | 1.0 |
| 5.0 | 5.0 | 4.0 | 4.0 | -3.0 | -1.0 |
| 5.5 | 4.5 | 4.0 | 3.5 | -3.5 | 0.0 |
| 6.0 | 5.0 | 3.0 | 3.0 | -1.0 | -2.0 |
| 6.0 | 5.0 | 3.0 | 5.0 | -4.0 | -1.0 |
| 6.0 | 5.5 | 2.5 | 2.0 | -0.5 | -1.5 |
| 6.0 | 6.0 | 3.0 | 5.0 | -5.0 | 0.0 |
| 6.5 | 4.5 | 3.0 | 2.5 | -1.5 | -1.0 |
| 6.5 | 5.0 | 2.5 | 1.5 | -1.0 | -0.5 |
| 6.5 | 5.0 | 2.5 | 4.5 | -3.0 | -1.5 |
| 6.5 | 6.0 | 1.5 | 2.5 | -2.0 | -0.5 |
| 6.5 | 6.0 | 4.5 | 4.5 | -5.0 | 0.5 |
| 7.0 | 6.0 | 2.0 | 4.0 | -3.0 | -1.0 |
| 7.0 | 7.0 | 6.0 | 4.0 | -6.0 | 2.0 |
| 7.0 | 7.0 | 6.0 | 6.0 | -4.0 | -2.0 |
| 7.5 | 6.0 | 3.5 | 6.5 | -5.0 | -1.5 |
| 7.5 | 6.5 | 3.0 | 3.5 | -1.5 | -2.0 |
| 7.5 | 6.5 | 5.0 | 6.5 | -4.5 | -2.0 |
| 7.5 | 7.5 | 5.0 | 5.5 | -6.5 | 1.0 |
| 7.5 | 7.5 | 5.0 | 6.5 | -5.5 | -1.0 |
| 8.0 | 6.0 | 3.0 | 3.0 | -2.0 | -1.0 |
| 8.0 | 6.0 | 3.0 | 6.0 | -4.0 | -2.0 |
| 8.0 | 6.0 | 5.0 | 6.0 | -5.0 | -1.0 |
| 8.0 | 6.0 | 6.0 | -5.0 | 0.0 | 5.0 |
| 8.0 | 6.0 | 6.0 | 5.0 | -5.0 | 0.0 |
| 8.0 | 6.0 | 6.0 | 5.0 | 0.0 | -5.0 |
| 8.0 | 7.0 | 5.0 | 6.0 | -6.0 | 0.0 |
| 8.0 | 7.5 | 1.5 | 3.0 | -2.5 | -0.5 |
| 8.0 | 7.5 | 3.5 | 7.0 | -6.5 | -0.5 |

Table 2.

The *inequivalent* zeros of degree 1 of the 3-j coefficient.

| $j_1$ | $j_2$ | $j_3$ | $m_1$ | $m_2$ | $m_3$ | $p_1$ | $p_2$ | $p_3$ | $n_1$ | $n_2$ | J |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 3.0 | 3.0 | 2.0 | 2.0 | - 2.0 | 0.0 | 4 | 1 | 1 | 1 | 1 | 8 |
| 4.5 | 4.0 | 2.5 | 3.5 | - 3.0 | -0.5 | 6 | 1 | 1 | 2 | 1 | 11 |
| 5.0 | 5.0 | 4.0 | 3.0 | - 4.0 | 1.0 | 6 | 2 | 1 | 3 | 2 | 14 |
| 6.0 | 5.0 | 3.0 | 5.0 | - 4.0 | -1.0 | 8 | 1 | 1 | 3 | 1 | 14 |
| 6.0 | 6.0 | 3.0 | 5.0 | - 5.0 | 0.0 | 9 | 1 | 1 | 2 | 2 | 15 |
| 6.5 | 6.0 | 4.5 | 4.5 | - 5.0 | 0.5 | 8 | 2 | 1 | 3 | 3 | 17 |
| 7.5 | 6.0 | 3.5 | 6.5 | - 5.0 | -1.5 | 10 | 1 | 1 | 4 | 1 | 17 |
| 7.5 | 6.5 | 5.0 | 6.5 | - 4.5 | -2.0 | 9 | 2 | 1 | 5 | 2 | 19 |
| 8.0 | 7.5 | 3.5 | 7.0 | - 6.5 | -0.5 | 12 | 1 | 1 | 3 | 2 | 19 |
| 7.0 | 7.0 | 6.0 | 4.0 | - 6.0 | 2.0 | 8 | 3 | 1 | 5 | 3 | 20 |
| 7.5 | 7.5 | 5.0 | 5.5 | - 6.5 | 1.0 | 10 | 2 | 1 | 4 | 3 | 20 |
| 9.0 | 7.0 | 4.0 | 8.0 | - 6.0 | -2.0 | 12 | 1 | 1 | 5 | 1 | 20 |
| 8.5 | 8.0 | 6.5 | 5.5 | - 7.0 | 1.5 | 10 | 3 | 1 | 5 | 4 | 23 |
| 9.0 | 8.5 | 5.5 | 8.0 | - 6.5 | -1.5 | 12 | 2 | 1 | 5 | 3 | 23 |
| 10.0 | 9.0 | 4.0 | 9.0 | - 8.0 | -1.0 | 15 | 1 | 1 | 4 | 2 | 23 |
| 10.5 | 8.0 | 4.5 | 9.5 | - 7.0 | -2.5 | 14 | 1 | 1 | 6 | 1 | 23 |
| 9.0 | 7.5 | 7.5 | -5.0 | - 1.5 | 6.5 | 9 | 4 | 1 | 5 | 5 | 24 |
| 10.0 | 8.0 | 6.0 | 9.0 | - 6.0 | -3.0 | 12 | 2 | 1 | 7 | 2 | 24 |
| 10.0 | 10.0 | 4.0 | 9.0 | - 9.0 | 0.0 | 16 | 1 | 1 | 3 | 3 | 24 |
| 9.0 | 9.0 | 8.0 | 5.0 | - 8.0 | 3.0 | 10 | 4 | 1 | 7 | 4 | 26 |
| 10.0 | 9.0 | 7.0 | 7.0 | - 8.0 | 1.0 | 12 | 3 | 1 | 5 | 5 | 26 |
| 10.5 | 9.5 | 6.0 | 9.5 | - 7.5 | -2.0 | 14 | 2 | 1 | 6 | 3 | 26 |
| 12.0 | 9.0 | 5.0 | 11.0 | - 8.0 | -3.0 | 16 | 1 | 1 | 7 | 1 | 26 |
| 10.5 | 9.0 | 7.5 | 9.5 | - 6.0 | -3.5 | 12 | 3 | 1 | 8 | 3 | 27 |
| 10.5 | 10.5 | 6.0 | 8.5 | - 9.5 | 1.0 | 15 | 2 | 1 | 5 | 4 | 27 |
| 12.0 | 10.5 | 4.5 | 11.0 | - 9.5 | -1.5 | 18 | 1 | 1 | 5 | 2 | 27 |
| 10.5 | 10.0 | 8.5 | 6.5 | - 9.0 | 2.5 | 12 | 4 | 1 | 7 | 5 | 29 |
| 11.0 | 10.5 | 7.5 | 8.0 | - 9.5 | 1.5 | 14 | 3 | 1 | 6 | 5 | 29 |
| 12.0 | 10.5 | 6.5 | 11.0 | - 8.5 | -2.5 | 16 | 2 | 1 | 7 | 3 | 29 |
| 12.5 | 9.5 | 7.0 | 11.5 | - 7.5 | -4.0 | 15 | 2 | 1 | 9 | 2 | 29 |
| 12.5 | 12.0 | 4.5 | 11.5 | -11.0 | -0.5 | 20 | 1 | 1 | 4 | 3 | 29 |
| 12.0 | 11.0 | 8.0 | 11.0 | - 8.0 | -3.0 | 15 | 3 | 1 | 8 | 4 | 31 |
| 12.5 | 12.0 | 6.5 | 10.5 | -11.0 | 0.5 | 18 | 2 | 1 | 5 | 5 | 31 |

Table 2 (continued).

| $j_1$ | $j_2$ | $j_3$ | $m_1$ | $m_2$ | $m_3$ | $p_1$ | $p_2$ | $p_3$ | $n_1$ | $n_2$ | J |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 11.0 | 11.0 | 10.0 | 6.0 | -10.0 | 4.0 | 12 | 5 | 1 | 9 | 5 | 32 |
| 12.0 | 11.0 | 9.0 | 8.0 | -10.0 | 2.0 | 14 | 4 | 1 | 7 | 6 | 32 |
| 12.0 | 12.0 | 8.0 | 9.0 | -11.0 | 2.0 | 16 | 3 | 1 | 7 | 5 | 32 |
| 12.5 | 11.0 | 10.5 | -6.5 | - 3.0 | 9.5 | 12 | 6 | 1 | 8 | 7 | 34 |
| 12.5 | 12.0 | 9.5 | 11.5 | - 8.0 | -3.5 | 15 | 4 | 1 | 9 | 5 | 34 |
| 12.5 | 12.0 | 10.5 | 7.5 | -11.0 | 3.5 | 14 | 5 | 1 | 9 | 6 | 35 |
| 13.0 | 13.0 | 12.0 | 7.0 | -12.0 | 5.0 | 14 | 6 | 1 | 11 | 6 | 38 |

Table 3

The *inequivalent* zeros of higher degrees of the 3-j coefficient.

Polynomial zeros of degree 2.

| $j_1$ | $j_2$ | $j_3$ | $m_1$ | $m_2$ | $m_3$ |
|---|---|---|---|---|---|
| 6.0 | 4.0 | 4.0 | 2.0 | -2.0 | 0.0 |
| 9.0 | 8.0 | 3.0 | 4.0 | -4.0 | 0.0 |
| 7.5 | 7.5 | 5.0 | 5.5 | -3.5 | -2.0 |
| 9.5 | 7.5 | 4.0 | 0.5 | -1.5 | 1.0 |
| 9.5 | 6.5 | 5.0 | 0.5 | -1.5 | 1.0 |
| 10.5 | 10.5 | 3.0 | 8.5 | -8.5 | 0.0 |
| 11.0 | 8.0 | 5.0 | 8.0 | -6.0 | -2.0 |
| 8.0 | 8.0 | 8.0 | 6.0 | -5.0 | -1.0 |
| 9.0 | 9.0 | 7.0 | 5.0 | 0.0 | -5.0 |
| 12.5 | 12.5 | 2.0 | 7.5 | 7.5 | 0.0 |
| 12.5 | 10.5 | 4.0 | 4.5 | -4.5 | 0.0 |
| 12.5 | 11.0 | 3.5 | 1.5 | 0.0 | -1.5 |
| 11.5 | 7.0 | 6.5 | 7.5 | -5.0 | -2.5 |
| Polynomial zeros of degree 4 | | | | | |
| 11.0 | 9.0 | 6.0 | 0.0 | 1.0 | -1.0 |
| 9.0 | 8.0 | 8.0 | -5.0 | 4.0 | 1.0 |

## Chapter 4

## Polynomial zeros of the 6-j coefficient

### 4.1 Introduction:

*Polynomial* (or *non-trivial*) zeros of the 6-j coefficient are defined as those which arise due to the polynomial part of the 6-j coefficient becoming zero when all the triangular inequalities involving the six angular momenta are satisfied. Such *polynomial* zeros of the 6-j coefficient have been classified by us according to their degree. Polynomial zeros of degree one, also referred to as weight-one zeros by Brudno, Bremner, Louck et. al. have been extensively studied in recent years.

In this chapter, the parametrisation developed by Jahn and Howell (1959) to characterise a 6-j coefficient in a unique manner is described first. Following this, the various approaches that have been used to study the *polynomial* zeros of degree 1 via either a formal binomial expansion or Diophantine equations or realisations of exceptional Lie algebras or orthogonal polynomials are discussed.

From a formal binomial expansion for the 6-j coefficient a closed form expression is obtained for the degree 1 zeros. Using the theorem due to E.T.Bell, stated in Chapter 1, for the homogeneous multiplicative Diophantine equation of degree 3: $xyz = uvw$, it is established that nine integral parameters ($a,b,c,d,e,f,g,h$ and $i$, say) are necessary and sufficient to obtain its complete set of solutions. An alternate proof based on induction with respect to N is also provided where N is given by: $x_1 x_2 \ldots x_n = u_1 \; u_2 \; \ldots \; u_n = N$. The equation $xyz = uvw$ constrained by $z = x + y + u + v + w$ is central to the discussion of the polynomial zeros of degree one of the 6-j coefficient. A theorem is established to show that eight parameters are necessary and sufficient to obtain the complete set of polynomial zeros of degree 1 of the 6-j coefficient. In the light of this theorem, the fewer parameter solutions obtained by other authors are shown to provide only a partial list of the complete set of solutions. The constraint equation: $ghi = abc + def + adg + beh + cfi$ has been reduced to two simpler forms of Diophantine equations :

viz. $\alpha gh = \beta g + \gamma h + \delta$ or $\alpha' a + \beta' e = \gamma'$ ,

for which solutions have been given by Brahmegupta (cf, Dickson 1952, p.64) and Paoli (cf. Dickson 1952, p.401) respectively. Two algorithms based on these solutions are presented here. From either of these, the complete set of polynomial zeros of degree one of the 6-j coefficient, upto I = 177, where I represents twice the sum of the six angular momenta, have been obtained.

## 4.2 Polynomial zeros of the 6-j coefficient

It is recalled that trivial zeros of the 6-j coefficient arise when the arguments violate one or more of the triangular inequalities implied by the four triads viz. $\Delta(j_1 j_2 j_3)$, $\Delta(j_3 \ell_1 \ell_2)$, $\Delta(j_1 \ell_2 \ell_3)$, $\Delta(\ell_1 j_2 \ell_3)$ to be satisfied by them. Apart from these trivial zeros, the 6-j coefficient possesses zeros for which all these triangular inequalities are satisfied. These are known as the *non-trivial* zeros. Koozekanani and Biedenharn (1974) tabulated these zeros for the first time by calculating the vanishing values of the 6-j coefficient using a computer program which resorted to an arithmetic based on powers of primes. Bowick (1976) reduced the table of Koozekanani and Biedenharn (1974) by eliminating the *equivalent* 6-j coefficients (i.e. coefficients related by any one of the 144 symmetries) and retaining only the *inequivalent* ones. To do this he used the parameters given by Jahn and Howell (1959) to characterise all 6-j coefficients related by the 144 symmetries in a unique way.

**4.3 Canonical parameters for the 6-j coefficient**

(i) Given a 6-j symbol :

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ \ell_1 & \ell_2 & \ell_3 \end{Bmatrix} ,$$

the parameters of Jahn and Howell (1959) are calculated in the following manner:

$$J_o = j_1+j_2+j_3,\; J_1 = j_1+\ell_2+\ell_3,\; J_2 = j_2+\ell_1+\ell_3,\; J_3 = j_3+\ell_1+\ell_2,$$
$$K_1 = j_2+\ell_2+j_3+\ell_3,\; K_2 = j_1+\ell_1+j_3+\ell_3,\; K_3 = j_1+\ell_1+j_2+\ell_2. \qquad (1)$$

The quantities $J_m$, $J_a$, $J_b$, $J_c$ and $K_a$, $K_b$, $K_c$ are defined such that

$$J_m \geq J_a \geq J_b \geq J_c = \text{ordered } (J_o,\ J_1,\ J_2,\ J_3)$$
$$K_a \geq K_b \geq K_c = \text{ordered } (K_1,\ K_2,\ K_3). \qquad (2)$$

In terms of these, six positive integral parameters are defined as:

$$n_1 = J_m - J_c \;,\quad n_2 = J_m - J_b \;,\quad n_3 = J_m - J_a \;,$$
$$p_1 = K_a - J_m \;,\quad p_2 = K_b - J_m \;,\quad p_3 = K_c - J_m \;, \qquad (3)$$

such that $$n_1 + n_2 + n_3 + p_1 + p_2 + p_3 = J_m . \tag{4}$$
From (2) it follows that
$$n_1 \geq n_2 \geq n_3 \quad ; \quad p_1 \geq p_2 \geq p_3 . \tag{5}$$
Hence each distinct 6-j symbol is characterised by an ordered partition of $J_m$ given by (4) and (5). It is to be noted that $J_o$, $J_1$, $J_2$, $J_3$ and $K_1$, $K_2$, $K_3$ in (1) are the same as the $\alpha$'s and $\beta$'s in (48) of Chapter 1.

(ii) Lockwood (1977) introduced certain parameters $q_x$, $q_y$, $q_z$, $q_w$ and $p_x$, $p_y$, $p_z$ which he called as intermediate parameters. These are the same as the $\alpha$'s and $\beta$'s introduced by Sato (1955) and are given in (48) of Chapter 1. After ordering the q's and p's as
$$q_w \leq q_x \leq q_y \leq q_z \quad ; \quad p_x \leq p_y \leq p_z , \tag{6}$$
Lockwood defined certain differences between these as:
$$\begin{aligned} n &= p_x - q_z , \quad a = q_z - q_y , \; b = q_z - q_x , \\ c &= q_z - q_w , \quad d = p_y - p_x , \; e = p_z - p_x . \end{aligned} \tag{7}$$
Using (7), after eliminating all but $q_z$ and substituting $(q_z + s)$ for the summation index in the expansion for the 6-j coefficient, Lockwood (1977) rewrote the 6-j coefficient as the product of a phase factor $P = (-1)^{3n+a+b+c+d+e}$, a numerical factor R and the series:
$$T = \sum_s (-)^s (3n + a + b + c + d + e + s + 1)!\{s!(s + a)! \times (s + b)!(s + c)!(n - s)!(n + d - s)!(n + e - s)!\}^{-1} . \tag{8}$$
Lockwood observed that P, R and T are invariant under the interchange of $a$, $b$ and $c$ and of $d$ and $e$ and concluded that the parameter n does not enter into the symmetry operations and that

there exists a 12 - element symmetry group for the 6-j coefficient. It was pointed out by Srinivasa Rao (1980) that P, R and T are infact invariant under the interchange of $a$, $b$ and $c$ and of n, n+$d$ and n+$e$. The series (8) thus exhibits 36 of the 144 symmetries of the 6-j coefficients and n *does* enter into the symmetry operations. Hence the conclusions drawn by Lockwood on the basis of his *canonical* parameters are not valid. If one must refer to some parameters as *canonical* parameters for the 6-j coefficient, then the ordered set of seven parameters $J_m$, $n_1$, $n_2$, $n_3$, $P_1$, $P_2$, $P_3$ introduced by Jahn and Howell are the canonical parameters.

**4.4 The 6-j coefficient as a formal binomial expansion:**

The explicit expression for the 6-j coefficient due to Regge (1959) given in (46) of Chapter 1 reads as:

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ \ell_1 & \ell_2 & \ell_3 \end{Bmatrix} = N' \sum_p (-1)^p (p+1)! \{ \prod_{i=1}^{4} (p-\alpha_i)! \prod_{j=1}^{3} (\beta_j - p)! \}^{-1}, \quad (9)$$

with

$$N' = \Delta(j_1 j_2 j_3).\ \Delta(j_3 \ell_1 \ell_2).\Delta(j_1 \ell_2 \ell_3).\Delta(\ell_1 j_2 \ell_3) ,$$

$$p_{min} \le p \le p_{max} ,$$

where

$$p_{min} = \max(\alpha_1, \alpha_2, \alpha_3, \alpha_4) \equiv \alpha_0 ,$$

and

$$p_{max} = \min(\beta_1, \beta_2, \beta_3) \equiv \beta_0 . \quad (10)$$

In (9) making the substitution:

$$p = \alpha_0 + k ,$$

Sato (1955) rewrote the 6-j coefficient as:

$$\left\{\begin{matrix} j_1 & j_2 & j_3 \\ \ell_1 & \ell_2 & \ell_3 \end{matrix}\right\} = N' \sum_{k=0}^{n} (-1)^{\alpha_0 + k} (\alpha_0 + 1 + k)! \{ k!(n-k)!(A_p + k)! \times (A_q + k)!(A_r + k)!(B_u - k)!(B_v - k)! \}^{-1} \quad (12)$$

where $n = \beta_0 - \alpha_0$, $A_i = \alpha_0 - \alpha_i$, $i = p,q,r$,

and $B_j = \beta_j - \alpha_0$, $j = u,v$. (13)

In (13) the indices p,q,r and u,v stand for those $\alpha$'s and $\beta$'s other than $\alpha_0$ and $\beta_0$ respectively.

Using the definitions:

$$p^{(\alpha)} = \frac{p!}{(p-\alpha)!} \quad \text{and} \quad p^{(-\alpha)} = \frac{(p+\alpha)!}{p!}, \quad (14)$$

the 6-j coefficient was rewritten as a formal binomial expansion by Sato (1955) as follows:

$$\left\{\begin{matrix} j_1 & j_2 & j_3 \\ \ell_1 & \ell_2 & \ell_3 \end{matrix}\right\} = N' (-1)^{\alpha_0} \Gamma(\alpha_0 + 2) \times$$

$$\times \{\Gamma(n+1, A_p+n+1, A_q+n+1, A_r+n+1, B_u+1, B_v+1)\}^{-1}$$

$$\times \{(A_p+n)(A_q+n)(A_r+n) - B_u B_v (\alpha_0+1)^{(-1)}\}^{(n)}. \quad (15)$$

Alternatively, by making the substitution:

$$p = \beta_0 - k$$

and using the symbolic notation:

$$p^{(\alpha)} = \frac{p!}{(p-\alpha)!} \quad \text{and} \quad p^{(-\alpha)} = \frac{1}{p^{(\alpha)}}, \quad (17)$$

in the place of (11) and (14), Srinivasa Rao and Venkatesh (1977) obtained the following symbolic binomial expansion for the 6-j coefficient:

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ \ell_1 & \ell_2 & \ell_3 \end{Bmatrix} = N' \ (-1)^{\beta_o} \Gamma(\beta_o + 2) \times$$

$$\times \ \{\Gamma(n+1, A_p+1, A_q+1, A_r+1, B_u+n+1, B_v+n+1)\}^{-1}$$

$$\times \ \{(B_u+n)(B_v+n) - A_p A_q A_r (\beta_o+1)^{(-1)}\}^{(n)} \ , \qquad (18)$$

with $A_i = \beta_o - \alpha_i$ , $i = p,q,r$ and $B_j = \beta_j - \beta_o$, $j = u,v$.

It is to be noted that for n = 1, (17) implies that

$$p^{(1)} = p \quad \text{and} \quad p^{(-1)} = 1/p \ , \qquad (20)$$

whereas (14) reads as:

$$p^{(1)} = p \quad \text{and} \quad p^{(-1)} = (p + 1). \qquad (21)$$

Hence atleast for n = 1, the generalised power (Ansary 1968 ) defined by (17) represents the *actual* power and the formal binomial expansion given by (18) is an exact binomial so that for X = Y this binomial expansion reveals some of the zeros of the 6-j coefficient. The X and Y referred above are given by:

$$X = (B_u + n)(B_v + n)(\beta_o + 1)$$

$$= (\beta_u - \alpha_o)(\beta_v - \alpha_o)(\beta_o + 1) \ , \qquad (22)$$

$$Y = (\beta_o - \alpha_p)(\beta_o - \alpha_q)(\beta_o - \alpha_r) \ . \qquad (23)$$

Based on the above mentioned criterion for the degree one zeros of the 6-j coefficient, viz:

$$(1 - \delta(n,1)\ \delta(X,Y)) \ , \qquad (24)$$

a computer program has been developed to generate these degree one zeros, with the same type of ordering for the arguments of the 6-j coefficients as has been done by Koozekanani and Biedenharn (1974). These degree one *polynomial* zeros have been generated for $j_i$, $\ell_i \le 18.5$ corresponding to the tables of Koozekanani and

Biedenharn (1974) and it is found that 1174 *out of the* 1420 *polynomial zeros listed by them are of degree one.* These majority of the zeros were seperated out and the remaining *polynomial* zeros tabulated by them were sorted out according to their degree given by $n = \beta_0 - \alpha_0$ (Srinivasa Rao and Rajeswari (1985a)). The first few entries of this sorted list of zeros of various degree are given in Tables 1,2 & 3. Using the parametrisation given by Jahn and Howell (1959) for the 6-j coefficient a FORTRAN program has been developed to sieve out the *inequivalent* 6-j coefficients from the *equivalent* ones. The *inequivalent* zeros of degree one given by Bowick (1976) was reproduced by the program. The details of this and other programs are given in Appendix B.

The condition for the degree one zeros given in (24) can also be simply interpreted in terms of the sets of ${}_4F_3(1)$s for the 6-j coefficient given by (54) and (60) of Chapter 1. In this case (n = 1) the expansion ends after the second term and the condition for the zeros reads as:

$$1 + \frac{A\ B\ C\ D}{E\ F\ G} = 0 \tag{25}$$

or,

$$A\ B\ C\ D = -\ E\ F\ G\ , \tag{26}$$

where, A, B, C, D, E, F and G are the numerator and denominator parameters of the ${}_4F_3(1)$ hypergeometric series, with A, B, C or D being $-1$.

### 4.5 Parametric formulae for the polynomial zeros of degree one of the 6-j coefficient

Brudno (1985) gave, for the first time, several parametric formulae for the *polynomial* zeros of degree one of the 6-j coefficient. He gave the following three one-parameter formulae:

$$\begin{Bmatrix} n+2 & n+1 & 2 \\ n & n+1 & n+1 \end{Bmatrix}, \tag{27}$$

$$\begin{Bmatrix} (3x+4)/2 & (3x+4)/2 & x+2 \\ (2x+3)/2 & 3/2 & (3x+3)/2 \end{Bmatrix}, \tag{28}$$

and

$$\begin{Bmatrix} J & 4J-1 & 3J \\ 2J+3/2 & J+1/2 & 2J-1/2 \end{Bmatrix} \tag{29}$$

Apart from these he gave a more general nine-parameter solution the derivation of which goes along the following lines: The condition for the zeros - eqn. (26) - in terms of the parameters of the ${}_4F_3(1)$ of set-I for the 6-j coefficient $\begin{Bmatrix} j_1 & j_2 & j_3 \\ \ell_1 & \ell_2 & \ell_3 \end{Bmatrix}$ (given by (18) of Chapter 1) when written explicitly reads as:

$$\begin{aligned} F &= (j_1+j_2-j_3)(-j_3+\ell_1+\ell_2)(j_1+\ell_2-\ell_3)(j_2+\ell_1-\ell_3), \\ &= (j_1+j_2+\ell_1+\ell_2+1)(j_3+\ell_3-j_1-\ell_1+1)(j_3+\ell_3-j_2-\ell_2+1). \end{aligned} \tag{30}$$

In (30) any one of the four integer quantities: $(j_1+j_2-j_3)$, $(-j_3+\ell_1+\ell_2)$, $(j_1+\ell_2-\ell_3)$ or $(j_2+\ell_1-\ell_3)$ could be equal to unity and without loss of generality it can be assumed that

$$-j_3+\ell_1+\ell_2 = 1 \tag{31a}$$

and F which is now a product of three integers is decomposed into nine integers:

$$F = a\,b\,c\,d\,e\,f\,g\,h\,i\,. \tag{32}$$

He considered the particular partition of F given by:

$$j_1+j_2-j_3 = a\,d\,g\,, \tag{31b}$$

$$j_1+\ell_2-\ell_3 = b\,e\,h\,, \tag{31c}$$

$$j_2+\ell_1-\ell_3 = c\,f\,i\,, \tag{31d}$$

$$j_1+j_2+\ell_1+\ell_2+1 = g\,h\,i\,, \tag{31e}$$

$$j_3 + \ell_3 - j_1 - \ell_1 + 1 \quad = \quad d\,e\,f\,, \tag{31f}$$

$$j_3 + \ell_3 - j_2 - \ell_2 + 1 \quad = \quad a\,b\,c\,. \tag{31g}$$

The seven equations (31a) - (31g) yield the solution for the 6-j coefficient as:

$$\begin{Bmatrix} (beh+abc+adg-1)/2 & (adg+cfi+def-1)/2 & (beh+abc+cfi+def-2)/2 \\ (cfi+abc)/2 & (beh+def)/2 & (abc+adg+def-1)/2 \end{Bmatrix}$$

along with the constraint: (33)

$$g\,h\,i \;=\; a\,b\,c \;+\; d\,e\,f \;+\; a\,d\,g \;+\; b\,e\,h \;+\; c\,f\,i\,, \tag{34}$$

with $a, b, c, d, \ldots\ldots, = 1, 2, \ldots$.In the above equations the identifications made are slightly different from those of Brudno (1985), and this has been done to fecilitate an uniform and consistent notation in the rest of the chapter.

Equation (30) can infact be written as:

$$F = u\,v\,w = x\,y\,z\,, \tag{35}$$

with the constraint (34) taking the form:

$$z = x + y + u + v + w\,, \tag{36}$$

where x, y, z, u, v and w are positive integers. It should be noted that eqn.(35) is a homogeneous multiplicative Diophantine equation of degree 3 the solution of which was given in terms of nine integer parameters $a$, $b$, $c$, $d$, $e$, $f$, $g$, $h$, $i$ by Brudno (1985). To establish that this nine-parameter formula gives all possible degree - one zeros, Brudno and Louck (1985) solved the multiplicative Diophantine equation (35) explicitly with the constraint (36). To this end eqns.(35) and (36) are transformed using the identity:

$$24\,ABC = (A+B+C)^3 + (A-B-C)^3 + (-A-B+C)^3 + (-A+B-C)^3 \tag{37}$$

and they are rewritten as a pair of Diophantine equations involving equal sums of like powers:

$$X^3 + Y^3 + Z^3 = U^3 + V^3 + W^3, \qquad (38)$$

and

$$X + Y + Z = U + V + W, \qquad (39)$$

where

$$\begin{aligned} X &= x - y + z, & U &= u + v - w, \\ Y &= -x + y + z, & V &= u - v + w, \\ Z &= u - v - w, & W &= x + y + z. \end{aligned} \qquad (40)$$

Brudno and Louck (1985) located a two-parameter solution to the system of equations (38) and (39) which was due to Gerardin (Dickson 1952, pp.565, 713). Bremner (1986) extended the investigation of (38) and (39) to produce two four-parameter solutions and related them to the Brudno and Louck solution of (35). Finally, Bremner and Brudno (1986) solved the same Diophantine equations to obtain another four-parameter solution which they claimed gave all degree-one zeros of the 6-j coefficients.

It is to be noted that using the theorem of Bell (1933) for the homogeneous multiplicative Diophantine equation stated and proved in Chapter 1, it can be established that the complete solution of (35) constrained by (36) requires eight integer parameters. Given below is an alternate proof provided for Bell's theorem. The various parametrisations of solutions referred to above are summarised and compared with the eight-parameter solution. It is shown (Srinivasa Rao, Rajeswari and King (1988a)) that all the parametric solutions with fewer than eight parameters are in a certain sense incomplete.

## 4.6 Alternate proof† of Bell's theorem

According to Bell's theorem, every solution of the multiplicative Diophantine equation:

$$x_1 x_2 \dots x_n = u_1 u_2 \dots u_n , \ (n > 1) \tag{41}$$

can be expressed in the form:

$$x_i = \prod_{j=1}^{n} \phi_{ij} \qquad \text{and} \qquad u_j = \prod_{i=1}^{n} \phi_{ij} , \tag{42}$$

where the $n^2$ independent parameters $\phi_{ij}$ with $i, j = 1, 2, \dots, n$ are positive integers which can be arranged in an $n \times n$ array $A(\phi)$ with $\phi_{ij}$ at the intersection of the ith row and the jth column subject to the greatest common divisor (g.c.d) conditions:

$$(x_i , u_i ) = \phi_{ii} , \tag{43}$$

for $i = 1, 2, \dots, n$ satisfied by the diagonal elements of the array. To prove the theorem for all values of n an inductive argument reminiscent of that used by Brudno and Louck (1985) is resorted to but taking into account the g. c. d conditions without allowing permutation of the components $x_i$ and $u_i$ for $i = 1, 2, \dots, n$. Let:

$$x_1 x_2 \dots x_n = u_1 u_2 \dots u_n = N , \tag{44}$$

and the induction argument is made with respect to the parameter N, keeping n fixed throughout.

Bell's theorem is obviously true for $N = 1$. The only solution is $x_i = u_i = 1$ for $i = 1, 2, \dots, n$ and correspondingly $\phi_{ij} = 1$ for all $i, j = 1, 2, \dots, n$. For the induction

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† The author wishes to thank Prof.R.C.King for this.

hypothesis it is assumed that all the solutions of (44) are given by Bell's theorem for $N = 1, 2, \ldots, M - 1$, with $M > 1$.

Now two cases arise: firstly any solution of (44) with $N = M$ for which

$$(x_i, u_i) = q \quad \text{with} \quad 1 < q \leq N \quad \text{for some } i \in \{ 1,2,\ldots,n \}. \tag{45}$$

Cancelling $q$ throughout (44) with $N = M$ gives an equation of the same type with $N = M/q$. By the induction hypothesis, all the solutions of this equation are given by Bell's theorem for some array $A(\phi')$. Having divided both $x_i$ and $u_i$ by $q$ it is clear that $\phi'_{ii} = 1$ . Simply multiplying this element at the intersection of the ith row and ith column of the array $A(\phi')$ by $q$ and leaving all the other elements unaltered gives the required array for the original solution of (44) with $N = M$. The g.c.d. conditions are automatically satisfied.

Secondly, there remains only the case for which

$$(x_i, u_i) = q = 1 \qquad \text{for all } i \in \{ 1,2,\ldots,n \}.$$

Since $M > 1$, it follows that there exists some prime $p > 1$ such that $p \mid M$. Correspondingly there exists $x_i$ and $u_j$ with $i \neq j$ such that $p \mid x_i$ and $p \mid u_j$. Cancelling $p$ throughout (44) with $N = M$ gives an equation of the type (44) with $N = M/p$. By the induction hypothesis, any solution of this equation gives an array $A(\phi')$ satisfying the g.c.d. conditions. In fact, by virtue of (46), all the diagonal entries are 1. Multiplying the entry $\phi'_{ij}$ at the intersection of the ith row and jth column by $p$ and again leaving all the other elements unaltered gives the array $A(\phi)$ required to represent the solution of (44) with $N = M$. The g.c.d condition is still satisfied because the diagonal entries are still just 1.

This completes the induction argument and Bell's theorem is proved provided it is shown that the $n^2$ parameters are genuinely independent. This can be seen most easily by considering those solutions of (41) of the form (42) for which the $n^2$ parameters $\phi_{ij}$ take on $n^2$ distinct prime values. It is obvious that to generate the complete set of such solutions for arbitrary $N$, all the $n^2$ parameters are required.

It is worth pointing out that in general for $n > 3$ it is not true that all distinct arrays $A(\phi)$ satisfying the g.c.d. conditions (43) give distinct solutions. However, this is the case for $n \leq 3$. This is trivial for $n = 1$ and $n = 2$. For $n = 3$ it can be proved by noting that if $A(\phi)$ and $A(\phi')$ are different but correspond to the same solution of (41) then there exists some prime $p > 1$ and some pair $(i, j)$ with $i \neq j$ such that

$$p \mid \phi_{ij} \quad , \quad p \nmid \phi'_{ij} \, . \tag{47}$$

In order that the arrays $A(\phi)$ and $A(\phi')$ correspond to the same solution the product of the elements in their $i$th rows must coincide, as must the products of the elements in their $j$th columns. Hence, taking into account the fact that their diagonal elements also coincide, there must exist $k$ such that

$$p \mid \phi'_{ik} \quad \text{with} \quad \{ i,j,k \} \subseteq \{ 1,2,\ldots,n \} \text{ and } k \neq i \neq j \neq k \tag{48}$$

and $m$ such that

$$p \mid \phi'_{mj} \quad \text{with} \quad \{ i,j,m \} \subseteq \{ 1,2,\ldots,n \} \text{ and } m \neq i \neq j \neq m \, .$$

It follows that if $n = 3$ then $k = m$. Hence

$$(x_k , u_k ) = \mu . p . \phi'_{kk} = \mu . p . (x_k , u_k) , \tag{50}$$

for some integer $\mu \geq 1$ , and we have a contradiction for $p > 1$. It follows that, for $n = 3$, distinct arrays $A(\phi)$ satisfying the g.c.d. conditions (43) lead by means of (42) to distinct solutions (41) and vice versa. Applying this result to the degree-one zeros discussed above leads to the following.

*Theorem:* The degree-one *polynomial* zeros of the 6-j coefficients are all given, upto symmetry transformations, by:

$$\left\{ \begin{matrix} (x+u+v-t)/2 & (y+u+w-t)/2 & (x+y+v+w-2t)/2 \\ (x+w)/2 & (y+v)/2 & (x+y+u-t)/2 \end{matrix} \right\}$$

$$= \left\| \begin{matrix} t & x & y \\ u & x+u-t & y+u-t \\ w & x+w-t & y+w-t \\ v & x+v-t & y+v-t \end{matrix} \right\| , \tag{51}$$

with $t = 1$ and $x\,y\,z = u\,v\,w$, where $z = x + y + u + v + w$. In (51) the right hand side represents the Bargmann - Shelepin array (Bargmann (1962), Shelepin (1964)) defined by (55) of Chapter 1. All possible solutions to these equations are specified by the distinct arrays of the form :

$$\begin{array}{c|ccc} & u & v & w \\ \hline x & a & b & c \\ y & d & e & f \\ z & g & h & i \end{array} , \tag{52}$$

where $(x, y, z, u, v, w)$ are given by the products of the elements in the appropriate rows and columns of this array. The entries $(a, b, c, d, e, f, g, h, i)$ take on all positive integer values consistent with the conditions:

and

$$g\,h\,i = a\,d\,g + b\,e\,h + c\,f\,i + a\,b\,c + d\,e\,f \tag{53}$$

$$\begin{aligned}(b,\ d) &= (b,\ g) = (b,\ f) = (c,\ d) = (c,\ g) = (c,\ h)\\ &= (d,\ h) = (f,\ g) = (f,\ h) = 1.\end{aligned} \tag{54}$$

This makes it obvious that the complete set of solutions of the equation (44) constrained by (43) requires a minimum of eight parameters (since (53) can be used to eliminate one of the nine parameters). Thus (33) can be explicitly written in terms of eight parameters alone (viz. x, y, u, v, $c$, $f$, $g$ and $h$ where $x = a\,b\,c$, $y = d\,e\,f$, $u = a\,d\,g$ and $v = b\,e\,h$) as:

$$\left\{\begin{matrix} (x+u+y+v-1) & (y+u+\dfrac{cf(x+y+u+v)}{(gh-cf)}-1) & (x+y+v-2+\dfrac{x+y+u+v}{(gh-cf)}) \\ (abc+\dfrac{cf(x+y+u+v)}{(gh-cf)}) & (y+v) & (x+y+u-1) \end{matrix}\right\} \tag{54a}$$

Though Brudno (1985) obtained a nine parameter solution, those parameters were not required to satisfy the g.c.d. conditions given by (54) nor did he realise the vital connection between *polynomial* zeros of degree 1 of the 6-j coefficient and the homogeneous multiplicative Diophantine equation of degree 3.

### 4.7 Comparison with other parametrisations

The three one-parameter formulae of Brudno (1985) given by (27), (28) and (29) are rewritten as:

$$\left\{\begin{matrix} n+2 & n+1 & 2 \\ n & n+1 & n+1 \end{matrix}\right\} \longrightarrow \left\{\begin{matrix} m+2 & m+1 & m+1 \\ m & 2 & m+1 \end{matrix}\right\}, \tag{55}$$

$$\left\{\begin{matrix} (3x+4)/2 & (3x+4)/2 & x+2 \\ (2x+3)/2 & 3/2 & (3x+3)/2 \end{matrix}\right\} \longrightarrow \left\{\begin{matrix} (3n+1)/2 & (3n+1)/2 & n+1 \\ (2n+1)/2 & 3/2 & 3n/2 \end{matrix}\right\}, \tag{56}$$

and

$$\begin{Bmatrix} J & 4J-1 & 3J \\ (4J+3)/2 & (2J+1)/2 & (4J-1)/2 \end{Bmatrix} \longrightarrow \begin{Bmatrix} (2b+5)/2 & 2b+1 & (2b+1)/2 \\ (b+1)/2 & (b+2)/2 & (3b+3)/2 \end{Bmatrix}, \qquad (57)$$

with $m, n, b = 1, 2, \ldots$ , where , in (55) and (57) the symmetries of the 6-j coefficient have been exploited to write them in the form (51) with $t = 1$. These three cases are covered in the notation of (52) by means of the arrays:

$$\begin{array}{c|ccc} & u & v & w \\ \hline x & 1 & 1 & m \\ y & 1 & 1 & 1 \\ z & m+2 & 3 & 1 \end{array}\ , \qquad \begin{array}{c|ccc} & u & v & w \\ \hline x & n & 1 & 1 \\ y & 1 & 1 & 1 \\ z & 2 & 2 & n+1 \end{array}\ , \qquad \begin{array}{c|ccc} & u & v & w \\ \hline x & 1 & 1 & 1 \\ y & 1 & 1 & b \\ z & (2b+3) & 2 & 1 \end{array}$$

respectively.

By solving the pair of Diophantine equations (38) and (39) for sums of like powers, Brudno and Louck (1985) determined the two-parameter solution specified by the array :

$$\begin{array}{c|ccc} & u & v & w \\ \hline x & q & 3q-2p & 1 \\ y & p/2 & 1 & q-p \\ z & 3 & (2q-p)/2 & 3q-p \end{array} \quad \Longrightarrow \quad \begin{array}{c|ccc} & u & v & w \\ \hline x & 2b+h & 2b+3h & 1 \\ y & b & 1 & h \\ z & 3 & b+h & 4b+3h \end{array}\ , \qquad (58)$$

with $b, h = 1, 2, \ldots$. By the same means Bremner (1986) obtained the solutions given by the arrays:

$$\begin{array}{c|ccc} & u & v & w \\ \hline x & \gamma-\delta & \beta & 2 \\ y & \alpha-2\beta & 1 & \delta \\ z & 1 & \gamma+2\delta & \alpha+\beta \end{array} \quad \Longrightarrow \quad \begin{array}{c|ccc} & u & v & w \\ \hline x & a & d & 2 \\ y & b & 1 & h \\ z & 1 & a+3h & b+3d \end{array}\ , \qquad (59)$$

with $a, b, d, h = 1, 2, \ldots$ and

$$
\begin{array}{c|ccc}
 & u & v & w \\
\hline
x & \alpha\gamma-4\alpha\delta+\beta\gamma-\beta\delta & (-\gamma+5\delta)/2 & \alpha \\
y & (\alpha\gamma-5\alpha\delta+\beta\gamma-2\beta\delta)/2 & 1 & -\alpha\gamma+5\alpha\delta-\beta\delta \\
z & 1 & -\alpha^2\gamma+5\alpha^2\delta+\beta^2\gamma-2\beta^2\delta & 3\delta/2
\end{array}
\longrightarrow
$$

$$
\longrightarrow
\begin{array}{c|ccc}
 & u & v & w \\
\hline
x & ps+3qr+4qs & r/2 & p \\
y & (-pr+2qr+3qs)/2 & 1 & pr-qr-qs \\
z & 1 & p^2r+2q^2r+3q^2s & (3r+3s)/2
\end{array}
\qquad (60)
$$

with p, q, r, s = 1, 2, ... subject to the constraint:

$$q\,(2r + 3s) \;>\; pr \;>\; q\,(r + s).$$

The culmination of this approach is the four-parameter formula of Bremner and Brudno (1986) which they claim gives the complete solution to the problem. However, it is not difficult to see that the array corresponding to their solution (Bremner and Brudno (1986), equation (27)) can be written in the form:

$$
\begin{array}{c|ccc}
 & u & v & w \\
\hline
x & r & 1 & pq-rs \\
y & s & pq-rs & 1 \\
z & p+q+r+s & p & q
\end{array}
\longrightarrow
\begin{array}{c|ccc}
 & u & v & w \\
\hline
x & a & 1 & fi-ab \\
y & b & fi-ab & 1 \\
z & a+b+f+i & f & i
\end{array}
\quad . \qquad (61)
$$

Clearly this solution is not complete in the sense that varying p, q, r and s over all positive integers subject to the obvious requirement $p\,q > r\,s$ does not generate all possible solutions. For example, the very well known first solution :

$$
\left\{ \begin{matrix} 2 & 2 & 2 \\ 3/2 & 3/2 & 3/2 \end{matrix} \right\} = 0 \qquad (62)
$$

corresponding to x = y = 1, u = v = w = 2 and z = 8, specified by the array :

| | u | v | w |
|---|---|---|---|
| x | 1 | 1 | 1 |
| y | 1 | 1 | 1 |
| z | 2 | 2 | 2 |

(63)

cannot be obtained from (61) with integer parameters. A clue to this omission comes from noticing that it may be recovered from (61) by setting :

$$p = q = 2.\left( \frac{1}{3} \right)^{1/3} \quad , \quad r = s = \left( \frac{1}{3} \right)^{1/3} \quad . \qquad (64)$$

The explanation for this lies in the fact that in deriving the solution (61) to (38) and (39) Bremner and Brudno (1986) have made successive transformations from the parameters (X, Y, Z, U, V, W) to ($\alpha$, $\beta$, $\gamma$, $\delta$) to (p, q, r, s). However, at one stage a denominator is removed, with the justification that their original equations (38) and (39) are homogeneous. Quite apart from the fact that such a step is not appropriate in dealing with Diophantine equations, the weight-one 6-j coefficients are not themselves homogeneous in any of the sets of parameters since their definition involves setting t = 1 in (51). In terms of the parameters (p, q, r, s) of Bremner and Brudno (1986), the hidden change of parameters is such that in their solution (27) these four parameters should be replaced by :

$$p' = p \{ 2(pq - rs) \}^{-1/3} \quad , \quad q' = q \{ 2(pq - rs) \}^{-1/3},$$
$$r' = r \{ 2(pq - rs) \}^{-1/3} \quad , \quad s' = s \{ 2(pq - rs) \}^{-1/3}. \qquad (65)$$

The substitution of the values p = q = 4 and r = s = 2 then gives $p' = q' = 2 \left(\frac{1}{3}\right)^{1/3}$ and $r' = s' = \left(\frac{1}{3}\right)^{1/3}$, which as noted in (64) enables (63) to be recovered from (61).

It is perhaps worth pointing out that a four-parameter solution very closely related to (61) may be very trivially obtained from the complete solution (52) merely by rearranging the elements as below, taking care to preserve all row and column products :

$$\begin{array}{c|ccc} & u & v & w \\ \hline x & abc & 1 & 1 \\ y & def & 1 & 1 \\ z & \dfrac{g}{bcef} & beh & cfi \end{array} \longrightarrow \begin{array}{c|ccc} & u & v & w \\ \hline x & a & 1 & 1 \\ y & d & 1 & 1 \\ z & \dfrac{a+d+h+i}{hi-ad} & h & i \end{array}$$

This is a four-parameter formula for the complete solution in which the parameters $a$, $d$, $h$, $i$ are positive integers. This same complete solution to the Diophantine equations (35) and (36) can be obtained even more trivially by setting x = a, y = d, v = h and w = i. Solving for z and u then gives

$$z = (a + d + h + i)\, hi \,/\, (hi - ad) \;, \quad u = adz\,/hi \qquad (67)$$

precisely as indicated in (66). For each set of such parameters it is necessary to check that z is a positive integer, which would ensure u being an integer. In terms of Bell's theorem (52), since $b = c = e = f = 1$, we have, in fact, a five-parameter solution, which reduces to a four-parameter solution due to the constraint equation (53). It should be noted that the fifth parameter $(a + d + h + i) / (hi - ad)$ will not always be an integer, e.g.

$$\begin{Bmatrix} 7 & 9/2 & 9/2 \\ 5/2 & 4 & 4 \end{Bmatrix} = \begin{Bmatrix} 9/2 & 9/2 & 7 \\ 4 & 4 & 5/2 \end{Bmatrix},$$

has the four-parameter solution

$$x = a = 2 \;, \quad y = d = 2 \;, \quad v = h = 6 \;, \quad w = i = 6 \;,$$

so that the fifth parameter is:

$$(a + d + h + i) \,/\, (hi - ad) = 1/2$$

which is an exceptional case referred to in Table 5.

The conclusion drawn from the above discussion is that the one-, two- and four-parametric solutions given by Brudno (55) - (57), Brudno and Louck (58), Bremner (59) and (60), and ourselves (66) do not yield all the polynomial zeros of degree one of the 6-j coefficient. To illustrate this explicitly, the minimum values of the parameters allowed in the one-, two-, four- and eight-parametric solutions given by different authors and the corresponding arguments of

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ \ell_1 & \ell_2 & \ell_3 \end{Bmatrix} = 0$$

with the value of the invariant

$$I = 2 \sum_{k=1}^{3} (j_k + \ell_k) = 3z + x + y - 5$$

are listed in Table 4. Note that

$$\begin{Bmatrix} 2 & 2 & 2 \\ 3/2 & 3/2 & 3/2 \end{Bmatrix} = 0$$

corresponding to I = 21 is the first polynomial zero of degree one given in Table 1.

Though, like the eight-parameter solution (52) and (53), the one-parameter and four-parameter formulae (56) and (66) also give rise to the first of the non-trivial degree-one zeros, unlike the eight-parameter case, (56) as well as the two other one-parameter formulae (55) and (57), the two-parameter formulae (58) and the four-parameter formulae (59) and (60), cannot generate the complete list of polynomial zeros of degree one. This is illustrated in Table 5 by listing the first fifteen Regge inequivalent polynomial zeros of degree one and indicating which of the parametric solutions given in Table 4 can account for them and which cannot.

### 4.8 Algorithms

In this section two algorithms are discussed to solve (53) and find all its solutions. To solve (53) completely, it is reduced to (i) a quadratic Diophantine equation (Srinivasa Rao and Rajeswari 1987) and (ii) a linear Diophantine equation, the solutions of which were given by Brahmegupta (of 6th Century A.D., c.f. Dickson, 1952, p.64) and Paoli (c.f. Dickson 1952, p.401) respectively, and these are described below:

**Algorithm 1** : Since the nine parameters in the array (52) can take non-zero integer values :

(i) Choose $a$, $b$, $c$, $d$, $e$ and $f$ to have values 1 to 10 (say), successively and arrange these into a nest of loops.

(ii) Choose a value of i, also to be 1 to 10 (say).

(iii) Equation (53) then reduces to the quadratic Diophantine equation :

$$\alpha x y = \beta x + \gamma y + \delta , \tag{68}$$

with $\alpha = i$, $x = g$, $y = h$, $\beta = ad$, $\gamma = be$ and $\delta = abc + def + cfi$.

(iv) The solutions of (68) were given by Brahmegupta as follows: Let $\varepsilon$ be an integer and let $\eta = (\alpha \delta + \beta \gamma)/\varepsilon$. Choosing only those integer values of $\varepsilon$ which will give integer values of $\eta$, the solutions for x and y are given by the two sets:

$\frac{1}{\alpha}$ [max $(\varepsilon,\eta)$ + min $(\beta,\gamma)$], $\frac{1}{\alpha}$ [min $(\varepsilon,\eta)$ + max $(\beta,\gamma)$], (69a)

$\frac{1}{\alpha}$ [max $(\varepsilon,\eta)$ + max $(\beta,\gamma)$], $\frac{1}{\alpha}$ [min $(\varepsilon,\eta)$ + min $(\beta,\gamma)$]. (69b)

In these sets (69a) and (69b), x is that containing $\gamma$ . Using this method, all allowed values of g and h for a given set of $a$, $b$, $c$, $d$, $e$, $f$ and $i$ in (53) are found out.

**Algorithm 2 :**

(i) Let seven of the nine parameters in (52) take successive values 1 to 10 (say) and these are arranged into a nest of loops. The two parameters excluded from this nest should belong to independent rows and columns, e.g. $(a,e)$, $(e,i)$, $(b,d)$, $(c,e)$, $(e,g)$ etc, in (52).

(ii) The nine relative prime conditions to be satisfied by the parameters, given by (54), are checked. (These conditions are the direct consequence of the three g.c.d. conditions).

(iii) The constraint equation (53) now reduces to the form of a linear Diophantine equation:

$$\alpha' x + \beta' y = \gamma' . \tag{70}$$

For instance, if x = $a$, y = $e$ then

$$\alpha' = bc + dg , \beta' = df + bh , \gamma' = i (gh - cf). \tag{71}$$

(iv) Solutions of (70) and (71) are sought such that $gh > cf$ and $i(gh - cf) \geq b (c + h) + d(f + g)$. Paoli (Dickson (1952)) noted that if (70) has integral solutions, any common factor of $\alpha'$ and $\beta'$ must divide $\gamma'$ and hence can be removed from every term. Hence, let $\alpha'$ and $\beta'$ be relatively prime and positive. Let $\varepsilon$ denote the least positive integer such that $(\gamma' - \alpha'\varepsilon)$ is divisible by $\beta'$. Then every solution is given by:

$$x = \varepsilon + \beta' m , \qquad y = (\gamma' - \alpha'\varepsilon)/\beta' - \alpha' m , \tag{72}$$

where the values of m making x and y positive are 0, 1, 2,...E; E being the largest integer less than $(\gamma' - \alpha'\varepsilon)/\alpha'\beta'$. Thus all the parameters subject to the constraint (70) are determined.

Determining the nine parameters of the array (52) using either of the algorithms given above x, y, z and u, v, w are found out (being the products of the row and column elements of (52) respectively). These values when used in (51) with t =1 gives the corresponding degree-one zero of the 6-j coefficient.

Alternatively, a simpler algorithm is the one which arises due to the four-parameter solution given in (66):

(i) Let all the four integer parameters, $a$, $d$, $h$, $i$ take successive values 1 to 10 (say) and these are arranged into a nest of loops;

(ii) Check for $hi > ad$, compute z given by (67), and

(iii) Check for z being an integer and compute u given in (67).

Having obtained the values of $x = a$, $y = d$, $v = h$ and $w = i$, as well as the values of u and z, the required degree-one polynomial zero is given by (51) with t = 1.

All the three algorithms mentioned above have been successfully tested on a computer to generate all the *inequivalent* polynomial zeros of degree 1 of the 6-j coefficient corresponding to the table of Biedenharn and Louck (1981b). These programs are described in Appendix B.

**4.9 Physical Significance of the zeros**

The *polynomial* zeros have also been studied using Group theoretical methods (Van den Berghe et al) and utilising the deep connection between the angular momentum coupling, recoupling coefficients and the orthogonal polynomial (Suslov et al). A few of the zeros have been explained using the seniority coupling scheme, quasi-spin model and the coefficients of fractional parentage. These are described briefly below.

One well-known example of a non-trivial zero of the 6-j coefficient known from the time of Racah (1942) is:

$$\begin{Bmatrix} 5 & 5 & 3 \\ 3 & 3 & 3 \end{Bmatrix}.$$

Biedenharn and Louck (1981b) have illustrated how this zero comes out as a consequence of the embedding of the exceptional Lie algebra $G_2$ in the algebra SO(1). Following their remark that it would be of considerable interest to examine the remaining exceptional groups by similar explicit results, Van den Berghe et. al. have discussed in series of papers (Van der Jeugt, Van den Berghe and De Meyer 1983; Van den Berghe, De Meyer and Van der Jeugt (1984); De Meyer, Van den Berghe and Van der Jeugt (1984)) the results for the exceptional groups $F_4$ and $E_6$. They have explained a few of the zeros from realisations of the exceptional Lie algebras $F_4$ and $E_6$. Their results are tabulated in Table 6. It is to be noted that of the 9 *inequivalent* 6-j zeros,8 are degree 1 zeros and only one is of a higher degree.

The connection between the 6-j coefficient and the Racah polynomial - which is an orthogonal polynomial (Wilson (1982)) of a discrete variable (polynomial orthogonal on a discrete set of points) - has been utilised by Smorodinskii and Suslov (1982a) in explaining some of the zeros. They look upon the zeros of these coefficients as the zeros of the Racah polynomial and have given a condition for these zeros which is the simplest condition for a root of the polynomial. In Table 7 the zeros explained by this method are listed.

Arfken, Biedenharn and Rose (1951) while investigating the possibility of competing radiations exhibiting different angular distributions (in the sense that one radiation is isotropic and another anisotropic) came across two singular cases, viz. the transitions: $3/2 \to 3/2$ and $5 \to 4$ by quadrupole emission. These transitions implied the non-trivial vanishing of the 6-j coefficients:

$$\begin{Bmatrix} 2 & 2 & 2 \\ 3/2 & 3/2 & 3/2 \end{Bmatrix} \quad \text{and} \quad \begin{Bmatrix} 5 & 5 & 2 \\ 2 & 2 & 4 \end{Bmatrix} .$$

Amos de-Shalit and Talmi (1963) have shown that the first of these is zero on the basis of the seniority scheme. An explanation for this vanishing has also been given by Biedenharn and Louck (1981b) who based their argument on the quasi-spin model. A brief description of the quasi - spin model and the explanation for the zero is presented below.

In the quasi-spin model, three operators viz. $Z_+$, $Z_-$ and $Z_o$

are defined in terms of the fermion creation and annihilation operators $b^{\dagger}_{j,m}$ and $b_{j,m}$ respectively as:

$$Z_{+} = \frac{1}{2} \sum_{m} (-1)^{j-m} b^{\dagger}_{j,m} b^{\dagger}_{j,-m} , \qquad (73)$$

$$Z_{-} \equiv (Z_{+})^{\dagger} = \frac{1}{2} \sum_{m} (-1)^{j-m} b_{j,-m} b_{j,m} . \qquad (74)$$

In (73) and (74) j, m denote the total angular momentum and projection quantum number of the fermion on which the operator $b_{j,m}$ operates. Using the anticommutation rules for the fermion operators, and assuming that (2j) is an odd integer one finds that:

$$[ Z_{+} , Z_{-} ] = 2 \sum (b^{\dagger}_{j,m} b_{j,m} - b_{j,m} b^{\dagger}_{j,m})/4 \equiv 2 Z_{o} . \qquad (75)$$

With $Z_o$ defined in the above manner, it can be shown that

$$[ Z_{o} , Z_{\pm} ] = \pm Z_{\pm} , \qquad (76)$$

which shows that the three operators, $Z_+$, $Z_-$, $Z_o$ obey the commutation rules characterising angular momentum. Hence these are called quasi-spin operators.

Combining the concept of seniority and the creation-annihilation property of the operators $Z_+$, $Z_-$ and $Z_o$ the eigenvalues of the operator $Z^2$ defined by:

$$Z^{2} = (Z_{+} Z_{-} + Z_{-} Z_{+}) + Z_{o}^{2} \qquad (77)$$

can be found out and it is given by:

$$z ( z + 1) \qquad (78)$$

where

$$z = \frac{2j+1}{4} - \frac{v}{2} , \qquad (79)$$

with v denoting the seniority of the many-particle nuclear state with angular momentum j. In (79) (2j + 1)/2 gives the total number of pairs (i.e. $J = 0$) that are allowed for a given j value and the seniority v gives the number of particles that are not paired (i.e not coupled to $J = 0$). The eigenvalue of $Z_o$ i.e. the *projection* of Z, is given by:

$$z_o = \frac{n}{2} - \frac{2j+1}{4}, \tag{80}$$

where n gives the total number of particles in the state j. Further, it can be shown that the tensor operators with odd angular momentum are quasi-scalars whereas the even tensor operators are quasi-vectors.

With these facts, let us look at the interaction energy of a quadrupolar one-body potential in the two-particle state (with $j = 3/2$) having $J = 2$. This has the form:

$$\begin{aligned} \langle E \rangle &= \langle (\tfrac{3}{2})^2, v = 2, J = 2, M \,|\, U_o^2 \,|\, (\tfrac{3}{2})^2, v = 2, J = 2, M \rangle \\ &\propto \begin{Bmatrix} 2 & 2 & 2 \\ 3/2 & 3/2 & 3/2 \end{Bmatrix} \end{aligned} \tag{81}$$

Since the one body potential $U_o^2$ is a quadrupole interaction it follows that it is a vector in quasi-spin space. The initial and final states belong to quasi-spin values:

$$\begin{aligned} z &= 0 \\ z_o &= 0 \end{aligned} \tag{82}$$

Hence the matrix element in (81) vanishes due to violation of quasi-spin $0 \not\subset 0 + 1$ and hence implies that the 6-j coefficient is zero though all the triangulr inequalities are satisfied for this.

Judd(1970) has related the following zeros:

$$\begin{Bmatrix} 5 & 5 & 2 \\ 2 & 2 & 4 \end{Bmatrix} \quad \text{and} \quad \begin{Bmatrix} 6 & 4 & 9 \\ 5 & 5 & 2 \end{Bmatrix}$$

to the vanishing of the fractional parentage coefficient in the atomic $g$ - shell.

## 4.10 Conclusion

To conclude, in this chapter

(i) We have shown that rewriting the 6-j coefficient as a formal binomial expansion, $(X - Y)^{(n)}$ the *polynomial* zeros of degree 1 of these coefficients can all be represented by the simple multiplicative factor :

$$(1 - \delta(n,1)\ \delta(X,Y)).$$

This criterion has been used to generate the complete list of degree one zeros.

(ii) Using Bell's theorem it has been established that eight parameters are necessary and sufficient for the complete solution of the homogeneous multiplicative Diophantine equation: $x\ y\ z = u\ v\ w$ along with the constraint $z = x + y + u + v + w$ which gives the condition for the *polynomial* zeros of degree 1 of the 6-j coefficient. The parametric formulae given by various authors for these degree 1 zeros in terms of fewer than eight parameters have been shown to generate only subsets of the complete set of zeros.

(iii) Two algorithms have been presented to solve the constraint equation $z = x + y + u + v + w$ which have been successfully tested on a computer to generate all the *polynomial* zeros of degree 1 of the 6-j coefficient.

Table 1

Polynomial zeros of degree one of the 6-j coefficient (equivalent ones).

| $j_1$ | $j_2$ | $j_3$ | $\ell_1$ | $\ell_2$ | $\ell_3$ | $j_1$ | $j_2$ | $j_3$ | $\ell_1$ | $\ell_2$ | $\ell_3$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 2.0 | 2.0 | 2.0 | 1.5 | 1.5 | 1.5 | 8.0 | 5.5 | 5.5 | 3.5 | 5.0 | 4.0 |
| 3.0 | 2.0 | 2.0 | 1.0 | 2.0 | 2.0 | 8.0 | 6.0 | 3.0 | 3.0 | 5.0 | 5.0 |
| 3.5 | 3.0 | 1.5 | 1.0 | 1.5 | 3.0 | 8.0 | 6.0 | 3.0 | 4.0 | 6.0 | 5.0 |
| 3.5 | 3.5 | 3.0 | 2.5 | 1.5 | 3.0 | 8.0 | 6.0 | 5.0 | 1.0 | 5.0 | 6.0 |
| 4.0 | 3.0 | 2.0 | 2.0 | 3.0 | 3.0 | 8.0 | 6.0 | 5.0 | 3.5 | 4.5 | 4.5 |
| 4.0 | 3.0 | 3.0 | 2.0 | 3.0 | 2.0 | 8.0 | 6.0 | 5.0 | 4.0 | 6.0 | 3.0 |
| 4.0 | 3.5 | 2.5 | 2.0 | 2.5 | 2.5 | 8.0 | 6.5 | 3.5 | 2.5 | 3.0 | 6.0 |
| 5.0 | 4.0 | 2.0 | 3.0 | 4.0 | 4.0 | 8.0 | 6.5 | 3.5 | 2.5 | 3.0 | 6.0 |
| 5.0 | 4.0 | 4.0 | 3.0 | 4.0 | 2.0 | 8.0 | 6.5 | 3 5 | 3.0 | 4.5 | 4.5 |
| 5.0 | 4.5 | 1.5 | 2.0 | 2.5 | 4.5 | 8.0 | 7.0 | 2.0 | 6.0 | 7.0 | 7.0 |
| 5.0 | 4.5 | 2.5 | 2.0 | 1.5 | 4.5 | 8.0 | 7.0 | 4.0 | 4.0 | 5.0 | 4.0 |
| 5.0 | 4.5 | 4.5 | 3.5 | 3.0 | 3.0 | 8.0 | 7.0 | 7.0 | 5.5 | 4.5 | 4.5 |
| 5.0 | 5.0 | 2.0 | 2.0 | 2.0 | 4.0 | 8.0 | 7.0 | 7.0 | 6.0 | 7.0 | 2.0 |
| 5.0 | 5.0 | 3.0 | 3.0 | 3.0 | 3.0 | 8.0 | 7.5 | 1.5 | 4.0 | 4.5 | 7.5 |
| 5.0 | 5.0 | 4.0 | 3.5 | 1.5 | 4.5 | 8.0 | 7.5 | 4.5 | 4.0 | 1.5 | 7.5 |
| 5.5 | 4.0 | 3.5 | 1.0 | 3.5 | 4.0 | 8.0 | 7.5 | 6.5 | 5.5 | 3.0 | 6.0 |
| 6.0 | 4.0 | 3.0 | 1.5 | 3.5 | 3.5 | 8.0 | 8.0 | 6.0 | 5.5 | 1.5 | 7.5 |
| 6.0 | 4.5 | 2.5 | 2.5 | 4.0 | 4.0 | 8.0 | 8.0 | 7.0 | 4.0 | 4.0 | 7.0 |
| 6.0 | 5.0 | 2.0 | 4.0 | 5.0 | 5.0 | 8.5 | 7.0 | 4.5 | 1.0 | 4.5 | 7.0 |
| 6.0 | 5.0 | 3.0 | 1.0 | 3.0 | 5.0 | 8.5 | 7.0 | 6.5 | 4.0 | 6.5 | 4.0 |
| 6.0 | 5.0 | 3.0 | 2.5 | 3.5 | 3.5 | 8.5 | 8.0 | 2.5 | 1.0 | 2.5 | 3.0 |
| 6.0 | 5.0 | 5.0 | 4.0 | 5.0 | 2.0 | 8.5 | 8.0 | 5.5 | 4.0 | 5.5 | 5.0 |
| 6.0 | 6.0 | 4.0 | 2.5 | 2.5 | 5.5 | 8.5 | 8.0 | 6.5 | 4.5 | 3.0 | 7.5 |
| 6.0 | 6.0 | 6.0 | 5.0 | 4.0 | 3.0 | 8.5 | 8.5 | 5.0 | 3.5 | 2.5 | 8.0 |
| 6.5 | 5.0 | 2.5 | 1.5 | 3.0 | 4.5 | 9.0 | 6.0 | 4.0 | 2.0 | 5.0 | 5.0 |
| 6.5 | 5.0 | 2.5 | 3.5 | 5.0 | 4.5 | 9.0 | 6.5 | 5.5 | 2.0 | 6.5 | 6.5 |
| 6.5 | 5.0 | 4.5 | 2.0 | 4.5 | 4.0 | 9.0 | 6.5 | 6.5 | 2.0 | 6.5 | 5.5 |
| 6.5 | 5.0 | 4.5 | 3.5 | 5.0 | 2.5 | 9.5 | 6.5 | 6.5 | 4.5 | 6.0 | 4.0 |
| 6.5 | 6.0 | 1.5 | 3.0 | 3.5 | 6.0 | 9.0 | 7.0 | 6.0 | 2.0 | 6.0 | 6.0 |

Table 1 (continued).

| $j_1$ | $j_2$ | $j_3$ | $\ell_1$ | $\ell_2$ | $\ell_3$ | $j_1$ | $j_2$ | $j_3$ | $\ell_1$ | $\ell_2$ | $\ell_3$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 6.5 | 6.0 | 3.5 | 3.0 | 1.5 | 6.0 | 9.0 | 7.5 | 2.5 | 3.0 | 4.5 | 6.5 |
| 6.5 | 6.0 | 3.5 | 3.0 | 2.5 | 5.0 | 9.0 | 7.5 | 2.5 | 5.0 | 6.5 | 6.5 |
| 6.5 | 6.0 | 3.5 | 3.5 | 4.0 | 3.5 | 9.0 | 7.5 | 3.5 | 4.0 | 6.5 | 7.5 |
| 6.5 | 6.0 | 5.5 | 3.5 | 5.0 | 3.5 | 9.0 | 7.5 | 5.5 | 4.5 | 5.0 | 5.0 |
| 6.5 | 6.0 | 5.5 | 4.5 | 3.0 | 4.5 | 9.0 | 7.5 | 6.5 | 4.0 | 3.5 | 7.5 |
| 6.5 | 6.5 | 5.0 | 4.5 | 1.5 | 6.0 | 9.0 | 8.0 | 2.0 | 1.5 | 2.5 | 7.5 |
| 6.5 | 6.5 | 5.0 | 4.5 | 3.5 | 4.0 | 9.0 | 8.0 | 2.0 | 5.5 | 6.5 | 7.5 |
| 6.5 | 6.5 | 5.0 | 5.0 | 5.0 | 2.5 | 9.0 | 8.0 | 2.0 | 7.0 | 8.0 | 8.0 |
| 7.0 | 4.5 | 4.5 | 2.5 | 4.0 | 4.0 | 9.0 | 8.0 | 3.0 | 3.0 | 4.0 | 6.0 |
| 7.0 | 5.5 | 5.5 | 4.0 | 4.5 | 3.5 | 9.0 | 8.0 | 3.0 | 3.0 | 5.0 | 8.0 |
| 7.0 | 6.0 | 2.0 | 2.5 | 3.5 | 5.5 | 9.0 | 8.0 | 5.0 | 3.0 | 3.0 | 8.0 |
| 7.0 | 6.0 | 2.0 | 5.0 | 6.0 | 6.0 | 9.0 | 8.0 | 6.0 | 5.0 | 3.0 | 7.0 |
| 7.0 | 6.0 | 5.0 | 4.0 | 4.0 | 4.0 | 9.0 | 8.0 | 6.0 | 5.0 | 4.0 | 6.0 |
| 7.0 | 6.0 | 6.0 | 2.5 | 5.5 | 4.5 | 9.0 | 8.0 | 6.0 | 6.0 | 7.0 | 3.0 |
| 7.0 | 6.0 | 6.0 | 5.0 | 6.0 | 2.0 | 9.0 | 8.0 | 8.0 | 1.5 | 7.5 | 7.5 |
| 7.0 | 6.5 | 2.5 | 2.5 | 3.0 | 5.0 | 9.0 | 8.0 | 8.0 | 5.5 | 7.5 | 3.5 |
| 7.0 | 6.5 | 4.5 | 4.5 | 5.0 | 3.0 | 9.0 | 8.0 | 8.0 | 7.0 | 8.0 | 2.0 |
| 7.0 | 6.5 | 5.5 | 2.5 | 5.0 | 5.0 | 9.0 | 8.5 | 4.5 | 4.0 | 2.5 | 7.5 |
| 7.5 | 6.0 | 5.5 | 3.0 | 5.5 | 4.0 | 9.0 | 8.5 | 8.5 | 7.0 | 5.5 | 4.5 |
| 7.5 | 6.5 | 3.0 | 2.0 | 4.0 | 6.5 | 9.0 | 9.0 | 4.0 | 4.0 | 3.0 | 7.0 |
| 7.5 | 6.5 | 4.0 | 2.0 | 3.0 | 6.5 | 9.0 | 9.0 | 4.0 | 5.0 | 5.0 | 5.0 |
| 7.5 | 6.5 | 5.0 | 3.0 | 5.0 | 4.5 | 9.0 | 9.0 | 5.0 | 5.0 | 4.0 | 6.0 |
| 7.5 | 7.0 | 3.5 | 2.0 | 3.5 | 6.0 | 9.0 | 9.0 | 5.0 | 6.0 | 6.0 | 4.0 |
| 7.5 | 7.5 | 7.0 | 5.0 | 3.0 | 6.5 | 9.0 | 9.0 | 8.0 | 6.0 | 3.0 | 8.0 |
| | | | | | | 9.0 | 9.0 | 8.0 | 7.0 | 5.0 | 5.0 |

Table - 2

Polynomial Zeros of degree 2 of the 6-j coefficient (equivalent ones).

| $j_1$ | $j_2$ | $j_3$ | $\ell_1$ | $\ell_2$ | $\ell_3$ |
|---|---|---|---|---|---|
| 6.0 | 6.0 | 3.0 | 6.0 | 5.0 | 6.0 |
| 6.0 | 6.0 | 5.0 | 6.0 | 3.0 | 6.0 |
| 6.0 | 6.0 | 6.0 | 6.0 | 5.0 | 3.0 |
| 6.5 | 6.0 | 5.5 | 5.5 | 3.0 | 5.5 |
| 7.0 | 6.0 | 4.0 | 4.0 | 6.0 | 5.0 |
| 7.0 | 6.0 | 5.0 | 4.0 | 6.0 | 4.0 |
| 7.0 | 6.5 | 4.5 | 4.0 | 5.5 | 4.5 |
| 7.5 | 5.5 | 4.0 | 4.5 | 5.5 | 5.0 |
| 7.5 | 5.5 | 5.0 | 4.5 | 5.5 | 4.0 |
| 7.5 | 6.0 | 4.5 | 4.5 | 5.0 | 4.5 |
| 8.0 | 8.0 | 3.0 | 6.5 | 5.5 | 7.5 |
| 8.5 | 7.5 | 3.0 | 6.0 | 6.0 | 7.5 |
| 8.5 | 7.5 | 6.0 | 6.0 | 3.0 | 7.5 |
| 8.5 | 8.0 | 2.5 | 4.0 | 3.5 | 8.0 |
| 8.5 | 8.0 | 3.5 | 4.0 | 2.5 | 8.0 |
| 8.5 | 8.5 | 3.0 | 4.0 | 3.0 | 7.5 |
| 9.0 | 8.0 | 3.0 | 3.5 | 3.5 | 7.5 |
| 9.0 | 8.0 | 4.0 | 4.5 | 6.5 | 6.5 |
| 9.0 | 8.0 | 8.0 | 7.5 | 5.5 | 5.5 |
| 9.0 | 8.5 | 4.5 | 4.5 | 6.0 | 6.0 |
| 9.0 | 9.0 | 5.0 | 3.5 | 3.5 | 7.5 |
| 9.0 | 9.0 | 5.0 | 7.5 | 7.5 | 3.5 |
| 9.0 | 9.0 | 8.0 | 8.0 | 7.5 | 3.5 |

Table - 3

Polynomial zeros of degree 3,4 and 5 of the 6-j coefficient (equivalent ones)

POLYNOMIAL ZEROS OF DEGREE 3

| $j_1$ | $j_2$ | $j_3$ | $\ell_1$ | $\ell_2$ | $\ell_3$ |
|---|---|---|---|---|---|
| 12.0 | 10 5 | 10.5 | 8.5 | 10.0 | 5.0 |
| 12.0 | 12.0 | 9.0 | 8.0 | 4.0 | 11.0 |
| 13.0 | 10.5 | 9.5 | 7.5 | 10.0 | 6.0 |
| 13.0 | 12.0 | 8.0 | 7.5 | 8.5 | 7.5 |
| 14.0 | 11.0 | 6.0 | 6.0 | 9.0 | 10.0 |
| 14.0 | 12.0 | 5.0 | 9.0 | 11.0 | 12.0 |
| 14.0 | 12.0 | 7.0 | 6.0 | 8.0 | 9.0 |
| 14.0 | 12.0 | 11.0 | 9.0 | 5.0 | 12.0 |
| 15.0 | 12.0 | 6.0 | 8.0 | 11.0 | 11.0 |
| 15.0 | 13.5 | 13.5 | 13.5 | 10.0 | 8.0 |
| 15.0 | 14.0 | 8.0 | 8.0 | 9.0 | 9.0 |
| 15.0 | 14.5 | 12.5 | 13.5 | 9.0 | 9.0 |
| 15.5 | 14.5 | 12.0 | 10.5 | 4.5 | 14.0 |
| 15.5 | 15.5 | 15.0 | 12.0 | 6.0 | 13.5 |
| 16.0 | 13.5 | 12.5 | 12.5 | 8.0 | 11.0 |
| 16.0 | 14.5 | 11.5 | 12.5 | 9.0 | 10.0 |
| 16.0 | 15.5 | 14.5 | 12.5 | 6.0 | 13.0 |
| POLYNOMIAL ZEROS OF DEGREE 4 | | | | | |
| 16.0 | 15.5 | 15.0 | 11.5 | 14.5 | 7.5 |
| 17.0 | 15.0 | 14.0 | 12.0 | 7.5 | 13.5 |
| 17.5 | 15.0 | 13.5 | 10.0 | 14.5 | 9.0 |
| 17.5 | 16.0 | 15.5 | 7.5 | 12.0 | 15.5 |
| 17.5 | 17.0 | 11.5 | 10.0 | 12.5 | 11.0 |
| 17.5 | 17.5 | 14.0 | 13.5 | 7.5 | 14.0 |
| 18.5 | 14.0 | 13.5 | 11.0 | 13.5 | 9.0 |
| 18.5 | 16.0 | 11.5 | 11.0 | 11.5 | 11.0 |
| 18.5 | 18.0 | 15.5 | 8.0 | 11.5 | 15.0 |

Table 3 (continued).

POLYNOMIAL ZEROS OF DEGREE 5

| $j_1$ | $j_2$ | $j_3$ | $\ell_1$ | $\ell_2$ | $\ell_3$ | $j_1$ | $j_2$ | $j_3$ | $\ell_1$ | $\ell_2$ | $\ell_3$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | 14.0 | | 13.5 | | 12.5 | 12.5 | | 10.0 | | 9.0 | |
| | 15.0 | | 12.5 | | 12.5 | 11.5 | | 11.0 | | 9.0 | |
| | 15.0 | | 13.5 | | 11.5 | 11.5 | | 10.0 | | 10.0 | |

Table - 4

Parametric solutions of the polynomial zeros of degree one of the 6-j coefficient.

| | | Parameters | | Racah coefficient | | | | | | Invariant |
|---|---|---|---|---|---|---|---|---|---|---|
| Sl. No. | Eqn | General | Minimum Values | $j_1$ | $j_2$ | $j_3$ | $\ell_1$ | $\ell_2$ | $\ell_3$ | I |
| 1 | (55) | m | 1 | 3.0 | 2.0 | 2.0 | 1.0 | 2.0 | 2.0 | 24 |
| 2 | (56) | n | 1 | 2.0 | 2.0 | 2.0 | 1.5 | 1.5 | 1.5 | 21 |
| 3 | (57) | b | 1 | 3.5 | 3.0 | 3.5 | 1.0 | 1.5 | 3.0 | 27 |
| 4 | (58) | (b,h) | (1,1) | 16.5 | 15.5 | 8.0 | 11.0 | 12.0 | 5.5 | 137 |
| 5 | (59) | (a,b,d,h) | (1,1,1,1) | 6.5 | 5.0 | 2.5 | 1.5 | 3.0 | 4.5 | 46 |
| 6 | (60) | (p,q,r,s) | (3,1,1,1) | 15.5 | 15.0 | 9.5 | 12.0 | 12.5 | 4.0 | 137 |
| 7 | (66) | (a,d,h,i) | (1,1,2,2) | 2.0 | 2.0 | 2.0 | 1.5 | 1.5 | 1.5 | 21 |
| 8 | (52) | (a,b,c,d, e,f,g,h,i) | (1,1,1,1, 1,1,2,2,2) | 2.0 | 2.0 | 2.0 | 1.5 | 1.5 | 1.5 | 21 |

Table 5

Parametric formulae and the first fifteen of the *inequivalent* polynomial zeros of degree one of the 6-j coefficient. ✓ indicates that the parametric formula accounts for the zero and x that it does not. * refers to exceptional case, given in text.

| | | | | | | Serial number of parametric solutions given in Table 4 (number of parameters). | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $j_1$ | $j_2$ | $j_3$ | $\ell_1$ | $\ell_2$ | $\ell_3$ | 1 (1) | 2 (1) | 3 (1) | 4 (2) | 5 (4) | 6 (4) | 7 (4) | 8 (8/9) |
| 2 | 2 | 2 | 3/2 | 3/2 | 3/2 | x | ✓ | x | x | x | x | ✓ | ✓ |
| 3 | 2 | 2 | 1 | 2 | 2 | ✓ | x | x | x | x | x | ✓ | ✓ |
| 7/2 | 3 | 3/2 | 1 | 3/2 | 3 | x | x | ✓ | x | x | x | ✓ | ✓ |
| 7/2 | 7/2 | 3 | 5/2 | 3/2 | 3 | ✓ | ✓ | x | x | x | x | ✓ | ✓ |
| 5 | 4 | 2 | 3 | 4 | 4 | ✓ | x | x | x | x | x | ✓ | ✓ |
| 5 | 9/2 | 3/2 | 2 | 5/2 | 9/2 | x | x | ✓ | x | x | x | ✓ | ✓ |
| 5 | 9/2 | 9/2 | 7/2 | 3 | 3 | x | x | x | x | x | x | ✓ | ✓ |
| 5 | 5 | 4 | 7/2 | 3/2 | 9/2 | x | ✓ | x | x | x | x | ✓ | ✓ |
| 11/2 | 4 | 7/2 | 1 | 7/2 | 4 | x | x | x | x | x | x | ✓ | ✓ |
| 6 | 5 | 3 | 1 | 3 | 5 | x | x | x | x | ✓ | x | ✓ | ✓ |
| 6 | 5 | 5 | 4 | 5 | 2 | ✓ | x | x | x | x | x | ✓ | ✓ |
| 6 | 6 | 4 | 5/2 | 5/2 | 11/2 | x | x | x | x | x | x | ✓ | ✓ |
| 13/2 | 6 | 7/2 | 3 | 3/2 | 6 | x | x | ✓ | x | x | x | ✓ | ✓ |
| 7 | 9/2 | 9/2 | 5/2 | 4 | 4 | x | x | x | x | x | x | * | ✓ |
| 15/2 | 7 | 7/2 | 2 | 7/2 | 6 | x | x | x | x | ✓ | x | ✓ | ✓ |

Table - 6

Polynomial zeros of the 6-j coefficient which can be explained from realizations of the exceptional Lie algebras $G_2$, $F_4$, and $E_6$.

| $j_1$ | $j_2$ | $j_3$ | $\ell_1$ | $\ell_2$ | $\ell_3$ | Algebra-subalgebra chain |
|---|---|---|---|---|---|---|
| 5.0 | 5.0 | 3.0 | 3.0 | 3.0 | 3.0 | $G_2 \supset SO(3)$ |
| 11.0 | 11.0 | 3.0 | 4.0 | 4.0 | 8.0 | |
| 11.0 | 11.0 | 9.0 | 8.0 | 4.0 | 8.0 | $F_4 \supset SO(3)$ |
| 3.0 | 2.0 | 2.0 | 1.0 | 2.0 | 2.0 | $F_4 \supset SO(3) \otimes G_2 \supset (SO(3) \otimes SO(3)$ |
| 4.5 | 4.5 | 7.0 | 4.0 | 4.0 | 2.5 | $F_4 \supset SO(3) \otimes Sp(6) \supset SO(3) \otimes SO(3)$ |
| 11.0 | 8.0 | 6.0 | 4.0 | 4.0 | 8.0 | $E_6 \supset F_4 \supset SO(3)$ |
| 7.0 | 6.0 | 5.0 | 4.0 | 6.0 | 4.0 | |
| 6.0 | 6.0 | 6.0 | 5.0 | 4.0 | 3.0 | $E_6 \supset Sp(8) \supset SO(3)$ |
| 9.0 | 6.0 | 4.0 | 2.0 | 5.0 | 5.0 | |

Table - 7

The zeros explained from the orthogonal polynomial approach

| $j_1$ | $j_2$ | $j_3$ | $\ell_1$ | $\ell_2$ | $\ell_3$ |
|---|---|---|---|---|---|
| 2.0 | 2.0 | 2.0 | 1.5 | 1.5 | 1.5 |
| 3.0 | 2.0 | 2.0 | 1.0 | 2.0 | 2.0 |
| 6.0 | 4.0 | 9.0 | 5.0 | 5.0 | 2.0 |
| 4.0 | 4.0 | 5.0 | 4.0 | 2.0 | 3.0 |
| 5.0 | 3.0 | 5.0 | 3.0 | 3.0 | 3.0 |

Chapter 5

# A New Fortran Program for the 9-j Angular Momentum coefficients.

## 5.1 Introduction

The need for angular momentum coupling coefficients, viz. 3-j, 6-j and 9-j coefficients, arises in nuclear shell model and nuclear reaction calculations (Amos de Shalit and Talmi (1963)), as well as in atomic and molecular physics calculations. The computation of the matrix elements requires these basic angular momentum coefficients. In this chapter we present a new FORTRAN program to compute the 9-j coefficient.

The conventional method of computing the 9-j coefficient makes use of its expansion in terms of a single sum over the product of three 6-j coefficients, due to Wigner (1940). Shapiro (1967) has written a program to compute arbitary 3n-j coefficients for SU(2) which are descrisbed through the graphical representation developed by Yutsis (1962). Tamura (1967) has developed codes based on the standard expressions for the 3n-j coefficients for $n \leq 3$. The program presented here makes use of the simplest form for the 9-j coefficient known in literature which is a triple - sum series due to Jucys and Bandzaitis (1977).

The triple sum series is identified with a triple hypergeometric series introduced by Srivastava (1967). The Horner scheme for polynomial evaluation (Lee (1966)) is then resorted to for computing this triple series. The conventional single sum series involving the product of three 6-j coefficients (each being a single sum series in turn) is also programmed for comparison. Three sum rules satisfied by the 9-j coefficient are evaluated to check the correctness of the code developed.

The mathematical formulae used are listed in the beginning, and the method of calculation described. Following this the program structure and its operation are described. The results and the relative merits of the programs are discussed at the end.

**5.2 Mathematical Formulae and Method of Calculation**

The conventional single sum expression for the 9-j coefficient derivable from the fundamental theorem of recoupling theory (Biedenharn 1953) was given in (68) of Chapter 1 and it reads as:

$$\begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix} = \sum_k (-1)^{2k}(2k+1) \begin{Bmatrix} a & d & g \\ h & i & k \end{Bmatrix} \begin{Bmatrix} b & e & h \\ d & k & f \end{Bmatrix} \begin{Bmatrix} c & f & i \\ k & a & b \end{Bmatrix}, \qquad (1)$$

where a, b, c, ...., i can take integral or half-integral values and the summation index k takes the values:

$$\max\,(|a-i|,\ |d-h|,\ |b-f|) \le k \le \min\,(a+i,\ d+h,\ b+f) \qquad (2)$$

The coefficients on the r.h.s. of (1) are the 6-j coefficients. The Fortran program WF to compute the 6-j coefficient based on the set I of ${}_4F_3(1)$s (discussed in Chapter 1) - due to Srinivasa Rao and Venkatesh (1978) and Srinivasa Rao (1981) - is employed in the function program WNINE for the 9-j coefficient given by (1).

The simplest known algebraic form for the 9-j coefficient due to Jucys and Bandzaitis (1977) was given in (69) of Chapter 1 and this after a slight change of notation reads as:

$$\left\{\begin{matrix} a & b & c \\ d & e & f \\ g & h & i \end{matrix}\right\} = (-1)^{x5} \frac{(d\ a\ g)\ (b\ e\ h)\ (i\ g\ h)}{(d\ e\ f)\ (b\ a\ c)\ (i\ c\ f)}$$

$$\times \frac{\Gamma(1+x1,\ 1+x2,\ 1+x3,\ 1+y1,\ 1+y2,\ 1+z1,\ 1+z2,\ 1+p1)}{\Gamma(1+x4, 1+x5, 1+y3, 1+y4, 1+y5, 1+z3, 1+z4, 1+z5, 1+p2, 1+p3)}$$

$$\times \sum_{x,y,z} \frac{1}{x!\ y!\ z!} \frac{(1+x2,x)\ (1+x3,x)\ (-x4,x)\ (-x5,x)}{(-x1,x)}$$

$$\times \frac{(1+y1,y)\ (1+y2,y)\ (-y4,y)\ (-y5,y)}{(1+y3,y)}$$

$$\times \frac{(1+z2,z)\ (-z3,z)\ (-z4,z)\ (-z5,z)}{(-z1,z)}$$

$$\times \frac{1}{(-p1,y+z)\ (1+p2,x+y)\ (1+p3,x+z)}, \quad (3)$$

where

$$0 \le x \le \min(-d+e+f,\ c+f-i) = XF,$$

$$0 \le y \le \min(\ g-h+i,\ b+e-h) = YF, \quad (4)$$

$$0 \le z \le \min(\ a-b+c,\ a+d-g) = ZF,$$

$$(\ a\ b\ c\ ) = \Delta(\ a\ b\ c\ ) \frac{(a+b+c+1)!}{(-a+b+c)!}. \quad (5)$$

and the symbol $(\lambda,k)$ as well as the quantities x1, ..., x5, y1,...,y5, z1, ...,z5, p1, p2 and p3 are defined in Chapter 1.

Study of multiple series in several variables was initiated by Appell (1926) who considered the product of two Gauss functions ($_2F_1$s) and showed that replacement of one or more of the pairs of (Pocchammer) products by a composite product leads to four double series: $F_1$, $F_2$, $F_3$ and $F_4$ which are called Appell functions in literature (1926) A generalization of this idea to products of $_pF_q$s is available and the book of Harold Exton(1976) on *Multiple hypergeometric series* summarizes the results published in several papers. The fact that the 9-j coefficient has been represented by

(1) and that each 6-j coefficient is a ${}_4F_3(1)$ suggests that the product of the following ${}_4F_3(1)$s be considered:

$$
{}_4F_3\left[\begin{matrix}1+x2, & 1+x3, & -x4, & -x5 \\ -x1, & 1+p2, & 1+p3 & \end{matrix};1\right]\; {}_4F_3\left[\begin{matrix}1+y1, & 1+y2, & -y4, & -y5 \\ 1+y3, & -p1, & 1+p2 & \end{matrix};1\right]
$$

$$
\times\; {}_4F_3\left[\begin{matrix}1+z2, & -z3, & -z4, & -z5 \\ -z1, & -p1, & 1+p3 & \end{matrix};1\right] = \sum_{x,y,z} \frac{1}{x!\,y!\,z!}
$$

$$
\times\; \frac{(1+x2,x)\,(1+x3,x)\,(-x4,x)\,(-x5,x)}{(-x1,x)\,(1+p2,x)\,(1+p3,x)}
$$

$$
\times\; \frac{(1+y1,y)\,(1+y2,y)\,(-y4,y)\,(-y5,y)}{(1+y3,y)\,(-p1,y)\,(1+p2,y)}
$$

$$
\times\; \frac{(1+z2,z)\,(-z3,z)\,(-z4,z)\,(-z5,z)}{(-z1,z)\,(-p1,z)\,(1+p3,z)}\,. \tag{6}
$$

In (6), the following replacements of the pairs of products:

$$
\begin{aligned}
&(1+p2,\ x)\ (1+p2,\ y) &&\text{by}&& (1+p2,\ x+y)\ ,\\
&(1+p3,\ x)\ (1+p3,\ z) &&\text{by}&& (1+p3,\ x+z)\ ,\\
&(-p1,\ y)\ (-p1,z) &&\text{by}&& (-p1,\ y+z),
\end{aligned} \tag{7}
$$

are made to make the identification with the triple series which occurs in (3) possible. The product of the three ${}_4F_3(1)$s given by (6), with the replacements given in (7) leads to the new function:

$$
F^{(3)}\left[\begin{matrix}(0):: & (0); & (0); & (0): & 1+x2,1+x3,-x4,-x5; & 1+y1,1+y2,-y4,-y5; \\ (0)::1+p2; & & -p1; & 1+p3: & -x1; & 1+y3;\end{matrix}\right.
$$

$$
\left.\begin{matrix}1+z2,-z3,-z4,-z5; & 1,1,1 \\ -z1 & \end{matrix}\right] \tag{8}
$$

which clearly is a particular case of the function defined in three variables by Srivastava (1967) and which is an elegant unification (Exton (1976)) of the triple hypergeometric functions of Lauricella-Saran (Lauricella (1893), Saran(1954)) and Srivastava(1964) functions. It is to be noted that the *new* generalised hypergeometric function in three variables:

$$
\phi^{(3)}(\alpha_{kl}\ ;\beta_i\ ,\ \gamma_m\ ;\ \omega_k)
$$

defined by Wu(1973) is the same as F(3) given in (8) above, which is a particular case of an extremely general hypergeometric series defined in three variables by Srivastava (1967) as:

$$F^{(3)}\left[\begin{matrix}(a)::(b);\ (b');\ (b''):\ (c);\ (c');\ (c'');\ x,\ y,\ z\\(e)::(f);\ (f');\ (f''):\ (g);\ (g');\ (g'')\end{matrix}\right] =$$

$$= \sum_{m,n,p} \frac{((a),m+n+p)\ ((b),m+n)\ ((b'),n+p)\ ((b''),p+m)}{((e),m+n+p)\ ((f),m+n)\ ((f'),n+p)\ ((f''),p+m)}$$

$$\times \frac{((c),m)\ ((c'),n)\ ((c''),p)\ x^m\ y^n\ z^p}{((g),m)\ ((g'),n)\ ((g''),p)\ m!\ n!\ p!}, \tag{9}$$

where (a) denotes a sequence of parameters (as in the notation of Srivastava (1967)).

The procedure adopted for the numerical computation of the triple sum series in (3) is as follows:

$$\begin{aligned}\sum_{x,y,z} \cdots &= \sum_x AS(x) \sum_y BS(y) \sum_z CS(x,y,z)\\ &= \sum_x AS(x) \sum_y BS(y)\ \phi(x,y)\\ &= \sum_x AS(x)\ f(x),\end{aligned} \tag{10}$$

where AS and BS are one-dimensional arrays and CS is a three-dimensional array. The summation over each one of the indices x,y and z is by adapting the Horner's rule (Lee 1966) for polynomial evaluation, viz:

$$a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n =$$

$$= a_0 \left(1 + \frac{a_1}{a_0} x \left(1 + \frac{a_2}{a_1} x \left(1 + \cdots + \frac{a_{n-1}}{a_{n-2}} x \left(1 + \frac{a_n}{a_{n-1}} x\right) \cdots\right)\right)\right). \tag{11}$$

The algorithm employed for evaluating (11) is:

$c := a_n$,

if $a_i \neq 0$, then $c := a_i\,(1 + c/a_i)$, (12)

for $i = n-1, n-2, \cdots, 1, 0$.

It is to be noted that (12) holds even when one or more of the $a_i$ are zero.

In the function programs which use either (1) or (3) the following special values for the 9-j coefficients have been incorporated:

$$\begin{Bmatrix} 0 & e & e \\ f & d & b \\ f & c & a \end{Bmatrix} = \begin{Bmatrix} e & 0 & e \\ c & f & a \\ d & f & b \end{Bmatrix} = \begin{Bmatrix} f & f & 0 \\ d & c & e \\ b & a & e \end{Bmatrix} = \begin{Bmatrix} f & b & d \\ 0 & e & e \\ f & a & c \end{Bmatrix}$$

$$\begin{Bmatrix} a & f & c \\ e & 0 & e \\ b & f & d \end{Bmatrix} = \begin{Bmatrix} b & a & e \\ f & f & 0 \\ d & c & e \end{Bmatrix} = \begin{Bmatrix} e & d & c \\ e & b & a \\ 0 & f & f \end{Bmatrix} = \begin{Bmatrix} c & e & d \\ a & e & b \\ f & 0 & f \end{Bmatrix}$$

$$\begin{Bmatrix} a & b & e \\ c & d & e \\ f & f & 0 \end{Bmatrix} = \frac{(-1)^{b+c+e+f}}{[e]\ [f]} \begin{Bmatrix} a & b & e \\ d & c & f \end{Bmatrix} . \qquad (13)$$

In the case of b = e = 1/2 in the 9-j coefficient, it is checked whether a = d and c = f; and if so, then

$$\begin{Bmatrix} a & 1/2 & c \\ a & 1/2 & c \\ g & h & i \end{Bmatrix} = 0,$$

if (g + h + i) is an odd integer.

The expressions (1) and (3) are used for calculating the 9-j coefficient and the corresponding function programs are named as WNINE and RNINE respectively. The function program WF is used to evaluate the 6-j coefficient.

In the past, sum rules were used often to check the correctness of tables of angular momentum coefficients. The following sum rules are satisfied by the 9-j coefficient (El Baz and Castel (1972)):

$$\sum_x (2x + 1)\ (2c + 1) \begin{Bmatrix} a & b & c \\ d & e & f \\ x & a & d \end{Bmatrix} = \delta_{c,e} \{a\ b\ c\}\ \{c\ d\ f\} , \qquad (14)$$

$$\sum_{x} (-1)^{b+c+e+f-x} (2x+1)(2b+1) \begin{Bmatrix} a & b & c \\ d & f & e \\ x & d & a \end{Bmatrix} = \delta_{b,e}\{a\ b\ c\}\{d\ e\ f\} \tag{15}$$

$$\sum_{x_1,x_2} (-1)^{c'+c+2a+x_1} (2x_1+1)(2x_2+1) \begin{Bmatrix} a & b & c \\ d & e & f \\ x_1 & x_2 & g \end{Bmatrix} \begin{Bmatrix} d & b & c' \\ a & e & f' \\ x_1 & x_2 & g \end{Bmatrix} = \begin{Bmatrix} a & b & c \\ f' & c' & g \\ e & d & f \end{Bmatrix} \tag{16}$$

where $\{a\ b\ c\}$ is defined by:

$$\{a\ b\ c\} = \begin{cases} 1 & \text{if } |a-c| \le b \le a+c\,, \\ 0 & \text{otherwise.} \end{cases} \tag{17}$$

An attempt has been made to see the usefulness of these sum rules in demonstrating the correctness of the numerical algorithm based on the triple sum series for the 9-j coefficient.

### 5.3 Program Structure and subprograms

The complete program comprises the main program which calls the function programs WNINE and RNINE for the 9-j coefficient. The time taken for a given set of parameters is noted with the help of system dependent routines. There are two main programs - PROGTEST and PROGSELECT - each of which makes use of seven function subprograms and nine subroutine subprograms.

#### Calling and operation of the main programs

Communication with the afore-mentioned function subprograms is established through the following statements:

WNINE (A, B, C, D, E, F, G, H, RI)

RNINE (A, B, C, D, E, F, G, H, RI)

where the arguments stand for the nine angular momenta: a, b, c, d, e, f, g, h and i.

At the very beginning the logarithms of the first 500 factorials are calculated and set-up as an array in a one-dimensional COMMON block, FCT(500). This is the conventional approach (see for e.g. Tamura (1967); Srinivasa Rao and Venkatesh (1978)) and has the advantage of not only being available for a look-up when needed but also prevents overflow due to products of large factorials, since multiplication of factorials is replaced by the sum of the corresponding logarithms, which is then exponentiated.

In noting the time required for execution, use is made of system dependent routines described later. Due to the limitations of these system dependent routines, reproducible timings were obtained only when the function program called is computed n times, n being 10 or 20 for the IBM-PC AT and 100 for the VAX-11/780, in a loop. In PROGTEST, since two functions are to be timed(viz. RNINE and WNINE), the system dependent routine is called twice for each of them - once before calling the function program and a second time after returning from the given function program. The difference in the two timings calculated is then divided by n to get the average time taken. The variable used for n is ITEST and this quantity is read in I3 format, after setting-up the FCT(500) array. The nine angular momenta are then read (either in the interactive mode or from a data file) in the F4.1 floating-point mode.

The subroutine SET is called which sets up a two-dimensional array R9 employed to keep track of the nine angular momenta treated as the elements of a 3x3 array. If any one of the elements of this array is equal to zero, then the value of the 9-j coefficient reduces to a 6-j coefficient, as given in (13). When the zero element is located, control is transferred to the function program VALUE which will return the special value of the 9-j coefficient.

Preliminary runs indicated that if b = e = 1/2, as in the case of the *ls-jj* transformation coefficients

$$\begin{Bmatrix} a & 1/2 & c \\ d & 1/2 & f \\ g & h & i \end{Bmatrix}$$

frequently encountered in quantum physics calculations, the RNINE function program, which uses the triple sum formula (3) is faster than the WNINE function program, which uses the single sum over the product of three 6-j coefficients given by (1). However, for arbitrary a,b......,i, subject only to the triangular inequalities, we found that depending upon the data, the number of terms involved in (1) or (3) indicates which of the two function programs is time-effective.

For this purpose, when none of the nine angular momenta is zero, the subroutine CHANGE is called and it searches for that symmetry of the 9-j coefficient for which the number of terms in the triple sum series is a minimum. The subprogram TERM evaluates the actual number of terms (NT1), which could occur in RNINE and the value (NT2) of the index k in (1) for WNINE, which when multiplied by three (NT3) gives the number of times the function WF will be called when (1) is employed for evaluating the 9-j coefficient. Using the values of NT1 and NT3, an ad hoc prescription is given to choose the time-effective program for the given data.

There are two main programs called PROGTEST and PROGSELECT. In the former, the computation for a given data is made using both RNINE and WNINE, the averages of the times taken are noted and the advantage factor computed. Control is then transferred to read the next set of input data. The main program PROGSELECT on the other hand differs from PROGTEST in that exiting from the subprogram TERM, based on the prescription, control is transferred to either RNINE or WNINE, so that the time-effective program alone is computed.

Subprograms

We now give a brief resume of the function programs used:

1. Function WNINE employs the single sum series (1) for the 9-j coefficient. A check is made to find whether the corresponding elements in the first and second rows of the 9-j coefficient are equal and if so, whether the sum of the elements in the third row (ICHK) is an odd or an even integer. If ICHK is odd, then the value of the 9-j coefficient is zero and hence no computation is required in this case. (This check is mainly because of the possibility which arises in quantum physics calculations, when two particles may be in the same $(n,\ell,s,j)$ orbit resulting in the 9-j coefficient being zero for the transition matrix element for certain special values of the operator involved). If ICHK is even or if any two of the

corresponding elements in the first and second rows are unequal, then the expression (1) is computed in a single DO loop for the variable k, in which for each term the function WF is called three times. The function WF calls the function programs TRIA and PHASE. The value of the 9-j coefficient is returned as WNINE.

2. The function subprogram WF (A,B,C,D,E,F) calculates the 6-j coefficient using the set I of three ${}_4F_3(1)$s given by (18) of Chapter 2. We check for the two denominator parameters being positive and accordingly select the parameter set (19), (20),or (21) for the ${}_4F_3(1)$. It is checked whether any of the numerator parameters is zero, and if so the ${}_4F_3(1)$ is set equal to 1. Otherwise, the number of terms in the series is found and the ${}_4F_3(1)$ calculated using the Horner's rule and the value of the 6-j coefficient is returned as WF. In Srinivasa Rao and Venkatesh(1978) WF denotes the Racah coefficient W(a b c d;e f) but in the present program WF denotes the 6-j coefficient $\begin{Bmatrix} a & b & e \\ d & c & f \end{Bmatrix}$. In this subprogram, there is only one exponentiation of the logarithmic sum in the last step.

   Function PHASE(N) is for finding the value of $(-1)^N$.

   Function TRIA(x,y,z) checks for the value of { x y z } being 1 or 0.

3. Function RNINE employs the triple sum series (3) evaluated using the scheme (10) which adopts the Horner's scheme for polynomial evaluation (11) - (12). The check for ICHK being

even or odd is made as in the function WNINE. The six triangular inequalities which must be satisfied by the nine angular momenta are then checked. Then, from (6) to (8), it is clear that for the series (3) to be well-defined the denominator zero (occuring due to the negative nature of -x1 and -z1) should not occur before the numerator zero (occuring due to the negative nature of -x4, -x5, -y4, -y5, -z4 and -z5). This requirement is then stipulated. The overall multiplicative constant factor (C1) and the overall phase factor (CONST) in (3) are computed next. The triple sum over the indices x, y and z starts by setting up the required one-dimensional arrays AS(x) and BS(y) and the three-dimensional array CS(x,y,z). The scheme stated in (11) for this triple-sum is then implemented in this function program, by suitably setting-up intermediate arrays - CZ(z), BY(y) and AX(x) - which are input to the Horner's scheme (11) being used for the indices z, y and x.

This function program RNINE calls besides TRIA (for checking the triangular inequalities to be satisfied by the triads of angular momenta) and PHASE (which computes $(-1)^n$), the function HORNER :

HORNER(KI, KF, A)

where KI and KF denote the index values of the first and last terms of the one-dimensional array A.It computes the folded sum of the non-zero terms of the array A, using the scheme(11), and algorithm (12).

4. The function subprogram

VALUE (A, B, C, D, E, F, G, H, RI, I, J)

where the nine angular momenta A,....,RI are the arguments of the 9-j coefficient and the two integer variables I and J are the two-dimensional array indices used to locate the position of the element which may be zero. The location of the zero helps in the use of (13) to express the special value of such a 9-j coefficient which is simply given by a 6-j coefficient multiplied by a phase factor and a numerical factor.

5. The subroutine subprogram

TERM (A, B, C, D, E, F, G, H, RI, NTI, NT2)

where A,...RI are the nine angular momenta in the 9-j coefficient and NT1 and NT2 are two integer parameters which determine, respectively, the actual number of terms which occur in (3), and the number of allowed values of k in (1). In this subprogram, the values of NT1 and NT2 are determined. Though k gives the number of terms in the expression (1), the fact that each term involves the function WF being called thrice, makes us consider 3k as the important index in reckoning the time taken per term of evaluation in what follows. The values of the variables x4, x5, y4, y5, z4, z5, p1, p2, p3 and their integer equivalents IX4,...,IP3, as well as the final values of the summation indices in (3) - viz. XF, YF and ZF (or, IXF, IYF and IZF) and of the initial and final values of k in (1) - viz. KI and KF - are required in the function programs RNINE or WNINE. So, they are put in COMMON blocks in this subprogram.

The times taken by RNINE and WNINE were noted for several input data including the following two sets of data:

(I) a=15, b=2, c=15, d=3, e=15, f=15, g=12, h=13, and 5≤ i ≤25

(II) a=15, b=15, c=15, d=15, e=3, f=15, g=15, h=18 and 5≤ i≤30

The data set (I) corresponds to a large number of allowed terms (210 for 5≤ i ≤21) for RNINE given by (3) but a small value of 3k (12 for 2≤ i ≤25) for WNINE given by (1). On the other hand, the data set (II) corresponds to a comparatively smaller number of allowed terms (64 for 15≤ i ≤27) for RNINE (3) and a larger value of 3k (between 48 and 84 for 8≤ i ≤30) for WNINE (1). For these specific data when we ran PROGTEST on a personal computer and on a VAX-11/780, we found the following absolute values for the average times (in seconds) per term of computation :

| Function program | PC - Fortran version 2.0 | PC - Fortran version 4.0 | VAX - 11/780 |
|---|---|---|---|
| RNINE | 0.00393 | 0.00258 | 0.0487 |
| WNINE | 0.0125 | 0.00829 | 0.0957 |
| Ratio | ~ 3 | ~ 3 | ~ 2 |

(Note: The timings shown here were obtained on an AT & T PC6300 which runs on an 8086 at 8 MHz supported by an 8 MHz 8087 Math-coprocessor and the timings given in the case of the VAX-11/780 are the CPU times found with the help of a lexical function discussed later, under System Dependent Routines. From these timings, we note that the use of the later version of Frotran compiler ver.4.0, instead of ver.2.0 reduces the absolute time of computation by a factor of ~ 1.5, though the ratio of the time taken per term of computation remains almost the same in both the cases. If we were to use these times as an index of the speed of computation of the 9-j coefficient using RNINE (3) and WNINE (1), then we can arrive at a prescription, that if NT1(number of terms in (3)) is less than 2 times 3k, NT3 (which corresponds to the number of calls of WF in (1)) then it would be advantageous to use RNINE. Otherwise, (viz. NT1 > 2 NT3) WNINE would be advantageous for computing the value of the given 9-j coefficient. This is the basis for our adhoc prescription referred to earlier. We found that if NT1 ≈ NT3 then the difference in times for computing the 9-j coefficient using RNINE or WNINE is not significant and hence either function program can be used. Also, to avoid numerical discrepancy in the value returned by RNINE, if the number of terms to be computed for any given nine arguments of the 9-j coefficient exceeds 200 on the PCs or 600 on the VAX-11/780, then the stable algorithm WNINE will be preferred to RNINE (since in RNINE exponentiation of the sums of logarithms is resorted for every term of computation and due to round off and truncation errors this causes the numerical discrepancies). These two prescriptions are incorporated in the main program PROGSLECT.

It is significant to note that when we ran PROGTEST with the call of CHANGE subroutine, the symmetry of the 9-j selected for computation in the case of the data set (I) reduced from 210 terms to a mere 3 terms, while in the case of the data set (II) the symmetry of the 9-j coefficient selected for computation had the same number of terms as before. This is mainly due to the fact that the formula (3) does not exhibit any of the 72 symmetries of the 9-j coefficient. For example, while

$$\left\{ \begin{matrix} 15 & 2 & 15 \\ 3 & 15 & 15 \\ 12 & 13 & 15 \end{matrix} \right\}$$

belonging to set (I) has

$$0 \le x \le 15, \quad 0 \le y \le 4 \quad \text{and} \quad 0 \le z \le 6,$$

its symmetry

$$\left\{ \begin{matrix} 3 & 15 & 12 \\ 15 & 2 & 13 \\ 15 & 15 & 15 \end{matrix} \right\}$$

has

$$x = 0, \quad 0 \le y \le 2 \quad \text{and} \quad z = 0.$$

The actual number of terms in the former case is 210 and in the latter case only 3. This is typical for large values of angular momenta. Since it is not possible to analytically find out that symmetry of the 9-j coefficient for which the number of terms in the triple-sum series is a minimum, we make use of a subroutine called CHANGE for this very purpose.

6. The subroutine subprogram

CHANGE (A, B, C, D, E, F, G, H, RI)

has A,...,RI as the nine angular momenta in the 9-j coefficient. The 72 symmetries of the given 9-j coefficient are those which arise due to 3! column permutations, 3! row permutations and the transposition of the 3 x 3 array. If $\sigma = a + b + c + d + e + f + g + h + i$, then the 9-j coefficient acquires a phase factor $(-1)^{\sigma}$ for odd column permutations and odd row permutations of the 9-j coefficient. These 72 symmetries are generated for the given 9-j coefficient by calling the function subprograms CINT for column permutation, RINT for row permutation and TRANS for transposition. For each of the symmetries generated, the values of XF, YF, ZF are found by calling a subroutine FXYZ - which calculates the quantities x4, x5, y4, y5, z4, z5 given a, b, ...i and the upper limits of the summation indices given by (9) - and the sum of XF + YF + ZF (IXYZ) is calculated. These 72 symmetries of the given 9-j coefficient and the value of the sum XF + YF + ZF for each one of them are then stored as one-dimensional arrays with array names: A1, B1, C1, D1, E1, F1, G1, H1, RI1 and IXYZ. These arrays are stored in a common block named AX. Also, the number of odd column and/or odd row permutations performed in the process of getting the symmetries of the given coefficient is noted in the one-dimensional array with the array name JSIG1, since it is necessary to keep track of the phase factor associated with the symmetries. The symmetry which yields a minimum of the sum XF + YF + ZF is a measure of the number of terms in the triple sum series. That symmetry is chosen by calling the subroutine ORDN which searches for the minimum value in the array IXYZ and returns it as IMINV. The 9-j coefficient parameters noted as A2, B2, C2, D2, E2, F2, G2, H2, RI2 correspond to that chosen symmetry for which XF + YF + ZF is a minimum (viz. IMINV). These nine values along with the number of odd column and/or odd row permutations which led to it from the given 9-j coefficient, noted as JSIG2 (for the chosen value of the element belonging to the array JSIG1) are placed in the common block named XX. The triple-sum series is evaluated only for this symmetry and it is multiplied by the phase factor, if $\sigma$ and JSIG2 are both odd. Thus, the use of the CHANGE subroutine converts the inherent disadvantage of the lack of symmetry in the triple sum series to an advantage! An extreme example is cited here to substantiate the importance of the CHANGE subroutine. In Table I are given some of the 72 symmetries of a 9-j coefficient and the corresponding values of XF, YF and ZF. The actual number of terms in the triple sum series is given in the last column.

Table 1.

| a | b | c | d | e | f | g | h | i | XF | YF | ZF | No. of terms |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 20 | 30 | 10 | 30 | 10 | 20 | 60 | 30 | 30 | 0 | 0 | 0 | 1 |
| 30 | 10 | 20 | 60 | 30 | 30 | 30 | 20 | 10 | 0 | 20 | 40 | 21 |
| 30 | 20 | 10 | 60 | 30 | 30 | 30 | 10 | 20 | 0 | 40 | 20 | 41 |
| 60 | 30 | 30 | 30 | 10 | 20 | 30 | 20 | 10 | 0 | 20 | 60 | 441 |
| 60 | 30 | 30 | 20 | 10 | 30 | 30 | 10 | 20 | 0 | 40 | 60 | 1681 |
| 30 | 30 | 60 | 20 | 10 | 30 | 10 | 20 | 30 | 20 | 20 | 40 | 9471 |
| 30 | 30 | 60 | 10 | 20 | 30 | 20 | 10 | 30 | 40 | 40 | 20 | 18081 |
| 20 | 10 | 30 | 30 | 30 | 60 | 10 | 20 | 30 | 60 | 20 | 40 | 33761 |

The actual number of terms given in the last column of this table is reckoned after taking into account the constraints on the ranges of x, y and z placed by p1, p2 and p3, viz.

$y+z \le p1$ and if $p2, p3 < 0$, then $x+y \ge |p2|$, $z+x \ge |p3|$.

Due to the search made by the CHANGE subroutine, the symmetry corresponding to the number of terms being one would be selected for the computation of RNINE whichever symmetry of the above example is read in. (The remaining 72 symmetries yield one or the other of the number of terms listed in the table for this specific example cited here). However, when the number of terms becomes large (above 200 for IBM-PC/AT and above 600 for VAX-11/780), we find that the program RNINE becomes numerically inaccurate due to the round-off and truncation errors caused by the repeated exponentiation of the terms involved in the x, y, z summations. On the other hand, the program WNINE is reliable, since it calls repeatedly (3k times) WF which is a single sum series and the exponentiation of the sum of the logarithms is made only once in WF. Consequently, in addition to using the subroutine CHANGE to get that symmetry which would make the number of terms to be summed in RNINE a minimum, the choice of RNINE or WNINE is made in PROGSELECT on the basis of the prescription given earlier.

In CHANGE, besides CINT, RINT, FXYZ, and ORDN two other simple subroutines SET and RESET are used. While SET sets the nine elements of the given 9-j coefficient: a, b, c, d, e, f, g, h, i, as the elements of a two dimensional array, RESET resets the two-dimensional array as a, b, ..., i.

7. The subroutine subprogram

ORDN (I1, IMINV)

has an integer parameter I1 which specifies the dimension of the one dimension arrays A1, B1, C1, D1, E1, F1, G1, H1, RI1, IXYZ and JSIG1 which are placed in the COMMON block (AX). This subroutine sorts and finds the minimum value of IXYZ out of the given list and returns this value as IMINV. The algorithm based on exchange of elements known as *bubble sort* (ref. Knuth 1973) is adapted to order the elements of the array IXYZ so that IXYZ(1) becomes the minimum value of XF + YF + ZF after the procedure is completed.

## System dependent routines

The timer routines used are system dependent. The IBM-PC/AT Fortran language Compiler version 2.00 allows the use of their GETTIM timer routine in the IBMFOR.LIB library. This subroutine

GETTIM(IH, IM, IS, IHS)

requires the variables IH, IM, IS and IHS (which represent the hour, minute, second and hundredth of a second) to be specified as type INTEGER*2 variables and at link time IBM-FOR.LIB must be linked along with the library 8087ONLY (which is for the 80287 Math Coprocessor). The VAX-11/780 computer allows the use of the SECNDS function subprogram which returns time in seconds as a single-precision floating-point value of its single-precision, floating-point argument. This function is used at the start of the segment to be timed with the Fortran statement: t1 = SECNDS(0.0) and at the end of the segment the use of a statement: time = SECNDS(t1) will return as the value of the variable *time* the elapsed time. Depending on the computer on which PROGTEST is to be run (viz. the IBM-PC/AT or the VAX-11/780, as the case may be) a certain set of statements are to be made comments in its main program because of the use of system dependent timer routines in it.

Furthermore, since the VAX-11/780 computer system is in a multi-user, time-sharing mode, no definite statements regarding the execution timings can be made when the SECNDS system routine is used. So, we made use of the lexical functions in a subroutine[1] to get the job-processor information. This subroutine uses those features of FORTRAN which are seldom used, if ever, by those users who are not System Analysts. This routine gave the CPU time for the execution of the function programs which was reliable when ITEST was set 100. These timings are the ones which are quoted in Table 2 .The details of the program PROGSELECT is given in Appendix C . In the case of PROGTEST the main program alone is given since the subprograms are common for both.

### 5.4 Results and discussion

For a chosen set of data with $b = e = 1/2$, the new 9-j coefficient program RNINE based on the triple-sum series shows considerable advantage factors over the conventional program WNINE. In this case, irrespective of the magnitude of the other angular momenta, it can be shown that the number of terms in the triple sum series is *at most* 8. In Table 2 a part of the output for the set of data used is reproduced. The number of terms (NT3 and NT1) for WNINE and RNINE, as well as the execution times in seconds (Z1 and Z2), along with the advantage factor (ZIDA = Z1/Z2), are given in the last three columns of this table. This demonstrates that the new Fortran program RNINE given here is advantageous in all quantum mechanical calculations which require the 9-j coefficient (with $b = e = 1/2$) and since the number of terms is at most 8 in these cases, RNINE is numerically reliable.

For large arguments of the 9-j coefficient, if the number of terms in RNINE exceeds 200 (for IBM-PC/AT) or 600 (for VAX-11/780) or when 3k (NT3) is much smaller than the actual number of terms occuring in the triple sum series (NT1), even after the CHANGE subrourine has been used, the conventional program WNINE based on (1) is to be preferred since it is always stable. The criterion of choosing either WNINE or RNINE, used in PROGSELECT, depending upon whether 2 x NT3 < NT1 or NT1 < 2 x NT3 has been found to hold for the 9-j coefficient data with b = e = 1/2 also (where the RNINE program is always advantageous as stated above). This ad hoc criterion is checked at the beginning of the main program. However, it is to be emphasised that for most, if not all of quantum physics calculations, the input angular momenta are not too large and further since b = e = 1/2 in those (*ls* - *jj*) coefficients, the upper bound on the number of terms is 12.

When contiguous allowed values of angular momentum - viz. a, a+1, a+2, . . . . ,a+8 - are used for the nine arguments of the 9-j coefficient as input to PROGTEST, it is found that for a = 3,4,5,6,7,8,9, and 10, the corresponding *minimum* number of terms to be computed in the triple sum series are: 6, 24, 60, 120, 210, 336, 504 and 720, respectively. This set of data revealed that the numerical values of RNINE deviate from those of WNINE for a > 9.

Further, in the 9-j coefficient $\left\{\begin{matrix} 8 & 9 & 7 \\ 6 & 7 & 10 \\ X & 8 & 6 \end{matrix}\right\}$, $2 \le X \le 14$.
As X is varied over this allowed range, the number of terms in the triple sum series starts from a minimum value (7), increases to a maximum value (196) when X is around its middle value (8), and then decreases.

Based on these two observations, a sample data set was used to check the correctness of the two codes RNINE and WNINE when used in the evaluation of the sum rules (14), (15) and (16). The sum rules could not pin-point the line of demarcation, in the allowed values for the nine arguments of the 9-j coefficient, for which the numerical values are right or wrong. In Tables 3, 4 and 5 a set of input data used for checking the sum rules (14), (15) and (16) as well as the numerical values obtained for the left side (summation) (and right side in the case of (16)) of the sum rules for RNINE and WNINE are given. The results were obtained on the Nelco Force 20 (XPS-20 of Honeywell-Bull) and the entries marked by (*) show the beginning of small deviations from the sum rules. These marked entries in Tables 3 and 4 correspond respectively to the maximum number of terms in the triple sum being > 1000. In the case of Table 5, one or more of the 9-j coefficients on the left hand side of the sum rule involves the number of terms in the triple sum being > 1000. This enables us to reiterate the earlier *ad hoc* criterion arrived at based on the number of terms to be summed in the triple sum series being used as an indicator to choose WNINE instead of RNINE in PROGSELECT.

## 5.5 Conclusion

The following results have been obtained in this chapter:

(i) The triple sum series for the 9-j coefficient given by Jycys and Bandzaitis has been identified with a triple hypergeometric series (Srinivasa Rao and Rajeswari (1988d)).

(ii) A new FORTRAN program RNINE has been developed to compute the 9-j coefficient, based on the triple sum series and the relative merits of this program in comparison to the conventional code WNINE are discussed. The execution time for the programs RNINE and WNINE are found to be proportional to the number of terms to be summed. Based on this observation a criterion is given to choose either of the programs for a given set of data. For the set of data considered, the new program RNINE has an advantage factor of 2 to 4 (for a, b, ...., i $\le$ 10 and an even larger advantage factor for larger values of angular momenta) over the conventional program *as long as* the number of terms to be summed in the triple sum series does not exceed 200 on the PCs or 600 on the VAX-11/780 computer(Srinivasa Rao, Rajeswari and Chiu (1988b)).

(Note: The numerical work on VAX-11/780 was done at the University of Texas, Austin, U.S.A. by my collaborators- Dr.K.Srinivasa Rao and Prof.Charles B.Chiu- and the details of this part of the work are included mainly for the sake of completeness).

Table 2

A part of the computer output from the VAX-11/780 for the sample data which includes the sets of values given by sets (I) and (II) of the text. WN and RN correspond to the functions WNINE and RNINE. The value of the 9-j coefficient is followed by the number of terms and the average (CPU) time taken in seconds. The last column gives the advantage factor of RNINE over WNINE.

ITEST = 100

| | | | |
|---|---|---|---|
| WN(1,0,0.5,0.5,1.0,0.5,1.5,2.0,1.0,2.0)= 0.645497-01 | 6 | 0.66 | |
| RN(1.0,0.5,0.5,1.0,0.5,1.5,2.0,1.0,2.0)= 0.645497-01 | 1 | 0.23 | 2.9 |
| WN(2.0,0.5,2.5,2.0,0.5,2.5,2.0,1.0,1.0)=-0.172133-01 | 6 | 0.63 | |
| RN(2.0,0.5,2.5,2.0,0.5,2.5,2.0,1.0,1.0)=-0.172133-01 | 1 | 0.20 | 3.1 |
| WN(3.0,0.5,3.5,2.0,0.5,2.5,1.0,1.0,2.0)= 0.267261-01 | 6 | 0.53 | |
| RN(3,0,0.5,3.5,2.0,0.5,2.5,1.0,1.0,2.0)= 0.267261-01 | 1 | 0.18 | 2.9 |
| WN(3.0,0.5,2.5,3.0,0.5,2.5,6.0,1.0,5.0)= 0.248682-01 | 6 | 0.55 | |
| RN(3,0,0.5,2.5,3.0,0.5,2.5,6.0,1.0,5.0)= 0.248682-01 | 1 | 0.18 | 3.1 |
| WN(4,0,0.5,3.5,2.0,0.5,2.5,6.0,1.0,6.0)= 0.166429-01 | 6 | 0.58 | |
| RN(4.0,0.5,3.5,2.0,0.5,2.5,6.0,1.0,6.0)= 0.166429-01 | 1 | 0.19 | 3.1 |
| WN(4.0,0.5,4.5,4.0,0.5,4.5,3.0,1.0,2.0)=-0.860663-02 | 6 | 0.58 | |
| RN(4.0,0.5,4.5,4.0,0.5,4.5,3.0,1.0,2.0)=-0.860663-02 | 1 | 0.16 | 3.6 |
| WN(5.0,0.5,5.5,1.0,0.5,1.5,5.0,1.0,6.0)= 0.211278-01 | 6 | 0.63 | |
| RN(5.0,0.5,5.5,1.0,0.5,1.5,5,0,1.0,6,0)= 0.211278-01 | 1 | 0.17 | 3.7 |
| WN(5.0,0.5,5.5,3.0,0.5,3.5,8.0,1.0,9.0)= 0.142915-01 | 3 | 0.32 | |
| RN(5.0,0.5,5.5,3.0,0.5,3.5,8.0,1.0,9.0)= 0.142915-01 | 1 | 0.15 | 2.1 |
| WN(5.0,0.5,4.5,5.0,0.5,5.5,8.0,1.0,7.0)= 0.423797-02 | 6 | 0.64 | |
| RN(5.0,0.5,4.5,5.0,0.5,5.5,8.0,1.0,7.0)= 0.423797-02 | 1 | 0.14 | 4.6 |
| WN(5.0,0.5,5.5,5.0,0.5,5.5,9.0,1.0,10.)= 0.105241-01 | 6 | 0.52 | |
| RN(5.0,0.5,5.5,5.0,0.5,5.5,9.0,1.0,10.)= 0.105241-01 | 1 | 0.16 | 3.3 |
| WN(3.0,0.5,2.5,1.0,0.5,0.5,3.0,1.0,3.0)=-0.158730-01 | 6 | 0.55 | |
| RN(3.0,0.5,2.5,1.0,0.5,0.5,3.0,1.0,3.0)=-0.158730-01 | 2 | 0.22 | 2.5 |
| WN(2.0,0.5,1.5,2.0,0.5,1.5,1.0,1.0,2.0)=-0.182574-01 | 6 | 0.54 | |
| RN(2.0,0.5,1.5,2.0,0.5,1.5,1.0,1.0,2.0)=-0.182574-01 | 1 | 0.19 | 2.8 |
| WN(2.0,0.5,1.5,2.0,0.5,1.5,2.0,1.0,1.0)= 0.483046-01 | 6 | 0.58 | |
| RN(2.0,0.5,1.5,2 0,0.5,1.5,2.0,1.0,1.0)= 0.483046-01 | 1 | 0.16 | 3.6 |

```
WN(2.0,0.5,1.5,2.0,0.5,1.5,2.0,1.0,3.0)=-0.845154-02  6   0.68
RN(2.0,0.5,1.5,2.0,0.5,1.5,2.0,1.0,3.0)=-0.845154-02  1   0.20   3.4

WN(2.0,0.5,1.5,2.0,0.5,1.5,3.0,1.0,2.0)= 0.447214-01  6   0.45
RN(2.0,0.5,1.5,2.0,0.5,1.5,3.0,1.0,2.0)= 0.447214-01  1   0.19   2.4

WN(2,0,0.5,1.5,2.0,0.5,1.5,4.0,1.0,3.0)= 0.436436-01  6   0.64
RN(2.0,0.5,1.5,2.0,0.5,1.5,4.0,1.0,3.0)= 0.436436-01  1   0.18   3.6

WN(15.,2.0,15.,3.0,15.,15.,12.,13.,5.0)=-0.292582-04 21   1.77
RN(15.,2.0,15.,3.0,15.,15.,12.,13.,5.0)=-0.292582-04  3   0.26   6.8

WN(15.,2.0,15.,3.0,15.,15.,12.,13.,10.)=-0.130119-03 21   1.83
RN(15.,2.0,15.,3.0,15.,15.,12.,13.,10.)=-0.130119-03  3   0.24   7.6

WN(15.,2.0,15.,3.0,15.,15.,12.,13.,15.)=-0.317425-03 21   1.83
RN(15.,2.0,15.,3.0,15.,15.,12.,13.,15.)=-0.317425-03  3   0.27   6.8

WN(15.,2.0,15.,3.0,15.,15.,12.,13.,20.)=-0.380328-03 21   1.85
RN(15.,2.0,15.,3.0,15.,15.,12.,13.,20.)=-0.380328-03  3   0.26   7.1

WN(15.,2.0,15.,3.0,15.,15.,12.,13.,25.)=-0.797602-04 21   1.82
RN(15.,2.0,15.,3.0,15.,15.,12.,13.,25.)=-0.797602-04  3   0.25   7.3

WN(15.,15.,15.,15.,3.0,15.,15.,18.,5.0)= 0.297649-04 33   2.94
RN(15.,15.,15.,15.,3.0,15.,15.,18.,5.0)= 0.297649-04 24   1.06   2.8

WN(15.,15.,15.,15.,3.0,15.,15.,18.,10.)=-0.778325-04 63   6.20
RN(15.,15.,15.,15.,3.0,15.,15.,18.,10.)=-0.778325-04 44   1.76   3.5

WN(15.,15.,15.,15.,3.0,15.,15.,18.,15.)= 0.833425-04 84   8.70
RN(15.,15.,15.,15.,3.0,15.,15.,15.,15.)= 0.833425-04 64   2.47   3.5

WN(15.,15.,15.,15.,3.0,15.,15.,18.,20.)=-0.229412-04 78   7.80
RN(15.,15.,15.,15.,3.0,15.,15.,18.,20.)=-0.229412-04 44   2.25   3.5

WN(15.,15.,15.,15.,3.0,15.,15.,18.,25.)=-0.428631-04 63   5.77
RN(15.,15.,15.,15.,3.0,15.,15.,18.,25.)=-0.428631-04 24   1.35   4.3

WN(15.,15.,15.,15.,3.0,15.,15.,18.,30.)=-0.643728-06 48   4.18
RN(15.,15.,15.,15.,3.0,15.,15.,18.,30.)=-0.643728-06  4   0.38  12.7

WN(30.,20.,10.,30.,10.,20.,60.,30.,30.)= 0.268745-03123  10.29
RN(30.,20.,10.,30.,10.,20.,60.,30.,30.)= 0.268745-03  1   0.14  73.5

WN(45.,30.,15.,45.,15.,30.,90.,45.,45.)= 0.120758-03183  15.56
RN(45.,30.,15.,45.,15.,30.,90.,45.,45.)= 0.120758-03  1   0.16  97.3
```

Table 3
Checking sum rule given by (14).

| a | b | c | d | e | f | RNINE | WNINE | |
|---|---|---|---|---|---|---|---|---|
| 1.0 | .5 | .5 | 2.0 | .5 | 1.5 | .1000000E+01 | .1000000E+01 | |
| 1.0 | 2.5 | 1.5 | .5 | 1.5 | 2.0 | .1000000E+01 | .1000000E+01 | |
| 2.0 | 3.0 | 4.0 | 3.5 | 4.0 | 5.5 | .1000000E+01 | .1000000E+01 | |
| 3.0 | 2.0 | 4.0 | 5.0 | 4.0 | 4.0 | .1000000E+01 | .1000000E+01 | |
| 7.0 | 8.0 | 11.0 | 6.0 | 11.0 | 9.0 | .1000000E+01 | .1000000E+01 | |
| 8.5 | 7.0 | 9.5 | 8.0 | 9.5 | 10.5 | .1000000E+01 | .1000000E+01 | |
| 8.0 | 9.0 | 7.0 | 6.0 | 7.0 | 10.5 | .1000000E+01 | .1000000E+01 | |
| 9.5 | 8.0 | 10.5 | 7.0 | 10.5 | 8.5 | .1000000E+01 | .1000000E+01 | |
| 10.0 | 9.0 | 8.0 | 14.0 | 8.0 | 20.5 | .1000000E+01 | .1000000E+01 | |
| 10.0 | 9.5 | 12.0 | 10.0 | 12.5 | 19.5 | .1000000E+01 | .1000000E+01 | |
| 15.0 | 13.0 | 12.0 | 10.0 | 12.0 | 14.0 | .9999571E+00 | .1000000E+01 | * |

Table 4
Checking sum rule given by (15).

| a | b | c | d | e | f | RNINE | WNINE | |
|---|---|---|---|---|---|---|---|---|
| 1.0 | .5 | .5 | 2.0 | .5 | 1.5 | .1000000E+01 | .1000000E+01 | |
| 1.0 | 1.5 | 2.5 | .5 | 1.5 | 2.0 | .1000000E+01 | .1000000E+01 | |
| 2.0 | 4.0 | 3.0 | 3.5 | 4.0 | 5.5 | .1000000E+01 | .1000000E+01 | |
| 3.0 | 4.0 | 2.0 | 5.0 | 4.0 | 4.5 | .1000000E+01 | .1000000E+01 | |
| 4.5 | 6.5 | 4.0 | 5.0 | 6.5 | 9.5 | .1000000E+01 | .1000000E+01 | |
| 7.0 | 11.0 | 8.0 | 6.0 | 11.0 | 9.0 | .1000000E+01 | .1000000E+01 | |
| 8.5 | 9.5 | 7.0 | 8.0 | 9.5 | 10.5 | .1000000E+01 | .1000000E+01 | |
| 8.0 | 7.0 | 9.0 | 6.0 | 7.0 | 10.5 | .1000000E+01 | .1000000E+01 | |
| 9.5 | 10.5 | 8.0 | 7.0 | 10.5 | 8.5 | .1000000E+01 | .1000000E+01 | |
| 10.0 | 8.0 | 9.0 | 14.0 | 8.0 | 20.0 | .1000000E+01 | .1000000E+01 | |
| 10.0 | 12.5 | 9.5 | 10.0 | 12.5 | 19.5 | .1000000E+01 | .1000000E+01 | |
| 15.0 | 12.0 | 13.0 | 10.0 | 12.0 | 14.0 | .9999651E+00 | .1000000E+01 | * |

Table - 5
Checking sum rule given by (16)

| a | b | c | d | e | f | g | h | i | RNINE | WNINE |
|---|---|---|---|---|---|---|---|---|---|---|
| 4.0 | 3.0 | 5.0 | 3.0 | 2.0 | 4.0 | 5.0 | 4.0 | 4.0 | -.276575-02 | -.276574-02 |
| 5.0 | 3.0 | 5.0 | 4.0 | 2.0 | 3.0 | 4.0 | 4.0 | 5.0 | -.178988-02 | -.178988-02 |
| 5.0 | 4.5 | 4.5 | 6.5 | 4.0 | 4.5 | 9.5 | 6.5 | 5.0 | .217731-03 | .217731-03 |
| 8.0 | 8.5 | 6.5 | 9.5 | 7.0 | 8.5 | 10.5 | 9.5 | 8.0 | .354854-05 | .354854-05 |
| 8.5 | 9.5 | 7.0 | 12.5 | 8.0 | 8.5 | 8.0 | 10.5 | 9.5 | .281298-03 | .281298-03 |
| 9.0 | 8.0 | 4.0 | 11.0 | 10.0 | 8.0 | 7.0 | 11.0 | 9.0 | -.985215-04 | -.985215-04 |
| 7.0 | 9.5 | 3.5 | 10.5 | 8.0 | 9.5 | 8.5 | 10.5 | 7.0 | .106378-03 | .106378-03 |
| 7.0 | 10.0 | 9.0 | 11.0 | 6.0 | 10.0 | 8.0 | 11.0 | 7.0 | -.104868-04 | -.104868-04 |
| 7.0 | 11.0 | 6.0 | 15.5 | 10.5 | 11.0 | 11.5 | 15.5 | 7.0 | .412024-05 | .412024-05 |
| 5.0 | 7.0 | 2.0 | 6.5 | 8.5 | 5.0 | 8.5 | 12.5 | 7.0 | .233157-03 | .233157-03 |
| 5.0 | 7.0 | 5.0 | 6.5 | 8.5 | 5.0 | 8.5 | 12.5 | 7.0 | -.610603-04 | -.610603-04 |
| 6.0 | 9.0 | 3.0 | 7.0 | 8.0 | 6.0 | 8.0 | 10.0 | 9.0 | .184965-03 | .184965-03 |
| 6.0 | 9.0 | 6.0 | 7.0 | 8.0 | 6.0 | 8.0 | 10.0 | 9.0 | .135267-03 | .135267-03 |
| 7.0 | 10.0 | 3.0 | 6.0 | 9.0 | 7.0 | 9.0 | 11.0 | 10.0 | .285535-05 | .285535-05 |
| 10.5 | 11.5 | 10.0 | 18.0 | 7.5 | 11.5 | 9.5 | 18.0 | 10.5 | .572775-05 | .572775-05 |
| 12.0 | 10.0 | 14.0 | 15.0 | 5.0 | 10.0 | 13.0 | 15.0 | 12.0 | .755133-05 | .755656-05 |

Note: The results for the left and right sides of this sum rule were the same for RNINE and WNINE in the computer output in all but the last line shown above. The entry for RNINE shown in the last line corresponds to the left side which deviates from the results for the right side and that for WNINE due to the large number of terms summed.

# Chapter - 6

## Polynomial zeros of the 9-j coefficient

### 6.1 Introduction

In earlier chapters the *polynomial* or (*non-trivial*) zeros of the 3-j and the 6-j coefficients - in particular zeros of degree 1 or weight 1 - were studied and a comparison was made with the studies made by various authors using different methods. In this chapter our study of the *polynomial* zeros of the 9-j coefficient is presented and this study is the first of its kind.

The *non-trivial* zeros of the 9-j coefficient are those zeros which arise even when the arguments satisfy all the triangular inequalities. A closed form expression is obtained for these zeros (of degree 1) using the triple sum series for the 9-j coefficient given by Jucys and Bandzaitis (1977). They are also studied from a set of parametric solutions to the homogeneous multiplicative Diophantine equations of degree 3, viz. $x_1\ x_2\ x_3 = u_1\ u_2\ u_3$. Using the closed form expression as well as the parametric formulae, the *polynomial* zeros of degree 1 of the 9-j coefficient were generated. However, unlike the single four-parameter solution of $x_1\ x_2 = u_1\ u_2$ which generated the complete set of degree one zeros of the 3-j coefficient and the single eight-parameter solution of $x_1\ x_2\ x_3 = u_1\ u_2\ u_3$ with the constraint $x_3 = x_1 + x_2 + u_1 + u_2 + u_3$, which generated the complete set of degree one zeros of the 6-j coefficient, it is found that a *set* of solutions of the equation $x_1\ x_2\ x_3 = u_1\ u_2\ u_3$ is necessary to generate the complete set of degree one zeros of the 9-j coefficient. This complex situation is a direct consequence of the fact that while single sum series representations hve been obtained by Wigner and Racah for the 3-j and the 6-j coefficients, the 9-j coefficient is represented, at best, by the triple sum series due to Jucys and Bandzaitis (1977).

### 6.2 Closed form expression for the degree one zeros

The triple sum series for the 9-j coefficient due to Jucys and Bandzaitis (1977) is:

$$\begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix} = (-1)^{x5} \frac{(d\ a\ g)\ (b\ e\ h)\ (i\ g\ h)}{(d\ e\ f)\ (b\ a\ c)\ (i\ c\ f)} \sum_{x,y,z} \frac{(-1)^{x+y+z}}{x!\ y!\ z!}$$
$$\times \frac{(x1-x)!(x2+x)!(x3+x)!}{(x4-x)!\ (x5-x)!} \frac{(y1+y)!\ (y2+y)!}{(y3+y)!(y4-y)!(y5-y)!}$$
$$\times \frac{(z1-z)!\ (z2+z)!}{(z3-z)!(z4-z)!(z5-z)!(P2+x+y)!(P3+x+z)!} (P1-y-z)! \qquad (1)$$

where

$$0 \le x \le \min(-d+e+f\ ,\ c+f-i) = XF\ ,$$
$$0 \le y \le \min\ (g-h+i\ ,\ b+e-h) = YF\ ,$$
$$0 \le z \le \min\ (a-b+c\ ,\ a+d-g) = ZF\ , \qquad (2)$$

$$(a\ b\ c) = \frac{(a+b+c+1)!\ \Delta(a\ b\ c)}{(-a+b+c)!}\ , \qquad (3)$$

and x1,...,x5,y1,...,y5,z1,...,z5, p1, p2, and p3 are defined in terms of the arguments a,b,...,i of the 9-j coefficient and are given explicitly in Chapter 1. If c is set equal to zero in the 9-j coefficient, the triangular inequalities to be satisfied will lead to f = i and a = b, and the triple sum series can be shown to reduce to a single sum series, which corresponds to a 6-j coefficient. The symmetries of the 9-j coefficient then leads to the well known special values of this coefficient (Edmonds 1957):

$$\begin{Bmatrix} 0 & e & e \\ f & d & b \\ f & c & a \end{Bmatrix} = \begin{Bmatrix} e & 0 & e \\ c & f & a \\ d & f & b \end{Bmatrix} = \begin{Bmatrix} f & f & 0 \\ d & c & e \\ b & a & e \end{Bmatrix} = \begin{Bmatrix} f & b & d \\ 0 & e & e \\ f & a & c \end{Bmatrix}$$
$$= \begin{Bmatrix} a & f & c \\ e & 0 & e \\ b & f & d \end{Bmatrix} = \begin{Bmatrix} b & a & e \\ f & f & 0 \\ d & c & e \end{Bmatrix} = \begin{Bmatrix} e & d & c \\ e & b & a \\ 0 & f & f \end{Bmatrix} = \begin{Bmatrix} c & e & d \\ a & e & b \\ f & 0 & f \end{Bmatrix}$$
$$= \begin{Bmatrix} a & b & e \\ c & d & e \\ f & f & 0 \end{Bmatrix} = \frac{(-1)^{b+c+e+f}}{[e]\,[f]} \begin{Bmatrix} a & b & e \\ d & c & f \end{Bmatrix} . \tag{4}$$

From (4) it is obvious that every polynomial zero of the 6-j coefficient would imply a polynomial zero of the 9-j coefficient. The degree of the polynomial zero would be the same in both the cases. However, the 9-j coefficient in this case is a special one with one of the nine angular momenta in it being zero and such 9-j zeros are not the subject of interest.

It was shown in the previous chapter that the triple sum series (1) for the 9-j coefficient can be identified with a hypergeometric series in three variables in contrast to the 3-j and the 6-j coefficients which are represented by hypergeometric series in a single variable. This triple hypergeometric series was also shown to be a particular case of an extremely general hypergeometric series defined in three variables by Srivastava (1967). Viz:

$$F^{(3)}\begin{bmatrix} (a)::(b);\ (b');\ (b''):\ (c);\ (c');\ (c'');\ x,\ y,\ z \\ (e)::(f);\ (f');\ (f''):\ (g);\ (g');\ (g'') \end{bmatrix} =$$
$$= \sum_{m,n,p} \frac{((a),m+n+p)\ ((b),m+n)\ ((b'),n+p)\ ((b''),p+m)}{((e),m+n+p)\ ((f),m+n)\ ((f'),n+p)\ ((f''),p+m)}$$
$$\times \frac{((c),m)\ ((c'),n)\ ((c''),p)\ x^m\ y^n\ z^p}{((g),m)\ ((g'),n)\ ((g''),p)\ m!\ n!\ p!} , \tag{5}$$

where (a) denotes a sequence of parameters (as in the notation of Srivastava (1967)).From (5) it is clear that the degree of the polynomial $F^{(3)}$ is given by the sum of the maximum values of m, n and p, and this corresponds to XF + YF + ZF in (1). While the conventional expression for the 9-j coefficient does not reveal the polynomial zeros of the 9-j coefficient, the above identification with a triple hypergeometric series enables us to find these zeros.

A closed form expression is derived for the zeros of degree 1, when the series (1) ends after the second term, and this could happen when :

(i) XF = 1, YF = 0, ZF = 0, or
(ii) XF = 0, YF = 1, ZF = 0, or
(iii) XF = 0, YF = 0, ZF = 1.

Using each one of the above conditions in (1) automatically leads to the following closed-form expression for the degree 1 zeros :

$$1 - \delta^{\alpha_1, X_F, Y_F, Z_F}_{\beta_1,\ 1,\ 0,\ 0} - \delta^{\alpha_2, X_F, Y_F, Z_F}_{\beta_2,\ 0,\ 1,\ 0} - \delta^{\alpha_3, X_F, Y_F, Z_F}_{\beta_3,\ 0,\ 0,\ 1}, \qquad (6)$$

where the following notation has been introduced:

$$\delta^{a,b,c,d}_{p,q,r,s} = \delta(a,p)\,\delta(b,q)\,\delta(c,r)\,\delta(d,s), \qquad (7)$$

the $\delta(a,p)$ etc., being the Kronecker delta functions. In (6) the $\alpha$'s and $\beta$'s are given by:

$$\begin{aligned}
\alpha 1 &= (x_2 + 1).(x_3 + 1).x_4.x_5, & \beta 1 &= x_1.(p_2 + 1).(p_3 + 1), \\
\alpha 2 &= (y_1 + 1).(y_2 + 1).y_4.y_5, & \beta 2 &= p_1.(p_2 + 1).(y_3 + 1), \\
\alpha 3 &= (z_2 + 1).\ z_3.\ z_4.\ z_5, & \beta 3 &= p_1.\ z_1.(p_3 + 1).
\end{aligned} \qquad (8)$$

and XF, YF and ZF are given by (2).

It should be pointed out that the triple sum series (1) does not exhibit the 72 symmetries of the 9-j coefficient. In the previous chapter while numerically evaluating the 9-j coefficient, using (1), it was shown that while the (extreme) example:

$$\left\{ \begin{matrix} 30 & 20 & 10 \\ 30 & 10 & 20 \\ 60 & 30 & 30 \end{matrix} \right\}$$

has XF + YF + ZF = 0, its symmetries can have XF + YF + ZF = 60, 80, 100 or 140. Correspondingly, the number of terms to be summed in the triple sum series, reckoned after taking into account the constraints on the ranges of x, y and z placed by p1, p2 and p3 (viz, $y + z \le p1$ and if $p2, p3 < 0$, then $x + y \ge |p2|$, $z + x \ge |p3|$), for the given 9-j coefficient and its symmetries can be 21, 41, 441, 1681, 9471, 18081 or 33761 terms! This is due to the inherent lack of symmetry of (1). On the basis of this observation, *the degree of the polynomial zero of the 9-j coefficient* can be defined as that given by *the minimum value of XF + YF + ZF for one or more of its symmetries.*

### 6.3 Multiplicative Diophantine equations

In the study of the polynomial zeros of degree one of the 6-j coefficient (in Chapter 4), it was shown that the complete set of zeros can be obtained only from the eight parameter solution of the multiplicative Diophantine equation: $x\ y\ z = u\ v\ w$ subject to the constraint $z = x + y + u + v + w$. The polynomial zeros of degree one of the 9-j coefficient can also be studied from the solutions of the homogeneous multiplicative Diophantine equations of degree 3, viz. $x\ y\ z = u\ v\ w$. Since (1) is a triple sum series ( and not a single sum series as in the case of the 6-j coefficient), the closed form expression (6) for the polynomial zeros of degree one contains four terms and this immediately suggests that the multiplicative Diophantine equations to be solved to generate the degree one zeros are:

$$\alpha 1 = \beta 1 , \quad \text{for} \quad XF = 1,\ YF = 0,\ ZF = 0, \tag{9}$$

$$\alpha 2 = \beta 2 , \quad \text{for} \quad XF = 0,\ YF = 1,\ ZF = 0, \tag{10}$$

$$\alpha 3 = \beta 3 , \quad \text{for} \quad XF = 0,\ YF = 0,\ ZF = 1, \tag{11}$$

where the $\alpha$'s and the $\beta$'s are products of three terms given in (8). Furthermore, from (2) it is obvious that XF = 1 (say) could arise due to $-d + e + f = 1$ and $c + f - i \geq 1$ or $c + f - i = 1$ and $-d + e + f \geq 1$; along with one of $g - h + i$ or $b + e - h$ being 0; and one of $a - b + c$ or $a + d - g$ being 0. There are therefore eight different cases which should be considered explicitly for each of the above three equations (9), (10) and (11), and these different possibilities are indicated in Table 1.

From the discussion of the homogeneous multiplicative Diophantine equation of degree n:

$$x_1\ x_2\ \ldots\ x_n = u_1\ u_2\ \ldots\ u_n,\ (n > 1) \tag{12}$$

in Chapter 1, it follows that if (12) is written as:

$$n_1\ n_2\ n_3 = n_4\ n_5\ n_6 \tag{13}$$

then the solution of (13) is represented by the array:

$$\begin{array}{c|ccc} & n_4 & n_5 & n_6 \\ \hline n_1 & \phi_{11} & \phi_{12} & \phi_{13} \\ n_2 & \phi_{21} & \phi_{22} & \phi_{23} \\ n_3 & \phi_{31} & \phi_{32} & \phi_{33} \end{array} \tag{14}$$

We first consider the case XF = 1. The solutions for the eight different cases can be grouped into two sets (I) and (II) of four solutions each:

$$(I)\quad \begin{Bmatrix} a & a+(2n_6-n_2)/2 & n_2/2 \\ (n_1-n_3+n_4-1)/2 & (n_1+n_3-1)/2 & n_4/2 \\ g & h & (n_2+n_4-2)/2 \end{Bmatrix}$$

where

$$n_6 = n_2,\ h = g + i,\ g = a + (n_1 - n_3 + n_4 - 2n_5 - 1)/2. \qquad (X1)$$

$$n_6 = (n_1 + n_2 + n_4 - n_3 - n_5 - 1),\ h = g + i,\ g = a + d. \qquad (X2)$$

$$n_6 = n_2, \qquad n_5 = n_1, \qquad h = b + e. \qquad (X3)$$

$$n_5 = n_1, \qquad h = b + e \qquad g = a + d. \qquad (X4)$$

$$(II)\quad \begin{Bmatrix} a & a+(2n_6+n_3-n_2-1)/2 & (n_2+n_3-1)/2 \\ (n_1+n_4-2)/2 & n_1/2 & n_4/2 \\ g & h & (n_2+n_4-n_3-1)/2 \end{Bmatrix}$$

where

$$n_6 = n_2,\ h = g + i,\ g = a + (2n_3 + 2n_5 - n_1 - n_4)/2. \qquad (X5)$$

$$n_6 = (n_1 + n_2 + n_4 - n_3 - n_5 - 1),\ h = g + i,\ g = a + d. \qquad (X6)$$

$$n_6 = n_2, \quad n_5 = n_1, \quad h = b + e. \qquad (X7)$$

$$n_5 = n_1, \quad h = b + e, g = a + d. \qquad (X8)$$

A detailed examination of these eight solutions, named as (X1), . . . ,(X8) reveals the following:

(a) The conditions given in (X2), (X3), (X6), (X7) are inconsistent with the triangular inequalities. This is demonstrated below:

(X2) In this case $c + f - i = 1$, $g - h + i = 0$, $a + d - g = 0$ and hence

$$\begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix} = \begin{Bmatrix} a & b & c \\ d & e & f \\ a+d & a+c+d+f-1 & c+f-1 \end{Bmatrix}$$

From the triangular inequalities for (b e h) and (a b c), we have:

$$b + e - (a + d + c + f - 1) \geq 0 \text{ and } a - b + c \geq 0$$

which together imply: $e - d - f + 1 \geq 0$, i.e $e = d + f$ or d + f - 1 only. Similarly, from the triangular inequalities for (b e h) and (d e f):

$$b + e - (a + d + c + f - 1) \geq 0 \quad \text{and} \quad d - e + f \geq 0,$$

implying: $b - a - c + 1 \geq 0$, i.e. $b = a + c$ or $a + c - 1$ only.

These restrictions on e and b lead to the following four cases:

**Case (i):** $e = d + f$ and $b = a + c$, which imply from (I):

$$n_3 = n_4 \quad \text{and} \quad n_2 = n_6 \tag{15}$$

These two together with $n_1n_2n_3 = n_4n_5n_6$ imply:

$$n_1 = n_5 \tag{16}$$

But the condition $n_6 = n_1 + n_2 + n_4 - n_3 - n_5 - 1$ along with (15) leads to:

$$n_1 = n_5 + 1 , \tag{17}$$

which is in contradiction to (16). Hence no solutions are possible in this case.

**Case (ii):** $e = d + f$ and $b = a + c - 1$. As in Case (i), these two conditions imply from (I):

$$n_3 = n_4 \quad \text{and} \quad n_6 = n_2 - 1 \tag{18}$$

Substituting these in $n_6 = n_1 + n_2 + n_4 - n_3 - n_5 - 1$ leads to:

$$n_1 = n_5 \tag{19}$$

The conditions $n_3 = n_4$ and $n_1 = n_5$ in $n_1n_2n_3 = n_4n_5n_6$ gives:

$$n_2 = n_6 \tag{20}$$

which is in contradiction with $n_6 = (n_2 - 1)$ given in (18).

Hence no solutions are possible in this case also.

**Case (iii):** $e = d + f - 1$ and $b = a + c$ . The arguments in case (ii) can be repeated here and it leads to the conditions:

$$n_3 = n_4 - 1 \quad \text{and} \quad n_3 = n_4$$

which contradict each other.

Case (iv): $e = d + f - 1$ and $b = a + c - 1$. Using these in :

$$b + e - h \geq 0$$

with $h = a + d + c + f - 1$ leads to:

$$-1 \geq 0$$

which again is a contradiction.

Hence (X2) cannot yield any degree-one zeros of the 9-j coefficient.

(X3) In this case $c + f - i = 1$, $b + e - h = 0$, $a - b + c = 0$.

From (I) we have $n_6 = n_2$, $n_5 = n_1$ and these two together with $n_1 n_2 n_3 = n_4 n_5 n_6$ imply $n_3 = n_4$. Substituting these in the 9-j coefficient given by (I) we get:

$$\begin{Bmatrix} a & a+c & c \\ d & e & f \\ g & a+c+e & c+f-1 \end{Bmatrix} = \begin{Bmatrix} a & a+n_2/2 & n_2/2 \\ (n_1-1)/2 & (n_1+n_3-1)/2 & n_3/2 \\ g & a+(n_1+n_2+n_3-1)/2 & (n_2+n_3-2)/2 \end{Bmatrix}. \quad (21)$$

The triangular inequalities for $(g\ h\ i)$ and $(a\ d\ g)$ imply:

$$(g - h + i) \geq 0 \quad \text{and} \quad (a + d - g) \geq 0 \qquad (22)$$

and these in terms of the solution in (20) read as:

$$\begin{aligned} g - a - n_1/2 - 1/2 &\geq 0 , \\ -g + a + n_1/2 - 1/2 &\geq 0. \end{aligned} \qquad (23)$$

These two together imply $-1 \geq 0$ which is a contradiction. Hence, (X3) does not yield any zeros.

(X6) In this case $-d + e + f = 1$, $g - h + i = 0$, $a + d - g = 0$, and hence

$$\begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix} = \begin{Bmatrix} a & b & c \\ e+f-1 & e & f \\ a+e+f-1 & a+e+f+i-1 & i \end{Bmatrix}$$

The triangular inequalities for $(b\ e\ h)$ and $(a\ b\ c)$ imply

$$b + e - (a + e + f + i - 1) \geq 0 \quad \text{and} \quad a - b + c \geq 0,$$

which together imply $(c - f - i + 1) \geq 0$ i.e.

$$c = f + i \quad \text{and} \quad c = f + i - 1 \quad \text{only} \qquad (24)$$

Similarly from the triangular inequalities for $(b\ e\ h)$ and $(c\ f\ i)$

we have:

$$b + e - (a + e + f + i - 1) \geq 0 \quad \text{and} \quad -c + f + i \geq 0$$

and these two together imply $b - a - c + 1 \geq 0$ or

$$b = a + c \quad \text{and} \quad b = a + c - 1 \quad \text{only} \tag{25}$$

These restrictions on b and c given by (25) and (24) lead to four cases and the arguments in these cases are similar to those given for the case(X2)and the conclusion is that (X6) cannot also yield any zeros.

(X7) Here we have: $-d + e + f = 1$, $b + e - h = 0$, $a - b + c = 0$, and the arguments are on the same lines as in (X3), thus leading to the conclusion that no zeros arise out of this parametric formula.

Thus (X2), (X3), (X6) and (X7)do not yield any polynomial zeros of degree-one of the 9-j coefficient.

(b) (X1), (X4), (X5) and (X8) are solutions in terms of fewer (than nine parameters) and have one of the angular momenta itself as a free parameter.

Next we consider the case YF = 1. The eight different solutions in this case are given by:

$$\text{(III)} \quad \left\{ \begin{array}{ccc} a & (-n_1+n_4)/2 & c \\ (n_2-n_3+2n_5-1)/2-a & n_1/2 & f \\ (n_2+n_3-1)/2 & (n_4-2)/2 & (-n_2+n_3+n_4-1)/2 \end{array} \right\}$$

where

$$a = (n_2-n_3+n_5-n_6)/2, \quad c = b - a, \quad f = i - c. \tag{Y1}$$

$$n_6 = n_1, \quad c = b - a, \quad f = d - e. \tag{Y2}$$

$$n_6 = n_1, \quad n_5 = n_3, \quad f = d - e. \tag{Y3}$$

$$n_5 = n_3, \quad c = i - f, \quad f = (n_1 + n_2 + n_3 - 2n_6 - 1)/2 - a. \tag{Y4}$$

$$
\text{(IV)}\quad \left\{ \begin{matrix} a & (-n_1+n_3+n_4-1)/2 & c \\ (n_2+2n_5-2)/2-a & (n_1+n_3-1)/2 & f \\ n_2/2 & (n_4-2)/2 & (-n_2+n_4)/2 \end{matrix} \right\}
$$

where

$$a = (n_2+n_5-n_6-1)/2, \quad c = b - a, \quad f = i - c. \qquad \text{(Y5)}$$

$$n_6 = n_1, \quad c = b - a, \quad f = d - e. \qquad \text{(Y6)}$$

$$n_6 = n_1, \quad n_5 = 1, \quad f = d - e. \qquad \text{(Y7)}$$

$$n_5 = 1, \quad c = i - f, \quad f = (n_1+n_2-n_3-2n_6+1)/2-a. \qquad \text{(Y8)}$$

The following conclusions are drawn from a study of these eight solutions:

(c) (Y1) and (Y5) are genuine nine parameter solutions, related by the symmetries of the 9-j coefficient and the interchange of $n_1$ by $n_2$.

(d) The conditions given in (Y2), (Y3), (Y6) and (Y7) are inconsistent with the triangular inequalities. This is demonstrated below:

(Y2) This corresponds to $b+e-h = 1$, $-d+e+f = 0$, $a-b+c = 0$. The condition $n_6 = n_1$ in $n_1n_2n_3 = n_4n_5n_6$ gives:

$$n_2n_3 = n_4n_5 \qquad (26)$$

From the triangular inequalities for (g h i) and (a d g) we have:

$$a + d - g \geq 0 \quad \text{and} \quad -g + h + i \geq 0$$

and these in terms of the solution given in (III) read as:

$$(n_5 - n_3) \geq 0 \quad \text{or} \quad n_5 \geq n_3\,, \qquad (27)$$

and

$$(n_4 - n_2 - 1) \geq 0 \quad \text{or} \quad n_4 \geq n_2 + 1. \qquad (28)$$

(27) in (26) implies:

$$n_4 \leq n_2 \quad \text{(or)} \quad (n_4 - n_2) \leq 0 \qquad (29)$$

Combining (29) and (28):

(i) $(n_4 - n_2) = 0$ in (28) leads to $-1 \geq 0$

(ii) $(n_4 - n_2) = -n$ in (28) leads to $(-n-1) \geq 0$

both of which are contradictions.

(Y3) In this case $b+e-h = 1$, $a+d-g = 0$, $e+f-d = 0$, and the arguments are similar to those for (X3) and (X7). In this case the condition :

$$-g + h + i \geq 0$$

which follows from the triangular inequalities for $(g\ h\ i)$ implies: $-1 \geq 0$ which is a contradiction.

(Y6) This corresponds to $g-h+i = 1$, $-d+e+f = 0$, $a-b+c = 0$, and the condition $n_6 = n_1$ in $n_1 n_2 n_3 = n_4 n_5 n_6$ leads to:

$$n_2 n_3 = n_4 n_5 \tag{30}$$

The triangular inequalities for $(c\ f\ i)$ implies $-c+f+i \geq 0$, or

$$n_5 - n_3 \geq 0\ , \quad \text{i.e.}\quad n_5 \geq n_3. \tag{31}$$

(31) in (30) leads to the condition:

$$n_4 \leq n_2. \tag{32}$$

Eqn. (32) leads to two seperate cases. These are:

(i) $n_4 = n_2$. In this case from (IV) it follows that $i = 0$. It has already been stated that when any one of the nine angular momenta is zero, the 9-j coefficient reduces to a 6-j coefficient as in (4) and the zeros of these special 9-j coefficients are a direct consequence of zeros of the 6-j coefficients and we are not interested in these, since they may be considered as derived polynomial zeros of the 9-j coefficient.

(ii) $n_4 < n_2$, (IV) implies $i < 0$ which is not allowed.

(Y7) In this case $g-h+i = 1$, $e+f-d = 0$, $a+d-g = 0$ and hence

$$\begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix} = \begin{Bmatrix} a & b & c \\ e+f & e & f \\ a+e+f & a+e+f+i-1 & i \end{Bmatrix}.$$

From the triangular inequalities for (b e h) and (a b c):

$$b + e - (a + e + f + i - 1) \geq 0 \quad \text{and} \quad a - b + c \geq 0$$

which together imply : $c - f - i + 1 \geq 0$, i.e.

$$c = f + i, \quad \text{or} \quad f + i - 1, \quad \text{only.}$$

Similarly, from the triangualr inequalities for (b e h) and (c f i):

$$b + e - (a + e + f + i - 1) \geq 0 \quad \text{and} \quad -c + f + i \geq 0,$$

implying: $b - a - c + 1 \geq 0$, or

$$b = a + c, \quad \text{or} \quad a + c - 1, \text{ only.}$$

These restrictions on c and b lead to the following four cases:

*Case (i)*: $c = f + i$ and $b = a + c$, which imply from (IV):

$$c = (-n_1 - n_3 + n_4 + 1)/2 \quad \text{and} \quad b = (-n_1 - n_3 + n_4 + 1)/2$$

But from (IV) we also have $b = (-n_1 + n_3 + n_4 - 1)/2$. So from both these expressions for b to be true, we require $n_3 = 1$. The conditions given in (Y7) already require $n_1 = n_6$ and $n_5 = 1$. These together with $n_3 = 1$ and the requirement $n_1n_2n_3 = n_4n_5n_6$ imply $n_2 = n_4$. From (IV), when $n_2 = n_4$, $i = 0$ and as mentioned before we are not interested in such cases.

*Case (ii)*: $c = f + i - 1$ and $b = a + c$, imply from (IV):

$$c = (-n_1 - n_3 + n_4 - 1)/2 - a \quad \text{and} \quad b = (-n_1 - n_3 + n_4 - 1)/2,$$

But from (IV) we also have $b = (-n_1 + n_3 + n_4 - 1)/2$. For both these expressions of b to be true, we require $n_3 = 0$. Since, by definition, each of the nine parameters in the solution for the multiplicative Diophantine equation take only positive non-zero integral values, we must have strictly $n_3 > 0$. Thus this case yields no zeros of degree 1.

*Case (iii):* $c = f + i$ and $b = a + c - 1 = a + f + i - 1$. The arguments for case (ii) can be repeated and they lead to $n_3 = 0$, and consequently to no zeros of degree 1.

*Case (iv):* $c = f + i - 1$ and $b = a + c - 1 = a + f + i - 2$, imply from (IV):

$$c = (-n_1 - n_3 + n_4 - 1)/2 - a \quad \text{and} \quad b = (-n_1 - n_3 + n_4 - 3)/2.$$

Also from (IV): $b = (-n_1 + n_3 + n_4 - 1)/2$. For both these expressions for $b$ to be true, we require $n_3 = -1$, which is forbidden.

Thus, (Y2), (Y3), (Y6) and (Y7) cannot yield any degree one zeros of the 9-j coefficient.

(e) (Y4) and (Y8) are solutions in terms of fewer (than nine) parameters with one of the angular momenta itself as a free parameter.

Finally $Z_F = 1$ is considered. The eight solutions in this case are given by:

$$\text{(V)} \quad \left\{ \begin{array}{ccc} n_4/2 & (n_1+n_4-n_3-1)/2 & (n_1+n_3-1)/2 \\ (n_2-n_4)/2 & e & i+(n_1-n_3-2n_6+1)/2 \\ (n_2-2)/2 & h & i \end{array} \right\}$$

where

$$i = (n_5 + n_6 - 1)/2, \quad e = d - f, \quad h = b + e. \tag{Z1}$$

$$n_5 = 1, \quad e = d - f, \quad h = g + i. \tag{Z2}$$

$$n_5 = 1, \; n_6 = n_1, \quad h = g + i. \tag{Z3}$$

$$n_6 = n_1, \quad h = b + e, \; e = i + (n_2 + n_3 - n_1 - n_4 - 2n_5 + 1)/2. \tag{Z4}$$

$$
(\mathrm{VI}) \qquad \left\{ \begin{array}{ccc} n_4/2 & (n_1+n_4-2)/2 & n_1/2 \\ (n_2+n_3-n_4-1)/2 & e & i+(n_1-2n_6)/2 \\ (n_2-n_3-1)/2 & h & i \end{array} \right\}
$$

where

$$i = (n_5 + n_6 - 1)/2, \quad e = d - f, \quad h = b + e . \tag{Z5}$$

$$n_3 = n_5, \quad e = d - f, \quad h = g + i . \tag{Z6}$$

$$n_3 = n_5, \quad n_1 = n_6, \quad h = g + i . \tag{Z7}$$

$$n_1 = n_6, \; h = b + e, \; e = i + (n_2 + n_3 - n_1 - n_4 - 2n_5 + 1)/2 \quad .\tag{Z8}$$

Of the eight solutions, (Z1) and (Z5) are genuine nine parameter solutions. The solutions given by (Z2), (Z3), (Z6) and (Z7) do not yield any polynomial zero of degree 1 due to violation of triangular inequalities as explained below and (Z4) and (Z8) are solutions in terms of fewer (than nine) parameters with one of the angular momenta itself as a free parameter.

(Z2): This corresponds to $a+d-g = 1$, $e+f-d = 0$, $g-h+i = 0$ and hence

$$
\left\{ \begin{array}{ccc} a & b & c \\ d & e & f \\ g & h & i \end{array} \right\} = \left\{ \begin{array}{ccc} a & b & c \\ e+f & e & f \\ a+e+f-1 & a+e+f+i-1 & i \end{array} \right\}
$$

The triangular inequalities for (b e h) and (a b c) imply:

$$b + e - (e + a + f + i - 1) \geq 0 \text{ and } a - b + c \geq 0$$

which together leads to : $c - f - i + 1 \geq 0$ , i.e.

$$c = f + i \quad \text{or} \quad c = f + i - 1$$

*Case (i):* $i = c - f$ in (V) yields:

$$i = (n_3 + n_6 - 1)/2 . \tag{33}$$

The triangular inequalities for (b e h) imply $(b + e - h) \geq 0$ and this condition in (V) along with i given by (32) in turn implies:

$$(-n_3 + 1) \geq 0 \tag{34}$$

The only value of $n_3$ consistent with (33) is $n_3 = 1$. The solution for (Z2) already has the condition $n_5 = 1$ and this along with $n_3 = 1$ reduces the equation $n_1 n_2 n_3 = n_4 n_5 n_6$ to:

$$n_1 n_2 = n_4 n_6 . \tag{35}$$

Also $i$ given by (32) now becomes :

$$i = (n_1 - n_6)/2 . \tag{36}$$

Since i should be greater than zero this implies:

$$n_1 > n_6 . \tag{37}$$

This condition applied to (35) requires $n_2 < n_4$. But $n_2 < n_4$ in (V) makes $d < 0$ and this is not allowed.

*Case (ii)*: $i = c - f + 1$ in the solution given by (V) leads to:

$$i = (n_3 + n_6)/2 \tag{38}$$

and this along with $(b + e - h) \geq 0$ in (V) implies:

$$-n_3 \geq 0$$

which is a contradiction.

(Z3): In this case $a + d - g = 1$, $c + f - i = 0$, $g - h + i = 0$ and hence

$$\begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix} = \begin{Bmatrix} a & b & c \\ d & e & f \\ a+d-1 & a+d+c+f-1 & c+f \end{Bmatrix},$$

and combining the relations:

$$b + e - (a + d + c + f - 1) \geq 0 \quad \text{and} \quad (d - e + f) \geq 0$$

which are implied by the triangular inequalities for (b e h) and (d e f) we get:

$$b = a + c \quad \text{or} \quad a + c - 1 .$$

*Case (i)*: $b = a + c$, in (V) implies:

$$b = (n_1 + n_3 + n_4 - 1)/2 . \tag{39}$$

From (V) b is also equal to:

$$(n_1 - n_3 + n_4 - 1)/2 \tag{40}$$

The two together imply $n_3 = 0$ which is forbidden.

*Case (ii)*: $b = a + c - 1$. In this case the same argument as above leads to:

$$n_3 = 1 \; . \tag{41}$$

This along with the other conditions ,viz. $n_5 = 1$ and $n_6 = n_1$, in $n_1\ n_2\ n_3 \;=\; n_4\ n_5\ n_6$ imply:

$$n_4 = n_2 \; . \tag{42}$$

But when $n_4 = n_2$, d becomes 0 and hence no non-trivial zeros result.

(Z6): This corresponds to $a-b+c = 1$, $-d+e+f = 0$, $g-h+i = 0$, and since $n_3 = n_5$, the condition $n_1\ n_2\ n_3 = n_4\ n_5\ n_6$ becomes :

$$n_1\ n_2 = n_4\ n_6 \; . \tag{43}$$

The conditions $(-b + e + h) \geq 0$ and $(c + f - i) \geq 0$ imply:

$$(n_2 + n_6) \geq (n_1 + n_4) \tag{44}$$

and

$$n_1 \geq n_6 \; , \tag{45}$$

respectively. The two together imply:

$$n_2 \geq n_4 \tag{46}$$

The only consistent solution for (43), (45) and (46) is:

$$n_1 = n_6 \text{ and } n_2 = n_4 \; . \tag{47}$$

But (46) in (VI) along with the condition :

$$-a + d + g \geq 0$$

leads to $-1 \geq 0$ , which is a contradiction.

(Z7): Here $a - b + c = 1$, $g - h + i = 0$, $c + f - i = 0$ and the arguments used in (X3)(also (X7) and (Y3)) can be repeated in this case. The condition: $-a + d + g \geq 0$, in this case leads to $-1 \geq 0$.

Hence (Z2), (Z3),(Z6) and (Z7) do not yield any zeros of degree 1.

To sum up of the 24 cases studied, 12 did not yield any degree one zeros because of inherent inconsistencies and of the remaining 12 studied, only four (two from (9) and two from (10)) are full nine parameter solutions, the other eight being fewer (than nine) parameter solutions having one of the angular momenta itself as a free parameter.

**6.4 Results and discussion**

The polynomial zeros of degree one of the 9-j coefficient were generated using both the closed form expression (6) and the set of 12 solutions of multiplicative diophantine equations discussed above. Using (6), the polynomial zeros of degree one for all non-zero arguments of the 9-j coefficient that arise when $0 < a, b, d, e \leq 5/2$, were listed on an IBM - PC/AT computer. This restricted range for the arguments was found to contain 447 polynomial zeros of degree one of the 9-j coefficient. The first 20 of these are given in Table-2. Also this range of arguments contained only three polynomial zeros of degree 1 of the 6-j coefficient, viz.

$$\begin{Bmatrix} 2 & 2 & 2 \\ 3/2 & 3/2 & 3/2 \end{Bmatrix}, \quad \begin{Bmatrix} 3 & 2 & 2 \\ 1 & 2 & 2 \end{Bmatrix} \quad \text{and} \quad \begin{Bmatrix} 4 & 7/2 & 5/2 \\ 2 & 5/2 & 5/2 \end{Bmatrix}$$

and (4) gives in this case all the corresponding polynomial zeros of degree one of the 9-j coefficient.

In Table 3 are listed the first few inequivalent polynomial zeros of degree one, for $12 \leq \sigma \leq 18$. These were generated from the 12 solutions of the multiplicative Diophantine equations discussed earlier. After generating the polynomial zeros, the results were further analysed with the help of a program by which the inequivalent 9-j coefficients were isolated (by dropping the equivalent ones, which are any of the 72 symmetries of the listed one). Since the symmetries of the 9-j coefficient are all generated only by column permutations, row permutations and transposition about the leading 'diagonal', (unlike in the case of 3-j and 6-j coefficient where in addition to permutations and/or exchanges, Regge symmetries also exist), the ones that are related by any one of the symmetries can be identified by inspection. Using these symmetries an ordering procedure has been arrived at to seperate the *inequivalent* ones. However, it was realised that a much simpler ordering prescription due to Howell (1959) can be used for ordering to get the inequivalent 9-j coefficients. The program used to obtain the list of *inequivalent* zeros based on Howell's prescription for $0 < a, b, d, e \leq 3$ is given in Appendix D. The significant point to be noted is that the nine parameter solutions *do not generate* all these listed zeros. This is obvious by a look at (6), since the nine parameter solutions are from (10) and (11) only which arise from the third or fourth terms of (6) being equal to 1, and these exclude the zeros that arise from the second term of (6). So, the set of 12 solutions of the multiplicative Diophantine equations is necessary to generate all the polynomial zeros of degree one of the 9-j coefficient. A scan of the tables of 9-j coefficients (Howell 1959) reveals a listing of 67 polynomial zeros and of these 60 are zeros of degree one.

**6.5 Conclusion:**

To conclude, based on the triple sum series for the 9-j coefficient, the polynomial zeros of degree one of this coefficient have been generated using:

(i) the closed form expression (6) ,or

(ii) a *set* of parametric formulae based on the solutions of 12 homogeneous multiplicative Diophantine equations of the type:

$$x_1\ x_2\ x_3 = u_1\ u_2\ u_3$$

Due to the relation (de-Shalit and Talmi 1963):

$$\langle \alpha_1\ j_1\ \alpha_2\ j_2\ J \parallel T^k \parallel \alpha'_1\ \ j'_1\ \ \alpha'_2\ \ j'_2\ \ J' \rangle = [J]\ [k]\ [J']$$

$$\times \left\{ \begin{matrix} j_1 & j_2 & J \\ j'_1 & j'_2 & J' \\ k_1 & k_2 & k \end{matrix} \right\} \langle \alpha_1 j_1 \parallel T^{k_1} \parallel \alpha'_1 j'_1 \rangle \ \langle \alpha_2 j_2 \parallel T^{k_2} \parallel \alpha'_2 j'_2 \rangle, (48)$$

it follows that the polynomial zeros of the 9-j coefficient imply that certain specific reduced matrix elements of the tensor product of two irreducible tensors taken between certain specific well-defined angular momentum states are zero. It is possible that these vanishing matrix elements have some quantum mechanical significance.

Table - 1

The 24 Parametric Solutions

| XF, YF, ZF | x4 =e+f-d | x5 =c+f-i | y4 =b+e-h | y5 =g-h+i | z4 =a+d-g | z5 =a-b+c | Resulting equation: |
|---|---|---|---|---|---|---|---|
| 1, 0, 0 | ≥ 1 | 1 | ≥ 0 | 0 | ≥ 0 | 0 | (X1) |
| | ≥ 1 | 1 | ≥ 0 | 0 | 0 | ≥ 0 | (X2) |
| | ≥ 1 | 1 | 0 | ≥ 0 | ≥ 0 | 0 | (X3) |
| | ≥ 1 | 1 | 0 | ≥ 0 | 0 | ≥ 0 | (X4) |
| | 1 | ≥ 1 | ≥ 0 | 0 | ≥ 0 | 0 | (X5) |
| | 1 | ≥ 1 | ≥ 0 | 0 | 0 | ≥ 0 | (X6) |
| | 1 | ≥ 1 | 0 | ≥ 0 | ≥ 0 | 0 | (X7) |
| | 1 | ≥ 1 | 0 | ≥ 0 | 0 | ≥ 0 | (X8) |
| 0, 1, 0 | ≥ 0 | 0 | 1 | ≥ 1 | ≥ 0 | 0 | (Y1) |
| | 0 | ≥ 0 | 1 | ≥ 1 | ≥ 0 | 0 | (Y2) |
| | 0 | ≥ 0 | 1 | ≥ 1 | 0 | ≥ 0 | (Y3) |
| | ≥ 0 | 0 | 1 | ≥ 1 | 0 | ≥ 0 | (Y4) |
| | ≥ 0 | 0 | ≥ 1 | 1 | ≥ 0 | 0 | (Y5) |
| | 0 | ≥ 0 | ≥ 1 | 1 | ≥ 0 | 0 | (Y6) |
| | 0 | ≥ 0 | ≥ 1 | 1 | 0 | ≥ 0 | (Y7) |
| | ≥ 0 | 0 | ≥ 1 | 1 | 0 | ≥ 0 | (Y8) |
| 0, 0, 1 | 0 | ≥ 0 | 0 | ≥ 0 | 1 | ≥ 1 | (Z1) |
| | 0 | ≥ 0 | ≥ 0 | 0 | 1 | ≥ 1 | (Z2) |
| | ≥ 0 | 0 | ≥ 0 | 0 | 1 | ≥ 1 | (Z3) |
| | ≥ 0 | 0 | 0 | ≥ 0 | 1 | ≥ 1 | (Z4) |
| | 0 | ≥ 0 | 0 | ≥ 0 | ≥ 1 | 1 | (Z5) |
| | 0 | ≥ 0 | ≥ 0 | 0 | ≥ 1 | 1 | (Z6) |
| | ≥ 0 | 0 | ≥ 0 | 0 | ≥ 1 | 1 | (Z7) |
| | ≥ 0 | 0 | 0 | ≥ 0 | ≥ 1 | 1 | (Z8) |

Table 2

The first 20 polynomial zeros of degree one of the 9-j coefficient, with $\sigma = a + b + c + d + e + f + g + h + i$ given in the last column.

| $a$ | $b$ | $c$ | $d$ | $e$ | $f$ | $g$ | $h$ | $i$ | $\sigma$ |
|---|---|---|---|---|---|---|---|---|---|
| 0.5 | 1.0 | 1.5 | 1.0 | 1.5 | 1.5 | 1.5 | 2.5 | 2.0 | 13 * |
| 0.5 | 1.0 | 1.5 | 1.0 | 2.0 | 3.0 | 1.5 | 3.0 | 3.5 | 17 |
| 0.5 | 1.0 | 1.5 | 1.5 | 0.5 | 2.0 | 2.0 | 1.5 | 1.5 | 12 * |
| 0.5 | 1.0 | 1.5 | 1.5 | 2.0 | 1.5 | 2.0 | 3.0 | 2.0 | 15 * |
| 0.5 | 1.0 | 1.5 | 1.5 | 2.5 | 3.0 | 2.0 | 3.5 | 3.5 | 19 |
| 0.5 | 1.0 | 1.5 | 2.0 | 1.0 | 2.0 | 2.5 | 2.0 | 1.5 | 14 |
| 0.5 | 1.0 | 1.5 | 2.0 | 2.5 | 1.5 | 2.5 | 3.5 | 2.0 | 17 * |
| 0.5 | 1.0 | 1.5 | 2.5 | 1.5 | 2.0 | 3.0 | 2.5 | 1.5 | 16 |
| 0.5 | 1.5 | 1.0 | 1.0 | 1.5 | 1.5 | 1.5 | 2.0 | 2.5 | 13 * |
| 0.5 | 1.5 | 1.0 | 1.5 | 1.5 | 2.0 | 2.0 | 2.0 | 3.0 | 15 * |
| 0.5 | 1.5 | 1.0 | 1.5 | 2.0 | 1.5 | 1.0 | 2.5 | 1.5 | 13 * |
| 0.5 | 1.5 | 1.0 | 2.0 | 1.5 | 1.5 | 1.5 | 2.0 | 0.5 | 12 * |
| 0.5 | 1.5 | 1.0 | 2.0 | 1.5 | 2.5 | 2.5 | 2.0 | 3.5 | 17 * |
| 0.5 | 1.5 | 1.0 | 2.5 | 1.5 | 3.0 | 3.0 | 2.0 | 4.0 | 19 |
| 0.5 | 1.5 | 2.0 | 1.0 | 0.5 | 1.5 | 1.5 | 2.0 | 1.5 | 12 * |
| 0.5 | 1.5 | 2.0 | 1.0 | 2.0 | 2.0 | 1.5 | 3.5 | 3.0 | 17 |
| 0.5 | 1.5 | 2.0 | 1.5 | 1.0 | 1.5 | 2.0 | 2.5 | 1.5 | 14 |
| 0.5 | 1.5 | 2.0 | 1.5 | 2.5 | 2.0 | 2.0 | 4.0 | 3.0 | 19 |
| 0.5 | 1.5 | 2.0 | 2.0 | 1.5 | 1.5 | 2.5 | 3.0 | 1.5 | 16 |
| 0.5 | 1.5 | 2.0 | 2.5 | 0.5 | 3.0 | 3.0 | 2.0 | 2.0 | 17 |

Table - 3

All the inequivalent polynomial zeros of degree 1 of the 9-j coefficient for $\sigma \leq 18$. The last three columns represent which of the 12 solutions of the multiplicative Diophantine equations give rise to the entries in this table. Column P represents the four 9 parameter solutions, column Q the four solutions of (15) and the column R represents the remaining four solutions. Y stands for YES and N for NO.

| $a$ | $b$ | $c$ | $d$ | $e$ | $f$ | $g$ | $h$ | $i$ | $\sigma$ | x | y | z | P | Q | R |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2.0 | 1.5 | 0.5 | 1.5 | 0.5 | 1.0 | 1.5 | 2.0 | 1.5 | 12 | 0 | 0 | 1 | Y | Y | Y |
| 1.5 | 2.5 | 1.0 | 1.0 | 1.5 | 0.5 | 1.5 | 2.0 | 1.5 | 13 | 0 | 1 | 0 | Y | Y | Y |
| 2.0 | 2.5 | 0.5 | 2.0 | 1.5 | 1.5 | 1.0 | 2.0 | 1.0 | 14 | 1 | 0 | 0 | Y | Y | Y |
| 2.0 | 1.5 | 0.5 | 1.5 | 1.0 | 1.5 | 1.5 | 2.5 | 2.0 | 14 | 0 | 0 | 1 | Y | Y | Y |
| 2.0 | 3.0 | 1.0 | 2.0 | 0.5 | 1.5 | 1.5 | 2.0 | 1.5 | 15 | 0 | 1 | 0 | Y | Y | Y |
| 2.5 | 3.0 | 0.5 | 2.0 | 1.5 | 1.5 | 1.5 | 2.5 | 1.0 | 16 | 1 | 0 | 0 | Y | Y | Y |
| 2.0 | 3.0 | 1.0 | 2.0 | 1.5 | 1.5 | 1.0 | 2.5 | 1.5 | 16 | 1 | 0 | 0 | N | Y | Y |
| 2.0 | 2.5 | 0.5 | 1.5 | 1.5 | 2.0 | 1.5 | 3.0 | 1.5 | 16 | 1 | 0 | 0 | Y | Y | Y |
| 2.0 | 1.5 | 0.5 | 2.5 | 1.0 | 1.5 | 2.5 | 2.5 | 2.5 | 16 | 0 | 0 | 1 | Y | Y | Y |
| 3.0 | 2.5 | 0.5 | 2.0 | 0.5 | 1.5 | 2.0 | 3.0 | 2.0 | 17 | 0 | 0 | 1 | Y | Y | Y |
| 3.0 | 2.0 | 1.0 | 1.5 | 1.0 | 0.5 | 3.5 | 3.0 | 1.5 | 17 | 0 | 0 | 1 | Y | Y | Y |
| 2.5 | 2.0 | 1.5 | 1.0 | 0.5 | 1.5 | 3.5 | 2.5 | 2.0 | 17 | 1 | 0 | 0 | Y | Y | Y |
| 2.0 | 2.0 | 1.0 | 2.0 | 1.5 | 0.5 | 3.0 | 3.5 | 1.5 | 17 | 0 | 0 | 1 | Y | Y | Y |
| 2.0 | 1.5 | 1.5 | 1.5 | 1.5 | 1.0 | 3.5 | 2.0 | 2.5 | 17 | 0 | 1 | 0 | N | Y | Y |
| 3.0 | 2.5 | 0.5 | 2.0 | 1.0 | 1.0 | 3.0 | 3.5 | 1.5 | 18 | 0 | 0 | 1 | Y | Y | Y |
| 2.5 | 3.5 | 0.5 | 1.5 | 2.0 | 1.5 | 2.0 | 3.0 | 2.0 | 18 | 0 | 1 | 0 | Y | N | N |
| 2.5 | 3.0 | 0.5 | 1.5 | 1.5 | 2.0 | 2.0 | 3.5 | 1.5 | 18 | 1 | 0 | 0 | Y | Y | Y |
| 2.0 | 3.0 | 2.0 | 1.5 | 0.5 | 1.0 | 1.5 | 3.5 | 3.0 | 18 | 0 | 0 | 1 | Y | Y | Y |
| 2.0 | 3.0 | 1.0 | 1.5 | 1.5 | 2.0 | 1.5 | 3.5 | 2.0 | 18 | 1 | 0 | 0 | N | Y | Y |
| 2.0 | 2.5 | 1.5 | 1.5 | 1.0 | 1.5 | 1.5 | 3.5 | 3.0 | 18 | 0 | 0 | 1 | N | Y | Y |
| 2.0 | 2.5 | 0.5 | 2.5 | 2.5 | 2.0 | 1.5 | 3.0 | 1.5 | 18 | 1 | 0 | 0 | N | Y | Y |
| 2.0 | 2.5 | 0.5 | 1.5 | 2.5 | 2.0 | 1.5 | 3.0 | 2.5 | 18 | 0 | 1 | 0 | Y | N | N |
| 2.0 | 2.0 | 1.0 | 2.5 | 1.0 | 1.5 | 2.5 | 3.5 | 2.5 | 18 | 0 | 0 | 1 | Y | Y | Y |

Chapter 7

# Hahn Polynomials and Recurrence Relations for 3-j coefficients.

## 7.1 Introduction

Recently, there has been a considerable interest in unravelling the deep connection between the basic quantities of the quantum theory of angular momentum - viz. the Clebsch-Gordan (or 3-j) coefficients and the Racah (or 6-j) coefficients and orthogonal polynomials of a discrete variable (i.e. polynomials which are orthogonal on a discrete set of points). Smorodinskii and Suslov (1982b), while determining the eigenvalues and eigenvectors of a Hermitian operator, were led to a relation between 3-j coefficients and discrete Hahn polynomials, "which are practically unknown to physicists". Wilson (1980) and Askey and Wilson (1979) related the 6-j coefficient to the orthogonal polynomial named as Racah polynomial, which contains as limiting cases the classical polynomials of Jacobi, Laguerre, and Hermite and their discrete analogues which go under the names of Hahn, Meixner, Krawtchouk and Charlier polynomials. Askey and Wilson (1980) discuss the classical type of orthogonal polynomials that can be given as hypergeometric polynomials and they provide also a chart showing their interrelationship.

In this chapter we relate the 3-j coefficient to the discrete orthogonal Hahn polynomial through a $3F_2(1)$ transformation due to Erdelyi and Weber (1952) which was discussed earlier in Chapter-2. The four recurrence relations (one old and three new) obtained by

Karlin and Mc Gregor (1961) for the Hahn polynomial are used to derive recurrence relations for the 3-j coefficient. Two of these recurrence relations have been found to be useful in the exact recursive revaluation of the 3-j coefficients by Schulten and Gordan (1975).

## 7.2 The Hahn Polynomial : Definition and Properties

The Hahn polynomials defined by Karlin and Mc Gregor (1961) are :

$$Q_n(x) \equiv Q_n(x;\ \alpha,\ \beta,\ N)$$
$$\qquad {}_3F_2(-n,\ -x,\ n+\alpha+\beta+1\ ;\ \alpha+1,\ -N+1\ ;\ 1) \tag{1}$$

for real $\alpha > -1$, $\beta > -1$ and positive integral N. The results of Karlin and McGregor, which are made use of here are obtained with this restriction of $\alpha$, $\beta$ to real values > -1.

This discrete polynomial has been shown (Karlin and McGregor, 1961) to satisfy the following orghogonality relations:

$$\sum_{x=0}^{N-1} Q_n(x)\ Q_m(x)\ \rho(x) = \frac{1}{\pi_n}\ \delta(m,n) \tag{2}$$

and

$$\sum_{n=0}^{N-1} Q_n(x)\ Q_n(y)\ \pi_n = \frac{1}{\rho(x)}\ \delta(x,y) \tag{3}$$

where $\delta(x,y)$ is the Kronecker delta function and the weight function are:

$$\rho(x) = \rho(x;\alpha,\beta,N) = \frac{\begin{bmatrix}\alpha+x\\ x\end{bmatrix}\begin{bmatrix}\beta+N-1-x\\ N-1-x\end{bmatrix}}{\begin{bmatrix}N+\alpha+\beta\\ N-1\end{bmatrix}}, \tag{4}$$

and

$$\pi_n = \pi_n(\alpha,\beta,N) = \frac{\begin{bmatrix}N-1\\ n\end{bmatrix}}{\begin{bmatrix}N+\alpha+\beta+n\\ n\end{bmatrix}}\ \frac{(2n+\alpha+\beta+1)}{(\alpha+\beta+1)}$$
$$\times \frac{\Gamma(\beta+1,\ n+\alpha+1,\ n+\alpha+\beta+1)}{\Gamma(\alpha+1,\ \alpha+\beta+1,\ n+\beta+1,\ n+1)} \tag{5}$$

with $\begin{bmatrix}n\\ r\end{bmatrix}$ representing the usual binomial coefficients. Karlin and McGregor call (3) as their new *Dual orthogonality relation.*

### 7.3 Hahn Polynomial and the 3-j coefficient

In Chapter 2 the 3-j coefficient was represented by the Van der Waerden set of ${}_3F_2(1)$s which for (p q r) = (1 2 3) reads as:

$$\begin{bmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{bmatrix} = \delta(m_1+m_2+m_3,0)\,(-1)^{j_1-j_2-m_3} \prod_{i,k=1}^{3} \{R_{ik}!/(J+1)!\}^{1/2}$$

$$\times \{\Gamma(1-A,1-B,1-C,D,E)\}^{-1}\ {}_3F_2(A,B,C;D,E;1), \qquad (6)$$

where

$A = -j_1+m_1, B = -j_2-m_2, C = -j_1-j_2+j_3, D = 1-j_1+j_3-m_2, E = 1-j_2+j_3+m_1$.

It was shown that using one of the transformations given by Erdelyi and Weber (1952) for the ${}_3F_2(1)$ viz.:

$${}_3F_2(\alpha,\beta,-n;\gamma,\delta;1) = \frac{\Gamma(\gamma,\ \gamma-\alpha+n)}{\Gamma(\gamma+n,\ \gamma-\alpha)}\ {}_3F_2(\alpha,\delta-\beta,-n;1+\alpha-\gamma-n,\delta;1). \quad (7)$$

to the right hand side of (6) with the identification:

$$\alpha = A,\ \beta = B,\ n = -C,\ \gamma = E \text{ and } \delta = D\ , \qquad (8)$$

leads to the Majumdar form of the 3-j coefficient:

$$\begin{bmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{bmatrix} = \delta(m_1+m_2+m_3\ ,0)(-1)^{2j_2-j_1-m_1} \prod_{i,k=1}^{3} \left(\frac{R_{ik}!}{(J+1)!}\right)^{1/2}$$

$$\times\ \Gamma(2j_3+1)\ \{\Gamma(1+j_3+m_3,\ 1+j_3-m_3,\ 1-j_1+j_2+j_3,$$

$$1+j_1-j_2+j_3,\ 1+j_2+m_2,\ 1+j_1-j_3-m_2)\}^{-1}$$

$$\times\ {}_3F_2(1+j_1+j_2-j_3,-j_3+m_3,j_1-j_2-j_3;-2j_3,1+j_1-j_3-m_2;1)$$

(9)

In this form, the ${}_3F_2(1)$ can be readily identified with the Hahn polynomial $Q_n(x)$ defined in (1) and this leads to:

$$Q_n(x) = (-1)^{j_1+m_2}\ \frac{(j_1-j_3-m_2)!}{(2j_3)!}\ \left\{ \frac{(2j_3-n)!\ n!\ (2j_1+n+1)!}{(2(j_1-j_3)+n)!(j_1+j_3+m_2-x)!} \right. \qquad (10)$$

$$\left. \times\ \frac{x!\ (2j_3-x)!\ (j_1-j_3+m_2+n\ )!}{(j_1-j_3-m_2+x)!(j_1-j_3-m_2+n)!} \right\}^{1/2} \begin{bmatrix} j_1 & j_1-j_3+n & j_3 \\ x-j_3-m_2 & m_2 & j_3-x \end{bmatrix}$$

where the following identifications have been made :

$$n = -j_1+j_2+j_3, x = j_3-m_3, N = 2j_3+1, \alpha = j_1-j_3-m_2, \beta = j_1-j_3+m_2. \quad (11)$$

Though, $\alpha = (j_1+m_1) - (j_3-m_3)$ and $\beta = (j_1-m_1) - (j_3+m_3)$, being differences between integer quantities, appear to be capable of taking positive or negative values: due to the 72 symmetries of the 3-j coefficient, it is *always* possible to choose a symmetry of the given 3-j coefficient for which both $\alpha$ and $\beta$ are $\geq 0$.. This restriction to non-negative real values of $\alpha$ and $\beta$ is required since we use the orthogonality properties for the Hahn and dual Hahn polynomials of Karlin and Mc Gregor (1961).

Using (7) over again, with the roles of $\gamma$ and $\delta$ interchanged to transform the right side of (7), Erdelyi and Weber (1952) obtained the transformation:

$$ {}_3F_2(\alpha,\beta,-n;\gamma,\delta;1) = \frac{\Gamma(\gamma,\ \delta,\ \gamma-\alpha+n,\ \delta+n-\alpha)}{\Gamma(\gamma+n,\ \delta+n,\ \gamma-\alpha,\ \delta-\alpha)}$$

$$\times\ {}_3F_2(\alpha, 1+\alpha+\beta-\gamma-\delta-n, -n; 1+\alpha-\gamma-n, 1+\alpha-\delta-n; 1). \quad (12)$$

Identifying:

$$\alpha = A,\ \beta = B,\ n = -C,\ \gamma = D \text{ and } \delta = E\ , \quad (13)$$

and applying (12) to the ${}_3F_2(1)$ in (6) leads to the following expression for the discrete Hahn polynomials:

$$Q_n(x) = \frac{(-1)^{j_1-j_2-m_3}}{(2j_1)!(j_1+j_2+m_3)!}\Big\{ \frac{n!\ (2j_1-n)!\ (2(j_1+j_2)-n+1)!}{(2j_2-n)!(j_1+j_2-m_3-n)!}$$

$$.\ x!\ (2j_1-x)!\ (j_1+j_2+m_3-x)!(-j_1+j_2-m_3+x)!(j_1+j_2+m_3-n)!\ \Big\}^{1/2}$$

$$\times \begin{bmatrix} j_1 & j_2 & j_1+j_2-n \\ j_1-x & -j_1-m_3+x & m_3 \end{bmatrix}, \quad (14)$$

with:

$$n = j_1+j_2-j_3,\ x=j_1-m_1,\ N=2j_1+1,\ \alpha=-j_1-j_2-m_3-1,\ \beta=-j_1-j_2+m_3-1. \quad (15)$$

This form (14) happens to be an equivalent way of relating the Hahn polynomial to the 3-j coefficient and is similar to that given by Smorodinskii and Suslov (1982b) who also made use of (12).

### 7.4 Recurrence relations

The first of the recurrence relations is due to Erdelyi and Weber (1952) which is:

$$[b_n + d_n - x]\, Q_n(x) = b_n Q_{n+1}(x) + d_n Q_{n-1}(x)\,, \tag{16}$$

where

$$b_n = \frac{(n+\alpha+\beta+1)\,(n+\alpha+1)\,(N-n-1)}{(2n+\alpha+\beta+1)\,(2n+\alpha+\beta+2)}\,, \tag{17}$$

$$d_n = \frac{n\,(n+\beta)\,(n+\alpha+\beta+N)}{(2n+\alpha+\beta)\,(2n+\alpha+\beta+1)}, \tag{18}$$

which is valid for complex values of $x$ if $n = 0, 1, 2, \ldots, N-2$ but is valid only for $X = 0, 1, 2, \ldots, N-1$ when $n = N-1$. Using (10), (17) and (18) in (16) after simplifying and rearranging leads to the following recurrence relation for the 3-j coefficient:

$$B(j_1, j_2, j_3)\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} + (j_1+1)\, A(j_1, j_2, j_3)\begin{pmatrix} j_1-1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$
$$+\, j_1\, A(j_1+1, j_2, j_3)\begin{pmatrix} j_1+1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = 0, \tag{19}$$

where

$$A(j_p, j_q, j_r) = [j_p^2 - (j_q - j_r)^2]^{1/2}\,[-j_p^2 + (j_q + j_r + 1)^2]^{1/2}\,[j_p^2 - m_p^2]^{1/2}, \tag{20}$$

$$B(j_p, j_q, j_r) = (2j_p+1)\{j_p(j_p+1)(m_r - m_q) - [j_q(j_q+1) - j_r(j_r+1)]m_p\}\,, \tag{21}$$

with $p \neq q \neq r$ being 1,2 or 3. These expressions, with minor notational modifications, correspond to (6a), (6b) and (6c) of Schulten and Gordan (1975), respectively.

The orthogonality relation (3) for the discrete Hahn polynomial, can be shown to imply the following normalisation condition for the 3-j coefficient:

$$\sum_{j_1} (2j_1 + 1) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}^2 = 1. \tag{22}$$

Schulten and Gordan (1975) have provided a numerical algorithm for the computation of the 3-j coefficient based on recursion equations relating coefficients in two different types of strings. They derived the recursion relations algebraically from certain sum rules satisfied by these coefficients. The orthogonality relation (22) along with the recurrence relation (19) has been shown by them to the adequate to determine (except for an overall phase factor), the values of the string of 3-j coefficients $\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$ for all allowed values of $j_1$.

The second difference equation derived by Karlin and McGregor for the Hahn polynomial is:

$$[B(x) + D(x) - \lambda_n]\, Q_n(x) = B(x)\, Q_n(x+1) + D(x)\, Q_n(x-1), \tag{23}$$

where

$$B(x) = (N-1-x)\,(\alpha+1+x),$$

$$D(x) = x(N+\beta-x),$$

$$\lambda_n = n(n+\alpha+\beta+1),$$

and (23) is valid for $n = 0, 1, \ldots, N-1$, for all complex value of $x$.

This recurrence relation implies for the 3-j coefficient :

$$C(m_2+1, m_3-1) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2+1 & m_3-1 \end{pmatrix} + D(m_2, m_3) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$
$$+ C(m_2, m_3) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2-1 & m_3+1 \end{pmatrix} = 0, \tag{24}$$

where

$$C(m_p, m_q) = [(j_p-m_p+1)(j_p+m_p)(j_q-m_q)(j_q+m_q+1)]^{1/2}, \tag{25}$$

and

$$D(m_p, m_q) = -j_r(j_r+1)+j_p(j_p+1)+j_q(j_q+1)+2m_p m_q \quad , \tag{26}$$

with $p \neq q \neq r$ being 1,2 or 3. These expressions correspond to the appropriately modified forms of 9(a), 9(b), and 9(c) of Schulten and Gordan (1975). The orthogonality relation (2) can be shown to imply the normalization condition :

$$\sum_{m_2} (2j_1+1) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}^2 = 1 \ , \tag{27}$$

which along with the recurrence relation (24), has been shown by Schulten and Gordan to determine (except for an overall phase factor)the values of the string of 3-j coefficients $\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_1-m_2 \end{pmatrix}$ for all allowed values of $m_2$.

Thus, the recurrence relation in $j_1$ and the recurrence relation in $m_2$, $m_3$ are found to be direct consequence of the corresponding recurrence relations satisfied by the discrete orthogonal Hahn polynomials. The derivations of (19) and (24) given here are a direct consequence of the definition of the 3-j coefficient in terms of $Q_n(x)$ given in (10), as opposed to the algebraic method resorted to by Schulten and Gordan of deriving them from certain other sum rules

Karlin and McGregor have given two *new* first - order difference-recurrence relations satisfied by the Hahn polynomial. These are :

$$\begin{aligned} &\{ (n+\alpha+\beta+1) \ [ \ (n+\beta+1) \ (x-n) \ - \ (n+\alpha+1) \ (N-1-x) \ ] \ + \\ &\quad + (2n+\alpha+\beta+2) \ (\alpha+1+x) \ (N-1-x) \ \} \ Q_n(x) \\ &- (2n+\alpha+\beta+2) \ (\alpha+1+x) \ (N-1-x) \ Q_n(x+1) \\ &+ (n+\alpha+\beta+1) \ (n+\alpha+1) \ (N-1-n) \ Q_{n+1}(x) \ = \ 0, \end{aligned} \tag{28}$$

and

$$\begin{aligned} \{ n\, [(n+\beta)\,(N-1-x) - (n+\alpha)\,(n+\alpha+\beta+x+1)\,] &+ \\ + (2n+\alpha+\beta)\,(\alpha+1+x)\,(N-1-x)\,\}\, Q_n(x) & \\ - (2n+\alpha+\beta)\,(\alpha+1+x)\,(N-1-x)\, Q_n(x+1) & \\ - n\,(n+\beta)\,(n+\alpha+\beta+N)\, Q_{n-1}(x) = 0. & \end{aligned} \tag{29}$$

While (16) is a three-term recurrence relation in n for $Q_n(x)$ and (23) is a three-term recurrence relation in x for $Q_n(x)$, it is to be noted that (28) and (29) are recurrence relations mixed in n and x. However, since a term involving $Q_n(x+1)$ is common in both (28) and (29), one can try to algebraically eliminate it. This results in (16) - a three-term recurrence relation in n. Therefore, we consider (28) and (29) along with (23) to be the fundamental recurrence-relations satisfied by $Q_n(x)$.

A straightforward use of (10) in (28) and (29), after simplifications, and rearrangements leads to the following recurrence-relations for the 3-j coefficient:

$$D(j_1, j_2, j_3) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} + 2(j_1+1)\; C(m_3, m_2) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2+1 & m_3-1 \end{pmatrix}$$
$$- A(j_1+1, j_2, j_3) \begin{pmatrix} j_1+1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = 0, \tag{30}$$

and

$$E(j_1, j_2, j_3) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} + 2j_1\; C(m_3, m_2) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2+1 & m_3-1 \end{pmatrix}$$
$$+ A(j_1, j_2, j_3) \begin{pmatrix} j_1-1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = 0 \quad , \tag{31}$$

where

$$D(j_p, j_q, j_r) = (j_p-j_q+j_r+1)[(j_p+1)(j_p+j_q-j_r-2m_q)+m_p(-j_p+j_q+j_r)], \tag{32}$$

and

$$E(j_p\; j_q\; j_r) = (-j_p-j_q+j_r)[j_p(j_p-j_q+j_r+2m_q+1)+m_p(j_p+j_q+j_r+1)]. \tag{33}$$

Multiplying (30) by $j_1$ and (31) by $(j_1+1)$ and subtracting, we would get the three-term recurrence relation in $j_1$ for the 3-j coefficient, with the constant factors obeying the condition:

$$(j_1+1)E(j_1,j_2,j_3) - j_1\, D(j_1,j_2,j_3) = B(j_1,j_2,j_3). \qquad (34)$$

It should be pointed out that the other two forms for the 3-j coefficient viz. the Wigner and Racah forms (discussed in Chapter 2) do not lead to the desired ranges for the indices x and n, to satisfy the known sum rules for the 3-j coefficients given in (22) and (27).

### 7.5 Conclusion

As a direct consequence of identifying the 3-j coefficient with a discrete orthogonal Hahn polynomial, corresponding to the four three-term recurrence relations due to Karlin and Mc Gregor, it was shown that four three-term recurrence relations can be derived for this coefficient. Of these, one is a linear combination of two others and the other three are fundamental recurrence relations for this coefficient and two of these appear to be new.

## CONCLUDING REMARKS

In this thesis the following results were established:

- Sets of six ${}_3F_2(1)$s corresponding to the single ${}_3F_2(1)$ due to van der Waerden ,Wigner, Racah and Majumdar were derived and these were shown to be related to each other via an Erdelyi - Weber transformation for the ${}_3F_2(1)$s.
- The 3-j coefficient was related to the Hahn polynomial and this led to three independent three-term recurrence relations for this coefficient, of which two appear to be new.
- The set I of three ${}_4F_3(1)$s and the set II of four ${}_4F_3(1)$s for the 6-j coefficient were shown to be related to each other by the *reversal of series* argument for the Saalschutzian ${}_4F_3(1)$s.
- Formal binomial expansions were derived for the 3-j and the 6-j coefficients, using which closed form expressions were derived for the polynomial zeros of degree 1 of these coefficients. These closed form expressions, as well as three algorithms based on solutions of multiplicative Diophantine equations were used to generate the complete set of the degree 1 zeros.
- The 9-j coefficient was related to a triple hypergeometric series and this led to an efficient *new* Fortran program for it and to a discussion of its polynomial zeros, for the first time.
- A closed form expression , as well as solutions to a set of multiplicative Diophantine equations were used to derive the complete set of polynomial zeros of degree 1 of the 9-j coefficient.

A study of the polynomial zeros of degree 2 of the 3-j and the 6-j coefficients in terms of the Orbit classification to solutions of the Pell equation is due to Louck and Stein(1987) and Beyer, Louck and Stein(1987). However, in the case of the 6-j coefficient, their algorithm for determining numerically the fundamental solutions of Pell's equation, does not generate *all* its polynomial zeros of degree 2. Exploiting the connection between the 3-j and the 6-j coefficients to sets of ${}_pF_q(1)$s, Srinivasa Rao and Chiu (1988) obtained closed form expressions which represent polynomial zeros of any degree n and they proposed simple algorithms based on the principle of factorization of integers, to generate numerically *all* the polynomial zeros of degree 2. It is considered that a study of the polynomial zeros of degree 2 for the 9-j coefficient can now be made exploiting the connection established between this coefficient and the triple hypergeometric series.

As has been suggested by Biedenharn and Louck (1981b)in their treatise on *Racah-Wigner Algebra in Quantum Theory* the distribution of the polynomial zeros of these angular momentum coefficients is basically a number-theoretic question and this is yet to be studied.

Suslov (1983) has suggested that the 9-j coefficient is an orthogonal polynomial in two variables. The connection between this and the triple hypergeometric series discussed at length in this thesis is to be studied.

Finally, the studies made till date on the polynomial zeros of these angular momentum coefficients will hopefully motivate an investigation into their physical significance.

## Appendix A

This is an Appendix to Chapter 3, which concerns the generation of polynomial zeros of degree one of the 3-j coefficient. All the equation numbers referred here belong to that chapter. The program ZERO1 generates the *equivalent* as well as the *inequivalent* zeros of degree 1 of the 3-j coefficient using either the closed form expression or the four parameter formula given by (17) and (26), respectively. The *equivalent* zeros of degree 1 using (17) are generated in a subroutine THREEJ and those using (26) are generated in a subroutine THREEB.

Of the two CALL statements in the main program ZERO1, one must be made a comment statement (by keying in C in the first column) at the very beginning to enable generation of the zeros by either THREEJ or THREEB. The one-dimensioned variables in the common block are set to 150 and for this case NN, the variable to be read in I3 format can be $\leq 26$. While in the case of THREEJ, the value of NN generates all the zeros for $j_1 \leq NN/2$; in the case of THREEB, the zeros corresponding to $a,b,c,d \leq NN$ are generated. The ordering prescription of Rotenberg et. al.(1959) is followed in the case of THREEJ. For every zero the canonical parameters $p_1$, $p_2$, $p_3$, $n_1$, $n_2$ and J are calculated by calling a subroutine CANON and the arguments of the 3-j coefficient corresponding to a zero along with its canonical parameters are stored in the one dimensional arrays AJ1, AJ2, AJ3, AM1, AM2, AM3, IP1, IP2, IP3, N1, N2 and J. The variable I1 gives the number of *equivalent* zeros generated. These entries are then ordered with respect to the parameter J in ascending values of J. The ordering is done by adapting the straight insertion sort Algorithm S given in Knuth (1973). After ordering, the minimum and maximum values of J are noted as JMIN and JMAX, respectively. The *inequivalent* ones are sieved out by making use of the fact that $p_1$, $p_2$, $p_3$, $n_1$, $n_2$ and J are the same for *equivalent* ones. The *inequivalent* zeros along with their canonical parameters are written down.

- SUBROUTINE CANON (IR, IP1, IP2, IP3, N1, N2) has the nine elements of the two dimensional array IR (I, K), I = 1, 2, 3 and K = 1, 2, 3 as its input elements. These are the elements $R_{ik}$'s of the Regge array (7) which are calculated in THREEJ (or THREEB). This subroutine calculates the canonical parameters $p_1$, $p_2$, $p_3$, $n_1$ and $n_2$ (J being calculated in THREEJ (or THREEB)), for a given 3-j coefficient by interpreting the parameters given by Bryant and Jahn (1960) in terms of the parameters of the set of six ${}_3F_2(1)$s given by (10).
- Function PHASE(N) calculates the value of $(-1)^N$.
- Function TRIA (X, Y, Z) checks for the triangular inequality being satisfied by X, Y and Z.
- Function PARITY (A, B, C, X, Y, Z) has the arguments of a 3-j coefficient - viz. A, B, C representing $j_1$, $j_2$, $j_3$ and X, Y, Z representing $m_1$, $m_2$, $m_3$ respectively - as its input parameters. It checks if any of the Regge symmetries of the

given 3-j coefficient is a parity 3-j coefficient. PARITY is used in THREEJ ( or THREEB ) to exclude parity 3-j coefficients from the list of zeros.

Subroutine ORDER (I1) has I1 as one of its input variables and the other input variable denoted by DUMS (which is a one dimensional array) along with the output variable KEY (which is also a one dimensional array) are stored in a COMMON block A4. This orders the array DUMS which has I1 elements in ascending order and stores the key sequence in the array KEY. This is adapted from the straight insert sort Algorithm S of Knuth (1973).

Subroutine ORDER2 (I, J, K, I1, I2, I3) orders the given three integers I, J,and K in descending order and returns them as I1, I2, and I3 so that I1 ≥ I2 ≥ I3.

```
****************************************************************************
      PROGRAM ZERO1
      IMPLICIT REAL*8(A-H,O-Z)
      LOGICAL LX,LY,LZ
      COMMON/A1/AJ1(150),AJ2(150),AJ3(150),AM1(150),AM2(150),AM3(150)
      COMMON/A2/IP1(150),IP2(150),IP3(150),N1(150),N2(150),J(150)
      COMMON/A3/JP1(72),JP2(72),JP3(72),JN1(72),JN2(72)
      COMMON/A4/DUMS(150),KEY(150)
      DIMENSION BJ1(150),BJ2(150),BJ3(150),BM1(150),BM2(150),BM3(150)
      DIMENSION KP1(150),KP2(150),KP3(150),M1(150),M2(150),N(150)
      READ(*,60) NN
 60   FORMAT(I3)
C     CALL THREEJ(NN,I1)
      CALL THREEB(NN,I1)
C     WRITE(*,10)(AJ1(I),AJ2(I),AJ3(I),AM1(I),AM2(I),AM3(I),I=1,I1)
 10   FORMAT(6(5X,F6.2))
      DO 11 I=1,I1
 11   DUMS(I)=J(I)
      CALL ORDER(I1)
      DO 13 I=1,I1
      IS=KEY(I)
      BJ1(I)=AJ1(IS)
      BJ2(I)=AJ2(IS)
      BJ3(I)=AJ3(IS)
      BM1(I)=AM1(IS)
      BM2(I)=AM2(IS)
```

```
      BM3(I)=AM3(IS)
      KP1(I)=IP1(IS)
      KP2(I)=IP2(IS)
      KP3(I)=IP3(IS)
      M1(I)=N1(IS)
      M2(I)=N2(IS)
      N(I) =J(IS)
 13   CONTINUE
      JMIN=N(1)
      JMAX=N(I1)
C     WRITE(*,12) JMIN,JMAX
 12   FORMAT(2I10)
C     WRITE(*,44) (AJ1(I),AJ2(I),AJ3(I),AM1(I),AM2(I),J(I),I=1,I1)
 44   FORMAT(5F6.2,I10)
      JM=JMIN
 14   I=1
      DO 50 L1=1,I1
      IF(JM  -N(L1)) 20,15,50
 15   JP1(I)=KP1(L1)
      JP2(I)=KP2(L1)
      JP3(I)=KP3(L1)
      JN1(I)=M1(L1)
      JN2(I)=M2(L1)
      IF(I.EQ.1) GO TO 25
      DO 30 K=1,I-1
      LX=(JP1(I).EQ.JP1(K)).AND.(JP2(I).EQ.JP2(K))
      LY=(JP3(I).EQ.JP3(K)).AND.(JN1(I).EQ.JN1(K))
      LZ=JN2(I).EQ.JN2(K)
      IF((LX.AND.LY).AND.LZ) GO TO 40
 30   CONTINUE
 25   AA=BJ1(L1)
      AB=BJ2(L1)
      AC=BJ3(L1)
      AD=BM1(L1)
      AE=BM2(L1)
      AF=BM3(L1)
      IA=KP1(L1)
      IB=KP2(L1)
      IC=KP3(L1)
      ID=M1(L1)
      IE=M2(L1)
      IG=N(L1)
      WRITE(*,35)AA,AB,AC,AD,AE,AF,IA,IB,IC,ID,IE,IG
 35   FORMAT(6(2X,F5.1),5(2X,I2),2X,I3)
 40   I=I+1
 50   CONTINUE
      GO TO 16
 20   JM=JM+1
      IF(JM.LE.JMAX) GO TO 14
 16   STOP
      END
C ------------------------------------------------------------------------
      SUBROUTINE THREEJ(N,I1)
      IMPLICIT REAL*8(A-H,O-Z)
      LOGICAL L1,L2
```

```
      COMMON /A1/AJ1(150), AJ2(150), AJ3(150), AM1(150), AM2(150), AM3(150)
      COMMON/A2/IP1(150),IP2(150),IP3(150),N1(150),N2(150),J(150)
      DIMENSION IR(3,3)
      I11=1
      DO 10 J1=1,N
      A=J1
      A11=A/2.0D0
      DO 15 J2=1,J1
      B=J2
      B11=B/2.0D0
      AMI3=DABS(A11-B11)
      AMA3=A11+B11
      C11=AMI3
20    IF(C11.GT.B11) GO TO 15
      AJ22=A11+B11+C11
      J22=AJ22
      T=TRIA(A11,B11,C11)
      IF(T.EQ.0.0) GO TO 25
      D11=-A11
22    E11=-B11
30    F11=-D11-E11
      AMOD=DABS(F11)
      IF(AMOD.GT.C11) GO TO 40
      S1=PHASE(J22)
      S2=-S1
      L1=(D11.EQ.0.0).AND.(E11.EQ.0.0)
      L2=(F11.EQ.0.0).AND.(S2.EQ.1.0D0)
      IF(L1.AND.L2) GO TO 40
      IR(1,1)=-A11+B11+C11
      IR(1,2)=A11-B11+C11
      IR(1,3)=A11+B11-C11
      IR(2,1)=A11-D11
      IR(2,2)=B11-E11
      IR(2,3)=C11-F11
      IR(3,1)=A11+D11
      IR(3,2)=B11+E11
      IR(3,3)=C11+F11
      DO 45 I=1,3
      DO 46 K=1,3
      IF(IR(I,K).EQ.1) GO TO 50
46    CONTINUE
45    CONTINUE
      GO TO 40
50    L3=IR(I,K)
      IF(I-2)52,54,56
52    I1=2
      I2=3
      GO TO 58
54    I1=1
      I2=3
      GO TO 58
56    I1=1
      I2=2
58    IF(K-2) 60,62,64
60    K1=2
      K2=3
```

```
      GO TO 66
 62   K1=1
      K2=3
      GO TO 66
 64   K1=1
      K2=2
 66   IX=IR(I1,K1)*IR(I2,K2)
      IY=IR(I1,K2)*IR(I2,K1)
      IF(IX.NE.IY) GO TO 40
      V=PARITY(A11,B11,C11,D11,E11,F11)
      IF((S2.EQ.1.0D0).AND.(V.EQ.0.0))GO TO 40
      CALL CANON(IR,IQ1,IQ2,IQ3,MN1,MN2)
      AJ1(I11)=A11
      AJ2(I11)=B11
      AJ3(I11)=C11
      AM1(I11)=D11
      AM2(I11)=E11
      AM3(I11)=F11
      IP1(I11)=IQ1
      IP2(I11)=IQ2
      IP3(I11)=IQ3
      N1(I11)=MN1
      N2(I11)=MN2
      J(I11)=J22
      I11=I11+1
 40   E11=E11+1.0D0
      IF(E11.LE.0.0) GO TO 30
 35   D11=D11+1.0D0
      IF(D11.LE.A11) GO TO 22
 25   C11=C11+1.0D0
      IF(C11.LE.AMA3) GO TO 20
 15   CONTINUE
 10   CONTINUE
      I1=I11-1
      RETURN
      END
C ---------------------------------------------------------------------
      SUBROUTINE CANON(IR,IP1,IP2,IP3,N1,N2)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION IR(3,3)
      DO 70 JP=1,3
      DO 71 JQ=1,3
      IF(JP.EQ.JQ) GO TO 71
      DO 72 JR=1,3
      IF((JQ.EQ.JR).OR.(JP.EQ.JR))GO TO 72
      JD=IR(3,JR)-IR(2,JP)
      IF(JD.LT.0)GO TO 72
      JE=IR(2,JR)-IR(3,JQ)
      IF(JE.LT.0) GO TO 72
      JA=IR(2,JP)
      JB=IR(3,JQ)
      JC=IR(1,JR)
      CALL ORDER2(JA,JB,JC,IP1,IP2,IP3)
      KA=IP1-IP3
      KB=IP2-IP3
```

```
      IF(JD.GT.JE) GO TO 75
      N1=JE
      N2=JD
      GO TO 76
 75   N1=JD
      N2=JE
 76   KAB=KA+KB
      KDE=JD+JE
      IF(KAB-KDE)72,73,74
 73   KAMB=KA-KB
      KDME=N1-N2
      IF(KAMB-KDME)72,74,74
 72   CONTINUE
 71   CONTINUE
 70   CONTINUE
 74   RETURN
      END
C ---------------------------------------------------------------------
      FUNCTION PHASE(N)
      IMPLICIT REAL*8(A-H,O-Z)
      PHASE = 1.0D0
      M=(N/2)*2
      IF(M.NE.N) PHASE = -1.0D0
      RETURN
      END
C ---------------------------------------------------------------------
      FUNCTION TRIA(X,Y,Z)
      IMPLICIT REAL*8(A-H,O-Z)
      TRIA=0.0
      X1=-X+Y+Z
      X2=X-Y+Z
      X3=X+Y-Z
      IF((X1.GE.0.0).AND.(X2.GE.0.0).AND.(X3.GE.0.0))TRIA=1.0D0
      RETURN
      END
C ---------------------------------------------------------------------
      FUNCTION PARITY(A,B,C,X,Y,Z)
      IMPLICIT REAL*8(A-H,O-Z)
      A0=0.5D0*(C-B+X)
      A1=B-C
      A2=A0+Y
      A3=A0+Z
      IF((A1.EQ.0.0).AND.(A2.EQ.0.0).AND.(A3.EQ.0.0))GO TO 75
      B0=0.5D0*(C-A+Y)
      B1=A-C
      B2=B0+X
      B3=B0+Z
      IF((B1.EQ.0.0).AND.(B2.EQ.0.0).AND.(B3.EQ.0.0))GO TO 75
      C0=0.5D0*(A-B+Z)
      C1=B-A
      C2=C0+X
      C3=C0+Y
      IF((C1.EQ.0.0).AND.(C2.EQ.0.0).AND.(C3.EQ.0.0))GO TO 75
      D1=C-0.5D0*(A+B+Z)
      D2=A-0.5D0*(B+C+X)
      D3=B-0.5D0*(A+C+Y)
      IF((D1.EQ.0.0).AND.(D2.EQ.0.0).AND.(D3.EQ.0.0))GO TO 75
```

```
      E1=0.5D0*(A+B-Z)-C
      E2=0.5D0*(B+C-X)-A
      E3=0.5D0*(A+C-Y)-B
      IF((E1.EQ.0.0).AND.(E2.EQ.0.0).AND.(E3.EQ.0.0))GO TO 75
      PARITY=1.0D0
      RETURN
 75   PARITY=0.0
      RETURN
      END
C ---------------------------------------------------------------------
      SUBROUTINE ORDER(I1)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/A4/ DUMS(150),KEY(150)
      DO 15 K=1,I1
 15   KEY(K)=K
      DO 45 J=2,I1
      X=DUMS(J)
      IY=KEY(J)
      DO 35 I=J-1,1,-1
      IF(X.GE.DUMS(I)) GO TO 40
      DUMS(I+1)=DUMS(I)
      KEY(I+1)=KEY(I)
 35   CONTINUE
 40   DUMS(I+1)=X
      KEY(I+1)=IY
 45   CONTINUE
      RETURN
      END
C ---------------------------------------------------------------------
      SUBROUTINE ORDER2(I,J,K,I1,I2,I3)
      IMPLICIT REAL*8(A-H,O-Z)
      I1=MAX0(I,J,K)
      IF(I1.EQ.I) GO TO 7
      IF(I1.EQ.J) GO TO 8
      IF(I1.EQ.K) GO TO 9
 7    I2=MAX0(J,K)
      IF(I2.EQ.J) I3=K
      IF(I2.EQ.K) I3=J
      RETURN
 8    I2=MAX0(I,K)
      IF(I2.EQ.I) I3=K
      IF(I2.EQ.K) I3=I
      RETURN
 9    I2=MAX0(I,J)
      IF(I2.EQ.I) I3=J
      IF(I2.EQ.J) I3=I
      RETURN
      END
C ---------------------------------------------------------------------
      SUBROUTINE THREEB(N,I1)
      IMPLICIT REAL*8(A-H,O-Z)
      LOGICAL L1,L2
      COMMON/A1/AJ1(150),AJ2(150),AJ3(150),AM1(150),AM2(150),AM3(150)
      COMMON/A2/IP1(150),IP2(150),IP3(150),N1(150),N2(150),J(150)
      DIMENSION IR(3,3)
      I11=1
```

```
      DO 10 IA=1,N
      A=IA
      DO 11 IB=1,N
      B=IB
      DO 12 IC=1,N
      C=IC
      DO 13 ID=1,N
      D=ID
      A11=A*(B+C)/2.D0
      B11=D*(B+C)/2.D0
      C11=(B+C)*(A+D)/2.D0-1.D0
      AJ22=A11+B11+C11
      J22=AJ22
      T=TRIA(A11,B11,C11)
      IF(T.EQ.0.0) GO TO 13
      D11=A*(C-B)/2.D0
      E11=D*(C-B)/2.D0
      F11=-D11-E11
      S1=PHASE(J22)
      S2=-S1
      L1=(D11.EQ.0.0).AND.(E11.EQ.0.0)
      L2=(F11.EQ.0.0).AND.(S2.EQ.1.0D0)
      IF(L1.AND.L2) GO TO 13
      IR(1,1)=-A11+B11+C11
      IR(1,2)=A11-B11+C11
      IR(1,3)=A11+B11-C11
      IR(2,1)=A11-D11
      IR(2,2)=B11-E11
      IR(2,3)=C11-F11
      IR(3,1)=A11+D11
      IR(3,2)=B11+E11
      IR(3,3)=C11+F11
      V=PARITY(A11,B11,C11,D11,E11,F11)
      IF((S2.EQ.1.0D0).AND.(V.EQ.0.0))GO TO 13
      CALL CANON(IR,IQ1,IQ2,IQ3,MN1,MN2)
      AJ1(I11)=A11
      AJ2(I11)=B11
      AJ3(I11)=C11
      AM1(I11)=D11
      AM2(I11)=E11
      AM3(I11)=F11
      IP1(I11)=IQ1
      IP2(I11)=IQ2
      IP3(I11)=IQ3
      N1(I11)=MN1
      N2(I11)=MN2
      J(I11)=J22
      I11=I11+1
13    CONTINUE
12    CONTINUE
11    CONTINUE
10    CONTINUE
      I1=I11-1
      RETURN
      END
```

## Appendix B

This is an Appendix to Chapter 4, which deals with the generation of the *equivalent* zeros of degree one of the 6-j coefficient, using:

i) the closed form expression (24);

ii) the algorithm based on the solution of Brahmegupta;

iii) the algorithm based on the solution of Paoli; or,

iv) the four-parameter solution given by (66) and (67).

(Note: all the equations referred here belong to Chapter 4). These four cases are computed in the subroutines SIXJ, SIXB, SIXP and SIXF, respectively.

At the outset, three of the four CALL statements in the main program ZERO2 are made into comment statements. The value of N is read in. In each of the subprograms, corresponding to every zero, the canonical parameters $n_1$, $n_2$, $n_3$, $p_1$, $p_2$, $p_3$ and $J_m$ are calculated by calling a subroutine CANON6 and the arguments of the 6-j coefficient along with the canonical parameters and the number of zeros generated, denoted by NC, are stored in a file ZERO2.OUT as AN, BN, EN, DN, CN, FN, N1, N2, N3, IP1, IP2, IP3, JM and NC. (The output can be stored in the file ZERO2.OUT either by redirecting at the time of running the program or by means of an OPEN statement). In these subroutines the ordering of the output parameters for the zeros of the 6-j coefficient is according to either the prescription of Koozekanani and Biedenharn (1974); or, that given in Rotenberg et.al (1959).

- Subroutine SIXJ (J) generates the equivalent zeros of degree 1 for $j_1 \le J/2$ using the closed form expression (24).

- Subroutine SIXF(N) generates the *equivalent* zeros of degree 1 based on the solution in terms of four integer parameter $a$, $d$, $h$ and $i$ each one taking the values 1,2,...N. The arguments of the 6-j coefficient are ordered by calling a subroutine ORDER3.
- Subroutine SIXB (J) generates the *equivalent* zeros of degree 1 based on the constraint equation (34) being reduced to utilize the algorithm (68) of Brahmegupta (of Dickson (1952) p.64). The zeros corresponding to each of the seven parameters $a$, $b$, $c$, $d$, $e$, $f$, *and* $i$ (called as IY, IU, IP, IZ, IV, IQ and IX) taking the values 1,2,...,J are generated, and the arguments of the 6-j coefficient are ordered using the subroutine ORDER3.
- Subroutine SIXP (N) uses the solution of Paoli (of. Dickson (1952) p.401) to solve the constraint equation (34) and generates the *equivalent* zeros of degree 1 corresponding to each of the seven parameters $b$, $c$, $d$, $f$, $g$, $h$ *and* $i$ (called as JB, JC, JD, JF, JG, JH and JI) taking the values 1,2,..,N. This subroutine makes use of a function subprogram IGCD (IX, IY) - which finds the greatest common divisor (g.c.d.) of IX and IY - to check for the nine relative prime conditions to be satisfied by the nine parameters (54). The arguments of the 6-j coefficient are

ordered using the subroutine ORDER3.

- Function IGCD (IX, IY) makes use of Euclid's algorithm (cf. Knuth (1973) p. ) to find the g.c.d. of IX and IY.
- Subroutine CANON6 (M0, M1, M2, M3, K1, K2, K3, N1, N2, N3, IP1, IP2, IP3, MM) has M0, M1, M2, M3, K1, K2, and K3 as its input variables which correspond to $J_0, J_1, J_2, J_3, K_1, K_2$, and $K_3$ given by (1) and computes $n_1$, $n_2$, $n_3$, $p_1$, $p_2$, $p_3$ and $J_m$ (named as N1, N2, N3, IP1, IP2, IP3 and MM respectively) given by (2) and (3).
- Subroutine ORDER3 (A, B, E, D, C, F, CJ1, CJ2, CL1, CL2, CL3) has the arguments of the 6-j coefficient as its input parameters and the output variables are ordered as in Rotenberg et.al.(1959) with the help of the 24 classial symmetries of the 6-j coefficient.

The output of ZERO2 stored in the file ZERO2.OUT serves as the input to the program ZERO3, which sieves out the *equivalent* 6-j coefficients generated in the program ZERO2 and retains only the *inequivalent* ones. The *inequivalent* ones are separated by making use of the fact that the parameters $n_1$, $n_2$, $n_3$, $p_1$, $p_2$, $p_3$ and $J_m$ are the same for *equivalent* ones.

```
*************************************************************************
C        PROGRAM ZERO2
         IMPLICIT REAL*8(A-H,O-Z)
         READ(*,10) N
 10      FORMAT(I3)
         CALL SIXJ(N)
C        CALL SIXB(N)
C        CALL SIXF(N)
C        CALL SIXP(N)
         STOP
         END
```

```
      SUBROUTINE SIXJ(J)
      IMPLICIT REAL*8(A-H,O-Z)
      LOGICAL LL1,LL2,LL3
      WRITE(*,95) J
 95   FORMAT(I3)
      NC=0
      M=1
      DO 60 M1= 1,J
      AN=M1
      AN=AN/2.0D0
      DO 50 M2=1,M1
      BN=M2
      BN=BN/2.0D0
      EMIN=DABS(AN-BN)
      EMAX=AN+BN
      EN=EMIN
 9    IF(BN.LT.EN) GO TO 50
 10   DO 40 M3=0,M1
      DN=M3
      DN=DN/2.0D0
      CMIN=DABS(EN-DN)
      CMAX=EN+DN
      CN=CMIN
 15   FMIN1=DABS(AN-CN)
      FMAX1=AN+CN
      FMIN2=DABS(BN-DN)
      FMAX2=BN+DN
      FMIN=DMAX1(FMIN1,FMIN2)
      FMAX=DMIN1(FMAX1,FMAX2)
      FN=FMIN
 35   AMX=DMAX1(CN,DN,FN)
      IF(AN.LT.AMX) GO TO 55
      X1=TRIA(AN,BN,EN)
      X2=TRIA(CN,DN,EN)
      X3=TRIA(AN,CN,FN)
      X4=TRIA(BN,DN,FN)
      IF(X1.EQ.0..OR.X2.EQ.0..OR.X3.EQ.0..OR.X4.EQ.0.)GO TO 55
C     GO TO 75
      L1=AN+BN+EN
      L2=CN+DN+EN
      L3=AN+CN+FN
      L4=BN+DN+FN
      LO=MAX0(L1,L2,L3,L4)
      LE1=AN+BN+CN+DN
```

```
      LE2=AN+DN+EN+FN
      LE3=BN+CN+EN+FN
      MO=MIN0(LE1,LE2,LE3)
      N=MO-LO
      CALL CANON6(L1,L2,L3,L4,LE1,LE2,LE3,N1,N2,N3,IP1,IP2,IP3,JM)
      IF(N.NE.1) GO TO 75
      IU=LE1-MO+N
      IV=LE2-MO+N
      IW=LE3-MO+N
      IX=IU*IV*IW
      IP=MO-L1
      IQ=MO-L2
      IR=MO-L3
      IS=MO-L4
      IY=IP*IQ*IR*IS/(MO+1)**N
102   CONTINUE
      XIY=IY
      AIN=IP*IQ*IR*IS
      AMO=MO
      AID=(AMO+1.0D0)**N
      AIY=AIN/AID
75    CH1=DMAX1(CN,FN)
      CH2=DMAX1(CN,DN)
      IF((AN.EQ.BN).AND.((CN.GT.DN).OR.(CH2.GT.BN))) GO TO 55
      IF((BN.EQ.EN).AND.((FN.GT.CN).OR.(CH1.GT.BN))) GO TO 55
      IF(((AN.GT.BN).AND.(BN.GT.EN)).AND.(CH1.GT.BN))GO TO 55
C     WRITE(*,444) AN,BN,EN,DN,CN,FN,M
C444  FORMAT(6(2X,F4.1),I10)
C     GO TO 54
      IF(N.NE.1) GO TO 54
      LL1=IX.EQ.IY
      LL2=AIY.EQ.XIY
      LL3=N.EQ.1
      IF(LL1.AND.LL2.AND.LL3) NC=NC+1
      IF(LL1.AND.LL2.AND.LL3) WRITE(*,65)AN,BN,EN,DN,CN,FN,N1,N2,
     1 N3,IP1,IP2,IP3,JM,NC
65    FORMAT(6(1X,F5.1),6(1X,I2),1X,I3,I5)
54    M=M+1
55    FN=FN+1.0D0
      IF(FN.LE.FMAX) GO TO 35
      CN=CN+1.0D0
      IF(CN.LE.CMAX) GO TO 15
40    CONTINUE
      EN=EN+1.0D0
      IF(EN.LE.EMAX) GO TO 9
50    CONTINUE
60    CONTINUE
      RETURN
      END
C     FUNCTION TRIA AND SUBROUTINE ORDER2 ARE GIVEN IN
C     APPENDIX A AND THEY ARE NOT REPEATED HERE
```

```
      SUBROUTINE SIXF(N)
      IMPLICIT REAL*8(A-H,O-Z)
      I11=1
      WRITE(*,75) N
 75   FORMAT(I5)
      DO 10 IA=1,N
      AA=IA
      DO 20 ID=1,N
      DD=ID
      DO 30 IH=1,N
      HH=IH
      DO 40 II=1,N
      AI=II
      DN=HH*AI-AA*DD
      IF((DN.LT.0.0).OR.(DN.EQ.0.0)) GO TO 40
      ANR=AA+DD+HH+AI
      NR=ANR
      NDR=DN
      Z=ANR*HH*AI/DN
      U=ANR*AA*DD/DN
      IZ=IDINT(Z)
      IU=IDINT(U)
      Z1=(IZ/2.0D0)*2.0D0
      U1=(IU/2.0D0)*2.0D0
      IF(Z1.NE.Z) GO TO 40
      X=AA
      Y=DD
      V=HH
      W=AI
      A=(X+U+V-1.0D0)/2.0D0
      B=(Y+U+W-1.0D0)/2.0D0
      E=(Z-U-2.0D0)/2.0D0
      D=(X+W)/2.0D0
      C=(Y+V)/2.0D0
      F=(X+Y+U-1.0D0)/2.0D0
      AMX=DMAX1(A,B,E,D,C,F)
      IF(AMX.GT.18.5D0) GO TO 40
      J0=A+B+E
      J1=C+D+E
      J2=A+C+F
      J3=B+D+F
      K1=A+B+C+D
      K2=A+D+E+F
      K3=B+C+E+F
      CALL CANON6(J0,J1,J2,J3,K1,K2,K3,N1,N2,N3,IP1,IP2,IP3,JM)
      CALL ORDER3(A,B,E,D,C,F,AJ1,AJ2,AJ3,AL1,AL2,AL3)
      WRITE(*,35)AJ1,AJ2,AJ3,AL1,AL2,AL3,N1,N2,N3,IP1,IP2,IP3,JM,I11
 35   FORMAT(6(1X,F5.1),6(1X,I2),1X,I3,I5)
C     WRITE(*,80) IA,ID,IH,II,NR,NDR
 80   FORMAT(5(1X,I2),1X,I3)
      I11=I11+1
```

```
40      CONTINUE
30      CONTINUE
20      CONTINUE
10      CONTINUE
        I1=I11-1
        RETURN
        END
       SUBROUTINE CANON6(M0,M1,M2,M3,K1,K2,K3,N1,N2,N3,IP1,IP2,IP3,MM)
        IMPLICIT REAL*8(A-H,O-Z)
        CALL ORDER2(K1,K2,K3,KA,KB,KC)
        MM=MAX0(M0,M1,M2,M3)
        IF(MM.EQ.M0) GO TO 66
        IF(MM.EQ.M1) GO TO 67
        IF(MM.EQ.M2) GO TO 68
        IF(MM.EQ.M3) GO TO 69
66      CALL ORDER2(M1,M2,M3,MA,MB,MC)
        GO TO 70
67      CALL ORDER2(M0,M2,M3,MA,MB,MC)
        GO TO 70
68      CALL ORDER2(M0,M1,M3,MA,MB,MC)
        GO TO 70
69      CALL ORDER2(M0,M1,M2,MA,MB,MC)
70      N1=MM-MC
        N2=MM-MB
        N3=MM-MA
        IP1=KA-MM
        IP2=KB-MM
        IP3=KC-MM
        RETURN
        END
C ---------------------------------------------------------------------
        SUBROUTINE ORDER3(A,B,E,D,C,F,CJ1,CJ2,CJ3,CL1,CL2,CL3)
        IMPLICIT REAL*8(A-H,O-Z)
        LOGICAL L1,L2
        AMX=DMAX1(A,B,E,D,C,F)
        IF(A.EQ.AMX) GO TO 13
        IF(B.EQ.AMX) GO TO 14
        IF(E.EQ.AMX) GO TO 15
        IF(D.EQ.AMX) GO TO 16
        IF(C.EQ.AMX) GO TO 17
        IF(F.EQ.AMX) GO TO 18
13      CJ1=A
        CL1=D
        GO TO 19
14      CJ1=B
        CL1=C
        B=A
        C=D
        GO TO 19
15      CJ1=E
        CL1=F
        E=A
```

```
      F=D
      GO TO 19
16    CJ1=D
      CL1=A
      G=B
      B=C
      C=G
      GO TO 19
17    CJ1=C
      CL1=B
      B=D
      C=A
      GO TO 19
18    CJ1=F
      CL1=E
      E=D
      F=A
19    BMX=DMAX1(B,C,E,F)
      IF(B.EQ.BMX) GO TO 21
      IF(C.EQ.BMX) GO TO 22
      IF(E.EQ.BMX) GO TO 23
      IF(F.EQ.BMX) GO TO 24
21    CJ2=B
      CL2=C
      CJ3=E
      CL3=F
      GO TO 25
22    CJ2=C
      CL2=B
      CJ3=F
      CL3=E
      GO TO 25
23    CJ2=E
      CL2=F
      CJ3=B
      CL3=C
      GO TO 25
24    CJ2=F
      CL2=E
      CJ3=C
      CL3=B
25    L1=((CJ2.EQ.CJ3).AND.(CL2.GE.CL3))
      L2=(CJ2.NE.CJ3)
      IF((CJ1.NE.CJ2).AND.(CJ2.NE.CJ3)) GO TO 26
      IF((CJ1.EQ.CJ2).AND.(CL1.LT.CL2)) GO TO 27
28    IF(L1.OR.L2) GO TO 26
      H=CL3
      CL3=CL2
      CL2=H
      GO TO 26
27    U=CL1
```

```
      CL1=CL2
      CL2=U
      GO TO 28
 26   RETURN
      END
C ---------------------------------------------------------------------
      SUBROUTINE SIXP(N)
      IMPLICIT REAL*8(A-H,O-Z)
      I11=1
      WRITE(*,75) N
 75   FORMAT(I5)
      DO 200 JB=1,N
      DO 190 JC=1,N
      DO 180 JD=1,N
      IF(IGCD(JB,JD).NE.1) GO TO 180
      IF(IGCD(JC,JD).NE.1) GO TO 180
        DO 170 JF=1,N
        IF(IGCD(JB,JF).NE.1) GO TO 170
        DO 160 JG=1,N
        IF(IGCD(JB,JG).NE.1) GO TO 160
        IF(IGCD(JC,JG).NE.1) GO TO 160
        IF(IGCD(JF,JG).NE.1) GO TO 160
        DO 150 JH=1,N
        IF(JC*JF.LE.JG*JH) GO TO 170
        IF(IGCD(JC,JH).NE.1) GO TO 150
        IF(IGCD(JD,JH).NE.1) GO TO 150
        IF(IGCD(JF,JH).NE.1) GO TO 150
        IA=JB*JC+JD*JG
        IB=JD*JF+JB*JH
        IS=IGCD(IA,IB)
        DO 140 JI=1,N
        IG=JI*(JC*JF-JG*JH)
        IX=IA+IB
        IF(IG.LT.IX) GO TO 140
        IF(IS*(IG/IS).NE.IG) GO TO 140
        IAP=IA/IS
        IBP=IB/IS
        IGP=IG/IS
        IEP=0
 130    IY=(IGP-IAP*IEP)
        IF(IBP*(IY/IBP).EQ.IY) GO TO 135
        IEP=IEP+1
        GO TO 130
 135    M=0
 250    JA=IEP+IBP*M
        IF(JA.LE.0) GO TO 137
        JE=IY/IBP-IAP*M
        IF(JE.LE.0) GO TO 140
C       WRITE(*,138) JA,JB,JC,JD,JE,JF,JG,JH,JI
C138    FORMAT(9I4)
        X1=JA*JB*JC
        X2=JD*JE*JF
```

```
      X3=JG*JH*JI
      U1=JA*JD*JG
      U2=JB*JE*JH
      U3=JC*JF*JI
      AX1=X1+X2+U1+U2
      A=0.5D0*(AX1- U2-1.0D0)
      B=0.5D0*(X1+U2+X3*AX1/IG-1.0D0)
      E=0.5D0*(U3*AX1/IG-X1-2.0D0)
      D=0.5D0*(U1+X3*AX1/IG)
      C=0.5D0*(X2+U2)
      F=0.5D0*(AX1-X2-1.0D0)
      AMX=DMAX1(A,B,E,D,C,F)
      IF(AMX.GT.18.5D0) GO TO 137
      J0=A+B+E
      J1=C+D+E
      J2=A+C+F
      J3=B+D+F
      K1=A+B+C+D
      K2=A+D+E+F
      K3=B+C+E+F
      CALL CANON6(J0,J1,J2,J3,K1,K2,K3,N1,N2,N3,IP1,IP2,IP3,JM)
      CALL ORDER3(A,B,E,D,C,F,AJ1,AJ2,AJ3,AL1,AL2,AL3)
      WRITE(*,35)AJ1,AJ2,AJ3,AL1,AL2,AL3,N1,N2,N3,IP1,IP2,
     1      IP3,JM,I11
 35   FORMAT(6(1X,F5.1),6(1X,I2),1X,I3,I5)
      I11=I11+1
 137  M=M+1
      GO TO 250
 140  CONTINUE
 150  CONTINUE
 160  CONTINUE
 170  CONTINUE
 180  CONTINUE
 190  CONTINUE
 200  CONTINUE
      I1=I11-1
      RETURN
      END
C ---------------------------------------------------------------------
      FUNCTION IGCD(IX,IY)
      IMPLICIT REAL*8(A-H,O-Z)
      IGCD=IX
      IF(IX.EQ.IY) RETURN
      IF(IX.GT.IY)  GO TO 10
      M=IY
      N=IX
      GO TO 20
 10   M=IX
      N=IY
 20   NQ=M/N
      IR=M-NQ*N
      IF(IR.EQ.0) GO TO 30
```

```
      M=N
      N=IR
      GO TO 20
30    IGCD=N
      RETURN
      END
C ---------------------------------------------------------------------
      SUBROUTINE SIXB(J)
      IMPLICIT REAL*8(A-H,O-Z)
      I11=1
      WRITE(*,75) J
75    FORMAT(I5)
      DO 20 IX=1,J
      AIX=IX
      DO 30 IA=1,J
      IP=IA
      DO 40 IB=1,J
      IQ=IB
      DO 7 IY=1,J
      AIY=IY
      DO 8 IZ=1,J
      AIZ=IZ
      DO 9 IU=1,J
      AIU=IU
      DO 11 IV=1,J
      AIV=IV
      ID=IP*IQ*IX+IP*IY*IU+IQ*IZ*IV
      ISB=IY*IZ
      ISC=IU*IV
      MABC=MAX0(ISB,ISC)
      MIBC=MIN0(ISB,ISC)
      AMABC=MABC
      AMIBC=MIBC
      N=IX*ID+ISB*ISC
      DO 50 IE=1,N
      AN=N
      AE=IE
      Q1=N/IE
      Q2=AN/AE
      IF(Q1.NE.Q2) GO TO 50
      IF(Q1.LT.AE) GO TO 11
      AMAQE=DMAX1(Q1,AE)
      AMIQE=DMIN1(Q1,AE)
      MAQE=AMAQE
      MIQE=AMIQE
      IF(MABC.EQ.ISC) GO TO 33
      AS1=(MAQE+MIBC)/IX
      S1 =(AMAQE+AMIBC)/AIX
      AT1=(MIQE+MABC)/IX
      T1 =(AMIQE+AMABC)/AIX
      AS2=(MIQE+MIBC)/IX
      S2 =(AMIQE+AMIBC)/AIX
```

```
      AT2=(MAQE+MABC)/IX
      T2 =(AMAQE+AMABC)/AIX
      GO TO 34
33    AS1=(MIQE+MABC)/IX
      S1 =(AMIQE+AMABC)/AIX
      AT1=(MAQE+MIBC)/IX
      T1 =(AMAQE+AMIBC)/AIX
      AS2=(MAQE+MABC)/IX
      S2 =(AMAQE+AMABC)/AIX
      AT2=(MIQE+MIBC)/IX
      T2 =(AMIQE+AMIBC)/AIX
34    IF((AS1.EQ.S1).AND.(AT1.EQ.T1)) GO TO 32
31    IF((AS2.NE.S2).OR.(AT2.NE.T2))  GO TO 50
      S=S2
      T=T2
      GO TO 10
32    S=S1
      T=T1
10    P=IP
      Q=IQ
      A=(P*Q*AIX+S*AIY*AIZ+Q*AIZ*AIV-1.D0)/2.D0
      B=(P*Q*AIX+P*AIY*AIU+T*AIU*AIV-1.D0)/2.D0
      E=(S*AIY*AIZ+T*AIU*AIV+P*AIY*AIU+Q*AIZ*AIV)/2.D0-1.D0
      D=(T*AIU*AIV+Q*AIZ*AIV)/2.D0
      C=(S*AIY*AIZ+P*AIY*AIU)/2.D0
      F=(P*Q*AIX+P*AIY*AIU+Q*AIZ*AIV-1.D0)/2.D0
      AMX=DMAX1(A,B,E,D,C,F)
      IF(AMX.GT.18.5D0) GO TO 50
      J0=A+B+E
      J1=C+D+E
      J2=A+C+F
      J3=B+D+F
      K1=A+B+C+D
      K2=A+D+E+F
      K3=B+C+E+F
      CALL CANON6(J0,J1,J2,J3,K1,K2,K3,N1,N2,N3,IP1,IP2,IP3,JM)
      CALL ORDER3(A,B,E,D,C,F,AJ1,AJ2,AJ3,AL1,AL2,AL3)
      WRITE(*,35)AJ1,AJ2,AJ3,AL1,AL2,AL3,N1,N2,N3,IP1,IP2,
     1 IP3,JM,I11
35    FORMAT(6(1X,F5.1),6(1X,I2),1X,I3,I5)
      I11=I11+1
      IF(S1.EQ.S2) GO TO 11
      IF(S.EQ.S1)  GO TO 31
50    CONTINUE
11    CONTINUE
9     CONTINUE
8     CONTINUE
7     CONTINUE
40    CONTINUE
30    CONTINUE
20    CONTINUE
```

```
      I1=I11-1
      RETURN
      END
C ------------------------------------------------------------------

C     PROGRAM ZERO3
C     PROGRAM TO OBTAIN THE 'INEQUIVALENT' 6J COEFFICIENTS FROM
C     A GIVEN LIST THAT INCLUDES  THE SYMMETRIES
      IMPLICIT REAL*8(A-H,O-Z)
      LOGICAL LX,LY,LZ
      DIMENSION JN1(1000),JN2(1000),JN3(1000)
      DIMENSION JP1(1000),JP2(1000),JP3(1000)
      OPEN(3,FILE='ZERO2.OUT')
      READ(*,50) JMIN,JMAX,I1
 50   FORMAT(2(I3),I6)
      WRITE(*,75) JMIN,JMAX,I1
 75   FORMAT(2(2X,I3),2X,I6)
      I11=1
      DO 10 J=JMIN,JMAX
      I=1
      REWIND 3
      READ(3,55) N
 55   FORMAT(I3)
 15   READ(3,2) A,B,E,D,C,F,N1,N2,N3,IP1,IP2,IP3,JM,MC
 2    FORMAT(6(1X,F5.1),6(1X,I2),1X,I3,I5)
      IF(J.NE.JM) GO TO 20
      JN1(I)=N1
      JN2(I)=N2
      JN3(I)=N3
      JP1(I)=IP1
      JP2(I)=IP2
      JP3(I)=IP3
      IF(I.EQ.1) GO TO 25
      M1=I-1
      DO 30 K=1,M1
      LX=(JN1(I).EQ.JN1(K).AND.JN2(I).EQ.JN2(K))
      LY=((JN3(I).EQ.JN3(K)).AND.(JP1(I).EQ.JP1(K)))
      LZ=((JP2(I).EQ.JP2(K)).AND.(JP3(I).EQ.JP3(K)))
      IF((LX.AND.LY).AND.LZ) GO TO 40
 30   CONTINUE
 25   WRITE(*,35) A,B,E,D,C,F,N1,N2,N3,IP1,IP2,IP3,JM,I11,MC
 35   FORMAT(6(2X,F4.1),7(2X,I3),I4,I6)
      I11=I11+1
 40   I=I+1
 20   IF(MC-I1)  15,10,10
 10   CONTINUE
      I2=I11-1
      WRITE(*,70) N,I2
 70   FORMAT(,/,' N=',I3,10X,' NO OF INEQUIVALENT ZEROS=',I5)
 200  STOP
      END
```

## Appendix C

This is an Appendix to Chapter 5 which gives a listing of the numerical code to compute the 9-j coefficient. The description of the main programs and various subroutines is given in detail in Chapter 5. While the complete listing of the program is given in the case of PROGSELECT, the main program alone is given for PROGTEST, since the other subroutines are common for both. Also, the subroutines that are already listed in Appendix A or B are not listed here.

```
*********************************************************************
        PROGRAM  PROGSELECT
C *******************************************************************
C MAIN PROGRAM TO COMPUTE RNINE(A,B,C,D,E,F,G,H,RI) AND
C WNINE(A,B,C,D,E,F,G,H,RI).THESE FUNCTION SUBPROGRAMS COMPUTE
C THE 9-J ANGULAR MOMENTUM COEFFICIENT. THE PROGRAM RNINE USES
C THE TRIPLE SUM FORMULA OF JUCYS AND BANDZAITIS IN ITS FOLD
C FORM,WHILE THE PROGRAM WNINE USES THE CONVENTIONAL SINGLE
C SUM OVER A PRODUCT OF THREE 6-J COEFFICIENTS, WHERE THE 6-J
C COEFFICIENT IS COMPUTED AS SET OF THREE HYPERGEOMETRIC
C FUNCTIONS OF UNIT ARGUMENT.
C THIS PROGRAM SELECTS EITHER WNINE OR RNINE DEPENDING UPON THE
C AD HOC PRESCRIPTION NT1.GT.2*NT3 OR WHEN THE NUMBER OF TERMS
C IN RNINE (NT1) EXCEEDS 200 (FOR IBM-PC/AT) OR 600 (FOR
C VAX-11/780).
C *******************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON FCT(500)
      COMMON/XX/A2,B2,C2,D2,E2,F2,G2,H2,RI2,JSIG2
      DIMENSION R9(3,3)
C     LOGARITHMS OF FACTORIALS SET UP IN A COMMON BLOCK
      FCT(1)=0.
      FCT(2)=0.
      DO 10 N=3,500
      AN=N-1
 10   FCT(N)=DLOG(AN)+FCT(N-1)
      WRITE(6,30)
 30   FORMAT(' INPUT DATA FOR A,B,...,RI, IN 9F4.1 FORMAT',//)
 40   READ(5,50) A,B,C,D,E.F,G,H,RI
 50   FORMAT(9F4.1)
      IF(A.LT.0) GO TO 190
      ISIG = A+B+C+D+E+F+G+H+RI
C CHECKING FOR ANY ONE OF THE ANGULAR MOMENTA BEING ZERO
      CALL SET(A,B,C,D,E,F,G,H,RI,R9)
```

```
      DO 70 I=1,3
      DO 70 J=1,3
      IF(R9(I,J).EQ.0.0) GO TO 80
 70   CONTINUE
      GO TO 90
 80   IK=I
      JK=J
C RNINEJ GIVES THE VALUE OF THE 9J-COEFFICIENT WHEN ONE OF
C ITS ARGUMENTS IS ZERO
      RNINEJ=VALUE(A,B,C,D,E,F,G,H,RI,IK,JK)
      GO TO 160
 90   CALL CHANGE(A,B,C,D,E,F,G,H,RI)
      CALL TERM(A2,B2,C2,D2,E2,F2,G2,H2,RI2,NT1,NT2)
      NT3=3*NT2
C     THE FOLLOWING IS A PRESCRIPTION FOR CHOOSING WNINE.
C $$  NOTE : FOR THE IBM-PC/AT MAKE THE NEXT STATEMENT C...
      IF(NT1.GT.2*NT3.OR.NT1.GT.600) GO TO 120
C $$  NOTE : FOR THE IBM-PC/AT REMOVE FROM THE NEXT STATEMENT C
C     IF(NT1.GT.2*NT3.OR.NT1.GT.200) GO TO 120
 100  RES1=RNINE(A2,B2,C2,D2,E2,F2,G2,H2,RI2)
      IF((ISIG/2)*2.NE.ISIG.AND.(JSIG2/2)*2.NE.JSIG2)
     1RES1 = PHASE(ISIG)*RES1
      WRITE(6,110) A,B,C,D,E,F,G,H,RI,RES1
 110  FORMAT(' RNINE(',8(F4.1,','),F4.1,')=',E13.6)
      GO TO 180
 120  RES2=WNINE(A2,B2,C2,D2,E2,F2,G2,H2,RI2)
      IF((ISIG/2)*2.NE.ISIG.AND.(JSIG2/2)*2.NE.JSIG2)
     1RES2 = PHASE(ISIG)*RES2
      WRITE(6,150) A,B,C,D,E,F,G,H,RI,RES2
 150  FORMAT(' WNINE(',8(F4.1,','),F4.1,')=',E13.6,/)
      GO TO 180
 160  WRITE(6,170) A,B,C,D,E,F,G,H,RI,RNINEJ
 170  FORMAT(' NINEJ(',8(F4.1,','),F4.1,')=',E13.6)
 180  GO TO 40
 190  STOP
      END
C -----------------------------------------------------------------------
      FUNCTION RNINE(A,B,C,D,E,F,G,H,RI)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION CS(30,30,30),BS(30),AS(30),AX(50),BY(50),CZ(50)
      COMMON FCT(500)
      COMMON/AA/X4,X5,IX4,IX5,Y4,Y5,IY4,IY5,Z4,Z5,IZ4,IZ5
      COMMON/AB/P1,P2,P3,IP1,IP2,IP3
      COMMON/AC/IXF,IYF,IZF,IXI,IYI,IZI
      RNINE=0.
C     THE FACTORS D1 TO D6 CHECK FOR THE TRIANGULAR INEQUALITIES
C     TO BE SATISFIED BY THE 9-J COEFFICIENT.
      IF(A.NE.D.OR.B.NE.E.OR.C.NE.F) GO TO 10
      ICHK=G+H+RI
      IF((ICHK/2)*2.NE.ICHK) RETURN
C     THE FACTORS D1 TO D6 CHECK FOR THE TRIANGULAR INEQUALITIES
C     TO BE SATISFIED BY THE 9-J COEFFICIENT.
 10   D1=TRIA(D,A,G)
      D2=TRIA(B,E,H)
      D3=TRIA(RI,G,H)
      D4=TRIA(D,E,F)
```

```
      D5=TRIA(B,A,C)
      D6=TRIA(RI,C,F)
      IF(D1.EQ.0..OR.D2.EQ.0..OR.D3.EQ.0..OR.D4.EQ.0..OR.D5.EQ.0..
     1  OR.D6.EQ.0.) RETURN
C     FACTORS X1 TO X3 (IX1 TO IX3) OCCUR IN X SUMMATION PART
      X1=2.0D0*F
      X2=D+E-F
      X3=C+RI-F
      X6=A+B-C
      X7=A+B+C+1.D0
      X8=-C+F+RI
      X9=C+F+RI+1.D0
      IX1=X1
      IX2=X2
      IX3=X3
      IX6=X6
      IX7=X7
      IX8=X8
      IX9=X9
C     FACTORS Y1 TO Y3 (IY1 TO IY3) OCCUR IN Y SUMMATION PART
      Y1=E+H-B
      Y2=G+H-RI
      Y3=2.0D0*H+1.0D0
      Y6=-G+H+RI
      Y7=G+H+RI+1.D0
      Y8=-E+F+D
      Y9=E+F+D+1.D0
      IY1=Y1
      IY2=Y2
      IY3=Y3
      IY6=Y6
      IY7=Y7
      IY8=Y8
      IY9=Y9
C     FACTORS Z1 TO Z3 (IZ1 TO IZ3) OCCUR IN Z SUMMATION PART
      Z1=2.0D0*A
      Z2=B+C-A
      Z3=A+D+G+1.0D0
      Z6=A-D+G
      Z7=-A+D+G
      Z8=B-E+H
      Z9=B+E+H+1.D0
      IZ1=Z1
      IZ2=Z2
      IZ3=Z3
      IZ6=Z6
      IZ7=Z7
      IZ8=Z8
      IZ9=Z9
C     CHECKING FOR THE DENOMINATOR ZERO NOT OCCURING BEFORE
C     THE NUMERATOR ZERO
 20   NN=DMIN1(X4,X5,Y4,Y5,Z4,Z5)
      ND=DMIN1(X1,Z1)
      IF(NN.GT.ND) RETURN
C     C1,C2,C3,C4,C5,C6,C7,C8 ARE CONSTANT TERMS
      C2=FCT(IX2+1)+FCT(IX3+1)-FCT(IX4+1)-FCT(IX5+1)
```

```
      C3=FCT(IY1+1)+FCT(IY2+1)-FCT(IY4+1)-FCT(IY5+1)
      C4=FCT(IZ2+1)-FCT(IZ3+1)-FCT(IZ4+1)-FCT(IZ5+1)
      C5=FCT(IX6+1)+FCT(IX7+1)+FCT(IX8+1)+FCT(IX9+1)
      C6=FCT(IY6+1)+FCT(IY7+1)-FCT(IY8+1)-FCT(IY9+1)
      C7=-FCT(IZ6+1)+FCT(IZ7+1)+FCT(IZ8+1)+FCT(IZ9+1)
      C8=FCT(IX1+1)-FCT(IY3+1)+FCT(IZ1+1)
      C1=0.5D0*(C2+C3+C4-C5+C6+C7)+C8
C     CONST IS THE OVERALL MULTIPLICATIVE CONSTANT PHASE FACTOR
      CONST=PHASE(IX5)
C     INITIALISATION OF THE ARRAYS AS,BS,CS,AX,BY,CZ
      DO 60  IX =IXI+1,IXF+1
      AS(IX)=1.D0
      AX(IX)=0.
      DO 50  IY=IYI+1,IYF+1
      BS(IY)=1.D0
      BY(IY)=0.
      DO 40  IZ=IZI+1,IZF+1
      CS(IX,IY,IZ)=0.
      CZ(IZ)=0.
 40   CONTINUE
 50   CONTINUE
 60   CONTINUE
      T1=1.0D0
      N1=1
      DO 170 IX=IXI+1,IXF+1
C     EVALUATION OF THE X-DEPENDENT FACTOR AS(IX)
      X=IX-1
      JX=X
      IF((JX.EQ.0).AND.(N1.EQ.1)) GO TO 80
      IF(N1.EQ.1)  THEN
              XT1=FCT(IX2+JX+1)+FCT(IX3+JX+1)+FCT(IX4+1)+FCT(IX5+1)
              XT1=XT1+FCT(IX1-JX+1)
              DXT=FCT(IX2+1)+FCT(IX3+1)+FCT(IX4-JX+1)+FCT(IX5-JX+1)
              DXT=DXT+FCT(IX1+1)+FCT(JX+1)
              T1=DEXP(XT1-DXT)
      ELSE
C             WRITE(6,66) IXI,IXF,IX,N1,X1,X2,X3,X4,X5,TM1,T1
C 66          FORMAT(//,4I5,/,7E11.4)
              TM1=(X4-X+1.0D0)*(X5-X+1.0D0)/(X1-X+1.0D0)
              T1=T1*(X2+X)*(X3+X)*TM1/X
      ENDIF
 80   AS(IX)=T1
      T2=1.D0
      N2=1
      DO 160 IY=IYI+1,IYF+1
C     EVALUATION OF THE Y-DEPENDENT FACTOR BS(IY)
      Y=IY-1
      JY=Y
      IF((JY.EQ.0).AND.(N2.EQ.1)) GO TO 100
      IF(N2.EQ.1)  THEN
              YT=FCT(IY4+1)+FCT(IY5+1)+FCT(IY1+JY+1)+FCT(IY2+JY+1)
              YT=YT+FCT(IY3+1)
              DYT=FCT(IY4-JY+1)+FCT(IY5-JY+1)+FCT(IY1+1)+FCT(IY2+1)
              DYT=DYT+FCT(IY3+JY+1)+FCT(JY+1)
              T2=DEXP(YT-DYT)
```

```
      ELSE
                  TM2=(Y4-Y+1.0D0)*(Y5-Y+1.0D0)
                  T2=T2*(Y1+Y)*(Y2+Y)*TM2/(Y*(Y3+Y))
      ENDIF
  100 BS(IY)=T2
      P2XY=P2+X+Y
      IF(P2XY.LT.0.) GO TO 150
      IP2XY=P2XY
      T3=1.D0
      N3=1
      DO 140 IZ=IZI+1,IZF+1
C     EVALUATION OF THE Z-DEPENDENT FACTOR T3
      Z=IZ-1
      JZ=Z
      IF((JZ.EQ.0).AND.(N3.EQ.1)) GO TO 110
      IF(N3.EQ.1)   THEN
                  ZT=FCT(IZ3+1)+FCT(IZ4+1)+FCT(IZ5+1)+FCT(IZ1-JZ+1)
                  ZT=ZT+FCT(IZ2+JZ+1)
                  DZT=FCT(IZ3-JZ+1)+FCT(IZ4-JZ+1)+FCT(IZ5-JZ+1)
                  DZT=DZT+FCT(IZ1+1)+FCT(IZ2+1)+FCT(JZ+1)
                  T3=DEXP(ZT-DZT)
      ELSE
                  TM3=(Z3-Z+1.0D0)*(Z4-Z+1.0D0)*(Z5-Z+1.0D0)/(Z1-Z+1.0D0)
                  T3=T3*(Z2+Z)*TM3/Z
      ENDIF
C     EVALUATION OF BILINEAR COUPLED FACTORS IN X,Y,Z
C     AND CS(IX,IY,IZ) ARRAY
  110 P1YZ=P1-Y-Z
      IP1YZ=P1YZ
      P3ZX=P3+Z+X
      IF(P3ZX.LT.0.) GO TO 130
      IP3ZX=P3ZX
      CC5=FCT(IP1YZ+1)-FCT(IP2XY+1)-FCT(IP3ZX+1) + C1
      IF(T3.EQ.0.) GO TO 130
      TT3 = DLOG(T3)
      CS(IX,IY,IZ)=PHASE(JX+JY+JZ)*DEXP(CC5+TT3)
  130 N3=N3+1
  140 CONTINUE
  150 N2=N2+1
  160 CONTINUE
      N1=N1+1
  170 CONTINUE
C     IMPLEMENTATION OF HORNER'S RULE FOR THE TRIPLE SUM SERIES.
      DO 210 IX=IXI+1,IXF+1
      DO 200 IY=IYI+1,IYF+1
      DO 190 IZ=IZI+1,IZF+1
      CZ(IZ)=CS(IX,IY,IZ)
  190 CONTINUE
C     SUMMATION OVER Z OF CS(X,Y,Z) USING HORNER
      BY(IY)=HORNER(IZI+1,IZF+1,CZ)*BS(IY)
  200 CONTINUE
C     SUMMATION OVER Y OF BY(Y) USING HORNER
      AX(IX)=HORNER(IYI+1,IYF+1,BY)*AS(IX)
  210 CONTINUE
```

```
C     SUMMATION OVER X OF AX(X) USING HORNER
      RNINE=CONST*HORNER(IXI+1,IXF+1,AX)
      RETURN
      END
C ----------------------------------------------------------------------
      FUNCTION HORNER(KI,KF,A)
      IMPLICIT REAL*8(A-H,O-Z)
C     FUNCTION HORNER COMPUTES THE FOLDED SUM OF THE NON-ZERO TERMS
C              OF THE GIVEN ARRAY.
      DIMENSION A(50)
      C=1.0D0
      IF(KI .EQ.0.AND.KF .EQ.0) GO TO 70
      IF(KI .EQ.KF ) GO TO 60
      C = A(KF)
      DO 50 I=KF-1,KI,-1
      IF(A(I).EQ.0.) GO TO 50
      C = A(I)*(1.D0 + C/A(I))
 50   CONTINUE
      HORNER = C
      RETURN
 60   HORNER=A(KI )*C
      RETURN
 70   HORNER=0.
      RETURN
      END
C ----------------------------------------------------------------------
      FUNCTION WNINE(A,B,C,D,E,F,G,H,RI)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON FCT(500)
      COMMON/AD/AKI,AKF
      SUM=0.0
      IF(A.NE.D.OR.B.NE.E.OR.C.NE.F) GO TO 10
      ICHK=G+H+RI
      IF((ICHK/2)*2.NE.ICHK) GO TO 30
 10   AK=AKI
 20   IC0=2.0D0*AK
      CC=PHASE(IC0)*(IC0+1.0D0)
      SUM=SUM+CC*WF(A,D,RI,H,G,AK)*WF(B,E,AK,D,H,F)*WF(C,F,A,AK,RI,B)
      AK=AK+1.0D0
      IF(AK.LE.AKF) GO TO 20
 30   WNINE=   SUM
      RETURN
      END
C ----------------------------------------------------------------------
      FUNCTION WF(A,B,C,D,E,F)
      IMPLICIT REAL*8(A-H,O-Z)
C  THE EQUATION NUMBERS IN THIS FUNCTION PROGRAM REFER TO THE ONES IN
C  COMP.PHYS.COMMUN.,VOL15 (1978) 227-235.
C  THE WF FUNCTION EMPLOYS THE SET I OF THREE HYPERGEOMETRIC
C  FUNCTIONS FOR THE RACAH COEFFICIENT GIVEN BY (2.18) TO (2.22).
      COMMON FCT(500)
      WF=0.
C  THE TRIANGULAR INEQUALITIES ARE CHECKED FIRST
      CHK1=TRIA(A,B,E)
```

```
      IF(CHK1.EQ.0.0) RETURN
      CHK2=TRIA(C,D,E)
      IF(CHK2.EQ.0.0) RETURN
      CHK3=TRIA(A,C,F)
      IF(CHK3.EQ.0.0) RETURN
      CHK4=TRIA(B,D,F)
      IF(CHK4.EQ.0.0) RETURN
      IF(B.EQ.0..OR.C.EQ.0..OR.E.EQ.0.) GO TO 70
      IF(A.EQ.0..OR.D.EQ.0..OR.F.EQ.0.) GO TO 80
      D1=E+F-A-D
      D2=E+F-B-C
C  THE POSITIVE NATURE OF THE DENOMINATOR PARAMETERS(D1,D2,D3) IS
C  CHECKED TO ENABLE THE SELECTION OF THE VALID 4F3 FUNCTION.
      IF(D1.GT.0..AND.D2.GT.0.) GO TO 10
      D3=A+D-B-C
      IF(D1.LE.0..AND.D3.GE.0.) GO TO 20
      IF(D2.LE.0..AND.D3.LE.0.) GO TO 30
C  THE NUMERATOR (N2 TO N5) AND DENOMINATOR (N1,N6,N7) PARAMETERS
C  OF THE 4F3 GIVEN BY (2.20).
 10   N1=A+B+C+D+1.0D0
      N2=A+B-E
      N3=C+D-E
      N4=A+C-F
      N5=B+D-F
      N6=D1+1.0D0
      N7=D2+1.0D0
      GO TO 40
C  THE NUMERATOR AND DENOMINATOR PARAMETERS OF THE 4F3 GIVEN BY(2.21)
 20   N1=B+C+E+F+1.0D0
      N2=B+F-D
      N3=B+E-A
      N4=C+E-D
      N5=C+F-A
      N6=-D1+1.0D0
      N7=D3+1.0D0
      GO TO 40
C  THE NUMERATOR AND DENOMINATOR PARAMETERS OF 4F3 GIVEN BY (2.22)
 30   N1=A+D+E+F+1.0D0
      N2=A+E-B
      N3=D+F-B
      N4=A+F-C
      N5=E+D-C
      N6=-D2+1.0D0
      N7=-D3+1.0D0
 40   F43=1.0D0
      I1=A+B+E
      I2=C+D+E
      I3=A+C+F
      I4=B+D+F
      I1X=-A+B+E
      I1Y=A-B+E
      I1Z=A+B-E
      I2X=-C+D+E
      I2Y=C-D+E
      I2Z=C+D-E
```

```
      I3X=-A+C+F
      I3Y=A-C+F
      I3Z=A+C-F
      I4X=-B+D+F
      I4Y=B-D+F
      I4Z=B+D-F
      C1=FCT(I1X+1)+FCT(I1Y+1)+FCT(I1Z+1)-FCT(I1+2)
      C2=FCT(I2X+1)+FCT(I2Y+1)+FCT(I2Z+1)-FCT(I2+2)
      C3=FCT(I3X+1)+FCT(I3Y+1)+FCT(I3Z+1)-FCT(I3+2)
      C4=FCT(I4X+1)+FCT(I4Y+1)+FCT(I4Z+1)-FCT(I4+2)
      CONST=0.5D0*(C1+C2+C3+C4)
C  IF ANY ONE OR MORE OF THE NUMERATOR PARAMETERS IS ZERO THEN THE
C  VALUE OF THE 4F3 IS SET EQUAL TO 1.0 AND THE PROGRAM SEGMENT FOR
C  COMPUTING IT IS CONVENIENTLY SKIPPED.
      IF(N2.EQ.0..OR.N3.EQ.0..OR.N4.EQ.0..OR.N5.EQ.0)GO TO 60
      N= MIN0(N2,N3,N4,N5)
      IX=N-1
 50   RN=(IX-N2)*(IX-N3)*(IX-N4)*(IX-N5)
      RND=(IX-N1)*(IX+N6)*(IX+N7)*(IX+1)
      F43=1.0D0+F43*RN/RND
      IX=IX-1
      IF(IX.GE.0) GO TO 50
 60   C5=FCT(N2+1)+FCT(N3+1)+FCT(N4+1)+FCT(N5+1)+FCT(N6)+FCT(N7)
      WF=PHASE(N1-1)*F43*DEXP(CONST+FCT(N1+1)-C5)
      RETURN
C  SPECIAL VALUES OF THE RACAH COEFFICIENT GIVEN BY (2.33).
 70   N=B+C+E+F
      WF=PHASE( N )/(AF(A)*AF(D))
      RETURN
 80   N=A+D+E+F
      WF=PHASE( N )/(AF(B)*AF(C))
      RETURN
      END
C -------------------------------------------------------------------
      SUBROUTINE TERM(A,B,C,D,E,F,G,H,RI,NT1,NT2)
      IMPLICIT REAL*8(A-H,O-Z)
C  SUBROUTINE TERM CALCULATES THE ACTUAL NUMBER OF TERMS CONTRIBUTING
C  TO THE SUM IN (3)AND THE NUMBER OF VALUES 'K' TAKES IN (1)
      COMMON/AA/X4,X5,IX4,IX5,Y4,Y5,IY4,IY5,Z4,Z5,IZ4,IZ5
      COMMON/AB/P1,P2,P3,IP1,IP2,IP3
      COMMON/AC/IXF,IYF,IZF,IXI,IYI,IZI
      COMMON/AD/AKI,AKF
C  SETTING THE LOWER LIMITS AND DETERMINING THE UPPER LIMITS OF
C  X (IXI,IXF), Y (IYI,IYF), Z (IZI,IZF) - (SUMMATION INDICES)
      IXI = 0
      IYI = 0
      IZI = 0
      CALL FXYZ(A,B,C,D,E,F,G,H,RI,IXF,IYF,IZF)
C  FACTORS P1,P2,P3 OCCUR WITH BILINEAR COMBINATIONS OF X,Y,Z
      P1=A+D+RI-H
      P2=D+H-B-F
      P3=B-F-A+RI
      IP1=P1
      IP2=P2
      IP3=P3
```

```
      IXI1=IXI
      IAP2=IABS(IP2)
      IAP3=IABS(IP3)
      IF(IP2.GE.0) GO TO 50
      IF(IAP2.LE.IXF)  THEN
                IF(IAP2.LE.IYF)  THEN
                           GO TO 50
                ELSE
                           IXI1=IAP2-IYF
                ENDIF
      ELSE
                IF(IAP2.LE.IYF)  THEN
                           IYI =IAP2-IXF
                ELSE
                           IXI1=IAP2-IYF
                           IYI=IAP2-IXF
                ENDIF
      ENDIF
50    IXI2=IXI
      IF(IP3.GE.0) GO TO 60
      IF(IAP3.LE.IXF)  THEN
              IF(IAP3.LE.IZF)   THEN
                      GO TO 60
              ELSE
                      IXI2=IAP3-IZF
              ENDIF
      ELSE
              IF(IAP3.LE.IZF)  THEN
                      IZI=IAP3-IXF
              ELSE
                      IXI2=IAP3-IZF
                      IZI=IAP3-IXF
              ENDIF
      ENDIF
60    IXI=MAX0(IXI1,IXI2)
      NT1=0
      DO 90  IXM=IXI+1,IXF+1
      IX=IXM-1
      DO 80  IYM=IYI+1,IYF+1
      IY=IYM-1
      IC1=IP2+IX+IY
      IF(IC1.LT.0) GO TO 80
      DO 70  IZM=IZI+1,IZF+1
      IZ=IZM-1
      IC2=IP3+IX+IZ
      IF(IC2.LT.0) GO TO 70
      NT1=NT1+1
70    CONTINUE
80    CONTINUE
90    CONTINUE
      AKI=DMAX1(DABS(A-RI),DABS(H-D),DABS(B-F))
      AKF=DMIN1(A+RI,H+D,B+F)
      T2=AKF-AKI+1.D0
      NT2=T2
      RETURN
```

```
      END
      FUNCTION VALUE(A,B,C,D,E,F,G,H,RI,IK,JK)
      IMPLICIT REAL*8(A-H,O-Z)
C   FUNCTION 'VALUE' EVALUATES THE 9J-COEFFICIENT WHEN ONE OF ITS
C                ARGUMENTS IS ZERO
      IF(IK.EQ.1.AND.JK.EQ.1) GO TO 10
      IF(IK.EQ.1.AND.JK.EQ.2) GO TO 20
      IF(IK.EQ.1.AND.JK.EQ.3) GO TO 30
      IF(IK.EQ.2.AND.JK.EQ.1) GO TO 40
      IF(IK.EQ.2.AND.JK.EQ.2) GO TO 50
      IF(IK.EQ.2.AND.JK.EQ.3) GO TO 60
      IF(IK.EQ.3.AND.JK.EQ.1) GO TO 70
      IF(IK.EQ.3.AND.JK.EQ.2) GO TO 80
      A1=A
      B1=B
      C1=D
      D1=E
      E1=C
      F1=G
      GO TO 90
 10   A1=RI
      B1=F
      C1=H
      D1=E
      E1=B
      F1=D
      GO TO 90
 20   A1=F
      B1=RI
      C1=D
      D1=G
      E1=A
      F1=E
      GO TO 90
 30    A1=H
       B1=G
       C1=E
       D1=D
       E1=F
       F1=A
       GO TO 90
 40     A1=H
        B1=B
        C1=RI
        D1=C
        E1=E
        F1=A
        GO TO 90
 50     A1=A
        B1=G
        C1=C
        D1=RI
        E1=D
        F1=H
        GO TO 90
```

```
60      A1=B
        B1=A
        C1=H
        D1=G
        E1=C
        F1=D
        GO TO 90
 70     A1=F
        B1=E
        C1=C
        D1=B
        E1=A
        F1=H
        GO TO 90
 80     A1=D
        B1=F
        C1=A
        D1=C
        E1=B
        F1=G
 90     N=B1+C1+E1+F1
        P1=2.0D0*E1+1.0D0
        P2=2.0D0*F1+1.0D0
        VALUE=PHASE(N)*WF(A1,B1,C1,D1,E1,F1)/DSQRT(P1*P2)
        RETURN
        END
C ------------------------------------------------------------------------
        SUBROUTINE CHANGE(A,B,C,D,E,F,G,H,RI)
        IMPLICIT REAL *8(A-H,O-Z)
        COMMON/XX/A2,B2,C2,D2,E2,F2,G2,H2,RI2,JSIG2
        COMMON/AX/A1(72),B1(72),C1(72),D1(72),E1(72),F1(72),G1(72),
     1  H1(72),RI1(72),IXYZ(72),JSIG1(72)
        DIMENSION R9(3,3),R91(3,3)
C THIS SUBROUTINE EXAMINES THE 72 SYMMETRIES OF THE 9-J COEFFICIENT
C AND SELECTS A SYMMETRY FIR WHICH XF+YF+ZF IS A MINIMUM.
        N = 1
        DO 120 I=1,3
        DO 120 J=1,3
        JS1 =0
        CALL SET(A,B,C,D,E,F,G,H,RI,R9)
        IF(I.EQ.J.AND.I.GT.1) GO TO 120
        IF(I.EQ.3.AND.J.EQ.1) GO TO 120
        IF(I.LT.J) CALL CINT(R9,3,I,J)
        IF(I.LT.J) JS1 = 1
        IF(I.EQ.2.AND.J.EQ.1) THEN
                CALL CINT(R9,3,2,1)
                CALL CINT(R9,3,3,2)
        ELSE
                IF(I.EQ.3.AND.J.EQ.2) THEN
                        CALL CINT(R9,3,3,2)
                        CALL CINT(R9,3,2,1)
                ELSE
                ENDIF
        ENDIF
        DO 50 L=1,3
```

```
      DO 50 M=1,3
50    R91(L,M) = R9(L,M)
      DO 110 I1=1,3
      DO 110 J1=1,3
      JS2 = 0
      DO 60 L=1,3
      DO 60 M=1,3
60    R9(L,M) = R91(L,M)
      IF(I1.EQ.J1.AND.I1.GT.1) GO TO 110
      IF(I1.EQ.3 .AND.J1.EQ.1) GO TO 110
      IF(I1.LT.J1) CALL RINT(R9,3,3,I1,J1)
      IF(I1.LT.J1) JS2 = 1
      IF(I1.EQ.2.AND.J1.EQ.1) THEN
                 CALL RINT(R9,3,3,2,1)
                 CALL RINT(R9,3,3,3,2)
      ELSE
                 IF(I1.EQ.3.AND.J1.EQ.2) THEN
                            CALL RINT(R9,3,3,3,2)
                            CALL RINT(R9,3,3,2,1)
                 ELSE
                 ENDIF
      ENDIF
      DO 100 K=1,2
      IF(K.EQ.2) CALL TRANS(R9,3)
      CALL RESET(A2,B2,C2,D2,E2,F2,G2,H2,RI2,R9)
      CALL FXYZ( A2,B2,C2,D2,E2,F2,G2,H2,RI2,IXF2,IYF2,IZF2)
 90   A1(N) =A2
      B1(N) =B2
      C1(N) =C2
      D1(N) =D2
      E1(N) =E2
      F1(N) =F2
      G1(N) =G2
      H1(N) =H2
      RI1(N) = RI2
      IXYZ(N) = IXF2+IYF2+IZF2
      JSIG1(N) = JS1 +JS2
 100  N = N+1
 110  CONTINUE
 120  CONTINUE
      N = N-1
      CALL ORDN(N,IMINV)
      DO 150 I=1,N
      IF(IMINV.NE.IXYZ(I)) GO TO 150
      GO TO 160
150   CONTINUE
160   A2 = A1(I)
      B2 = B1(I)
      C2 = C1(I)
      D2 = D1(I)
      E2 = E1(I)
      F2 = F1(I)
      G2 = G1(I)
      H2 = H1(I)
      RI2 = RI1(I)
```

```
      JSIG2 = JSIG1(I)
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE ORDN(I1,IMINV)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/AX/A1(72),B1(72),C1(72),D1(72),E1(72),F1(72),G1(72),
     1 H1(72),RI1(72),IXYZ(72),JSIG1(72)
C  THIS SUBROUTINE SORTS AND FINDS THE MINIMUM VALUE IN PLACE OF THE
C  GIVEN ARRAYS (ALGORITHM IS ADAPTED FROM THE ONE GIVEN IN
C  D.E.KNUTH "SORTING AND SEARCHING",VOL.3.
      DO 30 JL =2,I1
      K = JL
      I = JL - 1
      I1 = K
      K1 = I
 20   IF(IXYZ(K).GE.IXYZ(I)) GO TO 30
      A1(I) = A1(I1)
      A1(K) = A1(K1)
      B1(I) = B1(I1)
      B1(K) = B1(K1)
      C1(I) = C1(I1)
      C1(K) = C1(K1)
      D1(I) = D1(I1)
      D1(K) = D1(K1)
      E1(I) = E1(I1)
      E1(K) = E1(K1)
      F1(I) = F1(I1)
      F1(K) = F1(K1)
      G1(I) = G1(I1)
      G1(K) = G1(K1)
      H1(I) = H1(I1)
      H1(K) = H1(K1)
      RI1(I)= RI1(I1)
      RI1(K)= RI1(K1)
      IXYZ(I) = IXYZ(I1)
      IXYZ(K) = IXYZ(K1)
      JSIG1(I) = JSIG1(I1)
      JSIG1(K) = JSIG1(K1)
      K = K-1
      I = I-1
      IF(I.GE.1) GO TO 20
 30   IMINV = IXYZ(1)
      RETURN
      END
      SUBROUTINE SET(A,B,C,D,E,F,G,H,RI,R9)
      IMPLICIT REAL *8(A-H,O-Z)
      DIMENSION R9(3,3)
C  THE ELEMENTS A,B,...,RI ARE SET AS ELEMENTS OF THE ARRAY R9(3,3).
      R9(1,1) =A
      R9(1,2) =B
      R9(1,3) =C
      R9(2,1) =D
      R9(2,2) =E
      R9(2,3) =F
```

```
      R9(3,1) =G
      R9(3,2) =H
      R9(3,3) =RI
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE RESET(A,B,C,D,E,F,G,H,RI,R9)
      IMPLICIT REAL *8(A-H,O-Z)
      DIMENSION R9(3,3)
C THE ELEMENTS OF THE ARRAY R9(3,3) ARE RESET AS A,B,...,RI HERE.
      A = R9(1,1)
      B = R9(1,2)
      C = R9(1,3)
      D = R9(2,1)
      E = R9(2,2)
      F = R9(2,3)
      G = R9(3,1)
      H = R9(3,2)
      RI= R9(3,3)
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE CINT(A,N,LA,LB)
      IMPLICIT REAL *8(A-H,O-Z)
      DIMENSION A(1)
C THE COLUMN INTERCHANGE OF THE ELEMENTS OF THE ARRAY A IS PERFORMED.
      ILA = N*(LA -1)
      ILB = N*(LB -1)
      DO 10 I=1,N
      ILA = ILA +1
      ILB = ILB +1
      SAVE = A(ILA)
      A(ILA) = A(ILB)
   10 A(ILB) = SAVE
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE RINT(A,N,M,LA,LB)
      IMPLICIT REAL *8(A-H,O-Z)
      DIMENSION A(1)
C   THE ROW INTERCHANGE OF THE ELEMENTS OF THE ARRAY A IS PERFORMED.
      LAJ = LA -N
      LBJ = LB -N
      DO 10 J=1,M
      LAJ = LAJ + N
      LBJ = LBJ +N
      SAVE = A(LAJ)
      A(LAJ) =A(LBJ)
   10 A(LBJ) = SAVE
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE TRANS(A,N)
      IMPLICIT REAL *8(A-H,O-Z)
      DIMENSION A(3,3)
C   THE ARRAY A IS TRANSPOSED IN THIS SUBROUTINE.
      DO 10 I=1,N
```

```
      DO 10 J=1,N
      IF(I.GE.J) GO TO 10
      SAVE = A(J,I)
      A(J,I) = A(I,J)
      A(I,J) = SAVE
   10 CONTINUE
      RETURN
      END
C ----------------------------------------------------------------------
      SUBROUTINE FXYZ(A,B,C,D,E,F,G,H,RI,IXF,IYF,IZF)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/AA/X4,X5,IX4,IX5,Y4,Y5,IY4,IY5,Z4,Z5,IZ4,IZ5
C  THE UPPER LIMITS OF THE SUMMATION INDICES XF,YF AND ZF ARE
C       COMPUTED IN THIS SUBROUTINE.
      IX4=E+F-D
      IX5=C+F-RI
      X4 = IX4
      X5 = IX5
      IY4 = B+E-H
      IY5 = G+RI-H
      Y4 = IY4
      Y5 = IY5
      IZ4 = A+D-G
      IZ5 = A+C-B
      Z4 = IZ4
      Z5 = IZ5
      IXF = MIN0(IX4,IX5)
      IYF = MIN0(IY4,IY5)
      IZF = MIN0(IZ4,IZ5)
      RETURN
      END
***********************************************************************
      PROGRAM  PROGTEST
C     MAIN PROGRAM TO COMPUTE RNINE(A,B,C,D,E,F,G,H,RI) AND
C     WNINE(A,B,C,D,E,F,G,H,RI).THESE FUNCTION SUBPROGRAMS COMPUTE
C     THE 9-J ANGULAR MOMENTUM COEFFICIENT. THE PROGRAM RNINE USES
C     THE TRIPLE SUM FORMULA OF JUCYS AND BANDZAITIS IN ITS FOLD
C     FORM,WHILE THE PROGRAM WNINE USES THE CONVENTIONAL SINGLE
C     SUM OVER A PRODUCT OF THREE 6-J COEFFICIENTS, WHERE THE 6-J
C     COEFFICIENT IS COMPUTED AS SET OF THREE HYPERGEOMETRIC
C     FUNCTIONS.
C     THE SYSTEM DEPENDENT ROUTINES ARE NECESSARY ONLY WHEN THE
C     EXECUTION TIMES ARE NEEDED FOR THE FUNCTION PROGRAMS RNINE
C     AND WNINE. THE IBM-PC/AT REQUIRES INTEGER*2 DECLARATION AND
C     GETTIM ROUTINE FROM ITS LIBRARY IBMFOR.LIB (FORTRAN 77
C     VERSION 2.0). FOR VAX-11/780, THE ROUTINE REQUIRED IS THE
C     FUNCTION SUBPROGRAM SECNDS (NOTE THE SPELLING) WHICH RETURNS
C     THE SYSTEM TIME IN SECONDS AS A SINGLE-PRECISION FLOATING-
C     POINT ARGUMENT. COMMENTS WHICH START WITH $$ IN THE 4TH &
C     5TH COLUMN ACTS AS FLAGS TO NOTES WHICH INDICATE THE
C     STATEMENTS WHICH SHOULD BE CHANGED BEFORE COMPILING THE
C     PROGRAM ON THE IBM-PC/AT.
C     IN ITS PRESENT FORM THE PROGRAM WILL RUN ON THE VAX-11/780.
C     ***********************************************************
C  $$ NOTE: FOR IBM-PC/AT MAKE THE NEXT STATEMENT C...
```

```
      IMPLICIT REAL*8(A-H,O-Y)
C  $$ NOTE: FOR IBM-PC/AT REMOVE FROM THE NEXT TWO STATEMENTS C
C     IMPLICIT REAL*8(A-H,O-Z)
C     INTEGER *2 IH,IM1,IM2,IM3,IM4,IS1,IS2,IS3,IS4,IHS1,IHS2
C     INTEGER *2 IHS3,IHS4
      COMMON FCT(500)
      COMMON/XX/A2,B2,C2,D2,E2,F2,G2,H2,RI2,JSIG2
      DIMENSION R9(3,3)
C     LOGARITHMS OF FACTORIALS SET UP IN A COMMON BLOCK
      FCT(1)=0.
      FCT(2)=0.
      DO 10 N=3,500
      AN=N-1
 10   FCT(N)=DLOG(AN)+FCT(N-1)
      READ(5,20) ITEST
 20   FORMAT(I3)
      WRITE(6,30) ITEST
 30   FORMAT(' ITEST=',I3,//,)
 40   READ(5,50) A,B,C,D,E,F,G,H,RI
 50   FORMAT(9F4.1)
      IF(A.LT.0) GO TO 190
      ISIG = A+B+C+D+E+F+G+H+RI
C     CHECKING FOR ANY ONE OF THE NINE ANGULAR MOMENTA BEING ZERO.
      CALL SET(A,B,C,D,E,F,G,H,RI,R9)
      DO 70 I=1,3
      DO 70 J=1,3
      IF(R9(I,J).EQ.0.0) GO TO 80
 70   CONTINUE
      GO TO 90
 80   IK=I
      JK=J
C     RNINEJ GIVES THE VALUE OF THE 9J-COEFFICIENT WHEN ONE OF
C           ITS ARGUMENTS IS ZERO
      RNINEJ=VALUE(A,B,C,D,E,F,G,H,RI,IK,JK)
      GO TO 160
 90   CALL CHANGE(A,B,C,D,E,F,G,H,RI)
      CALL TERM(A2,B2,C2,D2,E2,F2,G2,H2,RI2,NT1,NT2)
      NT3=3*NT2
      ZTEST=ITEST
C  $$ NOTE: FOR IBM-PC/AT MAKE THE NEXT STATEMENT C...
      ZT1=SECNDS(0.0)
C  $$ NOTE : FOR IBM-PC/AT REMOVE FROM THE NEXT STATEMENT C
C     CALL GETTIM(IH,IM1,IS1,IHS1)
      DO 100 ITT=1,ITEST
 100  RES1=WNINE(A2,B2,C2,D2,E2,F2,G2,H2,RI2)
      IF((ISIG/2)*2.NE.ISIG.AND.(JSIG/2)*2.NE.JSIG2)
     1 RES1=PHASE(ISIG)*RES1
C  $$ NOTE: FOR IBM-PC/AT MAKE THE NEXT STATEMENT C ...
      Z1=SECNDS(ZT1)/ZTEST
C  $$ NOTE :FOR IBM-PC/AT REMOVE FROM THE NEXT THREE STATEMENTS C
C     CALL GETTIM(IH,IM2,IS2,IHS2)
C     AID1=((IM2-IM1)*60+(IS2-IS1))*100+(IHS2-IHS1)
C     Z1=AID1/(ZTEST*100.D0)
      WRITE(6,110)A,B,C,D,E,F,G,H,RI,RES1,NT3,Z1
 110  FORMAT(' WNINE(',8(F4.1,','),F4.1,')=',E13.6,I6,F10.5)
```

```
C       Z1 GIVES THE TIME TAKEN BY WNINE IN SECONDS
C   $$  NOTE: FOR IBM-PC/AT MAKE THE NEXT STATEMENT C...
        ZT2=SECNDS(0.0)
C   $$  NOTE: FOR IBM-PC/AT REMOVE FROM THE NEXT STATEMENT C
C       CALL GETTIM(IH,IM3,IS3,IHS3)
         DO 120 IT=1,ITEST
 120     RES2=RNINE(A2,B2,C2,D2,E2,F2,G2,H2,RI2)
         IF((ISIG/2)*2.NE.ISIG.AND.(JSIG2/2)*2.NE.JSIG2)
      1  RES2 = PHASE(ISIG)*RES2
C   $$   NOTE: FOR IBM-PC/AT MAKE THE NEXT STATEMENT C ...
        Z2=SECNDS(ZT2)/ZTEST
C   $$  NOTE: FOR IBM-PC/AT REMOVE FROM THE NEXT THREE STATEMENTS C
C       CALL GETTIM(IH,IM4,IS4,IHS4)
C       AID2=((IM4-IM3)*60+(IS4-IS3))*100+(IHS4-IHS3)
C       Z2=AID2/(TEST*100.0D0)
C       Z2 GIVES THE TIME TAKEN BY RNINE IN SECONDS
        ZIDA=Z1/Z2
C       ZIDA GIVES THE ADVANTAGE FACTOR OF RNINE OVER WNINE
        WRITE(6,150) A,B,C,D,E,F,G,H,RI,RES2,NT1,Z2,ZIDA
 150    FORMAT(' RNINE(',8(F4.1,','),F4.1,')=',E13.6,I6,2F10.5,/)
        GO TO 180
 160    WRITE(6,170) A,B,C,D,E,F,G,H,RI,RNINEJ
 170    FORMAT(' NINEJ(',8(F4.1,','),F4.1,')=',E13.6)
 180    GO TO 40
 190    STOP
        END
C --------------------------------------------------------------
```

## Appendix D

This is an Appendix to Chapter 6 which lists the programs used to generate the equivalent zeros of degree 1 of the 9-j coefficient and the one used to sieve out the inequivalent ones using the ordering prescription given by Howell (1959). The variables and equation numbers given here refer to those of Chapter 6.

Program NJ1 generates the equivalent zeros of the 9-j coefficient for the values $0 < a, b, d, e, \leq NN/2$, where NN is an input variable, using the closed-form expression given by (6). The argument of the 9-j coefficient a, b, ..., i, the maximum values of the summation indices XF, YF and ZF and $\sigma$, along with the serial number of the entry named as A, B, ..., RI, IXF, IYF, IZF, JS and N respectively are stored in a file 9J1.OUT. The output data is redirected to this file at the time of execution.

Program ORDER4 orders the data stored in 9J1.OUT in ascending order with respect to $\sigma$ (JS) so that when the execution is complete the first value of JS corresponds to its minimum value and the last one to its maximum value. The output of this is stored in ORDER4.OUT.

The output of ORDER4.OUT serves as input to the program SIEV. Before executing this program the minimum and maximum values of JS denoted by JMIN and JMAX and the total number of output data in ORDER4.OUT denoted by I1 should be provided in the appropriate places. The numbers given in the present case correspond to $0 < a, b, d, e \leq 3$.

The symmetries of the 9-j coefficient clearly indicate that while those having different values of $\sigma$ are certainly inequivalent ones, the ones with the same values of $\sigma$ may be either equivalent or inequivalent. Hence to separate the inequivalent ones, all the entries with the same value of $\sigma$ ie. JS are stored separately in one dimensional arrays, viz. A1, A2, ...., A9. This set of data is ordered with respect to A1 is ascending order. Following this the nine arguments of every 9-j coefficient are ordered amongst themselves in a particular fashion following the method of Howell (1959) (in the subprogram Howell) after which this ordered set of nine arguments will be the same for equivalent ones and different for inequivalent ones. Using this criterion the inequivalent ones are separated and written down. The ordering prescription given by Howell is as follows. Given a 9-j coefficient, with the nine arguments a,b,c...,i the following quantities calculated:

$$N_1 = a + b + c , \qquad N_4 = a + d + g ,$$
$$N_2 = d + e + f , \qquad N_5 = b + e + h ,$$
$$N_3 = g + h + i , \qquad N_6 = c + f + i .$$

and they are ordered using the symmetries of this coefficient such that the following conditions are satsified:

$$N_1 \geq N_2 \geq N_3 ,$$
$$N_1 \geq N_4 \geq N_5 \geq N_6 .$$

If $N_1 = N_2$ then $a \geq d$, if also $a = d$ then $b \geq e$.

If $N_2 = N_3$ then $d \geq g$, if also $d = g$ then $e \geq h$.

If $N_4 = N_5$ then $a \geq b$, if also $a = b$ then $d \geq e$.

If $N_5 = N_6$ then $b \geq c$, if also $b = c$ then $e \geq f$.

If $N_1 = N_4$ then $N_2 \geq N_5$ if also $N_2 = N_5$ then $b \geq d$.

If $N_1 = N_2$ and $N_4 = N_5$ then $a \geq e$, if also $a = e$ then $b \geq d$.

If $N_1 = N_2$ and $N_5 = N_6$ and $a = d$ then $b \geq f$.

If $N_2 = N_3$ and $N_4 = N_5$ and $a = b$ then $d \geq h$.

If $N_1 = N_2$ and $N_4 = N_5 = N_6$ then $a \geq f$, if also $a = f$ then $b \geq d, e$.

If $N_1 = N_2$ and $N_4 = N_5 = N_6$ and $a = e$, then $b \geq f$, if also $b = f$ then $b = c$.

If $N_2 = N_3$ and $N_4 = N_5 = N_6$ and $a = b = c$ then $d \geq i$.

If $N_1 = N_2$ $N_3 = N_4 = N_5 = N_6$ then $a \geq h$ if also $a = h$ then $b \geq e, i$.

If $N_1 = N_2 = N_3 = N_4 = N_5 = N_6$ then $a \geq i$, if also $a = i$ then $b \geq f, h$.

Note: In the programs NJ1 and SIEV the function TRIA,and the subroutines SET,RESET,CINT,RINT and TRANS that are already given in previous Appendices are not repeated. However, in the program SIEV, the subroutines SET and RESET are to be used without the list of variables being a part of the SUBROUTINE statement since they are to be placed in a COMMON block named YY in the main program. Similarly, the subroutines CINT and RINT should contain the statement COMMON /YY/ A(9),AA,B,C,...,RI and the subroutine TRANS should have the statement COMMON /YY/ R9(3,3),AA,B,C,...,RI.

******************************************************************

```
      PROGRAM NJ1
C     PROGRAM TO FIND THE 9-J ZEROS OF DEGREE 1
      IMPLICIT REAL*8(A-H,O-Z)
      OPEN(UNIT=3,FILE='9J1.OUT',STATUS='NEW')
      READ(*,5) NN
 5    FORMAT(I2)
      I=0
      I1=1
      DO 10 M1=1,NN
      AM1=M1
      A=AM1/2.0D0
      DO 20 M2=1,NN
      AM2=M2
      B=AM2/2.0D0
      CMIN=DABS(A-B)
      CMAX=A+B
      C=CMIN
 70   DO 30 M3=1,NN
      AM3=M3
      D=AM3/2.0D0
      DO 40 M4=1,NN
      AM4=M4
      E=AM4/2.0D0
      FMIN=DABS(D-E)
      FMAX=D+E
      F=FMIN
 80   GMIN=DABS(A-D)
      GMAX=A+D
      G=GMIN
 90   HMIN=DABS(B-E)
      HMAX=B+E
      H=HMIN
 100  DIF1=DABS(G-H)
      DIF2=DABS(C-F)
      RIMIN=DMAX1(DIF1,DIF2)
      RIMAX=DMIN1(G+H,C+F)
      RI=RIMIN
 110  D1=TRIA(A,B,C)
      D2=TRIA(D,E,F)
      D3=TRIA(G,H,RI)
      D4=TRIA(A,D,G)
      D5=TRIA(B,E,H)
      D6=TRIA(C,F,RI)
C     WRITE(*,200) D1,D2,D3,D4,D5,D6
C200  FORMAT(6F4.1)
      IF(D1.EQ.0..OR.D2.EQ.0..OR.D3.EQ.0..OR.D4.EQ.0.) GO TO 50
      IF(D5.EQ.0..OR.D6.EQ.0.) GO TO 50
      IX1=2.0D0*F
      IX2=D+E-F
      IX3=C+RI-F
      IX4=E+F-D
      IX5=C+F-RI
      IY1=E+H-B
      IY2=G+H-RI
      IY3=2.0D0*H+1.0D0
```

```
      IY4=B+E-H
      IY5=G+RI-H
      IZ1=2.0D0*A
      IZ2=B+C-A
      IZ3=A+D+G+1.0D0
      IZ4=A+D-G
      IZ5=A+C-B
      IP1=A+D+RI-H
      IP2=D+H-B-F
      IP3=B+RI-A-F
      IXF=MIN0(IX4,IX5)
      IYF=MIN0(IY4,IY5)
      IZF=MIN0(IZ4,IZ5)
      N1=A+B+C
      N2=D+E+F
      N3=G+H+RI
      N4=A+D+G
      N5=B+E+H
      N6=C+F+RI
      IF(IXF.EQ.1.AND.IYF.EQ.0.AND.IZF.EQ.0) GO TO 130
      IF(IXF.EQ.0.AND.IYF.EQ.1.AND.IZF.EQ.0) GO TO 140
      IF(IXF.EQ.0.AND.IYF.EQ.0.AND.IZF.EQ.1) GO TO 150
      GO TO 300
130   NDR=(IP2+1)*(IP3+1)
      IF(NDR.LT.0) GO TO 300
      IT1=(IX2+1)*(IX3+1)*IX4*IX5
      IT2=NDR*IX1
      IF(IT1.EQ.IT2) GO TO 160
      GO TO 300
140   NDR=IP1*(IP2+1)
      IF(NDR.LT.0) GO TO 300
      IT1=(IY1+1)*(IY2+1)*IY4*IY5
      IT2=(IY3+1)*NDR
      IF(IT1.EQ.IT2) GO TO 160
      GO TO 300
150   NDR=IP1*(IP3+1)
      IF(NDR.LT.0) GO TO 300
      IT1=(IZ2+1)*IZ3*IZ4*IZ5
      IT2=IZ1*IP1*(IP3+1)
      IF(IT1.NE.IT2) GO TO 300
160   IF(A.EQ.D.AND.B.EQ.E.AND.C.EQ.F.AND.(N3/2)*2.NE.N3)
     1   GO TO 300
      IF(D.EQ.G.AND.E.EQ.H.AND.F.EQ.RI.AND.(N1/2)*2.NE.N1)
     1   GO TO 300
      IF(A.EQ.G.AND.B.EQ.H.AND.C.EQ.RI.AND.(N2/2)*2.NE.N2)
     1   GO TO 300
      IF(A.EQ.B.AND.D.EQ.E.AND.G.EQ.H.AND.(N6/2)*2.NE.N6)
     1   GO TO 300
      IF(B.EQ.C.AND.E.EQ.F.AND.H.EQ.RI.AND.(N4/2)*2.NE.N4)
     1   GO TO 300
      IF(A.EQ.C.AND.D.EQ.F.AND.G.EQ.RI.AND.(N5/2)*2.NE.N5)
     1   GO TO 300
      IF(A.EQ.0.0.OR.B.EQ.0.0.OR.C.EQ.0.0.OR.D.EQ.0.0)
     1   GO TO 300
      IF(E.EQ.0.0.OR.F.EQ.0.0.OR.G.EQ.0.0.OR.H.EQ.0.0)
```

```
    1      GO TO 300
           IF(RI.EQ.0.0) GO TO 300
           JS=A+B+C+D+E+F+G+H+RI
           WRITE(3,60) A,B,C,D,E,F,G,H,RI,IT1,IT2,IXF,IYF,IZF,I,I1,JS
 60        FORMAT(9(2X,F4.1),2I4,5I2,I4)
           I1=I1+1
C          WRITE(*,120) IX1,IX2,IX3,IX4,IX5,IP2,IP3
C120       FORMAT(7I3)
 300       I=I+1
 50        RI=RI+1.0D0
           IF(RI.LE.RIMAX) GO TO 110
           H=H+1.0D0
           IF(H.LE.HMAX) GO TO 100
           G=G+1.0D0
           IF(G.LE.GMAX) GO TO 90
           F=F+1.0D0
           IF(F.LE.FMAX) GO TO 80
 40        CONTINUE
 30        CONTINUE
           C=C+1.0D0
           IF(C.LE.CMAX) GO TO 70
 20        CONTINUE
 10        CONTINUE
           STOP
           END
***********************************************************************
      PROGRAM ORDER4
C   PROGRAM TO LIST THE ZEROS OF THE 9-J ORDERED WITH RESPECT TO JS.
      IMPLICIT REAL*8(A-H,O-Z)
      OPEN(3,FILE='9J1.OUT')
      OPEN(4,FILE='ORDER4.OUT')
      READ(*,50) JMIN,JMAX,I1
 50   FORMAT(2(I3),I6)
      WRITE(4,75) JMIN,JMAX,I1
 75   FORMAT(2(2X,I3),2X,I6)
      I11=1
      DO 10 J=JMIN,JMAX
      REWIND 3
 15   READ(3,2) A,B,C,D,E,F,G,H,RI,IXF,IYF,IZF,JS,I
  2   FORMAT(9(2X,F4.1),3I2,2I4)
      IF(J.NE.JS) GO TO 20
      WRITE(4,2) A,B,C,D,E,F,G,H,RI,IXF,IYF,IZF,JS,I11
```

```
      I11=I11+1
20    IF(I-I1) 15,10,10
10    CONTINUE
      STOP
      END
C ----------------------------------------------------------------------
      PROGRAM SIEV
C  PROGRAM TO GET THE INEQUIVALENT LIST OF 9-J ,FROM A GIVEN LIST
C              THAT INCLUDES THE SYMMETRIES.
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/YY/R9(3,3),AA,AB,AC,AD,AE,AF,AG,AH,AI
      COMMON/XX/DUMS(200), KEY(200)
      COMMON/ZZ/N1,N2,N3,N4,N5,N6
      DIMENSION A1(200),A2(200),A3(200),A4(200),A5(200),A6(200)
      DIMENSION A7(200),A8(200),A9(200)
      DIMENSION B1(200),B2(200),B3(200),B4(200),B5(200),B6(200)
      DIMENSION B7(200),B8(200),B9(200)
      DIMENSION C1(200),C2(200),C3(200),C4(200),C5(200),C6(200)
      DIMENSION C7(200),C8(200),C9(200)
      LOGICAL FA,FB,FC
      OPEN(UNIT=3,FILE='ORDER4.OUT',STATUS='OLD')
      OPEN(UNIT=4,FILE='SIEV.OUT',STATUS='NEW')
      KK=1
      IX=1
      JMIN=12
      JMAX=41
      I1=1323
10    I=1
      JSOLD=JMIN
20    READ(3,30,END=45) A,B,C,D,E,F,G,H,RI,IXF,IYF,IZF,JS,N
30    FORMAT(1X,F4.1,8(2X,F4.1),3I2,2I4)
      JSNEW=JS
      IF(JSNEW-JSOLD) 20,33,35
33    A1(I)=A
      A2(I)=B
      A3(I)=C
      A4(I)=D
      A5(I)=E
      A6(I)=F
      A7(I)=G
      A8(I)=H
      A9(I)=RI
      JM=JSOLD
C     WRITE(*,2)A1(I),A2(I),A3(I),A4(I),A5(I),A6(I),A7(I),A8(I),A9(I)
 2    FORMAT(9(2X,F4.1))
C     WRITE(*,200)
C200  FORMAT(' STORING CONTINUES')
      I=I+1
      IX=IX+1
      GO TO 20
35    REWIND 3
```

```
      JMIN=JS
C     WRITE(*,210)
C210  FORMAT(' STORING COMPLETE')
 45   IM=I-1
C     IX=IX-1
      DO 40 k=1,IM
 40   DUMS(K)=A1(K)
      CALL ORDER(IM)
      DO 50 K=1,IM
      IS=KEY(K)
      B1(K)=A1(IS)
      B2(K)=A2(IS)
      B3(K)=A3(IS)
      B4(K)=A4(IS)
      B5(K)=A5(IS)
      B6(K)=A6(IS)
      B7(K)=A7(IS)
      B8(K)=A8(IS)
      B9(K)=A9(IS)
C     WRITE(*,220)
C220  FORMAT(' ORDERING CONTINUES')
C    WRITE(*,2)B1(K),B2(K),B3(K),B4(K),B5(K),B6(K),B7(K),B8(K),B9(K)
 50   CONTINUE
C     WRITE(*,230)
C230  FORMAT(' ORDERING COMPLETE')
      DO 100 L1=1,IM
      AA=B1(L1)
      AB=B2(L1)
      AC=B3(L1)
      AD=B4(L1)
      AE=B5(L1)
      AF=B6(L1)
      AG=B7(L1)
      AH=B8(L1)
      AI=B9(L1)
      CALL SET
      CALL  HOWELL
      CALL RESET
      C1(L1)=AA
      C2(L1)=AB
      C3(L1)=AC
      C4(L1)=AD
      C5(L1)=AE
      C6(L1)=AF
      C7(L1)=AG
      C8(L1)=AH
      C9(L1)=AI
C     WRITE(*,240)
C240  FORMAT(' INTERNAL ORDERING CONTINUES')
C     WRITE(*,2)C1(L),C2(L),C3(L),C4(L),C5(L),C6(L),C7(L),C8(L),C9(L)
 100  CONTINUE
C     WRITE(*,250)
C250  FORMAT(' INT.ORDER COMPL.')
      DO 150 L=IM,1,-1
      CA=C1(L)
```

```
      CB=C2(L)
      CC=C3(L)
      CD=C4(L)
      CE=C5(L)
      CF=C6(L)
      CG=C7(L)
      CH=C8(L)
      CI=C9(L)
c     WRITE(*,2) CA,CB,CC,CD,CE,CF,CG,CH,CI
      DA=B1(L)
      DB=B2(L)
      DC=B3(L)
      DD=B4(L)
      DE=B5(L)
      DF=B6(L)
      DG=B7(L)
      DH=B8(L)
      DI=B9(L)
      DO 140 LX=IM,L+1,-1
      BA=C1(LX)
      BB=C2(LX)
      BC=C3(LX)
      BD=C4(LX)
      BE=C5(LX)
      BF=C6(LX)
      BG=C7(LX)
      BH=C8(LX)
      BI=C9(LX)
      IF(LX.EQ.IM.AND.L.EQ.IM) GO TO 145
      FA=(CA.EQ.BA.AND.CB.EQ.BB.AND.CC.EQ.BC)
      FB=(CD.EQ.BD.AND.CE.EQ.BE.AND.CF.EQ.BF)
      FC=(CG.EQ.BG.AND.CH.EQ.BH.AND.CI.EQ.BI)
      IF(FA.AND.FB.AND.FC) GO TO 150
 140  CONTINUE
 145  WRITE(4,146) DA,DB,DC,DD,DE,DF,DG,DH,DI,N1,N2,N3,N4,N5,N6,JM,KK
 146  FORMAT(9(2X,F4.1),8I4)
      WRITE(4,400) CA,CB,CC,CD,CE,CF,CG,CH,CI
 400  FORMAT(9(2X,F4.1))
      KK=KK+1
 150  CONTINUE
      IF(JM.LT.JMAX) GO TO 10
      STOP
      END
C ---------------------------------------------------------------------
       SUBROUTINE HOWELL
       IMPLICIT REAL*8(A-H,O-Z)
       COMMON/YY/R9(3,3),A,B,C,D,E,F,G,H,RI
       COMMON/ZZ/N1,N2,N3,N4,N5,N6
       CALL N1TON6
       MX=MAX0(N1,N2,N3,N4,N5,N6)
       AMX=MX
       IF(AMX.EQ.N1.OR.AMX.EQ.N2.OR.AMX.EQ.N3) GO TO 10
       CALL TRANS(3)
       CALL N1TON6
 10    IF(N1.GE.N2) GO TO 20
```

```
      CALL RINT(3,3,1,2)
      CALL N1TON6
20    IF(N2.GE.N3) GO TO 30
      CALL RINT(3,3,2,3)
      CALL N1TON6
      IF(N1.GE.N2) GO TO 30
      CALL RINT(3,3,1,2)
      CALL N1TON6
30    IF(N4.GE.N5) GO TO 40
      CALL CINT(3,1,2)
      CALL N1TON6
40    IF(N5.GE.N6) GO TO 50
      CALL CINT(3,2,3)
      CALL N1TON6
      IF(N4.GE.N5) GO TO 50
      CALL CINT(3,1,2)
      CALL N1TON6
50    IF(N1.EQ.N2.AND.(A.LT.D.OR.(A.EQ.D.AND.B.LT.E)))
     1 CALL RINT(3,3,1,2)
      IF(N2.EQ.N3.AND.(D.LT.G.OR.(D.EQ.G.AND.E.LT.H)))
     1 CALL RINT(3,3,2,3)
      IF(N4.EQ.N5.AND.(A.LT.B.OR.(A.EQ.B.AND.D.LT.E)))
     1 CALL CINT(3,1,2)
      IF(N5.EQ.N6.AND.(B.LT.C.OR.(B.EQ.C.AND.E.LT.F)))
     1 CALL CINT(3,2,3)
      IF(N1.EQ.N4.AND.(N2.LT.N5.OR.(N2.EQ.N5.AND.B.LT.D)))
     1 CALL TRANS(3)
       CALL N1TON6
      IF(N1.EQ.N2.AND.N4.EQ.N5.AND.(A.LT.E.OR.(A.EQ.E.AND.
     1 B.LT.D))) THEN
               CALL RINT(3,3,1,2)
               CALL CINT(3,1,2)
      ELSE
      ENDIF
      IF(N1.EQ.N2.AND.N5.EQ.N6.AND.A.EQ.D.AND.B.LT.F) THEN
                     CALL RINT(3,3,1,2)
                     CALL CINT(3,2,3)
      ELSE
      ENDIF
      IF(N2.EQ.N3.AND.N4.EQ.N5.AND.A.EQ.B.AND.D.LT.H) THEN
               CALL RINT(3,3,2,3)
               CALL CINT(3,1,2)
      ELSE
      ENDIF
      IF(N1.EQ.N2.AND.N4.EQ.N5.AND.N5.EQ.N6.AND.A.LT.F)THEN
               CALL RINT(3,3,1,2)
               CALL CINT(3,1,3)
      ELSE
      ENDIF
      IF(N1.EQ.N2.AND.N4.EQ.N5.AND.N5.EQ.N6.AND.A.EQ.F) THEN
              CALL RINT(3,3,1,2)
              CALL CINT(3,2,3)
      ELSE
      ENDIF
      IF(N1.EQ.N2.AND.N4.EQ.N5.AND.N5.EQ.N6.AND.A.EQ.E
```

```
     1      .AND.B.LT.F)  THEN
               CALL RINT(3,3,1,2)
               CALL CINT(3,2,3)
            ELSE
            ENDIF
            IF(N2.EQ.N3.AND.N4.EQ.N5.AND.N5.EQ.N6.AND.A.EQ.B.AND.
     1      B.EQ.C.AND.D.LT.RI) THEN
               CALL RINT(3,3,2,3)
               CALL CINT(3,1,3)
            ELSE
            ENDIF
            IF(N1.EQ.N2.AND.N2.EQ.N3.AND.N3.EQ.N4.AND.N4.EQ.N5.
     1      AND.N5.EQ.N6.AND.A.LT.H) THEN
                CALL RINT(3,3,1,3)
                CALL CINT(3,1,2)
            ELSE
            ENDIF
            IF(N1.EQ.N2.AND.N2.EQ.N3.AND.N3.EQ.N4.AND.N4.EQ.N5.
     1      AND.N5.EQ.N6.AND.A.EQ.H.AND.B.LT.E) CALL RINT(3,3,1,2)
            IF(N1.EQ.N2.AND.N2.EQ.N3.AND.N3.EQ.N4.AND.N4.EQ.N5.
     1      AND.N5.EQ.N6.AND.A.EQ.H.AND.B.LT.RI) THEN
                 CALL RINT(3,3,1,3)
                 CALL CINT(3,2,3)
            ELSE
            ENDIF
            IF(N1.EQ.N2.AND.N2.EQ.N3.AND.N3.EQ.N4.AND.N4.EQ.N5.
     1      AND.N5.EQ.N6.AND.A.LT.RI) THEN
                CALL RINT(3,3,1,3)
                CALL CINT(3,1,3)
            ELSE
            ENDIF
            IF(N1.EQ.N2.AND.N2.EQ.N3.AND.N3.EQ.N4.AND.N4.EQ.N5
     1      .AND.N5.EQ.N6.AND.A.EQ.RI.AND.B.LT.F) THEN
                    CALL RINT(3,3,1,2)
                    CALL CINT(3,2,3)
            ELSE
            ENDIF
            IF(N1.EQ.N2.AND.N2.EQ.N3.AND.N3.EQ.N4.AND.N4.EQ.N5.
     1      AND.N5.EQ.N6.AND.A.EQ.RI.AND.B.LT.H) CALL RINT(3,3,1,3)
            RETURN
            END
            SUBROUTINE N1TON6
            IMPLICIT REAL*8(A-H,O-Z)
            COMMON/YY/R9(3,3),A,B,C,D,E,F,G,H,RI
            COMMON/ZZ/N1,N2,N3,N4,N5,N6
            N1=A+B+C
            N2=D+E+F
            N3=G+H+RI
            N4=A+D+G
            N5=B+E+H
            N6=C+F+RI
            RETURN
            END
************************************************************************
```

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## List of Symbols

In this thesis for the sake of ease in typing, a rigourous notation has not been adopted. The symbols used which are not further qualified, have the following significance:

| Symbol | Meaning |
| --- | --- |
| $a, b, c, \ldots, i$ | non-negative integer parameters |
| $\mathrm{a}, \mathrm{b}, \mathrm{c}, \ldots, \mathrm{i}$<br>$j_1, j_2, j_3, j_{12}, \ldots, J, \ell_k$<br>$m_1, m_2, m_3, m_{12}, \ldots, M$ | half-integral and integral values of angular momenta |
| $J_1, J_2, J_3, J_{12}, \ldots, J$ | angular momentum operators |
| $b^{\dagger}_{j,m}, b_{j,m}$ | creation, annihilation operators |
| $Z_+, Z_-, Z_0$ | quasi-spin operators |
| $\binom{n}{r}$ | binomial coefficient |
| $Q_n(x) \equiv Q_n(x; \alpha, \beta, N)$ | Hahn polynomial, (1) of Chapter 7. |
| $\delta(x, y)$ | Kronecker delta function |
| $\lvert j,m\rangle$ , $\langle j,m\rvert$ | Dirac ket, bra notation for angular momentum states |
| $\langle j, m\rvert T^k_q \lvert j', m'\rangle$ | matrix element of tensor $T^k_q$ |
| $\langle j \Vert T^k \Vert j'\rangle$ | reduced matrix element |
| $A^R(\phi)$ | reciprocal of the array $A(\phi)$ |
| $x\mid y$ | x divides y (or, x/y is an integer) |
| $(x, n)$ | Pocchammer symbol (n an integer) |
| $(a, b)$ | g.c.d. of $a$, $b$ (in the context of multiplicative Diophantine equations *only*) |
| $[x]$ | $(2x + 1)^{1/2}$ |
| $[J/3]$ | largest integer < J/3 (Chapter 3) |
| $\{a\ b\ c\}$ | defined in eq.(17) of Chapter 5 |

| | |
|---|---|
| $C(j_1, j_2, j_3; m_1, m_2, m_3)$ | Clebsch-Gordan coefficient |
| $\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$ | 3-j coefficient (or 3-j symbol) |
| $\Delta(j_1\ j_2\ j_3)$ | defined on p.19 of Chapter 1 |
| $(a\ b\ c)$ | eqn.(72) of Chapter 1. |
| $\left\Vert \begin{matrix} -j_1+j_2+j_3 & j_1-j_2+j_3 & j_1+j_2-j_3 \\ j_1-m_1 & j_2-m_2 & j_3-m_3 \\ j_1+m_1 & j_2+m_2 & j_3+m_3 \end{matrix} \right\Vert$ | Regge 3 × 3 array |
| $\Vert R_{ik} \Vert$ | Regge array ,(27) of Chapter 1 |
| $U(j_1 j_2 J\ j_3; j_{12} j_{23})$ | recoupling coefficient,(41)of Ch.1 |
| $W(abcd;\ ef)$ | Racah coefficient |
| $\begin{Bmatrix} a & b & e \\ d & c & f \end{Bmatrix}$ | 6-j coefficient (6-j symbol) |
| ${}_2F_1(a,b;c;z)$ | Gauss hypergeometric series |
| $(\alpha_p)$ | $\alpha_1, \alpha_2, \ldots, \alpha_p$ :integer parameters |
| $(\beta_q)$ | $\beta_1, \beta_2, \ldots, \beta_q$ :integer parameters |
| ${}_pF_q((\alpha_p);(\beta_q);z)$ | generalized hypergeometric series |
| $F^{(3)}\left[\begin{matrix} (a)::(b);(b');(b''):(c);(c');(c'');x,y,z \\ (e)::(f);(f');(f''):(g);(g');(g'') \end{matrix}\right]$ | : triple hypergeometric series. |
| $\begin{bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & J \end{bmatrix}$ | *ls - jj* transformation coefficient |
| $\begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix}$ | 9-j coefficient |
| $\left\Vert \begin{matrix} \beta_1-\alpha_1 & \beta_2-\alpha_1 & \beta_3-\alpha_1 \\ \beta_1-\alpha_2 & \beta_2-\alpha_2 & \beta_3-\alpha_2 \\ \beta_1-\alpha_3 & \beta_2-\alpha_3 & \beta_3-\alpha_3 \\ \beta_1-\alpha_4 & \beta_2-\alpha_4 & \beta_3-\alpha_4 \end{matrix} \right\Vert$ | Bargmann - Shelepin array |

(Note: Standard mathematical notation is used as far as possible and these symbols are naturally not listed herein).