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2004 J. Phys. A: Math. Gen. 37 3259

(http://iopscience.iop.org/0305-4470/37/9/014)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **37** (2004) 3259–3269 PII: S0305-4470(04)69457-1

Universal factorization of $3n$-j ($j > 2$) symbols of the first and second kinds for $SU(2)$ group and their direct and exact calculation and tabulation

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Received 24 September 2003, in final form 22 December 2003
Published 18 February 2004
Online at stacks.iop.org/JPhysA/37/3259 (DOI: 10.1088/0305-4470/37/9/014)

Abstract

We show that general $3n$-j ($n > 2$) symbols of the first and second kinds for the group $SU(2)$ can be reformulated in terms of binomial coefficients. The proof is based on the graphical technique established by Yutsis *et al* and through a definition of a reduced 6-j symbol. The resulting $3n$-j symbols thereby take a combinatorial form which is simply the product of two factors. The one is an integer or polynomial which is the single sum over the products of reduced 6-j symbols. They are in the form of summing over the products of binomial coefficients. The other is a multiplication of all the triangle relations appearing in the symbols, which can also be rewritten using binomial coefficients. The new formulation indicates that the intrinsic structure for the general recoupling coefficients is much nicer and simpler, which might serve as a bridge for study with other fields. Along with our newly developed algorithms, this also provides a basis for a direct, exact and efficient calculation or tabulation of all the $3n$-j symbols of the $SU(2)$ group for all the range of quantum angular momentum arguments. As an illustration, we present the results for the 12-j symbols of the first kind.

PACS numbers: 03.65.Fd, 02.20.Uw

1. Introduction

The quantum theory of angular momentum is a fundamental field in sciences. In particular, the topic of angular momentum coupling scheme, which is an indication of the geometric aspect of an interacting many-body system, plays a paramount role in a variety of disciplines [1–4]. In the mathematical front line of development, there exists a close relation for the coupling or recoupling coefficients of angular momenta with its various branches such as combinatorial analysis, special functions, calculus of finite difference, algebra and topology [5]. The investigation of their properties and relations should always have great implications or impact on those fields. For example, the Clebsch–Gordan coefficients, Racah coefficients and other coefficients are expressible in terms of generalized hypergeometric functions of many variables [1, 5, 6]. These functions are related to the discrete orthogonal polynomial, which has wide applications in areas from numerical analysis, to solutions of differential equation in physics, and to topological study. The applications of the vector coupling coefficients also abound in physical sciences including the fields of quantum chemistry and quantum molecular dynamics. The Clebsch–Gordan coefficients and Racah coefficients, for instance, are the basic mathematical apparatus in the formulation of rovibrational spectra, quantum scattering process and photodissociation dynamics for polyatomic molecules or molecular complexes [3, 7–9]. They are also very useful for the evaluation of molecular integrals in electronic structure calculation, where the primary basis functions are chosen to be the spherical harmonics or solid harmonics [10]. The myriad applications of coupling theory of quantum angular momentum in the traditional fields of atomic physics, nuclear physics and elementary particle physics are well known. A noticeable recent development is their role in the study of quantum integrable systems. One example is that the products of two wavefunctions for a Calogero–Sutherland system with a potential $v(x) = \sin^{-2} x$ are proved to be identical with the Clebsch–Gordan coefficients [11].

In most of the applications described above, the exact determination of angular momentum coupling and recoupling coefficients for all ranges of quantum angular momentum arguments is often very critical. In the first place, it is obvious that the domain of definition for these quantum numbers occurring in the coefficients should be the full range for the investigation in mathematical applications. Semiclassical limits of coupling and recoupling coefficients also play very important roles in modern physics. This includes the famous Ponzano and Regge's relation of the asymptotic 6-j symbols with the partition function for three-dimensional quantum gravity [12]. The Heisenberg correspondence limits or asymptotic approximations of these coefficients are also useful in the study of scattering cross section and Rydberg states of molecules [13, 14]. Furthermore, in quantum molecular scattering study for the chemical reactions, the angular momentum coupling coefficients naturally arise in the evaluation of interaction matrix elements between the channels corresponding to different chemical arrangements. When the collision energy increases, the channels with large angular momentum become energetically accessible, and the accurate computation of their coupling coefficients is important for a correct description of the chemical dynamic processes [15].

Recently, we have independently shown that all the 3-j, 6-j and 9-j symbols can be reformulated as a common combinatorial form by utilization of binomial coefficients [16]. The intrinsic structure of these symbols is found to be much nicer and simpler than thought before, which is simply the product of a polynomial and a square root of integer multiplication and division. This opens an avenue for the symbolic study of these symbols, and also lays the foundation for an exact, direct and fast numerical calculation or tabulation of each coupling or recoupling coefficient. In addition, it provides a convenient numerical approach for exactly locating all the structural and non-trivial zeros of angular momentum coupling or recoupling coefficients since these zeros can be determined exclusively by the polynomial part from our schemes. Although it is still an interesting work to identify their physical implication, a few non-trivial zeros do show obvious associated physical meaning [1].

This paper aims at a generalization of methods we developed previously for the work on the direct and exact calculation and tabulation of 3-j, 6-j and 9-j symbols to the case of $3n$-j ($n > 2$) symbols of the first kind and the second kind [16]. The concentration is more on the analysis of their intrinsic structure. In section 2, we begin with a review of the general theory about $3n$-j symbols, their calculation and their decomposition in particular. By utilizing the graphic technique, developed by Yutsis *et al* and via a definition of reduced

6-j symbols, we give a formal description and detailed proof about the statement that *all the* $3n$-j $(n > 2)$ *symbols of the first and second kinds can be factorized into a prefactor and an integer or a polynomial part*. The latter is simply the single sum over the products of reduced 6-j symbols. In section 3, we concretize our development in section 2 and give the calculation results for the 12-j symbols of the first kind. Section 4 is a discussion and conclusion.

2. Factorization of $3n$-j symbols with binomial coefficients

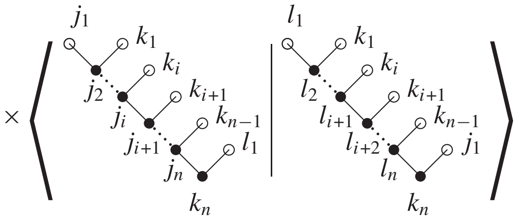
The angular momentum coupling leading to a total angular momentum of a composite system can be characterized by a binary tree. Each binary coupling scheme corresponds to a way for constructing the basis vectors for the tensor product Hilbert space. The general angular momentum recoupling coefficients $3n$-j for a system with $n + 1$ degrees of freedom are the unitary transformation matrix elements connecting these different pairwise and sequential angular momentum coupling schemes. These coefficients have been formulated in different manners including explicit algebraic expressions, the formulae in terms of Clebsch–Gordan coefficients or Racah coefficients, and graphic representations, etc, serving for different purposes [2]. From the computational point of view, however, the forms of these different expressions really matter considering the requirements of accuracy, efficiency or convenience for their practical evaluation. For example, the explicit algebraic expressions were most often used in numerical calculations in the early years. But it is well known that they suffer serious numerical instability and overflow or underflow are occurring issues. The recursive relations for the coupling or recoupling coefficients are used in the accurate calculation. However, it is not a direct and efficient approach either [17, 18]. Other methods based on the hyper-geometric series expansions or graphical techniques have been developed, but the programmes are usually too complicated to be practical. The representations of the general recoupling coefficients in terms of 6-j symbols are also employed for computation, but similar problems exist as for those using algebraic expressions [4]. Recently, we have developed an approach for direct and exact computation and tabulation of 3-j, 6-j and 9-j symbols for all ranges of angular momentum arguments. The calculation scheme is based on the reformulation of these symbols by utilization of binomial coefficients. The resulting formulae are simply the product of two factors, which lay the foundation for a symbolic study as well as for a direct and exact calculation of its numerical values. Furthermore, it gives a deeper understanding of the intrinsic structure of these coupling or recoupling coefficients, and establishes a link for the study with the other branches of the fields. Encouraged by this work, we believe that the statement that a recoupling coefficient can be factorized into an integer or a polynomial part times a multiplication of all the triangle relations appearing in the coefficient might generally hold for any number or any kind of angular momentum coupling. Motivated by getting a better understanding of their intrinsic structure including their connection to other fields, and giving a unified exact calculation scheme, it is very natural to extend previous work to the case of the general $3n$-j symbols.

In our previous work on the 3-j and 6-j symbols, the derivation is from their algebraic expressions. For 9-j symbols, however, the derivation is from their expression in terms of 6-j symbols rather than the explicit triple-sum formula. In fact, for the general $3n$-j $(n > 2)$ recoupling coefficients, which include 9-j symbols as a special case, there is a well-known fundamental theorem which states that they can be written as multiple sums over the products of 6-j symbols. The soundness of this theorem is based on the recognition that there are only two basic operations: commutation or association in the binary coupling theory which can transfer one binary coupling scheme to another. The operation of sequences of these two operations will either change the phase of basis vectors or introduce an additional factor of

Racah coefficients or 6-j symbols. From the derivation for 9-j symbols, it seems obvious that a general $3n$-j symbol can be reformulated in terms of reduced 6-j symbols defined in [16] similar to that for 9-j symbols. However, an unpleasant fact about these transformations is that there exist different paths from a given binary coupling scheme to another. In addition, what kind of actual form to which a recoupling coefficient can be reduced depends on the type of that coefficient. For the special types, the $3n$-j symbols of the first and second kinds, which are most commonly used and most important up to the present time, things look much more obvious and we do achieve our goals here.

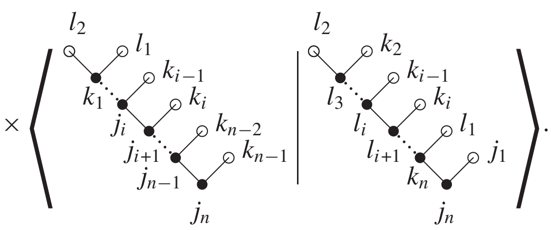
The $3n$-j symbols of the first kind are proportional to the unitary transformation matrix elements between two basis vectors associated with two different coupling schemes, defined by

$$\begin{Bmatrix} j_1 & & j_2 & & \cdots & j_n & \\ & k_1 & & k_2 & \cdots & & k_n \\ l_1 & & l_2 & & \cdots & l_n & \end{Bmatrix}_1 \equiv \frac{(-1)^{j_1+l_n-j_n-l_1}}{\left[\Pi_{\alpha=2}^{n}(2j_\alpha+1)(2l_\alpha+1)\right]^{1/2}} \tag{1}$$



where the phase and proportional coefficients are introduced so that the symbols possess the maximal symmetry. They contain the 6-j symbols and the 9-j symbols as special cases except for possible phase factors. Similarly, the $3n$-j symbols of the second kind are related to the transformation matrix elements between two different coupling schemes in the following way,

$$\begin{Bmatrix} j_1 & & j_2 & & \cdots & j_n & \\ & k_1 & & k_2 & \cdots & & k_n \\ l_1 & & l_2 & & \cdots & l_n & \end{Bmatrix}_2 \equiv \frac{(-1)^{j_2-j_1-k_1+k_n-l_n-l_1}}{\left[(k_1+1)(k_n+1)\Pi_{\alpha=2}^{n-1}(2j_\alpha+1)(2l_{\alpha+1}+1)\right]^{1/2}} \tag{2}$$



The study of their properties such as reduction is best performed through the graphical technique developed by Yutsis *et al* [19–23]. It merits a simple and clear presentation of angular momentum relations and facilitates their general analysis. In the graphical method, a general $3n$-j symbol is represented by a closed diagram or polygon with $3n$ line segments representing the angular momenta and the $2n$ vertices being their Clebsch–Gordan coupling coefficients. It is formed by combining the free ends of the line segments with the same angular momentum arguments for the coupling coefficients. For the reduction process we are studying, however, it is the opposite process, which corresponds to the separation of a diagram into its several sub-diagrams. Some rules have been developed guiding this decomposition, which can be classified into two types of situation. The first one is the case when the diagram is separable on one, two or three lines. The diagram can therefore be decomposed into two independent parts. The second one is the situation when the diagram is separable on four or more lines. The decomposition of this diagram will bring one or more summation indices, depending on the number of connected lines. The reduction process of an angular momentum diagram is a repeating and sequential application of the above rules. This also leads to the fundamental theorem in quantum angular momentum theory we mentioned earlier.

For the $3n$-j symbols of the first kind we are studying, their diagram is a Mobius band or a band *with* braiding, while the diagram for the second kind is a band *without* braiding as shown in [24]. The common feature of these diagrams is that after utilization of the orthogonal relation for the coupled states, which introduces a summation index, they both become ones separable on three lines. Repeating and sequential application of the rule for the diagram separable on three lines then leads to the complete reduction of the diagram, for example, for the $3n$-j symbols of the first kind, in terms of the diagrams for the 6-j symbols. Analytically, this process indicates the following relation,

$$\begin{Bmatrix} j_1 & & j_2 & & \dots & j_n & \\ & k_1 & & k_2 & \dots & & k_n \\ l_1 & & l_2 & & \dots & l_n & \end{Bmatrix}_1 = \sum_x (-1)^{S+(n-1)x}(2x+1) \begin{Bmatrix} j_1 & l_1 & x \\ l_2 & j_2 & k_1 \end{Bmatrix}$$
$$\times \begin{Bmatrix} j_2 & l_2 & x \\ l_3 & j_3 & k_2 \end{Bmatrix} \dots \begin{Bmatrix} j_{n-1} & l_{n-1} & x \\ l_n & j_n & k_{n-1} \end{Bmatrix} \begin{Bmatrix} j_n & l_n & x \\ j_1 & l_1 & k_n \end{Bmatrix} \tag{3}$$

which is just the single sum over the products of 6-j symbols. The same procedure also yields the relation for the $3n$-j symbols of the second kind,

$$\begin{Bmatrix} j_1 & & j_2 & & \dots & j_n & \\ & k_1 & & k_2 & \dots & & k_n \\ l_1 & & l_2 & & \dots & l_n & \end{Bmatrix}_2 = \sum_x (-1)^{S+nx}(2x+1) \begin{Bmatrix} j_1 & l_1 & x \\ l_2 & j_2 & k_1 \end{Bmatrix}$$
$$\times \begin{Bmatrix} j_2 & l_2 & x \\ l_3 & j_3 & k_2 \end{Bmatrix} \dots \begin{Bmatrix} j_{n-1} & l_{n-1} & x \\ l_n & j_n & k_{n-1} \end{Bmatrix} \begin{Bmatrix} j_n & l_n & x \\ l_1 & j_1 & k_n \end{Bmatrix} \tag{4}$$

where

$$S = \sum_{i=1}^{n} (j_i + k_i + l_i). \tag{5}$$

Two points are noticeable in the above diagram decomposition. First, any triangle relation arising from the diagram separation will always appear in both separated parts. Second, for the $3n$-j symbols of the first and second kinds, all the 6-j symbols are symmetric in the sense that summation is single fold and only one summation index appears in each of the 6-j symbols. These are critical in the current reformulation.

Now, we define an integer factor or polynomial by

$$\begin{bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{bmatrix} \equiv \sum_k (-1)^k \begin{pmatrix} k+1 \\ k-j_1-j_2-j_3 \end{pmatrix} \begin{pmatrix} j_1+j_2-j_3 \\ k-j_3-j_4-j_5 \end{pmatrix}$$
$$\times \begin{pmatrix} j_1-j_2+j_3 \\ k-j_2-j_4-j_6 \end{pmatrix} \begin{pmatrix} -j_1+j_2+j_3 \\ k-j_1-j_5-j_6 \end{pmatrix} \tag{6}$$

which is the sum over the products of four binomial coefficients. It relates to the 6-j symbol in the following way,

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix} = \frac{\Delta(j_3j_4j_5)\Delta(j_2j_4j_6)\Delta(j_1j_5j_6)}{\Delta(j_1j_2j_3)} \begin{bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{bmatrix}. \tag{7}$$

It is simply the polynomial part of the 6-j symbol but nevertheless has its full symmetry. In addition, the triangle relation appearing in the denominator can be any one of the four triangle relations for the 6-j symbol. Because of its status as a fundamental building block in all following formulation, we call it the *reduced* 6-j *symbol*. Substitution of equation (7) into equation (3) or (4) yields the following two formulae,

$$\begin{Bmatrix} j_1 & & j_2 & & \cdots & j_n & \\ & k_1 & & k_2 & \cdots & & k_n \\ l_1 & & l_2 & & \cdots & l_n & \end{Bmatrix}_1 = \Delta(j_1j_2k_1)\Delta(l_2l_1k_1)\Delta(j_2j_3k_2)\Delta(l_3l_2k_2)$$
$$\times\cdots\times\Delta(j_{n-1}j_nk_{n-1})\Delta(l_nl_{n-1}k_{n-1})\Delta(j_nl_1k_n)\Delta(j_1l_nk_n)$$
$$\times\begin{bmatrix} j_1 & & j_2 & & \cdots & j_n & \\ & k_1 & & k_2 & \cdots & & k_n \\ l_1 & & l_2 & & \cdots & l_n & \end{bmatrix}_1 \tag{8}$$

where

$$\begin{bmatrix} j_1 & & j_2 & & \cdots & j_n & \\ & k_1 & & k_2 & \cdots & & k_n \\ l_1 & & l_2 & & \cdots & l_n & \end{bmatrix}_1 \equiv \sum_x (-1)^{S+(n-1)x}(2x+1)\begin{bmatrix} j_1 & l_1 & x \\ l_2 & j_2 & k_1 \end{bmatrix}$$
$$\times\begin{bmatrix} j_2 & l_2 & x \\ l_3 & j_3 & k_2 \end{bmatrix}\cdots\begin{bmatrix} j_{n-1} & l_{n-1} & x \\ l_n & j_n & k_{n-1} \end{bmatrix}\begin{bmatrix} j_n & l_n & x \\ j_1 & l_1 & k_n \end{bmatrix} \tag{9}$$

and

$$\begin{Bmatrix} j_1 & & j_2 & & \cdots & j_n & \\ & k_1 & & k_2 & \cdots & & k_n \\ l_1 & & l_2 & & \cdots & l_n & \end{Bmatrix}_2 = \Delta(j_1j_2k_1)\Delta(l_2l_1k_1)\Delta(j_2j_3k_2)\Delta(l_3l_2k_2)$$
$$\times\cdots\times\Delta(j_{n-1}j_nk_{n-1})\Delta(l_nl_{n-1}k_{n-1})\Delta(j_nl_1k_n)\Delta(j_1l_nk_n)$$
$$\times\begin{bmatrix} j_1 & & j_2 & & \cdots & j_n & \\ & k_1 & & k_2 & \cdots & & k_n \\ l_1 & & l_2 & & \cdots & l_n & \end{bmatrix}_2 \tag{10}$$

where

$$\begin{bmatrix} j_1 & & j_2 & & \cdots & j_n & \\ & k_1 & & k_2 & \cdots & & k_n \\ l_1 & & l_2 & & \cdots & l_n & \end{bmatrix}_2 \equiv \sum_x (-1)^{S+nx}(2x+1)\begin{bmatrix} j_1 & l_1 & x \\ l_2 & j_2 & k_1 \end{bmatrix}$$
$$\times\begin{bmatrix} j_2 & l_2 & x \\ l_3 & j_3 & k_2 \end{bmatrix}\cdots\begin{bmatrix} j_{n-1} & l_{n-1} & x \\ l_n & j_n & k_{n-1} \end{bmatrix}\begin{bmatrix} j_n & l_n & x \\ l_1 & j_1 & k_n \end{bmatrix}. \tag{11}$$

Equations (8)–(11) constitute the final results of this section. By utilization of binomial coefficients, the $3n$-j ($n > 2$) symbols of the first and second kinds are now in a separated form with one factor being the product of all the triangle relations occurring in the symbol, and the other being an integer or polynomial. It is in the form of a *two*-fold summation, and the corresponding actual polynomial form is a topic for further study.

It should be mentioned that the graphical technique of Yutsis *et al* utilized here for the angular momentum coupling has proved to be a powerful tool in the theory for quantum many-body particles in general. In recent years, for instance, some researchers have employed it for the study of complex spectra [25]. Extended to the approach of unitary group $U(n)$ from $SU(2)$, they not only use the graphical technique for the coupling of states but also for the representation of matrix elements of the generators and their product. Similar rules for the graphical decomposition have also been developed. In addition, the factorization of the matrix elements of the generator product via the graphical decomposition rules has been achieved even though it is for different purposes and in different contexts.

3. Examples: 12-j symbols of the first kind

As an illustration of the power of the methods and algorithms discussed previously for the reformulation and exact calculation of angular momentum recoupling coefficients, we present the results for the 12-j symbols of the first kind. The 12-j symbols arise in the recoupling of five angular momenta [2, 24, 26, 27]. They are related to the theory of the fractional parentage coefficients (fpc), which are used, for example, in the construction of wavefunctions for N identical particles and for the evaluation of their matrix elements for operators from the counterparts for $N-1$ identical particles coupled with one more particle [28]. Recently, it was found that the well-known Ponzano and Regge's formula, which connects the asymptotic form of the Racah–Wigner 6-j symbols with the partition function for three-dimensional quantum gravity mentioned at the beginning, can be extended to the physically significant four-dimensional case by utilization of the 12-j symbols [29]. There are five distinct types of abstract cubic graphs associated with the coupling of five angular momenta. However, three of those correspond to the recoupling coefficients which can be directly factorized into the products of 6-j symbols or 9-j symbols according to the rules for the first case discussed in the previous section. Therefore, the actual number of 12-j symbols is two [1, 2]. The 12-j symbols of the first kind, for example, are the transformation of the following two coupling schemes,

$$\begin{Bmatrix} j_1 & & j_6 & & j_7 & & j_8 & \\ & j_2 & & j_3 & & j_4 & & j \\ j_5 & & j_6' & & j_7' & & j_8' & \end{Bmatrix}_1 \equiv \frac{(-1)^{j_1-j_5-j_8+j_8'}}{[(2j_6+1)(2j_7+1)(2j_8+1)(2j_6'+1)(2j_7'+1)(2j_8'+1)]^{1/2}} \times \langle\{[\langle(j_1j_2)j_6, j_3\rangle j_7, j_4]j_8, j_5\}j|\{[\langle(j_5j_2)j_6', j_3\rangle j_7', j_4]j_8', j_1\}j\rangle. \tag{12}$$

From the results of the last section, they can be formulated in the factorized form as follows,

$$\begin{Bmatrix} j_1 & & j_6 & & j_7 & & j_8 & \\ & j_2 & & j_3 & & j_4 & & j \\ j_5 & & j_6' & & j_7' & & j_8' & \end{Bmatrix}_1 = \Delta(j_1j_2j_6)\Delta(j_6j_3j_7)\Delta(j_7j_4j_8)\Delta(j_8j_5j) \times\Delta(j_5j_2j_6')\Delta(j_6'j_3j_7')\Delta(j_7'j_4j_8')\Delta(j_8'j_1j) \times\begin{bmatrix} j_1 & & j_6 & & j_7 & & j_8 & \\ & j_2 & & j_3 & & j_4 & & j \\ j_5 & & j_6' & & j_7' & & j_8' & \end{bmatrix}_1 \tag{13}$$

Table 1. A table of 12-j symbols and corresponding decimal values.

$\left\{\begin{matrix} j_1 & & j_6 & & j_7 & & j_8 & \\ & j_2 & & j_3 & & j_4 & & j \\ j_5 & & j_6' & & j_7' & & j_8' & \end{matrix}\right\}$	Tabulation	Exact decimal values
$\left\{\begin{matrix} 0 & & 1 & & 1 & & 1 & \\ & 1 & & 1 & & 0 & & 1 \\ 1 & & 1 & & 1 & & 1 & \end{matrix}\right\}$	$2^4 3^{-6} \times (1)$	0.148 148 148 148 148
$\left\{\begin{matrix} 1 & & 1 & & 2 & & 2 & \\ & 2 & & 2 & & 2 & & 1 \\ 1 & & 2 & & 1 & & 2 & \end{matrix}\right\}$	$-2^{-2} 3^{-3} 5^{-8} 7^{-1} 89^2 \times (1)$	$-5.179\,037\,928\,267\,551 \times 10^{-3}$
$\left\{\begin{matrix} 2 & & 1 & & 2 & & 1 & \\ & 2 & & 2 & & 1 & & 2 \\ 1 & & 1 & & 2 & & 2 & \end{matrix}\right\}$	$2^{-6} 3^1 5^{-8} 7^1 41^2 \times (1)$	$3.757\,712\,069\,863\,789 \times 10^{-2}$
$\left\{\begin{matrix} 3 & & 3 & & 5 & & 4 & \\ & 2 & & 4 & & 5 & & 3 \\ 4 & & 2 & & 4 & & 5 & \end{matrix}\right\}$	$-2^{-14} 3^{-16} 5^{-7} 7^{-10}$ $\times 11^{-6} 13^{-3} 743^2$ $\times (471, 15\,204, 19\,117)$	$-1.528\,195\,512\,735\,275 \times 10^{-3}$
$\left\{\begin{matrix} 4 & & 3 & & 5 & & 6 & \\ & 3 & & 5 & & 6 & & 4 \\ 2 & & 4 & & 3 & & 5 & \end{matrix}\right\}$	$3^{-14} 5^{-2} 7^{-2} 11^{-7}$ $\times 13^{-6} 17^{-1}$ $\times (20\,891, 18\,501)$	$2.236\,532\,215\,249\,387 \times 10^{-4}$
$\left\{\begin{matrix} 5 & & 5 & & 4 & & 3 & \\ & 6 & & 4 & & 6 & & 4 \\ 2 & & 4 & & 7 & & 5 & \end{matrix}\right\}$	$2^{-16} 3^{-6} 5^3 7^{-7} 11^{-5}$ $\times 13^{-5} 19^1 109^1 521^2$ $\times (2467)$	$-4.451\,211\,337\,906\,913 \times 10^{-3}$
$\left\{\begin{matrix} 6 & & 4 & & 7 & & 4 & \\ & 2 & & 5 & & 7 & & 6 \\ 4 & & 5 & & 6 & & 3 & \end{matrix}\right\}$	$2^{-1} 3^{-8} 5^{-3} 7^{-6} 11^{-6}$ $\times 13^{-7} 17^{-2} 19^{-1}$ $\times (10\,963, 3214, 29\,879)$	$3.429\,876\,771\,358\,886 \times 10^{-2}$
$\left\{\begin{matrix} 7 & & 8 & & 9 & & 10 & \\ & 8 & & 6 & & 4 & & 6 \\ 7 & & 9 & & 7 & & 5 & \end{matrix}\right\}$	$-2^{-30} 3^{-3} 5^3 7^{-3} 11^{-9}$ $\times 13^{-5} 17^{-8} 19^{-7}$ $\times 23^{-6} 41^2 1153^2$ $\times (3297, 6491, 22\,005,$ $\times 31\,646, 20\,367)$	$-0.708\,747\,948\,235\,219$
$\left\{\begin{matrix} 10 & & 7 & & 8 & & 6 & \\ & 9 & & 10 & & 6 & & 8 \\ 7 & & 9 & & 10 & & 7 & \end{matrix}\right\}$	$-2^7 3^{-7} 5^{-9} 7^{-3} 11^{-7}$ $\times 13^{-11} 17^{-8} 19^{-8} 29^1 47^2$ $\times 179^2 \times (42, 6600,$ $\times 31\,323, 17\,916, 4465)$	$-0.320\,311\,506\,498\,916$
$\left\{\begin{matrix} 20 & & 15 & & 9 & & 10 & \\ & 14 & & 18 & & 15 & & 15 \\ 9 & & 8 & & 10 & & 12 & \end{matrix}\right\}$	$2^3 3^{-13} 5^{-19} 7^{-3} 11^{-5}$ $\times 17^{-6} 19^1 23^{-4} 29^{-8}$ $\times 31^{-8} 37^{-1} 41^{-1} 43^{-1}$ $\times 263^2 \times (20\,491, 6148,$ $\times 19\,764, 6941)$	$1.315\,510\,402\,031\,053 \times 10^{-13}$

where the integer or polynomial part is the sum over products of reduced 6-j symbols defined by

$$\left[\begin{matrix} j_1 & & j_6 & & j_7 & & j_8 & \\ & j_2 & & j_3 & & j_4 & & j \\ j_5 & & j_6' & & j_7' & & j_8' & \end{matrix}\right]_1 = \sum_x (-1)^{S-x}(2x+1) \begin{bmatrix} j_1 & j_5 & x \\ j_6' & j_6 & j_2 \end{bmatrix} \times \begin{bmatrix} j_6 & j_6' & x \\ j_7' & j_7 & j_3 \end{bmatrix} \begin{bmatrix} j_7 & j_7' & x \\ j_8' & j_8 & j_4 \end{bmatrix} \begin{bmatrix} j_8 & j_8' & x \\ j_1 & j_5 & j \end{bmatrix} \quad (14)$$

Table 2. Ten examples of structural or accidental zeros of 12-j symbols with small angular momentum arguments.

$\begin{Bmatrix} j_1 & & j_6 & & j_7 & & j_8 & \\ & j_2 & & j_3 & & j_4 & & j \\ j_5 & & j_6' & & j_7' & & j_8' & \end{Bmatrix}$	$\begin{Bmatrix} j_1 & & j_6 & & j_7 & & j_8 & \\ & j_2 & & j_3 & & j_4 & & j \\ j_5 & & j_6' & & j_7' & & j_8' & \end{Bmatrix}$
$\begin{Bmatrix} 3 & & 2 & & 2 & & 2 & \\ & 2 & & 1 & & 0 & & 3 \\ 2 & & 1 & & 0 & & 0 & \end{Bmatrix}$	$\begin{Bmatrix} 2 & & 3 & & 2 & & 2 & \\ & 2 & & 2 & & 0 & & 2 \\ 1 & & 2 & & 0 & & 0 & \end{Bmatrix}$
$\begin{Bmatrix} 2 & & 2 & & 3 & & 3 & \\ & 1 & & 2 & & 0 & & 2 \\ 2 & & 2 & & 0 & & 0 & \end{Bmatrix}$	$\begin{Bmatrix} 2 & & 2 & & 1 & & 1 & \\ & 3 & & 2 & & 0 & & 2 \\ 2 & & 2 & & 0 & & 0 & \end{Bmatrix}$
$\begin{Bmatrix} 2 & & 1 & & 2 & & 2 & \\ & 2 & & 2 & & 0 & & 2 \\ 3 & & 2 & & 0 & & 0 & \end{Bmatrix}$	$\begin{Bmatrix} 1 & & 2 & & 2 & & 2 & \\ & 2 & & 3 & & 0 & & 1 \\ 2 & & 3 & & 0 & & 0 & \end{Bmatrix}$
$\begin{Bmatrix} 3 & & 2 & & 2 & & 2 & \\ & 2 & & 0 & & 1 & & 3 \\ 2 & & 1 & & 1 & & 0 & \end{Bmatrix}$	$\begin{Bmatrix} 3 & & 2 & & 1 & & 2 & \\ & 2 & & 1 & & 1 & & 3 \\ 2 & & 1 & & 1 & & 0 & \end{Bmatrix}$
$\begin{Bmatrix} 3 & & 2 & & 2 & & 2 & \\ & 2 & & 1 & & 1 & & 3 \\ 2 & & 1 & & 1 & & 0 & \end{Bmatrix}$	$\begin{Bmatrix} 3 & & 2 & & 3 & & 2 & \\ & 2 & & 1 & & 1 & & 3 \\ 2 & & 1 & & 1 & & 0 & \end{Bmatrix}$
$\begin{Bmatrix} 3 & & 2 & & 1 & & 2 & \\ & 2 & & 2 & & 1 & & 3 \\ 2 & & 1 & & 1 & & 0 & \end{Bmatrix}$	$\begin{Bmatrix} 3 & & 2 & & 2 & & 2 & \\ & 2 & & 2 & & 1 & & 3 \\ 2 & & 1 & & 1 & & 0 & \end{Bmatrix}$
$\begin{Bmatrix} 3 & & 2 & & 3 & & 2 & \\ & 2 & & 2 & & 1 & & 3 \\ 2 & & 1 & & 1 & & 0 & \end{Bmatrix}$	$\begin{Bmatrix} 2 & & 3 & & 2 & & 2 & \\ & 2 & & 2 & & 1 & & 2 \\ 0 & & 2 & & 1 & & 0 & \end{Bmatrix}$
$\begin{Bmatrix} 1 & & 3 & & 2 & & 2 & \\ & 2 & & 2 & & 1 & & 1 \\ 1 & & 2 & & 1 & & 0 & \end{Bmatrix}$	$\begin{Bmatrix} 1 & & 3 & & 2 & & 2 & \\ & 3 & & 2 & & 1 & & 1 \\ 1 & & 2 & & 1 & & 0 & \end{Bmatrix}$
$\begin{Bmatrix} 2 & & 3 & & 2 & & 2 & \\ & 2 & & 1 & & 1 & & 2 \\ 1 & & 2 & & 1 & & 0 & \end{Bmatrix}$	$\begin{Bmatrix} 2 & & 3 & & 3 & & 2 & \\ & 2 & & 1 & & 1 & & 2 \\ 1 & & 2 & & 1 & & 0 & \end{Bmatrix}$
$\begin{Bmatrix} 2 & & 3 & & 2 & & 2 & \\ & 1 & & 2 & & 1 & & 2 \\ 1 & & 2 & & 1 & & 0 & \end{Bmatrix}$	$\begin{Bmatrix} 2 & & 3 & & 1 & & 2 & \\ & 2 & & 2 & & 1 & & 2 \\ 1 & & 2 & & 1 & & 0 & \end{Bmatrix}$

where the S, as defined before, is the sum of all 12 angular momentum arguments. It is a function of all 12 angular momentum arguments. However, unlike the cases for the rotation matrices and 3-j and 6-j symbols, the actual form of the corresponding polynomial with the defined arguments is unknown. As already demonstrated, the rotational matrices are expressible in terms of the Jacobi polynomial [1], the 3-j symbols are proportional to the Hahn polynomial [5] and the 6-j symbols are related to the Racah polynomial [5]. The polynomial that the 9-j symbols correspond to and is expressible as an orthogonal one in two discrete variables has been identified [30]. Nevertheless, it is expected that the same level of theory as those for the 3-j and 6-j symbols can be developed also for the 9-j symbols [30, 31].

Having rewritten the 12-j symbols of the first kind in the desired form, we are now in a position to calculate and tabulate their numerical values. One of the major advantages in our formulation is in the realization of a *direct* and *exact* calculation and tabulation of *all* recoupling coefficients of the first and second kinds for *all* ranges of angular momentum arguments. In the summation step, we have developed a series of algebraic operation routines for large integer, where integer algebraic addition and multiplication are performed in a basis of 32 768. The array for the integer is arranged in order of increasing power so that the rounding-off error can be avoided when converting to the decimal values and final results are exact. In addition, we evaluate binomial coefficients recursively rather than doing the calculation by definition. This avoids the numerical errors from computation while increasing the efficiency of computation. In table 1, we list a table of 12-j symbols and corresponding decimal values.

The structural zeros and accidental zeros of the 12-j symbols can also be easily and safely determined by our schemes, which are just the zeros of the corresponding integer or polynomial part. Obviously, exploration of the mathematical or physical meaning of these zeros should be an interesting and valuable investigation. We list in table 2 some of the structural or accidental zeros in order that future researchers might have a comparative study.

4. Discussion and conclusion

In this paper, we have factorized the $3n$-j symbols of the first and second kinds in a form which is a prefactor times an integer or a polynomial. The immediate benefit of this reformulation is that, when combined with our developed algorithms, it provides an analytical foundation for a direct, exact and fast calculation of all the $3n$-j symbols of the first and second kinds. It also gives a convenient and exact approach for determining all their structural or accidental zeros. It is really very significant considering their wide applications in a variety of fields.

Furthermore, from the analytical point of view, the reformulation indicates a simpler algebraic structure for the recoupling coefficients which will serve as a bridge for the study with other fields. The actual form of the integer or polynomial part with identified arguments needs to be explored. Their properties including the relations to the other areas are expected to be investigated.

Just like the case when the building block for recoupling coefficients has been changed from the fundamental Clebsch–Gordan coefficients to the Racah coefficients which is indicated in the fundamental theorem of quantum angular momentum, it is also a surprise that the reduced 6-j symbol, as we have defined it, can serve as a similar building block for the $3n$-j symbols of the first and second kinds, where the general relation with a polynomial has been established. Nevertheless, for the general recoupling coefficients, which cover the cases of the third or higher kinds, things do not look so clear. The endeavour to explore the similar structure seems elusive. Even though we can always transfer a $3n$-j symbol to the multiple sum over the products of 6-j symbols, it is by no means obvious that we might reformulate it as the multiple sum over the products of reduced 6-j symbols with one factor being an integer or polynomial. What kind of role does the binomial coefficient play in the current reformulation? What is the building block for all the recoupling coefficients when they have the desired factorization? These are the questions to be answered. We have more discoveries to make and we will have more to understand about their intrinsic structure.

Acknowledgments

This work was partially supported by the National Science Foundation through a grant for the Institute for Theoretical Atomic, Molecular and Optical Physics at Harvard University and Smithsonian Astrophysical Observatory. The authors would like to thank the referees for pointing out the work cited in [25, 30].

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