JOURNAL OF COMPUTATIONAL PHYSICS **139,** 137–165 (1998)
ARTICLE NO. CP975867

Efficient Evaluation of Vector Translation Coefficients in Multiparticle Light-Scattering Theories

Yu-lin Xu

Department of Astronomy, P.O. Box 112055, University of Florida, Gainesville, Florida 32611-2055
E-mail: shu@astro.ufl.edu

Received May 15, 1997; revised October 1, 1997

Vector addition theorems are a necessary ingredient in the analytical solution of electromagnetic multiparticle-scattering problems. These theorems include a large number of vector addition coefficients. There exist three basic types of analytical expressions for vector translation coefficients: Stein's (*Quart. Appl. Math*. **19**, 15 (1961)), Cruzan's (*Quart. Appl. Math*. **20**, 33 (1962)), and Xu's (*J. Comput. Phys*. **127**, 285 (1996)). Stein's formulation relates vector translation coefficients with scalar translation coefficients. Cruzan's formulas use the Wigner 3jm symbol. Xu's expressions are based on the Gaunt coefficient. Since the scalar translation coefficient can also be expressed in terms of the Gaunt coefficient, the key to the expeditious and reliable calculation of vector translation coefficients is the fast and accurate evaluation of the Wigner 3jm symbol or the Gaunt coefficient. We present highly efficient recursive approaches to accurately evaluating Wigner 3jm symbols and Gaunt coefficients. Armed with these recursive approaches, we discuss several schemes for the calculation of the vector translation coefficients, using the three general types of formulation, respectively. Our systematic test calculations show that the three types of formulas produce generally the same numerical results except that the algorithm of Stein's type is less accurate in some particular cases. These extensive test calculations also show that the scheme using the formulation based on the Gaunt coefficient is the most efficient in practical computations.

Key Words: electromagnetic multiparticle-scattering; vector spherical harmonics; vector addition theorems; vector translation coefficients; Wigner 3jm symbols; Gaunt coefficients; computational efficiency; computational method.

I. INTRODUCTION

Vector translational addition theorems are a useful analytic tool to translate a multipole expansion of an electromagnetic field from one to an other coordinate system. These theorems have many practical applications in the solution to various scientific problems involving multiple sources or multiple particles, including electromagnetic multiparticle-scattering problems. Use of these theorems introduces a large number of vector translation coefficients [1, 2]. In multisphere light-scattering calculations, the vector translation coefficients appear in a linear system as the coefficients of unknown partial interactive scattering coefficients of each individual spheres [3–7]. These addition coefficients are also required in the determination of the scattering cross section and asymmetry parameter of an arbitrary multiparticle configuration [8]. Starting with the work by Stein [1] and Cruzan [2] in early 1960s, considerable efforts have been devoted to the formulation and evaluation of these vector addition coefficients.

Vector translation coefficients have basically three forms of analytical expressions in terms of the scalar translation coefficient [9], the Wigner 3jm symbol [10], and the Gaunt coefficient [11], respectively. Stein [1] showed that vector translation coefficients can be evaluated from pertinent scalar translation coefficients. Kim [12] and Mackowski [13] derived their own expressions of Stein's type. Cruzan [2] formulated the translation coefficients using the Wigner 3jm symbol. Xu [14] provided a set of expressions in terms of the Gaunt coefficient. As shown in the present paper, all these three types of formulas are equivalent in view of numerical results. Making use of the formulas of Stein's type, one needs to compute relevant scalar translation coefficients, which, in turn, calls for the evaluation of the related Gaunt coefficients. Implementation of Xu's formulas requires also the computation of the Gaunt coefficient. The use of Cruzan's formulas demands the evaluation of the Wigner 3jm symbol. An adequate numerical technique for the evaluation of the Wigner 3jm symbol or the Gaunt coefficient is thus of key importance to obtaining reliable numerical values of vector translation coefficients in practical scattering calculations.

The Wigner 3jm symbol, one of the angular momentum coupling coefficients extensively used in quantum mechanics, is defined by [15, 16]

$$\begin{aligned}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} &= (-1)^{j_1+j_2+m_3} \\ &\times \left[\frac{(j_1-m_1)!(j_1+m_1)!(j_2-m_2)!(j_2+m_2)!(j_3-m_3)!(j_3+m_3)!}{(j_1+j_2-j_3)!(j_1-j_2+j_3)!(-j_1+j_2+j_3)!(j_1+j_2+j_3+1)!}\right]^{1/2} \\ &\times \sum_{k=k_{\min}}^{k_{\max}} (-1)^k \begin{pmatrix} j_1+j_2-j_3 \\ k \end{pmatrix} \begin{pmatrix} j_1-j_2+j_3 \\ j_1-m_1-k \end{pmatrix} \begin{pmatrix} -j_1+j_2+j_3 \\ j_2+m_2-k \end{pmatrix}, \end{aligned} \tag{1}$$

where $\binom{j}{k}$ represents the binomial coefficient, and

$$k_{\min} = \max(0,\, j_2 - j_3 - m_1,\, j_1 - j_3 + m_2), \tag{2}$$

$$k_{\max} = \min(j_1 + j_2 - j_3,\, j_1 - m_1,\, j_2 + m_2). \tag{3}$$

The Wigner 3jm symbol (or called the Wigner 3jm coefficient) vanishes unless $m_1 + m_2 + m_3 = 0$ and j_3 satisfies the triangle condition $j_{3_{\min}} \le j_3 \le j_1 + j_2$, where $j_{3_{\min}} = \max(|j_1 - j_2|, |m_1 + m_2|)$. For the evaluation of Wigner 3jm symbols, there are several published computer programs, which provide numerical results either in exact numerical expressions or in decimal approximations. The former includes the computer codes written by Lai and Chiu [16] and by Fang and Shriner [17], which are designed to evaluate the

Wigner 3jm symbol individually and to express the numerical result in an integer prime-factor and rational-fraction form. These programs are excellent whenever an exact numerical expression is needed and the involved j-value is not large. But this kind of programs is not suitable for the general use in multiparticle-scattering calculations because its purpose is not for an extensive use in a simultaneous calculation of a large number of the coefficients, especially when large j-values are involved. Fang and Shriner's program overflows at large j-values and Lai and Chiu's program switches to decimal approximations when $j > 30$. Nearly all existing computer codes, including Lai and Chiu's, Fang and Shriner's, and those in decimal approximations, are based on the direct use of Eq. (1). This causes an accuracy problem when the value of j is not small. In practical calculations, no matter what numerical representation is used, this direct use of the definition equation must evaluate the sum over k. This summation occurred in Eq. (1) takes all values of k for which the factorial arguments are nonnegative. It implies delicate cancellations between successive terms that alternate in sign. For large j-values, the individual terms in the summation become much larger than their sum and the accuracy of their sum will be very poor. Also, direct evaluation of factorials and binomial coefficients in each term of an individual k will easily cause an overflow. The only exception from this method of direct calculation seems to be the work by Schulten and Gordon [18, 19]. These two authors derived a very useful recurrence relation and provided a recursion scheme for the evaluation of the 3jm symbols [19]. Their recursive approach proceeds with an arbitrary starting value in both forward and backward recursions. Matching an intermediate 3jm symbol in the forward and backward recursion series leaves all values of the group of 3jm symbols off by a constant factor. This factor is then determined by the unitary property of Wigner 3jm symbols and the phase convention. Schulten and Gordon's work is an important example showing that recursive evaluation of Wigner 3jm symbols is practically feasible. Recursive approach is much more efficient and more accurate than the method of direct calculation. Based on the recurrence relation formulated by Schulten and Gordon, we devise a recursion scheme that allows one to fast and accurately evaluate Wigner 3jm symbols.

The Gaunt coefficient is closely related to the Wigner 3jm symbol and defined by [11]

$$a(m, n, \mu, \nu, p) = \frac{(2p+1)}{2}\frac{(p-m-\mu)!}{(p+m+\mu)!}\int_{-1}^{1} P_n^m(x)P_\nu^\mu(x)P_p^{m+\mu}(x)\,dx, \tag{4}$$

where m, n, μ, ν, p are integers, $|m| \le n$, $|\mu| \le \nu$, P_n^m represents the associated Legendre function of the first kind. Cruzan's formula [2] relating the Gaunt coefficient and the 3jm symbol is

$$a(m, n, \mu, \nu, p) = (-1)^{m+\mu}(2p+1)\left[\frac{(n+m)!(\nu+\mu)!(p-m-\mu)!}{(n-m)!(\nu-\mu)!(p+m+\mu)!}\right]^{1/2} \times \begin{pmatrix} n & \nu & p \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} n & \nu & p \\ m & \mu & -m-\mu \end{pmatrix}. \tag{5}$$

Gaunt coefficients can be either directly calculated using Eq. (5) with an appropriate algorithm to compute Wigner 3jm symbols or recursively evaluated by their recurrence relations. Bruning and Lo [3] published a three-term recurrence relation for some particular Gaunt coefficients with $\mu = -m$. Bruning [20] and Fuller [21] tried to derive general recurrence relations. Recently, Xu [22] devised an algorithm for the fast evaluation of Gaunt coefficients by solving a lower triangular linear system. The linearization algorithm has been further developed to a general recursion scheme [23]. The present paper discusses this recursion scheme and systematically compares its numerical results with those from Cruzan's 3jm formula Eq. (5). Our extensive numerical tests show that the numerical results from both methods are in excellent agreement. But the recursive approach is more time-effective, especially for the computation of a large number of Gaunt coefficients in multiparticle light-scattering calculations.

With Wigner 3jm symbols and Gaunt coefficients evaluated with satisfactory accuracy, vector translation coefficients can be computed using either one of the existing analytical expressions. Our systematic numerical tests indicate that the three basic types of formulas provide in general the same numerical results. Only in some particular cases, Stein's algorithm, which is based on the scalar translation coefficient, is less accurate. In [13], Mackowski provided an indirect recursion scheme for the calculation of scalar translation coefficients, which has been also discussed in detail in [14]. Numerical results from Mackowski's formulas, which are of Stein's type, and his indirect recursive approach to evaluating scalar translation coefficients are also in good agreement with those from the schemes using Stein's, Cruzan's, and Xu's formulas. However, there is literature containing a conclusion that one of Cruzan's formulas is incorrect. In addition to the experimental validation by Xu and Gustafson [24], we demonstrate here by our test calculations that, although one of the two equations for the two classes of vector translation coefficients needs some clarification, Cruzan's overall formulation is right, indeed.

II. RECURSIVE EVALUATION OF WIGNER 3jm SYMBOLS

Wigner 3jm symbols can be evaluated, in principle, directly from Eq. (1). It seems that, to date, the main stream of existing computer codes has been following this method of direct calculation. This is, however, probably not a good approach in practical calculations unless the involved j-values are small. In this section, we present a useful recursion scheme capable of computing accurately Wigner 3jm symbols from low to very high j-values. This recursion scheme is stable, accurate, and highly efficient.

A. *Exact Numerical Expression*

As Eq. (1) shows explicitly, numerical values of Wigner 3jm symbols can be expressed exactly in terms of prime factors since the square of each 3jm symbol is rational. Any rational number can be specified by two integers and every positive integer has a unique factorization to primes. In practical programming the rational-fraction and prime-factor method can be implemented by an array containing the exponents of the prime factors and the phase. Lai and Chiu [16] express the numerical value of a 3jm symbol by a sign and two arrays. One array stores the prime factors and the other stores the corresponding powers of each prime number. Fang and Shriner [17] use the form of $(a/b)\sqrt{c/d}$, where a, b, c, and d are integers. Readers are referred to Refs. [16, 17, 25] for the detailed description of the exact calculation of the 3jm symbols. In practical calculations, the largest j-value, for which an exact numerical expression for the 3jm symbol can be obtained, is limited by the length of computer word in use. When the exact numerical value of some quantity in manipulation exceeds the number of digits that a computer word can represent, the truncation error introduces a certain degree of approximation. Problems also occur when performing the summation over k. The overflow problem hampers Fang and Shriner's program in going to large j-values. Lai and Chiu's program switches to decimal approximations when $j > 30$. Lai and Chiu's program is written in quadruple-precision and demands significantly more computing time than lower precision arithmetic. Although Lai and Chiu's program works well for fairly large j-values, similar to other existing programs, it also loses accuracy when computing the sum over k. Because Lai and Chiu's and Fang and Shriner's programs are designed to calculate the 3jm symbol separately and do not make use of relationships between the values of contiguous coefficients, they are too time-consuming for the extensive use in multiparticle-scattering calculations where numerous sets of the coupling coefficients need to be determined at the same time. Nevertheless, these programs can be used in mutual tests for our new recursion scheme.

B. *Recursive Evaluation*

There exists an algorithm for the evaluation of Wigner 3jm symbols based on the exact solution of recurrence relations. Schulton and Gordon [18, 19] provided the three-term recurrence relation,

$$j_3 C(j_3+1)\begin{pmatrix} j_1 & j_2 & j_3+1 \\ m_1 & m_2 & m_3 \end{pmatrix} + D(j_3)\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} + (j_3+1)C(j_3)\begin{pmatrix} j_1 & j_2 & j_3-1 \\ m_1 & m_2 & m_3 \end{pmatrix} = 0, \tag{6}$$

where

$$\begin{aligned} C(j_3) &= \{[(j_3)^2-(j_1-j_2)^2][(j_1+j_2+1)^2-(j_3)^2][(j_3)^2-(m_3)^2]\}^{1/2}, \\ D(j_3) &= -(2j_3+1)[j_1(j_1+1)m_3 - j_2(j_2+1)m_3 - j_3(j_3+1)(m_2-m_1)]. \end{aligned} \tag{7}$$

This recurrence relation follows directly from the eigenvalue problems that define the coupling coefficients. It is also solved in a way similar to the integration of bound state Schrödinger equations. The linear three-term recurrence relation Eq. (6) reduces to two terms at the boundaries $j_{3_{\min}} = |j_1 - j_2|$ or $|m_1 + m_2|$ and $j_{3_{\max}} = j_1 + j_2$,

$$\begin{aligned} \begin{pmatrix} j_1 & j_2 & j_1+j_2-1 \\ m_1 & m_2 & m_3 \end{pmatrix} &= \frac{D(j_1+j_2)}{(j_1+j_2+1)C(j_1+j_2)}\begin{pmatrix} j_1 & j_2 & j_1+j_2 \\ m_1 & m_2 & m_3 \end{pmatrix}, \\ \begin{pmatrix} j_1 & j_2 & j_{3_{\min}}+1 \\ m_1 & m_2 & m_3 \end{pmatrix} &= \frac{D\left(j_{3_{\min}}\right)}{\left(j_{3_{\min}}\right)C\left(j_{3_{\min}}+1\right)}\begin{pmatrix} j_1 & j_2 & j_{3_{\min}} \\ m_1 & m_2 & m_3 \end{pmatrix}. \end{aligned} \tag{8}$$

Hence, the recurrence process can start with a single starting value in either forward or backward recursion. For an integer combination of (j_1, j_2, m_1, m_2), the total number of 3jm symbols is determined by

$$N_t = j_1 + j_2 + 1 - \max(|j_1 - j_2|, |m_1 + m_2|). \tag{9}$$

1. *Calculation of starting values.* For backward recursion (i.e., the recursion with j_3 decreasing), the starting value is $\left(\begin{smallmatrix} j_1 & j_2 & j_1+j_2 \\ m_1 & m_2 & -m_1-m_2 \end{smallmatrix}\right)$. For this particular 3jm symbol, since

$$k_{\min} = k_{\max} = 0 \tag{10}$$

by Eqs. (2) and (3), Eq. (1) becomes

$$\begin{pmatrix} j_1 & j_2 & j_1+j_2 \\ m_1 & m_2 & -m_1-m_2 \end{pmatrix} = (-1)^{j_1+j_2+m_1+m_2} \times \left[\frac{(2j_1)!(2j_2)!(j_1+j_2-m_1-m_2)!(j_1+j_2+m_1+m_2)!}{(2j_1+2j_2+1)!(j_1-m_1)!(j_1+m_1)!(j_2-m_2)!(j_2+m_2)!} \right]^{1/2}. \quad (11)$$

For forward recursion (with j_3 increasing), the starting value is $\begin{pmatrix} j_1 & j_2 & j_{3_{\min}} \\ m_1 & m_2 & -m_1-m_2 \end{pmatrix}$. There are in total four possibilities for the value of $j_{3_{\min}}$:

$$j_{3_{\min}} = |j_1 - j_2|, \quad (12)$$

or

$$j_{3_{\min}} = |m_1 + m_2|. \quad (13)$$

Similar to Eq. (11), the analytical expressions for $\begin{pmatrix} j_1 & j_2 & j_{3_{\min}} \\ m_1 & m_2 & -m_1-m_2 \end{pmatrix}$ corresponding to these four cases are, respectively,

$$\begin{pmatrix} j_1 & j_2 & j_1-j_2 \\ m_1 & m_2 & -m_1-m_2 \end{pmatrix} = (-1)^{j_1+m_1} \times \left[\frac{(j_1-m_1)!(j_1+m_1)!(2j_1-2j_2)!(2j_2)!}{(j_2-m_2)!(j_2+m_2)!(j_1-j_2-m_1-m_2)!(j_1-j_2+m_1+m_2)!(2j_1+1)!} \right]^{1/2}, \quad (14)$$

$$\begin{pmatrix} j_1 & j_2 & j_2-j_1 \\ m_1 & m_2 & -m_1-m_2 \end{pmatrix} = (-1)^{j_2+m_2} \times \left[\frac{(j_2-m_2)!(j_2+m_2)!(2j_2-2j_1)!(2j_1)!}{(j_1-m_1)!(j_1+m_1)!(j_2-j_1-m_1-m_2)!(j_2-j_1+m_1+m_2)!(2j_2+1)!} \right]^{1/2}, \quad (15)$$

$$\begin{pmatrix} j_1 & j_2 & m_1+m_2 \\ m_1 & m_2 & -m_1-m_2 \end{pmatrix} = (-1)^{j_2+m_2} \times \left[\frac{(j_1+m_1)!(j_2+m_2)!(j_1+j_2-m_1-m_2)!(2m_1+2m_2)!}{(j_1-m_1)!(j_2-m_2)!(j_1-j_2+m_1+m_2)!(j_2-j_1+m_1+m_2)!(j_1+j_2+m_1+m_2+1)!} \right]^{1/2}, \quad (16)$$

$$\begin{pmatrix} j_1 & j_2 & -m_1-m_2 \\ m_1 & m_2 & -m_1-m_2 \end{pmatrix} = (-1)^{j_1+m_1} \times \left[\frac{(j_1-m_1)!(j_2-m_2)!(j_1+j_2+m_1+m_2)!(-2m_1-2m_2)!}{(j_1+m_1)!(j_2+m_2)!(j_1-j_2-m_1-m_2)!(j_2-j_1-m_1-m_2)!(j_1+j_2-m_1-m_2+1)!} \right]^{1/2}. \quad (17)$$

All Eqs. (11) and (14–17) imply a single value of k. In other words, accurate starting values can be obtained directly using Eq. (1) because these particular cases do not have the problem of losing accuracy in the summation over k.

2. *Stability and efficiency of the forward and backward recursions.* We use the unitary property of the Wigner 3jm symbol

$$\sum_{j_3=j_{3_{\min}}}^{j_1+j_2} (2j_3+1)\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}^2 = 1 \tag{18}$$

to systematically check the accuracy of the numerical results from both forward and backward recursion procedures, the method of direct calculation, and Lai and Chiu's program. The residual

$$R = \left| 1 - \sum_{j_3=j_{3_{\min}}}^{j_1+j_2} (2j_3+1)\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}^2 \right| \tag{19}$$

is the direct measure of the accuracy. In this accuracy test, all our calculations are in quadruple precision, the same as in Lai and Chiu's program. Table 1 shows the accuracy-test results for the four schemes: backward recursion (BR), forward recursion (FR), the method of direct calculation (DC), and Lai and Chiu's program (Lai90). From Table 1 we see that the method of direct calculation using Eq. (1) and Lai and Chiu's program start to lose accuracy at around $j \approx 20$ and that neither backward nor forward recursion is satisfactorily accurate, although the backward recursion seems to be more stable. As pointed out by Schulton and Gordon [19], both backward and forward recursion procedures are stable only in the

TABLE 1

Computational Accuracy of Four Methods for the Calculation of Wigner 3jm Symbols Using Quadruple-Precision Arithmetic

		Largest residual $R_{\max}$ [c]			
$j_{\max}$ [a]	N [b]	BR [d]	FR [e]	DC [f]	Lai90 [g]
10	128,843	0.338994E-32	0.377964E-32	0.114352E-32	0.722224E-33
20	3,267,285	0.670027E-32	0.772177E-32	0.394575E-31	0.883360E-33
30	22,903,327	0.116300E-31	0.171656E-31	0.403632E-29	0.363135E-29
40	92,684,969	0.126091E-31	0.213693E-22	0.318329E-27	0.283796E-27
50	276,020,211	0.165525E-31	0.171587E-10	0.276811E-25	—
60	675,677,053	0.190997E-31	—	—	—
70	1,443,383,495	0.716262E-28	—	—	—
80	2,789,427,537	0.331044E-22	—	—	—

[a] The largest value of j_1 and j_2 reached in the test calculations, $j_{\max} = j_{1\max} = j_{2\max}$. The same applies to Tables 2, 4, and 7.

[b] The total number of all possible groups of (j_1, j_2, m_1, m_2) when j_1 and j_2 reach $j_{\max}$. The same applies to Tables 2, 4, and 7.

[c] The residual R, defined by Eq. (19), is the direct measure of the numerical accuracy of calculated Wigner 3jm symbols. The same applies to Table 4.

[d] Backward recursion, i.e., the recursion in the direction with j_3 decreasing.

[e] Forward recursion, i.e., the recursion in the direction with j_3 increasing.

[f] The method of direct calculation using Eq. (1). The same applies to Tables 2, 4, and 7.

[g] Lai and Chiu's computer code [16].

direction of increasing coupling coefficients. For large j-values, the 3jm symbols drop exponentially at both end regions of the recursion domain (so-called nonclassical domains) towards the boundaries. These two nonclassical domains are separated by an intermediate region (so-called classical domain), where the values of the 3jm symbols oscillate rapidly. Schulton and Gordon's recursion scheme [19] proceeds simultaneously forward and backward from the two nonclassical domains towards an intermediate coefficient that lies in the classical domain of larger coupling coefficients. In their program, starting values for both recursion directions are arbitrary. Their scheme requires, therefore, finding an appropriate intermediate value of j_3 at which both recursion series meet and using the appropriate numerical factors to rescale recursion series in the determination of the actual numerical values of 3jm symbols.

Table 2 lists the CPU times required by the four different schemes. Table 2 shows that the method of direct calculation and, especially, Lai and Chiu's program are much more CPU time-demanding than the recursion procedures. This is not surprising because the method of direct calculation and Lai and Chiu's program calculate the 3jm symbol individually.

3. *A practically useful recursion scheme.* As indicated in Table 1, our test calculations show that the backward recursion is more accurate than the forward recursion, although no one alone works satisfactorily well. For the backward recursion, problems occur at the end region of $j_{3_{\min}}$, where the forward recursion is stable. We propose a recursion scheme that is: (i) using the analytical expressions Eqs. (11) and (14–17) to directly calculate two starting values at $j_{3_{\max}}$ and $j_{3_{\min}}$, (ii) using the two-term relations Eqs. (8) to calculate the next coefficient at both ends, (iii) using Schulton and Gordon's recurrence relation Eq. (6) to generate the backward recursion series, and (iv) calculating in the forward direction for only the 3jm symbols that monotonically increase and replacing those in the backward series. Unlike Schulton and Gordon's program, this scheme does not use arbitrary starting values and does not require the determination of an intermediate value of j_3 as well as rescaling factors.

4. *Calculation of factorials.* We need to address here the problem of the calculation of factorials. Although using Eqs. (11) and (14–17) to determine starting values does not have

TABLE 2

CPU Time Required by the Same Four Schemes as in Table 1 in Quadruple-Precision Calculations of Wigner 3jm Symbols[a]

		CPU (s) on DEC ALphaStation 600 5/333			
$j_{\max}$	N	BR	FR	DC	Lai90
10	128,843	4.91	4.75	11.34	120.91
20	3,267,285	127.20	122.68	585.54	8,340.21
30	22,903,327	906.01	874.30	6,929.53	104,549.61
40	92,684,969	3,678.46	3,546.22	42,576.03	631,109.01
50	276,020,211	11,014.74	10,623.30	178,450.70	—
60	675,677,053	26,961.18	—	—	—
70	1,443,383,495	57,676.91	—	—	—
80	2,789,427,537	111,891.44	—	—	—

[a] See the footnotes of Table 1 for the meaning of headings.

the problem of losing accuracy in the summation over k, these equations involve the calculation of a quite large number of factorials. Quadruple-precision calculations can handle very large numbers. But it is much more time-consuming than lower precision. Usually, we use double-precision arithmetic, where 171! overflows floating point representation. This will occur at around $j_1 = j_2 = 42$ in Eq. (11). To avoid the overflow problem, logarithms of factorials can be used in decimal calculations. There is a very neat approximation derived by Lanczos [26] specifically to the gamma function:

$$z! = \sqrt{2\pi}\left(z+\gamma+\frac{1}{2}\right)^{z+1/2} e^{-(z+\gamma+1/2)} A_\gamma(z), \tag{20}$$

where

$$A_\gamma(z) = \frac{1}{2}\rho_0 + \rho_1\frac{z}{z+1} + \rho_2\frac{z(z-1)}{(z+1)(z+2)} + \cdots \tag{21}$$

with

$$\begin{aligned}\rho_k &= \sum_{\alpha=0}^{k} C_{2\alpha}^{2k} F(\alpha),\\ F(\alpha) &= \frac{\sqrt{2}}{\pi}\left(\alpha-\frac{1}{2}\right)!\left(\alpha+\gamma+\frac{1}{2}\right)^{-\alpha-1/2} e^{\alpha+\gamma+1/2},\end{aligned} \tag{22}$$

and $C_{2\alpha}^{2k}$s are the coefficients of the Chebyshev polynomial. The logarithm of a factorial can be calculated from the equation

$$\begin{aligned}\ln(z!) = {}& \frac{\ln(2\pi)}{2} - \left(z+\gamma+\frac{1}{2}\right) + \left(z+\frac{1}{2}\right)\ln\left(z+\gamma+\frac{1}{2}\right)\\ &+ \ln\left(c_0 + \frac{c_1}{z+1} + \frac{c_2}{z+2} + \cdots + \frac{c_N}{z+N} + \epsilon\right),\end{aligned} \tag{23}$$

where ϵ is the truncation error. There is a published subroutine using Lanczos' approximation method in the book "Numerical Recipes" [27], which uses $\gamma = 5$ and $N = 6$ that result in $|\epsilon| < 2 \times 10^{-10}$. To apply Lanczos' approximation in double-precision calculations, we use $\gamma = 10$ and $N = 11$, and consequently, $|\epsilon| < 1.4 \times 10^{-17}$. The corresponding values of c's are given in Table 3.

C. *Accuracy and Timing Tests*

Based on Schulton and Gordon's recurrence relation, we have devised a recursive approach to computing Wigner 3jm symbols. In our practical programming, we use double precision. Our systematic accuracy test indicates that this recursion scheme (REC-W) works well from low to very high j-values, while the method of direct calculation using Eq. (1) (DC) and the forward recursion (FR) work well only for $j \approx 10$ or smaller and are unable to provide accurate results even at quite modest values of j such as $j \approx 20$, not to mention larger j-values. The backward recursion (BR) works reasonably well until $j = 20{\sim}30$. Similar to Table 1, Table 4 shows the largest residuals $R_{\max}$ (see Eq. (19) for the definition of R) occurred in the double-precision calculations of Wigner 3jm symbols using the four

TABLE 3

***c*-Coefficients in Lanczos' Approximation (Eq. (23)) when γ = 10 and *N* = 11**

c_0	0.10000000000000000d1	c_1	0.16427423239836267d5
c_2	−0.48589401600331902d5	c_3	0.55557391003815523d5
c_4	−0.30964901015912058d5	c_5	0.87287202992571788d4
c_6	−0.11714474574532352d4	c_7	0.63103078123601037d2
c_8	−0.93060589791758878d0	c_9	0.13919002438227877d-2
c_{10}	−0.45006835613027859d-8	c_{11}	0.13069587914063262d-9

different schemes: our recursion scheme (REC-W), the method of direct calculation (DC), the forward recursion (FR), and the backward recursion (BR). As examples for practical computations, Tables 5 and 6 provide the numerical values of all Wigner 3jm symbols with $(j_1, j_2, m_1, m_2) = (98, 115, -69, -100)$ and (260, 280, 228, 268) calculated by the recursion scheme REC-W. Table 7 is the timing-test results, which show that our recursive approach is much more efficient, especially at large j-values. The computing time required by our recursion scheme is only a few percentages of that of the method of direct calculation.

III. RECURSIVE EVALUATION OF GAUNT COEFFICIENTS

As defined by Eq. (4), the Gaunt coefficient can be expressed using the definite integrals of the product of three associated Legendre functions. Alternatively, Gaunt coefficients can be also defined by the equation [22]

$$P_n^m(x)P_\nu^\mu(x) = \sum_{q=0}^{q_{\max}} a_q P_{n+\nu-2q}^{m+\mu}(x), \tag{24}$$

TABLE 4

Numerical Accuracy of the Wigner 3jm Symbols Computed by the Recursion Scheme Proposed in the Present Paper (REC-W), the Backward (BR) and Forward (FR) Recursions, and the Method of Direct Calculation (DC) Using Double-Precision Arithmetic[a]

		Largest residual $R_{\max}$			
$j_{\max}$	N	REC-W	BR	FR	DC
10	128,843	0.1650E-12	0.2391E-12	0.3192E-12	0.1539E-12
20	3,267,285	0.4125E-12	0.4441E-12	0.1095E-06	0.6831E-11
30	22,903,327	0.4125E-12	0.4730E-12	—	0.8050E-09
40	92,684,969	0.4784E-12	0.3717E-10	—	0.7658E-07
50	276,020,211	0.6483E-12	0.2538E-04	—	0.8140E-05
60	675,677,053	0.7675E-12	—	—	0.6197E-03
70	1,443,383,495	0.9029E-12	—	—	—
80	2,789,427,537	0.1103E-11	—	—	—
90	4,992,257,179	0.1247E-11	—	—	—
100	8,408,080,421	0.1381E-11	—	—	—

[a] See the footnotes of Table 1 for the meaning of headings.

TABLE 5
Wigner 3jm Symbols $\begin{pmatrix} 98 & 115 & j_3 \\ -69 & -100 & 169 \end{pmatrix}$ Calculated by the Recursion Scheme (REC-W) Proposed in the Present Paper

j_3	$\begin{pmatrix} 98 & 115 & j_3 \\ -69 & -100 & 169 \end{pmatrix}$	j_3	$\begin{pmatrix} 98 & 115 & j_3 \\ -69 & -100 & 169 \end{pmatrix}$
213	0.247807608975E-02	190	−0.766670865870E-02
212	0.693884894548E-02	189	0.183623427214E-02
211	0.119894874087E-01	188	0.885978296144E-02
210	0.137159251054E-01	187	0.360339675896E-02
209	0.878978201272E-02	186	−0.675539815610E-02
208	−0.134879420191E-02	185	−0.775155593324E-02
207	−0.970595957126E-02	184	0.217581459579E-02
206	−0.914594140187E-02	183	0.920466519730E-02
205	0.198440813258E-04	182	0.332904024036E-02
204	0.878311425522E-02	181	−0.741474620815E-02
203	0.793425707299E-02	180	−0.792886358693E-02
202	−0.164593319164E-02	179	0.278789882553E-02
201	−0.910034650419E-02	178	0.995072010456E-02
200	−0.569261339324E-02	177	0.338584101796E-02
199	0.451366658452E-02	176	−0.824790063946E-02
198	0.900428915783E-02	175	−0.908913611839E-02
197	0.213839293164E-02	174	0.249530288372E-02
196	−0.738662641847E-02	173	0.116922354185E-01
195	−0.727334991775E-02	172	0.649086743310E-02
194	0.238138717955E-02	171	−0.766439796219E-02
193	0.884240026286E-02	170	−0.158289171853E-01
192	0.343404012778E-02	169	−0.115821629971E-01
191	−0.662762854015E-02		$R = 0.19706459\text{E-}13$

where a_q is an abbreviated notation of the Gaunt coefficient $a(m, n, \mu, \nu, n + \nu - 2q)$ and

$$q_{\max} = \min\left(n, \nu, \frac{n + \nu - |m + \mu|}{2}\right). \tag{25}$$

There are two ways to calculate the Gaunt coefficient. With Wigner 3jm symbols accurately calculated using the recursion scheme developed in the last section, Gaunt coefficients can be evaluated by Eq. (5) formulated by Cruzan. Gaunt coefficients can also be recursively calculated in terms of their general recurrence relations [23].

A. *General Recurrence Relations*

Gaunt coefficients can be solved in a lower triangular linear system [22]:

$$\begin{aligned} a_q = {} & a_0 \frac{(p + 1/2)_{2q}}{(-n_4)_{2q}} \sum_{k=0}^{q} \frac{(m - n)_{2k}(\mu - \nu)_{2q-2k}}{k!(q - k)!(-n + 1/2)_k(-\nu + 1/2)_{q-k}} \\ & - \sum_{j=0}^{q-1} \frac{(-p - q + j + 1/2)_{q-j}}{(q - j)!} a_j. \end{aligned} \tag{26}$$

TABLE 6

Wigner 3jm Symbols $\begin{pmatrix} 260 & 280 & j_3 \\ 228 & 268 & -496 \end{pmatrix}$ Calculated by the Recursion Scheme (REC-W) Proposed in the Present Paper

j_3	$\begin{pmatrix} 260 & 280 & j_3 \\ 228 & 268 & -496 \end{pmatrix}$	j_3	$\begin{pmatrix} 260 & 280 & j_3 \\ 228 & 268 & -496 \end{pmatrix}$
540	0.646538800496E-03	517	−0.547290382597E-02
539	−0.215500549372E-02	516	0.174964877782E-02
538	0.465411076035E-02	515	0.394504283491E-02
537	−0.731061039588E-02	514	−0.527216572521E-02
536	0.838427599069E-02	513	0.724931930634E-03
535	−0.626797503117E-02	512	0.468182444016E-02
534	0.111598158779E-02	511	−0.496946357969E-02
533	0.440871782946E-02	510	−0.217788430018E-03
532	−0.656221561371E-02	509	0.526678411373E-02
531	0.357812146408E-02	508	−0.473156768970E-02
530	0.224745743079E-02	507	−0.865329202847E-03
529	−0.592844996838E-02	506	0.572304021206E-02
528	0.410199707330E-02	505	−0.488192167706E-02
527	0.156337294749E-02	504	−0.859257546078E-03
526	−0.558989788105E-02	503	0.604575462241E-02
525	0.395146634823E-02	502	−0.598098779693E-02
524	0.170679604185E-02	501	0.773481764641E-03
523	−0.551972978223E-02	500	0.547061798683E-02
522	0.345323154487E-02	499	−0.866216228838E-02
521	0.230286994591E-02	498	0.777640385675E-02
520	−0.553203800308E-02	497	−0.465713579139E-02
519	0.269624934600E-02	496	0.173119327070E-02
518	0.310961234591E-02		$R = 0.10780049\text{E-}12$

From this linearization algorithm, we obtained an analytical expression for any individual Gaunt coefficient,

$$a_q = a_0 \frac{2p+1}{2} \sum_{i=0}^{q} \frac{(p+q-i+3/2)_{q+i-1}}{(q-i)!(n_4-2i+1)_{2i}} \times \sum_{j=0}^{i} \frac{(m-n)_{2j}(\mu-\nu)_{2i-2j}}{j!(i-j)!(-n+1/2)_j(-\nu+1/2)_{i-j}}, \tag{27}$$

where $q = 1, 2, \ldots, q_{\max}$, $n_4 = n + \nu - m - \mu$, and

$$p = n + \nu - 2q. \tag{28}$$

Based on this algorithm, we have also derived the general recurrence formulas for Gaunt coefficients [23], which are shown in the Appendix. Another and easier way to derive the recurrence relations is to use Eqs. (5) and (6). Denote that

$$W_p = \begin{pmatrix} n & \nu & p \\ m & \mu & -m-\mu \end{pmatrix}, \tag{29}$$

$$W_p^0 = \begin{pmatrix} n & \nu & p \\ 0 & 0 & 0 \end{pmatrix}, \tag{30}$$

TABLE 7
CPU Time Required by Two Schemes REC-W and DC in Double-Precision Calculations of Wigner 3jm Symbols

j_{max}	N	CPU (s) on DEC AlphaStation 600 5/333	
		REC-W	DC
10	128,843	0.87	5.54
20	3,267,285	14.57	197.22
30	22,903,327	83.30	1,785.18
40	92,684,969	295.84	8,868.34
50	276,020,211	808.66	31,285.43
60	675,677,053	1,861.11	88,516.61
70	1,443,383,495	3,794.23	—
80	2,789,427,537	7,065.23	—
90	4,992,257,179	12,270.59	—
100	8,408,080,421	20,159.84	—

$$\beta_p = \{[p^2 - (n-\nu)^2][(n+\nu+1)^2 - p^2]\}^{1/2}, \tag{31}$$

$$\xi_p = [(p-m-\mu)(p+m+\mu)]^{1/2}, \tag{32}$$

$$A_p = p(p-1)(m-\mu) - (m+\mu)(n-\nu)(n+\nu+1). \tag{33}$$

With the use of these notations, Eqs. (5) and (6) become, respectively,

$$a_p = a(m,n,\mu,\nu,p) = \frac{(-1)^{m+u}(2p+1)\xi_p}{(p+m+\mu)!}\left[\frac{(n+m)!(\nu+\mu)!}{(n-m)!(\nu-\mu)!}\right]^{1/2} W_p^0 W_p, \tag{34}$$

$$(p+2)\beta_{p+1}\xi_{p+1}W_p = (2p+3)A_{p+2}W_{p+1} - (p+1)\beta_{p+2}\xi_{p+2}W_{p+2}. \tag{35}$$

Equation (35) is equivalent to

$$C_0 W_p = C_2 W_{p+2} + C_4 W_{p+4}, \tag{36}$$

where

$$C_0 = (p+2)(p+3)\beta_{p+1}\beta_{p+2}\xi_{p+1}\xi_{p+2}(2p+7)A_{p+4}, \tag{37}$$

$$\begin{aligned} C_2 = {} & (2p+3)(2p+5)(2p+7)A_{p+2}A_{p+3}A_{p+4} \\ & - (p+1)(p+3)\beta_{p+2}^2\xi_{p+2}^2(2p+7)A_{p+4} \\ & - (p+2)(p+4)\beta_{p+3}^2\xi_{p+3}^2(2p+3)A_{p+2}, \end{aligned} \tag{38}$$

$$C_4 = -(p+2)(p+3)\beta_{p+3}\beta_{p+4}\xi_{p+3}\xi_{p+4}(2p+3)A_{p+2}. \tag{39}$$

For the special case of W_p^0, $A_p \equiv 0$, $\xi_p = p$, and then

$$W_p^0 = -\frac{\beta_{p+2}}{\beta_{p+1}} W_{p+2}^0. \tag{40}$$

Equations (34)–(40) result in the recurrence relation

$$
\begin{aligned}
&(p+2)(p+3)(p_1+1)(p_1+2)\frac{\beta_{p+1}^2}{(2p+1)(2p+3)}A_{p+4}a_p \\
&= -a_{p+2}\Bigg[A_{p+2}A_{p+3}A_{p+4} \\
&\quad -(p+1)(p+3)(p_1+2)(p_2+2)\frac{\beta_{p+2}^2}{(2p+3)(2p+5)}A_{p+4} \\
&\quad -(p+2)(p+4)(p_1+3)(p_2+3)\frac{\beta_{p+3}^2}{(2p+5)(2p+7)}A_{p+2}\Bigg] \\
&\quad -(p+2)(p+3)(p_2+3)(p_2+4)\frac{\beta_{p+4}^2}{(2p+7)(2p+9)}A_{p+2}a_{p+4},
\end{aligned} \tag{41}
$$

where

$$
p_1 = p - m - \mu, \quad p_2 = p + m + \mu. \tag{42}
$$

Now, we define that $\alpha_p = \beta_p^2/(1-4p^2)$, i.e.,

$$
\alpha_p = [p^2 - (n-\nu)^2][p^2 - (n+\nu+1)^2]/(4p^2-1). \tag{43}
$$

Then, we can rewrite Eq. (41) in the form

$$
\begin{aligned}
&(p+2)(p+3)(p_1+1)(p_1+2)\alpha_{p+1}A_{p+4}a_p \\
&= [A_{p+2}A_{p+3}A_{p+4} + (p+1)(p+3)(p_1+2)(p_2+2)\alpha_{p+2}A_{p+4} \\
&\quad + (p+2)(p+4)(p_1+3)(p_2+3)\alpha_{p+3}A_{p+2}]a_{p+2} \\
&\quad - (p+2)(p+3)(p_2+3)(p_2+4)\alpha_{p+4}A_{p+2}a_{p+4},
\end{aligned} \tag{44}
$$

which is exactly the same as Eqs. (A1) with (A2) in Appendix. From this three-term relation, a four-term recurrence relation without the factor A_{p+4} can be derived (see Eqs. (A5) and (A6) in Appendix), which applies to the case of $A_{p+4} = 0$, where the three-term recurrence relation Eq. (44) is not applicable.

The recursion scheme for Gaunt coefficients based on their recurrence relations requires only a single starting value for both forward and backward recursions, because all recurrence formulas reduce to two-term relations at both ends. Necessary equations for the calculation of starting values are also given in Appendix. Similar to the case of the recursive evaluation of Wigner 3jm symbols, neither forward nor backward recursion alone is satisfactorily accurate although, again, the backward recurrence is more stable. A practically applicable recursion scheme for Gaunt coefficients must also combine forward and backward recurrence procedures, like the one for Wigner 3jm symbols. In practical programming, we first generate the recursion series with q increasing and then calculate in the opposite direction with q decreasing until a coefficient is reached for which the numerical values obtained by both recursions are in satisfactory agreement.

B. *Numerical Test*

We calculated all possible Gaunt coefficients up to $n_{\max} = \nu_{\max} = 120$ using both the recursion scheme (REC-G) discussed above and the 3jm approach using Cruzan's formula Eq. (5) with Wigner 3jm symbols computed by the recursive scheme (REC-W) developed in the last section. The numerical results from these two schemes are in excellent agreement. Both methods generally have more than 11 digits agreeable. This means that the relative deviation is usually less than 10^{-12}. For illustration, the numerical values of the Gaunt coefficients with $(m, n, \mu, \nu) = (-15, 55, -58, 72)$ and $(100, 112, 99, 143)$ obtained by both methods are given in Table 8. Larger relative deviations occur at some particular cases. Table 9 shows some practical examples of such cases where a smaller coefficient is inlaid in much larger neighboring coefficients. Table 10 lists the largest relative deviations among all Gaunt coefficients with $n \le n_{\max}$ and $\nu \le \nu_{\max}$ ($n_{\max} = \nu_{\max}$) for different values of $n(\nu)_{\max}$. These relative deviations are the indication of the best accuracy that can be achieved in double-precision calculation of the Gaunt coefficient. If more accurate numerical values are needed, it probably needs to go to higher precision arithmetic, yet considerable computing time will be required.

As stated in [23], several other tests can be used to check the stability of the recursion scheme:

(i) When $\mu = -m$ and $\nu = n$, the last Gaunt coefficient $a_{q_{\max}}$ is explicitly given by

$$a(m, n, -m, n, 0) = \frac{(-1)^m}{2n+1}. \tag{45}$$

(ii) From Eq. (24) it is obvious that when $\mu = -m$, $\sum_{q=0}^{q_{\max}} a(m, n, -m, \nu, n+\nu-2q) = \delta_{m0}$, where δ_{m0} is the Krönecker delta symbol.

(iii) From Eq. (24) it is also obvious that when $n+m$ and $\mu+\nu$ are both odd,

$$\sum_{q=0}^{q_{\max}} a_q \frac{(-1)^{(n+\nu-2q-m-\mu)/2}(n+\nu-2q+m+\mu)!}{2^{n+\nu-2q}[(n_4-2q)/2]![(n+\nu-2q+m+\mu)/2]!} = 0, \tag{46}$$

i.e., $\sum_{q=0}^{q_{\max}} a_q P_{n+\nu-2q}^{m+\mu}(0) = 0$, and when $n+m$ and $\mu+\nu$ are both even,

$$\sum_{q=0}^{q_{\max}} a_q \frac{(-1)^{(n+\nu-2q-m-\mu)/2}(n+\nu-2q+m+\mu)!}{2^{n+\nu-2q}[(n_4-2q)/2]![(n+\nu-2q+m+\mu)/2]!} = \frac{(-1)^{(n+\nu-m-\mu)/2}(n+m)!(\nu+\mu)!}{2^{n+\nu-m-\mu}[(n-m)/2]![(n+m)/2]![(\nu-\mu)/2]![(\nu+\mu)/2]!}, \tag{47}$$

i.e., $\sum_{q=0}^{q_{\max}} a_q P_{n+\nu-2q}^{m+\mu}(0) = P_n^m(0) P_\nu^\mu(0)$.

(iv) In general, the numerical values of all Gaunt coefficients in the set of $a(m, n, \mu, \nu, p)$ for an integer group (m, n, μ, ν) must satisfy Eq. (24) for any value of x $(0 \le |x| \le 1)$. All our test calculations using above criteria are satisfactory and show that the recursion scheme for the Gaunt coefficient is satisfactorily stable [23].

TABLE 8

The Gaunt Coefficients $a(-15, 55, -58, 72, p)$ and $a(100, 112, 99, 143, p)$ Calculated by Both Cruzan's 3jm Formula Eq. (5) and the Recursion Scheme (REC-G) Using Double-Precision Arithmetic

q	p	$a(-15, 55, -58, 72, p)$	p	$a(100, 112, 99, 143, p)$
0	127	0.2646565853203E+18	255	0.9014801412620E-64
1	125	−0.9020609422680E+18	253	−0.4454291036755E-62
2	123	0.1261206946319E+19	251	0.8111679090489E-61
3	121	−0.9081541876029E+18	249	−0.4865717151971E-60
4	119	0.3328773378798E+18	247	−0.2865747624629E-59
5	117	−0.3999023716726E+17	245	0.2872507671244E-58
6	115	−0.9370424600630E+16	243	0.2910460460651E-57
7	113	0.1937954274150E+16	241	−0.1000363901943E-56
8	111	0.4151474435389E+15	239	−0.3299666103578E-55
9	109	−0.4503345686430E+14	237	−0.1346893095521E-54
10	107	−0.1873104702543E+14	235	0.2734024566471E-53
11	105	−0.6892824708879E+12	233	0.4243593635563E-52
12	103	0.4706522197096E+12	231	0.1415220328564E-52
13	101	0.8362386532752E+11	229	−0.6940324016290E-50
14	99	0.3331711456707E+09	227	−0.7931615430226E-49
15	97	−0.1793741596315E+10	225	0.6094455105485E-48
16	95	−0.2623374312346E+09	223	0.2730320093940E-46
17	93	−0.5949690414500E+07	221	0.1403572183265E-45
18	91	0.3036193424123E+07	219	−0.8069100849572E-44
19	89	0.4523897047862E+06	217	−0.1467294635946E-42
20	87	0.2132756927936E+05	215	0.2945238881000E-41
21	85	−0.1468293231304E+04	213	0.1164727483072E-39
22	83	−0.2692135114944E+03	211	−0.2533890338350E-38
23	81	−0.1397178728905E+02	209	−0.1158929585758E-36
24	79	0.9600863474247E-02	207	0.7915615134293E-35
25	77	0.2934252243338E-01	205	−0.2548737638735E-33
26	75	0.8107892805619E-03	203	0.5844941612434E-32
27	73	−0.5910928044174E-05	201	−0.1070823713196E-30
28			199	0.1654077641495E-29

C. *Timing Test*

Table 11 compares the computing times required by the recursive (REC-G) and the 3jm approaches. It shows that the recursion scheme is around five times faster.

IV. CALCULATION OF VECTOR TRANSLATION COEFFICIENTS

Suppose that an electromagnetic field is represented by an infinite series in terms of vector spherical wave functions in an original lth coordinate system. Its alternative multipole expansion in a displaced jth coordinate system is connected with the original expansion in the lth coordinate system by vector translational addition theorems. Introduced by the addition theorems are a large number of vector translation coefficients $A^{lj}_{mn\mu\nu}$ and $B^{lj}_{mn\mu\nu}$, where m, n, μ, ν are integers and $n \geq 0$, $\nu \geq 0$, $|m| \leq n$, $|\mu| \leq \nu$. Based on the techniques developed in the last two sections, this section discusses the calculation of these vector translation coefficients.

TABLE 9

Numerical Examples Showing a Certain Degree of Discrepancy between the Gaunt Coefficients Calculated by Cruzan's 3jm Formulation and the Recursion Scheme (REC-G) Using Double-Precision Arithmetic[a]

	q	p	$a(m, n, \mu, \nu, p)$ 3jm	REC-G
$m = 7$	33	20	−0.200951835283E-04	−0.200951835283E-04
$n = 42$	34	18	−0.468041626714E-05	−0.468041626714E-05
$\mu = -15$	35	16	0.5753587**03497**E-12	0.5753587**16715**E-12
$\nu = 44$	36	14	0.550968182890E-06	0.550968182890E-06
	37	12	0.256949806872E-06	0.256949806872E-06
$m = 6$	34	44	0.182562971139E+00	0.182562971137E+00
$n = 50$	35	42	0.191236492753E+00	0.191236492748E+00
$\mu = 8$	36	40	−0.513681**002248**E-05	−0.513681**858330**E-05
$\nu = 62$	37	38	−0.918115021080E+00	−0.918115021097E+00
	38	36	−0.420617949011E+01	−0.420617949015E+01
$m = 20$	38	74	0.113220844079E+02	0.113220844079E+02
$n = 66$	39	72	0.481866384456E+02	0.481866384457E+02
$\mu = 36$	40	70	0.629412**856959**E-03	0.62941**3919494**E-03
$\nu = 84$	41	68	−0.449898083589E+04	−0.449898083588E+04
	42	66	−0.981044427713E+05	−0.981044427713E+05
$m = 24$	66	89	−0.998195574121E+04	−0.998195574089E+04
$n = 105$	67	87	−0.225862452960E+05	−0.225862452946E+05
$\mu = 31$	68	85	0.38999**3630823**E+01	0.38999**4300697**E+01
$\nu = 116$	69	83	0.529145427253E+06	0.529145427285E+06
	70	81	0.550520830612E+07	0.550520830628E+07

[a] The highlights (bold style) indicate the discrepancies on the numerical values of the Gaunt coefficients obtained by Cruzan's 3jm formulation and Xu's recursive scheme presented in this paper. Note that the highlighted Gaunt coefficients are a few magnitude smaller than the neighboring coefficients.

TABLE 10

The Largest Relative Deviation δ_{max} between the Numerical Values of Gaunt Coefficients $a(m, n, \mu, \nu, p)$ Calculated by Cruzan's 3jm Formulation and Xu's Recurrence Scheme (REC-G) Using Double-Precision Arithmetic[a]

$n(\nu)_{max}$	δ_{max}	m	n	μ	ν	$n(\nu)_{max}$	δ_{max}	m	n	μ	ν
10	2.472E-13	−1	9	−1	9	70	1.667E-06	6	50	8	62
20	9.607E-12	−3	10	−5	16	80	1.667E-06	6	50	8	62
30	1.360E-10	−3	12	−6	23	90	1.688E-06	20	66	36	84
40	1.375E-09	4	30	6	40	100	1.688E-06	20	66	36	84
50	2.297E-08	7	42	−15	44	110	1.688E-06	20	66	36	84
60	2.297E-08	7	42	−15	44	120	1.718E-06	24	105	31	116

[a] The numbers in the four columns under m, n, μ, and ν show the integer group of (m, n, μ, ν) at which the largest relative deviation occurs. The same applies to Table 13.

TABLE 11

CPU Time Required by Cruzan's 3jm Formulation and the Recursion Scheme (REC-G) for the Calculation of Gaunt Coefficients Using Double-Precision Arithmetic

$n(\nu)_{\max}$	N^a	CPU (s) on DEC AlphaStation 600 5/333 REC-G	CPU (s) on DEC AlphaStation 600 5/333 3jm
20	915,166	4.36	17.32
40	24,593,932	77.88	351.39
60	175,876,298	453.03	2,217.19
80	718,962,264	1,627.10	8,410.96
100	2,254,211,830	4,450.56	24,010.40

[a] The total number of all possible Gaunt coefficients when n and ν reach $n(\nu)_{\max}$.

A. *Formulas of Stein's Type*

Stein's formulas relate the vector translation coefficients $A^{lj}_{mn\mu\nu}$ and $B^{lj}_{mn\mu\nu}$ with seven scalar translation coefficients [1]:

$$\begin{aligned}A^{lj}_{mn\mu\nu} &= E_{mn\mu\nu}\Bigg(C^{lj}_{mn\mu\nu} + kd_{lj}\cos\theta_{lj}\left[\frac{(n-m)C^{lj}_{mn-1\mu\nu}}{n(2n-1)} + \frac{(n+m+1)C^{lj}_{mn+1\mu\nu}}{(2n+3)(n+1)}\right] \\ &\quad + \frac{kd_{lj}}{2}\sin\theta_{lj}\left\{\left[\frac{C^{lj}_{m-1n-1\mu\nu}}{n(2n-1)} - \frac{C^{lj}_{m-1n+1\mu\nu}}{(2n+3)(n+1)}\right]\exp(-i\phi_{lj})\right. \\ &\quad - \left[\frac{(n-m-1)(n-m)C^{lj}_{m+1n-1\mu\nu}}{n(2n-1)}\right. \\ &\quad \left.\left. - \frac{(n+m+2)(n+m+1)C^{lj}_{m+1n+1\mu\nu}}{(2n+3)(n+1)}\right]\exp(i\phi_{lj})\right\}\Bigg),\end{aligned} \tag{48}$$

$$\begin{aligned}B^{lj}_{mn\mu\nu} &= \frac{ikd_{lj}E_{mn\mu\nu}}{2n(n+1)}\left\{2mC^{lj}_{mn\mu\nu}\cos\theta_{lj} - \left[C^{lj}_{m-1n-1\mu\nu}\exp(-i\phi_{lj})\right.\right. \\ &\quad \left.\left. + (n+m+1)(n-m)C^{lj}_{m+1n-1\mu\nu}\exp(i\phi_{lj})\right]\sin\theta_{lj}\right\},\end{aligned} \tag{49}$$

where [6]

$$E_{mn\mu\nu} = i^{\nu-n}\frac{(2\nu+1)(n+m)!(\nu-\mu)!}{(2n+1)(n-m)!(\nu+\mu)!}. \tag{50}$$

In Eqs. (48) and (49), k is the wave number and $(d_{lj}, \theta_{lj}, \phi_{lj})$ are the spherical coordinates of the origin of the jth coordinate system in the lth coordinate system. Mackowski's equations are [13]

$$\begin{aligned}A^{lj}_{mn\mu\nu} &= \frac{E_{mn\mu\nu}}{2n(n+1)}\left[(n-m)(n+m+1)C^{lj}_{m+1n\mu+1\nu}\right. \\ &\quad \left. + 2\mu mC^{lj}_{mn\mu\nu} + (\nu+\mu)(\nu-\mu+1)C^{lj}_{m-1n\mu-1\nu}\right],\end{aligned} \tag{51}$$

$$B^{lj}_{mn\mu\nu} = -\frac{i(2n+1)E_{mn\mu\nu}}{2n(n+1)(2n-1)}\big[(n-m)(n-m-1)C^{lj}_{m+1n-1\mu+1\nu} + 2\mu(n-m)C^{lj}_{mn-1\mu\nu} - (\nu+\mu)(\nu-\mu+1)C^{lj}_{m-1n-1\mu-1\nu}\big], \tag{52}$$

or alternatively,

$$B^{lj}_{mn\mu\nu} = \frac{i(2n+1)E_{mn\mu\nu}}{2n(n+1)(2n+3)}\big[(n+m+1)(n+m+2)C^{lj}_{m+1n+1\mu+1\nu} - 2\mu(n+m+1)C^{lj}_{mn+1\mu\nu} - (\nu+\mu)(\nu-\mu+1)C^{lj}_{m-1n+1\mu-1\nu}\big]. \tag{53}$$

The scalar translation coefficient is given by [9]

$$C^{lj}_{-mn\mu\nu} = (-1)^m(2n+1)i^{n-\nu}\sum_{q=0}^{q_{\max}} i^p a_q \begin{bmatrix} h_p^{(1)}(kd_{lj}) \\ j_p(kd_{lj}) \end{bmatrix} \times P_p^{\mu+m}(\cos\theta_{lj})\exp[i(\mu+m)\phi_{lj}] \quad \begin{pmatrix} r \le d_{lj} \\ r > d_{lj} \end{pmatrix}, \tag{54}$$

where $h_p^{(1)}$ represents the Hankel function of the first kind and j_p is the Bessel function of the first kind. Evaluation of the scalar translation coefficient using Eq. (54) requires the determination of a complete set of the Gaunt coefficient $a(m, n, \mu, \nu, p)$. With Gaunt coefficients calculated using the numerical techniques developed in the last section, the evaluation of scalar translation coefficients and, therefore, the vector translation coefficients becomes an easy task through the use of Eqs. (48)–(49), (51)–(52), or (53). There is also an other way to calculate the scalar translation coefficient using Mackowski's recurrence relations [13]:

$$\frac{C^{lj}_{mn\mu\nu-1} + C^{lj}_{mn\mu\nu+1}}{2\nu+1} = \frac{C^{lj}_{m-1n-1\mu-1\nu}}{2n-1} + \frac{C^{lj}_{m-1n+1\mu-1\nu}}{2n+3}, \tag{55}$$

$$\frac{(\nu+\mu)(\nu+\mu+1)C^{lj}_{mn\mu\nu-1} + (\nu-\mu)(\nu-\mu+1)C^{lj}_{mn\mu\nu+1}}{2\nu+1} = \frac{(n-m)(n-m-1)}{2n-1}C^{lj}_{m+1n-1\mu+1\nu} + \frac{(n+m+1)(n+m+3)}{2n+3}C^{lj}_{m+1n+1\mu+1\nu}, \tag{56}$$

$$\frac{(\nu+\mu)C^{lj}_{mn\mu\nu-1} - (\nu-\mu+1)C^{lj}_{mn\mu\nu+1}}{2\nu+1} = -\frac{n-m}{2n-1}C^{lj}_{mn-1\mu\nu} + \frac{n+m+1}{2n+3}C^{lj}_{mn+1\mu\nu}. \tag{57}$$

The procedure of calculating the scalar translation coefficient by Eqs. (55)–(57) has been discussed in detail in [14].

B. *Cruzan's 3jm Formulation*

Cruzan's analytical expressions for $A^{lj}_{mn\mu\nu}$ and $B^{lj}_{mn\mu\nu}$ can be written in the following revised form [7, 14]:

$$
\begin{aligned}
A^{lj}_{-mn\mu\nu} = (-1)^m \frac{(2\nu+1)(n-m)!(\nu-\mu)!}{2n(n+1)(n+m)!(\nu+\mu)!} \exp[i(\mu+m)\phi_{lj}] \\
\times \sum_{q=0}^{q_{\max}} i^p [n(n+1)+\nu(\nu+1)-p(p+1)] a_q \\
\times \begin{bmatrix} h_p^{(1)}(kd_{lj}) \\ j_p(kd_{lj}) \end{bmatrix} P_p^{\mu+m}(\cos\theta_{lj}) \quad \begin{pmatrix} r \le d_{lj} \\ r > d_{lj} \end{pmatrix},
\end{aligned}
\tag{58}
$$

$$
\begin{aligned}
B^{lj}_{-mn\mu\nu} = (-1)^{m+1} \frac{(2\nu+1)(n-m)!(\nu-\mu)!}{2n(n+1)(n+m)!(\nu+\mu)!} \exp[i(\mu+m)\phi_{lj}] \\
\times \sum_{q=1}^{Q_{\max}} i^{p+1} \{[(p+1)^2-(n-\nu)^2][(n+\nu+1)^2-(p+1)^2]\}^{1/2} \\
\times b(m,n,\mu,\nu,p+1,p) \begin{bmatrix} h_{p+1}^{(1)}(kd_{lj}) \\ j_{p+1}(kd_{lj}) \end{bmatrix} P_{p+1}^{\mu+m}(\cos\theta_{lj}) \quad \begin{pmatrix} r \le d_{lj} \\ r > d_{lj} \end{pmatrix},
\end{aligned}
\tag{59}
$$

where p, $q_{\max}$, and $a_q = a(m,n,\mu,\nu,p)$ are the same as defined by Eqs. (28), (25), and (5), respectively, and

$$
Q_{\max} = \min[n, \nu, (n+\nu+1-|m+\mu|)/2], \tag{60}
$$

$$
\begin{aligned}
b(m,n,\mu,\nu,p+1,p) = (-1)^{\mu+m}(2p+3) \left[\frac{(n+m)!(\nu+\mu)!(p-m-\mu+1)!}{(n-m)!(\nu-\mu)!(p+m+\mu+1)!} \right]^{1/2} \\
\times \begin{pmatrix} n & \nu & p+1 \\ m & \mu & -m-\mu \end{pmatrix} \begin{pmatrix} n & \nu & p \\ 0 & 0 & 0 \end{pmatrix}.
\end{aligned}
\tag{61}
$$

Eqs. (58)–(61) are not Cruzan's original formulas in [2]. These equations specify explicitly the exact summation range over q (equivalently, the range of p) and include the factor of $E_{mn\mu\nu}$ defined by Eq. (50). In Eqs. (58) and (59) for $A^{lj}_{mn\mu\nu}$ and $B^{lj}_{mn\mu\nu}$, p has exactly the same definition and takes the same set of numerical values. It is worth emphasizing here that, despite these minor revisions, the set of equations given above has no difference from Cruzan's original work.

Evaluating vector translation coefficients by Cruzan's 3jm formulation Eqs. (58) and (59) needs two complete sets of Wigner 3jm symbols $\left(\begin{smallmatrix} n & \nu & p \\ 0 & 0 & 0 \end{smallmatrix}\right)$ and $\left(\begin{smallmatrix} n & \nu & p \\ m & \mu & -m-\mu \end{smallmatrix}\right)$, the calculation of which has been discussed in detail in Section II.

C. *Xu's Formulas*

Vector translation coefficients can also be expressed in terms of the Gaunt coefficient, as derived in [14]. The formulas given in [14] involve three sets of Gaunt coefficients. It can be further simplified to the form that requires only a single set of Gaunt coefficients in both equations for $A^{lj}_{mn\mu\nu}$ and $B^{lj}_{mn\mu\nu}$,

$$A^{lj}_{-mn\mu\nu} = (-1)^m \frac{(n+2)_{n-1}(\nu+2)_{\nu+1}(n+\nu-m-\mu)!}{4n(n+\nu+1)_{n+\nu}(n+m)!(\nu+\mu)!} \exp[i(\mu+m)\phi_{lj}] \times \sum_{q=0}^{q_{\max}} i^p[n(n+1)+\nu(\nu+1)-p(p+1)] \times \tilde{a}_q \begin{bmatrix} h_p^{(1)}(kd_{lj}) \\ j_p(kd_{lj}) \end{bmatrix} P_p^{\mu+m}(\cos\theta_{lj}) \quad \begin{pmatrix} r \le d_{lj} \\ r > d_{lj} \end{pmatrix}, \tag{62}$$

$$B^{lj}_{-mn\mu\nu} = (-1)^m \frac{(n+2)_{n-1}(\nu+2)_{\nu+1}(n+\nu-m-\mu)!}{4n(n+\nu+1)_{n+\nu}(n+m)!(\nu+\mu)!} \exp[i(\mu+m)\phi_{lj}] \times \sum_{q=1}^{Q_{\max}} i^{p+1} b_q \begin{bmatrix} h_{p+1}^{(1)}(kd_{lj}) \\ j_{p+1}(kd_{lj}) \end{bmatrix} P_{p+1}^{\mu+m}(\cos\theta_{lj}) \quad \begin{pmatrix} r \le d_{lj} \\ r > d_{lj} \end{pmatrix}, \tag{63}$$

where

$$b_q = \frac{2p+3}{A_{p+2}}[(p+2)(p_1+1)\alpha_{p+1}\tilde{a}_q - (p+1)(p_2+2)\alpha_{p+2}\tilde{a}_{q-1}], \quad A_{p+2} \ne 0, \tag{64}$$

$$b_q = \frac{2p+3}{(p+3)(p_1+2)A_{p+4}} \times \{[A_{p+3}A_{p+4} + (p+2)(p+4)(p_1+3)(p_2+3)\alpha_{p+3}]\tilde{a}_{q-1} - (p+2)(p+3)(p_2+3)(p_2+4)\alpha_{p+4}\tilde{a}_{q-2}\}, \quad A_{p+2} = 0; \tag{65}$$

$\tilde{a}_q$ stands for the normalized Gaunt coefficient defined by $\tilde{a}_q = a_q/a_0$, A_p, p_1, p_2, α_p, and $Q_{\max}$ have been defined by Eqs. (33), (42), (43), and (60), respectively. When $A_{p+2} = A_{p+4} = 0$, i.e., A_p vanishes independently of the value of p, $B^{lj}_{-mn\mu\nu} \equiv 0$. This includes the cases: (i) $\mu = m = 0$ and (ii) $\mu = m$ and $n = \nu$. In addition, there are other special cases where $B^{lj}_{mn\mu\nu} \equiv 0$, which include (i) $m = n$ and $\mu = -\nu$, and (ii) $m = -n$ and $\mu = \nu$. Also, in the following cases the expression for b_q is rather simple:

(i) $q = 1$,

$$b_1 = \frac{(2p+3)A_{p+3}}{(p+3)(p_1+2)}; \tag{66}$$

(ii) $q = q_{\max}$ and $n + \nu - 2q_{\max} = |n-\nu|, |m-\mu|$,

$$b_{q_{\max}} = -\frac{(2p+3)A_{p+1}}{p(p_2+1)}\tilde{a}_{q_{\max}}; \tag{67}$$

(iii) $q = q_{\max}+1$, $n+\nu-2q_{\max} = |m-\mu|+1$, and $A_{p+2} \ne 0$,

$$b_{q_{\max}+1} = -\frac{(2p+3)(p+1)(p_2+2)\alpha_{p+2}}{A_{p+2}}\tilde{a}_{q_{\max}}. \tag{68}$$

Both Eqs. (62) and (63) involve the same set of Gaunt coefficients. Equation (62) will be exactly the same as Cruzan's formula Eq. (58) if the normalized Gaunt coefficient $\tilde{a}_q$

is replaced by the normal Gaunt coefficient a_q. Equation (63) is equivalent to Cruzan's formula Eq. (59), since it can be directly derived from Eq. (59) through the use of Eq. (6).

D. *Numerical Results*

We calculated all possible vector translation coefficients of $A^{lj}_{mn\mu\nu}$ and $B^{lj}_{mn\mu\nu}$ ($kd_{lj} = 2.0$ and $\theta_{lj} = \phi_{lj} = 0.5$) from $n_{\min} = \nu_{\min} = 1$ up to $n_{\max} = \nu_{\max} = 45$ using four different schemes. All of our test calculations use $h^{(1)}_p$, the Hankel function, in the equations for the vector translation coefficients. The first scheme (referred to as SX) uses Stein's formulas and the recursive approach (REC-G) developed in Section III to computing the Gaunt coefficients. The second (CX) employs Cruzan's formulas. Wigner 3jm symbols are calculated by the recursive scheme (REC-W) developed in Section II. The third (MM) utilizes Mackowski's formulas, together with Mackowski's recursion scheme for the calculation of scalar translation coefficients. The fourth (XU) is based on Xu's formulas and the recursive approach (REC-G) to calculating Gaunt coefficients. In general, these four schemes produce same numerical results (but maybe with different accuracies). Table 12 provides some sample numerical values of $A^{lj}_{mn\mu\nu}$ and $B^{lj}_{mn\mu\nu}$ for which all four schemes obtain identical results for all the digits shown. But the numerical results from the four approaches are not always precisely the same. In some cases, larger relative deviation shows up. The largest

TABLE 12

Sample Numerical Values of Vector Translation Coefficients $A^{lj}_{mn\mu\nu}$ and $B^{lj}_{mn\mu\nu}$ with (kd_{lj}, θ_{lj}, ϕ_{lj}) = (2, 0.5, 0.5) for Which All Four Schemes (SX, CX, MM, XU) Obtain More Than 12 Digits Exactly the Same Using Double-Precision Arithmetic

				$A^{lj}_{mn\mu\nu}$		$B^{lj}_{mn\mu\nu}$	
m	n	μ	ν	Real	Imag.	Real	Imag.
8	10	−9	12	.3663964990E+35	−.2762412192E+35	−.8370892023E+32	−.1110285257E+32
0	10	0	10	.2969682019E+00	−.1928601440E+18	.0000000000E+00	.0000000000E+00
−2	11	3	9	.7726121583E+12	.1034255820E+13	.1222239141E+11	−.9130398908E+10
−12	13	10	15	.3290937356E+01	.1456483748E-01	−.1763167849E-03	.3983892680E-01
−15	16	17	18	.3793897303E-08	−.1261972860E-07	−.3042702016E-11	−.9147343290E-12
−5	20	5	20	.4040625669E+34	−.1195269260E+34	.0000000000E+00	.0000000000E+00
10	18	15	22	−.6206840651E+36	−.8308775621E+36	−.3610252125E+35	.2696938836E+35
10	30	−10	30	.1807705110+110	.2788115866+110	.0000000000E+00	.0000000000E+00
18	33	20	38	.3343492687E+92	.5207181338E+92	.1759309957E+91	−.1129639932E+91
−35	36	11	12	−.1901528547E-15	.1197320691E-15	−.1618572254E-18	−.2570540515E-18
36	36	−38	38	.4146334728+191	−.4931584782+191	.0000000000E+00	.0000000000E+00
−35	40	35	40	−.6514262216E-05	.1374854333E-04	.0000000000E+00	.0000000000E+00
32	35	−43	45	.2762232925+212	−.1368895313+213	.8373862584+209	.1689724460+209
38	42	−39	45	−.2298689786+235	.2371029493+235	.1277697908+232	.1238711556+232
−42	42	45	45	.3488835702E-28	−.1826524477E-28	.0000000000E+00	.0000000000E+00
−43	45	41	42	.5178100899E-22	.1186503822E-21	.3274958627E-25	−.1429246656E-25
48	50	−30	49	.3393827523+267	−.1226717423+268	−.5718637033+265	−.1582113973+265
−72	72	1	3	.6946365327E-42	−.1782022552E-41	.1833377882E-43	.7146549596E-44
42	52	9	81	.3656934399+271	.3705813223+271	−.4499925012+269	−.4440572037+269
18	100	−5	45	.4118769973+293	.7460688240+293	.5914795871+291	−.3265339985+291

TABLE 13

The Largest Relative Deviation δ_{max} of the Numerical Values of Vector Translation Coefficients $A^{lj}_{mn\mu\nu}$ and $B^{lj}_{mn\mu\nu}$ with $(kd_{lj}, \theta_{lj}, \phi_{lj}) = (2,0.5,0.5)$ Obtained by Two Schemes CX and XU Using Double-Precision Arithmetic

$n(\nu)_{max}$	δ_{max}	m	n	μ	ν	$n(\nu)_{max}$	δ_{max}	m	n	μ	ν
5	2.283E-13	0	3	1	5	30	1.331E-10	−9	20	−21	30
10	2.412E-12	−3	6	4	8	35	1.331E-10	−9	20	−21	30
15	2.412E-12	−3	6	4	8	40	1.331E-10	−9	20	−21	30
20	5.135E-12	−1	18	−1	18	45	1.331E-10	−9	20	−21	30
25	5.686E-11	−21	22	−14	22						

relative deviations of the numerical values obtained by CX and XU schemes are shown in Table 13 for different values of $n(\nu)_{max}$. The values of (m, n, μ, ν), where the largest relative deviations occur, are also given. The test results tell us that for all $A^{lj}_{mn\mu\nu}$ and $B^{lj}_{mn\mu\nu}$ we calculated, CX and XU schemes are satisfactorily accurate. The results also tell us that the algorithm of Stein's type is less accurate in some circumstances, although the numerical results given by all four schemes are usually in good agreement. Some examples are shown in Table 14.

TABLE 14

Numerical Examples of Vector Translation Coefficients $A^{lj}_{mn\mu\nu}$ and $B^{lj}_{mn\mu\nu}$ Showing the Formulation of Stein's Type Is Less Accurate

$kd = 2.0$, $\theta = \phi = 0.5$ rad		$A_{mn\mu\nu}$ Real	$A_{mn\mu\nu}$ Imag.	$B_{mn\mu\nu}$ Real	$B_{mn\mu\nu}$ Imag.
$m = -2$	SX	.1**415553297**E-01	.2385575934E+13	−.3282035237E+12	.15**05192773**E-02
$n = 6$	CX	.1377011649E-01	.2385575934E+13	−.3282035237E+12	.1587043209E-02
$\mu = -2$	MM	.1377011649E-01	.2385575934E+13	−.3282035237E+12	.1587043209E-02
$\nu = 10$	XU	.1377011649E-01	.2385575934E+13	−.3282035237E+12	.1587043209E-02
$m = -15$	SX	**.4484065575**E-01	−.2653706899E+36	−.5072175010E+35	**.6893509830E+19**
$n = 16$	CX	.2074318970E-01	−.2653706899E+36	−.5072175010E+35	.9852438545E-02
$\mu = -15$	MM	.2074318970E-01	−.2653706899E+36	−.5072175010E+35	.9852438545E-02
$\nu = 20$	XU	.2074318970E-01	−.2653706899E+36	−.5072175010E+35	.9852438545E-02
$m = -20$	SX	**.1171318929+100**	−.4993981811+115	−.2073152255+114	**.3718472789E+98**
$n = 35$	CX	.1851837652E-05	−.4993981811+115	−.2073152255+114	.4193366215E-07
$\mu = -20$	MM	.1851837652E-05	−.4993981811+115	−.2073152255+114	.4193366215E-07
$\nu = 45$	XU	.1851837652E-05	−.4993981811+115	−.2073152255+114	.4193366215E-07
$m = 41$	SX	**.5274527123+243**	**.6806046183+243**	**−.1036557371+246**	**.8033077975+245**
$n = 45$	CX	.2276246420+247	.2937180509+247	−.8692874643+243	.6736775193+243
$\mu = -42$	MM	**−.5984438460+241**	**−.7722088366+241**	**.7496750010+238**	**−.5809806487+238**
$\nu = 45$	XU	.2276246420+247	.2937180509+247	−.8692874643+243	.6736775193+243
$m = 45$	SX	**−.3850764003+250**	**.2984252330+250**	**.8048935394+247**	**.10386035512+248**
$n = 57$	CX	−.4293609827+274	.3327447520+274	−.4939385256+271	−.6373592055+271
$\mu = -38$	MM	**−.2482905385+243**	**.1924193790+243**	**.1512629781+246**	**.1951839076+246**
$\nu = 42$	XU	−.4293609827+274	.3327447520+274	−.4939385256+271	−.6373592055+271

TABLE 15
CPU Time Required by SX, CX, MM, XU Schemes in Double-Precision Calculations of Vector Translation Coefficients $A_{mn\mu\nu}$ and $B_{mn\mu\nu}$

		CPU (s) on DEC AlphaStation 600 5/333			
$n(\nu)_{\max}$	N^a	SX	MM	CX	XU
10	14,400	9.46	4.11	3.30	1.85
15	65,025	57.34	30.30	19.48	11.43
20	193,600	217.13	131.57	72.85	44.43
25	455,625	632.71	422.81	208.52	131.78
30	921,600	1,551.08	1,119.16	503.19	327.12
35	1,677,025	3,354.16	2,559.29	1,073.56	715.46
40	2,822,400	6,603.60	5,290.66	2,083.63	1,421.09
45	4,473,225	12,101.05	10,059.45	3,770.67	2,621.65

[a] The total number of vector translation coefficients with $(kd_{lj}, \theta_{lj}, \phi_{lj})$ specified when n and ν reach $n(\nu)_{\max}$.

It is noticed that the values of $A^{lj}_{mn\mu\nu}$ and $B^{lj}_{mn\mu\nu}$ dramatically increase with n and ν increasing. When the values of n and ν are larger than 45, the values of certain $A^{lj}_{mn\mu\nu}$ or $B^{lj}_{mn\mu\nu}$ overflow double-precision float point representation. For the calculation of the vector translation coefficients with n and ν larger than 45, higher precision arithmetic may be needed although it will demand significantly more computing time.

E. *Timing Test*

Table 15 shows the timing-test results. Among the four schemes to calculate vector translation coefficients, SX, CX, MM, and XU, the schemes using the formulas of Stein's type (SX and MM) are slower than the others. The 3jm-approach (CX) and the approach (XU) using the Gaunt coefficient is comparable, but the latter is a bit more efficient.

V. EXAMPLES FOR PRACTICAL APPLICATION IN MULTISPHERE LIGHT-SCATTERING CALCULATIONS

We have implemented the algorithms described in this paper, together with our multi-sphere light-scattering formulation, in a working computer code. Comparison of the theoretical results from our multisphere-scattering calculations with experimental data for various aggregates of spheres are successful [7, 14, 24]. For illustration, Figs. 1 and 2 show two practical examples. In 1983, Wang and Gustafson [28] published the microwave-scattering measurement results of phase functions and the degree of polarization for 12 sets of dumbbells and linear chains, each consisting of 2, 3, or 5 identical spheres in various intersphere separations. In addition to the measurements for some principal fixed orientations, their data include the measurements of phase function at random-orientation average by taking the arithmetic mean of 35 orientations uniformly distributed over an octant of space. Figure 1 refers to a bisphere system (target ID#542000 in Ref. [28]). The two identical spheres in #542000 with a complex refractive index $\approx 1.63 - 0.01i$ are in contact. The size parameter, i.e., the circumference to wavelength ratio, of each sphere is 4.346. The two spheres in the bisphere system (target ID#542002 in Ref. [28]) shown in Fig. 2 are the

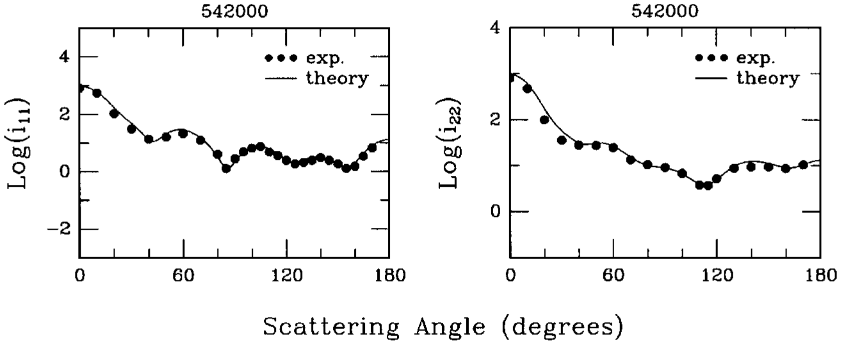

FIG. 1. Angular distribution of polarization components of scattered intensity by randomly oriented two contacting identical spheres of refractive index $1.63 - i0.01$ and size parameter 4.346 (ID#542000 in Ref. [28]). i_{11} and i_{22} correspond to the scattered-field components, perpendicular and parallel to the scattering plane, respectively. The laboratory microwave scattering data are measured by Wang and Gustafson [28].

same as in #542000. The difference between the bisphere systems #542000 and #542002 is only that the two spheres in the latter are not in contact, which have a center-to-center separation s with $ks = 9.94$. The microwave-scattering measurements shown in Figs. 1 and 2 are random-orientation average of the phase functions i_{11} and i_{22} of the targets #542000 and #542002, respectively. i_{11} and i_{22} are the scattered-field components, perpendicular and parallel to the scattering plane, respectively. Figures 1 and 2 show that our theoretical calculations are in good agreement with experimental data.

VI. CLOSING REMARKS

We have shown that all Stein's, Cruzan's, Mackowski's, and Xu's formulas produce generally the same numerical results for vector translation coefficients. But the numerical accuracies of the four different schemes are not always competitive in some cases, especially for the calculation of high-degree coefficients. The two schemes based on the Wigner 3jm symbol and the Gaunt coefficient are satisfactorily accurate and more efficient than the other two.

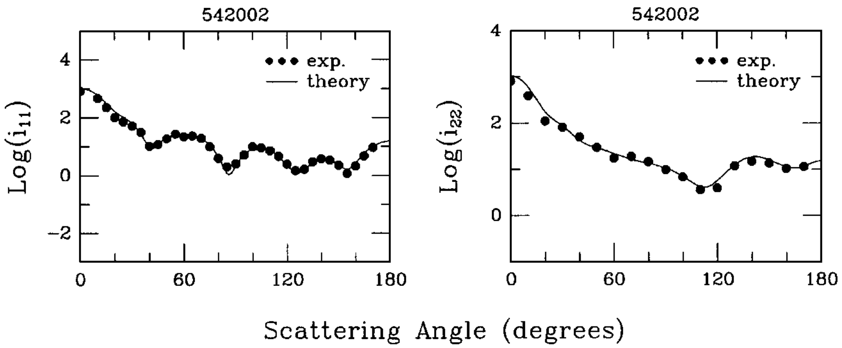

FIG. 2. Same as in Fig. 1, but for the randomly oriented sphere system #542002 [28] of two separated identical spheres.

Our thorough numerical test concludes that, from the point of view of numerical results, Cruzan's formulas are equivalent to the formulas of others, including Stein's and Xu's. This clears up the long-existing ambiguity in the analytical representation of vector translation coefficients and rules out the criticism on Cruzan's equation.

The recursive approach presented in this paper to calculating Wigner 3jm symbols is implemented in decimal approximations. But in principle, Schulten and Gordon's recursion relation can also apply to the exact calculation of the Wigner coefficients, which may be more efficient than the existing computer codes. Also, with a slight modification, this recursive approach can also be applied to the calculation of Clebsch–Gordan coefficients.

APPENDIX: RECURRENCE RELATIONS OF GAUNT COEFFICIENTS

Gaunt coefficients, $a_q = a(m, n, \mu, \nu, n+\nu-2q)$, where q is an integer and $q = 0, 1, \ldots, q_{\max}$ with $q_{\max} = \min[n, \nu, (n+\nu-|m+\mu|)/2]$, have the following three-term recurrence relation [23],

$$c_0 a_q = c_1 a_{q-1} + c_2 a_{q-2}, \tag{A1}$$

where

$$\begin{aligned} c_0 &= (p+2)(p+3)(p_1+1)(p_1+2)A_{p+4}\alpha_{p+1}, \\ c_1 &= A_{p+2}A_{p+3}A_{p+4} + (p+1)(p+3)(p_1+2)(p_2+2)A_{p+4}\alpha_{p+2} \\ &\quad + (p+2)(p+4)(p_1+3)(p_2+3)A_{p+2}\alpha_{p+3}, \\ c_2 &= -(p+2)(p+3)(p_2+3)(p_2+4)A_{p+2}\alpha_{p+4}, \end{aligned} \tag{A2}$$

with p, A_p, p_1, p_2, and α_p defined by Eqs. (28), (33), (42), and (43), respectively. When $\mu = m$ and $\nu = n$, A_p vanishes independently of p so that the three-term relation Eq. (A1) reduces to two-terms:

$$(p+2)(p_1+1)\alpha_{p+1}a_q = (p+1)(p_2+2)\alpha_{p+2}a_{q-1}. \tag{A3}$$

Especially, when $\mu = m = 0$, the above two-term relation further reduces to

$$\alpha_{p+1}a_q = \alpha_{p+2}a_{q-1}. \tag{A4}$$

When $A_{p+4} = 0$ but $A_{p+6} \neq 0$, the four-term recurrence formula,

$$c_0 a_q = c_1 a_{q-1} + c_2 a_{q-2} + c_3 a_{q-3}, \tag{A5}$$

can be used, where

$$\begin{aligned} c_0 &= (p+2)(p+3)(p+5)(p_1+1)(p_1+2)(p_1+4)A_{p+6}\alpha_{p+1}, \\ c_1 &= (p+5)(p_1+4)A_{p+6}\left[A_{p+2}A_{p+3} + (p+1)(p+3)(p_1+2)(p_2+2)\alpha_{p+2}\right], \\ c_2 &= (p+2)(p_2+3)A_{p+2}\left[A_{p+5}A_{p+6} + (p+4)(p+6)(p_1+5)(p_2+5)\alpha_{p+5}\right], \\ c_3 &= -(p+2)(p+4)(p+5)(p_2+3)(p_2+5)(p_2+6)A_{p+2}\alpha_{p+6}. \end{aligned} \tag{A6}$$

For both backward and forward recursions, the implementation of either the three-term or the four-term recurrence relation, (A1) or (A5), requires only one single starting value. In the backward recursion, i.e., the recurrence direction of p decreasing (q increasing), for the second Gaunt coefficient a_1 the three-term relation (A1) reduces to two terms: $c_0 a_1 = c_1 a_0$. It is similar for forward recursion. Also, the four-term recurrence relation (A5) reduces to two terms at boundaries for a_1 or $a_{q_{\max}-1}$ and to three terms for the third coefficient a_2 or $a_{q_{\max}-2}$. This is just because all Gaunt coefficients out of range (i.e., $q < 0$ or $q > q_{\max}$) are a null set. The first Gaunt coefficient in the backward recurrence direction with $p_{\max} = n + \nu$ is given by [20–22]

$$a_0 = a(m, n, \mu, \nu, n + \nu) = \frac{(n+1)_n (\nu+1)_\nu}{(n+\nu+1)_{n+\nu}} \frac{(n+\nu-m-\mu)!}{(n-m)!(\nu-\mu)!}. \tag{A7}$$

In the forward recurrence direction with p increasing, the starting value at $p_{\min} = n + \nu - 2_{q_{\max}}$ can be computed by one of the following equations:

(i) $p_{\min} = n - \nu$,

$$a_{q_{\max}} = \frac{(-1)^\mu (\nu+1)_\nu (n+m)!(2p_{\min}+1)!}{(n+1)_{n+1}(\nu-\mu)!(n-\nu)!(p_{\min}+m+\mu)!}; \tag{A8}$$

(ii) $p_{\min} = \nu - n$,

$$a_{q_{\max}} = \frac{(-1)^m (n+1)_n (\nu+\mu)!(2p_{\min}+1)!}{(\nu+1)_{\nu+1}(n-m)!(\nu-n)!(p_{\min}+m+\mu)!}; \tag{A9}$$

(iii) $p_{\min} = m + \mu$,

$$\begin{aligned} a_{q_{\max}} &= (-1)^{n+m-q_{\max}}(2p_{\min}+1)(q_{\max}+1)_{q_{\max}} \\ &\quad \times \frac{(n+\nu-q_{\max})!(n+m)!(\nu+\mu)!}{(n-q_{\max})!(\nu-q_{\max})!(n-m)!(\nu-\mu)!(n+\nu+p_{\min}+1)!}; \end{aligned} \tag{A10}$$

(iv) $p_{\min} = -m - \mu$,

$$\begin{aligned} a_{q_{\max}} &= (-1)^{\nu+\mu-q_{\max}}(2p_{\min}+1)(q_{\max}+1)_{q_{\max}} \\ &\quad \times \frac{(n+\nu-q_{\max})!(p_{\min}-m-\mu)!}{(n-q_{\max})!(\nu-q_{\max})!(n+\nu+p_{\min}+1)!}; \end{aligned} \tag{A11}$$

(v) $p_{\min} = m + \mu + 1$,

$$\begin{aligned} a_{q_{\max}} &= \frac{(-1)^{n+m-q_{\max}} A_{p_{\min}} (2p_{\min}+1)(q_{\max}+1)_{q_{\max}}}{(p_{\min}-1)(n+\nu+p_{\min}+1)!} \\ &\quad \times \frac{(n+\nu-q_{\max})!(n+m)!(\nu+\mu)!}{(n-q_{\max})!(\nu-q_{\max})!(n-m)!(\nu-\mu)!}. \end{aligned} \tag{A12}$$

In this case, when $A_{p_{\min}} = 0$, $a_{q_{\max}} = 0$, the next coefficient must be provided, which is

$$a_{q_{\max}-1} = \frac{(-1)^{m+n-q_{\max}} A_{p_{\min}+2}(2p_{\min}+3)(2p_{\min}+5)(q_{\max}+1)_{q_{\max}+1}}{p_{\min}(n+\nu+p_{\min}+3)(n+\nu+p_{\min})!} \times \frac{(n-q_{\max})(\nu-q_{\max})(2q_{\max}+1)}{(p_{\min}+m+\mu+1)(p_{\min}+m+\mu+2)(2q_{\max}-1)} \times \frac{(n+\nu-q_{\max})!(n+m)!(\nu+\mu)!}{(n-q_{\max}+1)!(\nu-q_{\max}+1)!(n-m)!(\nu-\mu)!}, \tag{A13}$$

where $A_{p_{\min}+2}$ is always nonzero when $A_{p_{\min}} = 0$.

(vi) $p_{\min} = -m - \mu + 1$,

$$a_{q_{\max}} = \frac{(-1)^{\nu+\mu-q_{\max}} A_{p_{\min}}(2p_{\min}+1)(q_{\max}+1)_{q_{\max}}}{(p_{\min}-1)(n+\nu+p_{\min}+1)!} \times \frac{(n+\nu-q_{\max})!(p_{\min}-m-\mu)!}{(n-q_{\max})!(\nu-q_{\max})!}. \tag{A14}$$

When $A_{p_{\min}} = 0$,

$$a_{q_{\max}-1} = \frac{(-1)^{\nu+\mu-q_{\max}} A_{p_{\min}+2}(2p_{\min}+3)(2p_{\min}+5)(q_{\max}+1)_{q_{\max}+1}}{6p_{\min}(n+\nu+p_{\min}+3)(n+\nu+p_{\min})!} \times \frac{(n-q_{\max})(\nu-q_{\max})(n+\nu-q_{\max})!(p_{\min}-m-\mu)!}{(2q_{\max}-1)(n-q_{\max}+1)!(\nu-q_{\max}+1)!}. \tag{A15}$$

ACKNOWLEDGMENTS

This work was supported by NSF through Grant AST-9619539 and by NASA through Grants NAGW-2482 and 1923.

REFERENCES

1. S. Stein, *Quart. Appl. Math.* **19**, 15 (1961).
2. O. R. Cruzan, *Quart. Appl. Math.* **20**, 33 (1962).
3. J. H. Bruning and Y. T. Lo, *IEEE Trans. Ant. Prop.* **AP-19**, 378 (1971).
4. K. A. Fuller and G. W. Kattawar, *Opt. Lett.* **13**, 90 (1988).
5. K. A. Fuller and G. W. Kattawar, *Opt. Lett.* **13**, 1063 (1988).
6. Y.-l. Xu, *Appl. Opt.* **34**, 4573 (1995).
7. Y.-l. Xu, *Appl. Opt.* **36**, 9496 (1997).
8. Y.-l. Xu, *Appl. Opt.*, in press.
9. B. Friedman and J. Russek, *Quart. Appl. Math.* **12**, 13 (1954).
10. E. P. Wigner, in *Quantum Theory of Angular Momentum*, edited by L. C. Biedenharn and H. van Dam (Academic Press, New York, 1965), p. 89.
11. J. A. Gaunt, *Philos. Trans. Roy. Soc. (London) Ser. A* **228**, 151 (1929).
12. K. T. Kim, *IEEE Trans. Ant. Prop.* **44**, 1482 (1996).
13. D. W. Mackowski, *Proc. R. Soc. London Ser. A* **433**, 599 (1991).
14. Y.-l. Xu, *J. Comput. Phys.* **127**, 285 (1996) [Erratum, *ibid.* **134**, 200 (1997)].
15. M. Rotenberg, R. Bivins, N. Metropolis, and J. K. Wooten Jr., *The 3-j and 6-j Symbols* (Technology Press, MIT, Cambridge, MA, 1959).

16. S.-T. Lai and Y.-N. Chiu, *Comput. Phys. Commun.* **61**, 350 (1990).
17. D. F. Fang and J. F. Shriner Jr., *Comput. Phys. Commun.* **70**, 147 (1992).
18. K. Schulten and R. G. Gordon, *J. Math. Phys.* **16**, 1961 (1975).
19. K. Schulten and R. G. Gordon, *Comput. Phys. Commun.* **11**, 269 (1976).
20. J. H. Bruning, Ph.D. dissertation, Department of Electrical Engineering, University of Illinois, 1969.
21. K. A. Fuller, Ph.D. dissertation, Department of Physics, Texas A&M University, 1987.
22. Y.-l. Xu, *Math. Comput.* **65**, 1601 (1996).
23. Y.-l. Xu, *J. Comput. Appl. Math.* **85**, 53 (1997).
24. Y.-l. Xu and B. Å. S. Gustafson, *Appl. Opt.* **36**, 8026 (1997).
25. W. J. Thompson, *Angular Momentum* (Wiley, New York, 1994), Chap. 7, p. 270.
26. C. Lanczos, *J. SIAM. Numer. Anal. Ser. B* **1**, 86 (1964).
27. W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes* (Cambridge University Press, Cambridge, New York, 1992).
28. R. T. Wang and B. Å. S. Gustafson, in *Proceedings, 1983 CRDC Scientific Conference on Obscuration and Aerosol Research*, edited by J. Farmer and R. Kohl (U.S. Army CRDC-SP-84009, Aberdeen, MD, 1984), p. 237.