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FAST EVALUATION OF THE GAUNT COEFFICIENTS

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Abstract. Addition theorems for vector spherical harmonics require the determination of the Gaunt coefficients that appear in a linearization expansion of the product of two associated Legendre functions. This paper presents an algorithm for the efficient calculation of these coefficients through solving the most appropriate (lower triangular) linear system and derives all relevant recurrence relations needed in the calculation. This algorithm is also applicable to the calculation of the Clebsch-Gordan coefficients that are closely related to the Gaunt coefficients and are frequently encountered in the quantum theory of angular momentum. The new method described in this paper reduces the computing time to $\sim 1\%$, compared to the existing formulation that is widely used. This new method can be applied to the calculation of both low- and high-degree coefficients, while the existing formulation works well only for low degrees.

1. Introduction

Theoretical study of electromagnetic scattering by interacting spheres has been an active area during the last few decades [2, 3, 4, 5, 6, 10, 11, 12, 13, 15, 16, 17, 18, 19, 20, 21, 23, 26, 27, 28, 29, 31, 33]. The problem requires the use of addition theorems to relocate the vector spherical wave functions from one coordinate system centered on a scatterer to other reference systems centered on other scatterers. In the derivation of such addition theorems [7, 9, 24] there occurs a product of two associated Legendre functions, which can be expressed in terms of the linearization expansion

$$P_n^m(\cos\theta)P_\nu^\mu(\cos\theta) = \sum_{p=|n-\nu|}^{n+\nu} a(m,n,\mu,\nu,p)P_p^{m+\mu}(\cos\theta), \tag{1}$$

where $a(m,n,\mu,\nu,p)$ is the so-called Gaunt coefficient [14]. Gaunt coefficients are closely related to the Clebsch-Gordan coefficients [1, 22] that are extensively used in the quantum theory of angular momentum and play an important role in the decomposition of reducible representations of a rotation group into irreducible representations. Clebsch-Gordan coefficients are usually expressed in terms of the Winger $3jm$ symbols [8, 30, 34]. Cruzan [7] provided a similar expression for the

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Gaunt coefficient:

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

where the Winger $3jm$ symbol is defined by [25]

$$
\begin{aligned}
&\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \delta_{m_1+m_2+m_3,0}(-1)^{j_1-j_2-m_3} \\
&\times\left[\frac{(j_3+j_1-j_2)!\,(j_3-j_1+j_2)!\,(j_1+j_2-j_3)!\,(j_3-m_3)!\,(j_3+m_3)!}{(j_1+j_2+j_3+1)!\,(j_1-m_1)!\,(j_1+m_1)!\,(j_2-m_2)!\,(j_2+m_2)!}\right]^{1/2} \\
&\times\sum_k \frac{(-1)^{k+j_2+m_2}(j_2+j_3-m_1-k)!\,(j_1-m_1+k)!}{k!\,(j_3-j_1+j_2-k)!\,(j_3-m_3-k)!\,(k+j_1-j_2+m_3)!}.
\end{aligned}
\tag{3}
$$

The summation over k is over all integers for which the factorials are nonnegative. In quantum mechanics, the product of two Winger $3jm$ symbols is associated with the coupling of two angular momentum vectors. Some tables of the values of the Clebsch-Gordan coefficients exist. These tabulated values are, however, limited to only low degrees and hardly suffice for any practical use in the study of the multisphere scattering problems. Even if one were able to tabulate all the necessary values, any practical computation involving the addition theorems, except for the lowest degrees, would require a prohibitively large computer memory. Furthermore, using the $3jm$ formulation for the calculation of the addition coefficients that occur in the addition theorems requires a rather cumbersome summation of multitudinous factorials. One can appreciate the complexity in trying to compute even a single Gaunt coefficient, not to mention the huge number of these coefficients that are required in practical problems. Significant efforts have been made towards the calculation of high-degree coefficients and the reduction of the computing time and computer memory usage. Bruning [5] and Fuller [11] derived some three-term recursion relations for the Gaunt coefficients. In his research on the multisphere scattering problem, Mackowski [21] developed a technique for implementing the addition theorems that completely avoids the evaluation of the Gaunt coefficients.

In this paper, we present an efficient approach to computing the Gaunt coefficients through solving a lower triangular linear system. We also derive the relevant recurrence formulae from which all elements of the coefficient matrix and the constant vector in the linear system can be easily obtained.

2. Expansion of the associated Legendre function of the first kind

We recall that the associated Legendre function of the first kind is defined by

$$
P_n^m(x) = \frac{1}{2^n n!}(1-x^2)^{\frac{m}{2}}\frac{d^{n+m}}{dx^{n+m}}[(x^2-1)^n].
\tag{4}
$$

The right-hand side of Eq. (4) is well defined for all integers m satisfying $-n \le m \le n$. When $|m| > n$, necessarily $P_n^m(x) = 0$. An alternative definition of the associated Legendre function differs from the definition (4) by a factor of $(-1)^m$. Any one of the two definitions serves equally well for the purpose of this paper.

Considering the binomial series

$$(x^2-1)^n = \sum_{k=0}^{n} (-1)^k \binom{n}{k} x^{2n-2k} \tag{5}$$

and noting that

$$\frac{d^{n+m}}{dx^{n+m}}(x^{2n-2k}) = \begin{cases} \frac{(2n-2k)!}{(n-m-2k)!} x^{n-m-2k}, & 2k \le n-m, \\ 0, & 2k > n-m, \end{cases} \tag{6}$$

we infer

$$\frac{d^{n+m}}{dx^{n+m}}[(x^2-1)^n] = \sum_{k=0}^{n} (-1)^k \binom{n}{k} \frac{(2n-2k)!}{(n-m-2k)!} x^{n-m-2k}, \tag{7}$$

from which it follows that

$$P_n^m(x) = \frac{2^{-n}(n+1)_n}{(n-m)!}(1-x^2)^{\frac{m}{2}} x^{n-m} F^{mn}, \tag{8}$$

where

$$F^{mn} = F\left(\frac{m-n}{2}, \frac{m-n+1}{2}; \frac{1-2n}{2}; \frac{1}{x^2}\right) \tag{9}$$

is a truncated hypergeometric function and takes only the leading $\frac{n-m}{2}+1$ terms.

3. The Gaunt coefficient

The Gaunt coefficient $a(m,n,\mu,\nu,p)$ is defined by

$$a(m,n,\mu,\nu,p) = \frac{(2p+1)}{2} \frac{(p-m-\mu)!}{(p+m+\mu)!} \int_{-1}^{1} P_n^m(x) P_\nu^\mu(x) P_p^{m+\mu}(x)\, dx. \tag{10}$$

Such integrals were first given by Gaunt in 1929 in his study of the triplets of helium. But the formulas that he gave for their evaluation are of little use in the extended cases such as in the multisphere scattering problems when many such integrals need to be evaluated simultaneously.

An alternative definition, equivalent to Eq. (10), has been given above in Eq. (1). It is obvious that p on the right-hand side of Eq. (1) should be increased in steps of 2 because the power of x in the expansion (8) has an increment of -2. Thus, the Gaunt coefficients must vanish whenever $p = n+\nu-1, n+\nu-3, \ldots,$ etc. For convenience in practical applications, we reformulate the definition (1) and thus write

$$P_n^m(x) P_\nu^\mu(x) = \sum_{q=0}^{q_{\max}} a_q P_{n+\nu-2q}^{m+\mu}(x), \tag{11}$$

where a_q is an abbreviated notation for the Gaunt coefficient $a(m,n,\mu,\nu,n+\nu-2q)$, and $q_{\max}$ is given by

$$q_{\max} = \min\left(n, \nu, \frac{n+\nu-|m+\mu|}{2}\right). \tag{12}$$

While q takes the values of successive natural numbers, i.e., $q = 0,1,2,\ldots,q_{\max}$, the values of $(n+\nu-2q)$ change now in steps of -2.

4. An expression of the Gaunt coefficients for practical calculation

By applying Eq. (8) to $P_\nu^\mu(x)$ and $P_{n+\nu-2q}^{m+\mu}(x)$, we have

$$P_\nu^\mu(x) = \frac{2^{-\nu}(\nu+1)_\nu}{(\nu-\mu)!}(1-x^2)^{\frac{\mu}{2}} x^{\nu-\mu} F^{\mu\nu} \tag{13}$$

and

$$P_{n+\nu-2q}^{m+\mu}(x) = \frac{2^{2q-n-\nu}(n+\nu-2q+1)_{n+\nu-2q}}{(n_4-2q)!}(1-x^2)^{\frac{m+\mu}{2}} x^{n_4-2q} F^q, \tag{14}$$

where $n_4 = n+\nu-m-\mu, F^{\mu\nu}$ and F^q are also truncated hypergeometric series given by

$$F^{\mu\nu} = F\left(\frac{\mu-\nu}{2}, \frac{\mu-\nu+1}{2}; \frac{1-2\nu}{2}; \frac{1}{x^2}\right) \tag{15}$$

and

$$F^q = F\left(\frac{-n_4+2q}{2}, \frac{-n_4+2q+1}{2}; \frac{4q+1-2n-2\nu}{2}; \frac{1}{x^2}\right). \tag{16}$$

The number of terms in $F^{\mu\nu}$ and F^q is $\frac{\nu-\mu}{2}+1$ and $\frac{n_4-2q}{2}+1$, respectively. With the use of Eqs. (8), (13) and (14), Eq. (11) gives rise to

$$\frac{(n+1)_n(\nu+1)_\nu}{(n-m)!\,(\nu-\mu)!} F^{mn} F^{\mu\nu} = \sum_{q=0}^{q_{\max}} a_q \frac{4^q(n+\nu-2q+1)_{n+\nu-2q}}{(n_4-2q)!} x^{-2q} F^q. \tag{17}$$

Matching the coefficients of like terms on both sides of Eq. (17), we obtain a general expression containing the Gaunt coefficients $(a_0, a_1, \ldots, a_q)$:

$$\frac{(n+1)_n(\nu+1)_\nu}{(n-m)!\,(\nu-\mu)!} \sum_{k=0}^{q} c_{k+1}^{mn} c_{q-k+1}^{\mu\nu} = \sum_{k=0}^{q} a_k \frac{4^k(n+\nu-2k+1)_{n+\nu-2k}}{(n_4-2k)!} c_{q-k+1}^{k}, \tag{18}$$

where c_{k+1}^{mn} stands for the coefficient of the power x^{-2k} in the $(k+1)$st term of the hypergeometric series F^{mn}, and similarly for $c_{q-k+1}^{\mu\nu}$ and c_{q-k+1}^{k}. Explicitly, these three coefficients are given by

$$c_{k+1}^{mn} = 4^{-k}\frac{(m-n)_{2k}}{k!\,(-n+1/2)_k}, \qquad 1 \le k \le \frac{n-m}{2}, \tag{19}$$

$$c_{q-k+1}^{\mu\nu} = 4^{k-q}\frac{(\mu-\nu)_{2q-2k}}{(q-k)!\,(-\nu+1/2)_{q-k}}, \qquad 1 \le q-k \le \frac{\nu-\mu}{2}, \tag{20}$$

$$c_{q-k+1}^{k} = 4^{k-q}\frac{(2k-n_4)_{2q-2k}}{(q-k)!\,(-n-\nu+2k+1/2)_{q-k}}, \qquad 1 \le k \le q-1, \tag{21}$$

respectively, and by definition (9)

$$c_1^{mn} = c_1^{\mu\nu} = c_1^k \equiv 1. \tag{22}$$

5. New approach to evaluating the Gaunt coefficients

From Eqs. (18) and (22) we find immediately

$$a_0 = \frac{(n+1)_n(\nu+1)_\nu}{(n+\nu+1)_{n+\nu}} \frac{(n+\nu-m-\mu)!}{(n-m)!\,(\nu-\mu)!}. \tag{23}$$

We now define "normalized" Gaunt coefficients by

$$\tilde{a}_k = \frac{a_k}{a_0}. \tag{24}$$

In terms of these, Eq. (18) becomes

$$\sum_{k=0}^{q} c_{k+1}^{mn} c_{q-k+1}^{\mu\nu} = \sum_{k=0}^{q} \tilde{a}_k \frac{4^k (n+\nu-2k+1)_{n+\nu-2k}(n_4)!}{(n+\nu+1)_{n+\nu}(n_4-2k)!} c_{q-k+1}^{k}. \tag{25}$$

Using the notations

$$A_{qk} = \frac{4^k (n+\nu-2k+1)_{n+\nu-2k}(n_4)!}{(n+\nu+1)_{n+\nu}(n_4-2k)!} c_{q-k+1}^{k} \tag{26}$$

and

$$B_q = \sum_{k=0}^{q} b_{qk}, \tag{27}$$

where

$$b_{qk} = c_{k+1}^{mn} c_{q-k+1}^{\mu\nu}, \tag{28}$$

we can rewrite Eq. (25) in the form

$$\sum_{k=0}^{q} A_{qk} \tilde{a}_k = B_q, \qquad 0 \le q \le q_{\max}, \tag{29}$$

which is equivalent to a linear system containing all $q_{\max}+1$ nonzero Gaunt coefficients for an integer group (m, n, μ, ν). This linear system can be written in matrix form as

$$\mathbf{A}\tilde{\mathbf{a}} = \mathbf{B}, \tag{30}$$

where $\mathbf{A} = (A_{ij})$ is lower triangular, $\tilde{\mathbf{a}} = (\tilde{a}_i)$ and $\mathbf{B} = (B_j)$; the order of the system is $q+1$.

As seen above, there are $q_{\max}+1$ Gaunt coefficients for given integers (m, n, μ, ν), where $q_{\max}$ is given by Eq. (12). To calculate the normalized Gaunt coefficients, one must first set up the matrix $\mathbf{A}$ and the vector $\mathbf{B}$. Some useful recurrence formulas can be derived for the determination of the elements of $\mathbf{A}$ and $\mathbf{B}$. Eqs. (21), (22) and (26) show that

$$A_{i0} = c_{i+1}^{0}, \tag{31}$$

where

$$c_{i+1}^{0} = \frac{4^{-i}(-n_4)_{2i}}{i!\,(-n-\nu+1/2)_i}. \tag{32}$$

This leads to a recurrence relation

$$A_{i0} = A_{i-1,0} \frac{-(n_4-2i+2)(n_4-2i+1)}{2i(2n+2\nu-2i+1)}. \tag{33}$$

Also, from the definition (26), together with Eq. (21), we have

$$A_{ij} = \frac{4^j (n+\nu-2j+1)_{n+\nu-2j}(n_4)!}{(n+\nu+1)_{n+\nu}(n_4-2j)!} c^j_{i-j+1}, \tag{34}$$

and

$$c^{j+1}_{i-(j+1)+1} = c^j_{i-j+1} \frac{-2(i-j)(2n+2\nu-4j-1)(2n+2\nu-4j-3)}{(n_4-2j)(n_4-2j-1)(2n+2\nu-2i-2j-1)}, \tag{35}$$

whence

$$A_{ij} = A_{ij-1} \frac{2(j-i-1)}{(2n+2\nu-2i-2j+1)}, \qquad j \geq 1. \tag{36}$$

Similarly, from the expression

$$b_{ij} = c^{mn}_{j+1} c^{\mu\nu}_{i-j+1} = \frac{4^{-i}(m-n)_{2j}(\mu-\nu)_{2i-2j}}{j!\,(i-j)!\,(-n+1/2)_j(-\nu+1/2)_{i-j}} \tag{37}$$

we easily find that

$$b_{ij} = b_{i-1j} \frac{-(\nu-\mu-2i+2j+2)(\nu-\mu-2i+2j+1)}{2(i-j)(2\nu-2i+2j+1)}, \qquad j < i, \tag{38}$$

and

$$b_{ii} = b_{i-1i-1} \frac{-(n-m-2i+2)(n-m-2i+1)}{2i(2n-2i+1)}. \tag{39}$$

These four recurrence relations (33), (36), (38) and (39) are very useful for the efficient calculation of the Gaunt coefficients. With all b_{qk} $(k = 0, 1, 2, \ldots, q)$ for a given q known, B_q, the $(q+1)$st element of the column vector $\mathbf{B}$, can be calculated by employing Eq. (27) but can be written as

$$B_q = \sum_{k=k_{\min}}^{k_{\max}} b_{qk}, \tag{40}$$

where

$$k_{\min} = \max\left(0, q - \frac{\nu-\mu}{2}\right), \quad k_{\max} = \min\left(q, \frac{n-m}{2}\right), \tag{41}$$

by noticing that when $q > \frac{\nu-\mu}{2}$ and $q-k > \frac{\nu-\mu}{2}$, or $k > \frac{n-m}{2}$ (for any q),

$$b_{qk} \equiv 0. \tag{42}$$

6. Summary of the new algorithm

All $q_{\max}+1$ nonzero Gaunt coefficients $(a_0, a_1, a_2, \ldots, a_{q_{\max}})$ for a given integer group (m, n, μ, ν) can be evaluated one by one as follows.

(i) The first coefficient a_0 is obtained directly from Eq. (23).

(ii) The normalized Gaunt coefficients [see Eq. (24)] are therefore

$$\tilde{a}_q = \frac{a_q}{a_0} = \frac{a(m,n,\mu,\nu,n+\nu-2q)}{a(m,n,\mu,\nu,n+\nu)}.$$

Obviously, $\tilde{a}_0 \equiv 1$.

(iii) Starting from

$$A_{00} = b_{00} = B_0 = \tilde{a}_0 = 1,$$

we obtain the normalized Gaunt coefficients $(\tilde{a}_1, \tilde{a}_2, \ldots, \tilde{a}_{q_{\max}})$ by successively solving the linear equations

$$\tilde{a}_q = \frac{1}{A_{qq}} \left(B_q - \sum_{k=0}^{q-1} A_{qk} \tilde{a}_k \right), \qquad q = 1, 2, \ldots, q_{\max}. \tag{43}$$

All coefficients A_{qk} $(k = 0, 1, \ldots, q)$ in the linear equation for $\tilde{a}_q$ can be calculated from the known value of $A_{q-1,0}$ using the two-term recurrence relations (33) and (36). The constant term B_q is computed from Eq. (40) with $k_{\min}$ and $k_{\max}$ determined by Eqs. (41), and all b_{qk} $(k = k_{\min}, \ldots, k_{\max})$ can be computed from the known values of $b_{q-1,k}$ by using the two-term recurrence relation (38) [or (39) with $k = q$]. For example, with the initial values $\tilde{a}_0 = 1$ and $A_{00} = b_{00} = B_0 = 1$, $\tilde{a}_1$ is given by

$$\tilde{a}_1 = \frac{B_1 - A_{10}}{A_{11}},$$

where

$$A_{10} = \frac{-n_4(n_4 - 1)}{2(2n + 2\nu - 1)}, \qquad A_{11} = A_{10} \frac{-2}{(2n + 2\nu - 3)},$$

and $B_1 = b_{10} + b_{11}$ (taking the general case of $k_{\min} = 0$ and $k_{\max} = 1$) with

$$b_{10} = \frac{-(\nu - \mu)(\nu - \mu - 1)}{2(2\nu - 1)}, \qquad b_{11} = \frac{-(n - m)(n - m - 1)}{2(2n - 1)}.$$

With $\tilde{a}_0$ and $\tilde{a}_1$ known, $\tilde{a}_2$ can be calculated by

$$\tilde{a}_2 = \frac{B_2 - A_{20} - A_{21}\tilde{a}_1}{A_{22}},$$

where A_{20}, A_{21} and A_{22} can be calculated from A_{10} by the use of Eqs. (33) and (36), and B_2 can be computed from b_{10} and b_{11} by the use of Eqs. (38), (39), (40), (41). Generally, with $(\tilde{a}_0, \tilde{a}_1, \ldots, \tilde{a}_{q-1})$ known, $\tilde{a}_q$ can be easily found by

$$\begin{aligned} \tilde{a}_q = \frac{(n + \nu - 2q + 1/2)_{2q}}{(-n_4)_{2q}} & \sum_{k=0}^{q} \frac{(m - n)_{2k}(\mu - \nu)_{2q-2k}}{k!\,(q-k)!\,(-n + 1/2)_k(-\nu + 1/2)_{q-k}} \\ & - \sum_{j=0}^{q-1} \frac{(-n - \nu + q + j + 1/2)_{q-j}}{(q-j)!} \tilde{a}_j. \end{aligned} \tag{44}$$

(iv) Then, the Gaunt coefficients are restored by $a_q = a_0 \tilde{a}_q$. In fact, only normalized Gaunt coefficients are involved in practical multisphere scattering calculations.

7. Timing tests

Extensive timing and numerical tests have been carried out on an IBM RS6000-340 Workstation. Table I gives some comparison for the computational times (in seconds) required by our algorithm and Cruzan's $3jm$ formulation represented by Eqs. (2) and (3). In Table I, the first column is the highest degree $n_{\max}$ $(\nu_{\max})$ reached in the computation; the second column is the total number of nonzero Gaunt coefficients computed, which is the number of all possible nonzero Gaunt coefficients for all possible combinations of (m, n, μ, ν) from the lowest degree $n = \nu = 0$ to the highest degree $n_{\max} = \nu_{\max}$; the next two columns list the CPU time spent by the corresponding algorithm. Table I indicates that the required computing time for our algorithm is only $\sim 1\%$ of that for Cruzan's algorithm.

TABLE I. Timing tests for the calculation of the Gaunt coefficients

$n_{\max}(=\nu_{\max})$	N_g [1]	CPU (in seconds) on IBM RS6000-340 Workstation	
		Xu [2]	Cruzan [3]
10	69082	1	86
15	440810	8	725
20	1697663	34	3479
25	4903641	97	12631
30	11757744	239	33667

[1] total number of nonzero Gaunt coefficients calculated.
[2] The calculation used Xu's algorithm, i.e., the new algorithm presented in this paper.
[3] The calculation used Cruzan's $3jm$ formulation, i.e., Eqs. (2) and (3).

8. Numerical tests

(i) We performed the first test by comparing the numerical values of the Gaunt coefficients determined by our algorithm with those converted from the Clebsch-Gordan coefficients tabulated by Varshalovich et al. [32]. Varshalovich et al. defined the coefficients by

$$C^{j_3 m_3}_{j_1 m_1 j_2 m_2} = (-1)^{j_1 - j_2 + m_3} \sqrt{2j_3+1} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3 \end{pmatrix}. \tag{45}$$

Thus, the Gaunt coefficient can also be computed by

$$a(m,n,\mu,\nu,p) = \left[\frac{(n+m)!\,(\nu+\mu)!\,(p-m-\mu)!}{(n-m)!\,(\nu-\mu)!\,(p+m+\mu)!}\right]^{1/2} C^{p0}_{n0\nu0} C^{pm+\mu}_{nm\nu\mu}. \tag{46}$$

All numerical values of the Gaunt coefficients obtained by these two methods are identical, note, however, that the tabulated Clebsch-Gordan coefficients are available for low degrees only.

(ii) The second test consisted of a direct comparison of both sides of Eq. (11). For any integer combination (m,n,μ,ν) in a range of degrees from $n=\nu$ to $n_{\max} = \nu_{\max} = 20$, we first computed the $q_{\max}+1$ nonzero Gaunt coefficients by our algorithm, the associated Legendre functions $P^m_n(x), P^\mu_\nu(x)$ and $P^{m+\mu}_{n+\nu-2q}(x)$ for all q, and then performed the summation check to examine if Eq. (11) holds. For all cases we calculated, the results of this test were satisfactory within the precision allowed by the computer.

(iii) The numerical values of the Gaunt coefficients calculated by our algorithm were also systematically compared with those calculated by the $3jm$ formulation. This was simultaneously carried out with the timing tests described in §7. This comparison shows that (a) for low degrees from $n=\nu=0$ to $n=\nu=5$, all the corresponding numerical values obtained by both methods agree with each other, (b) for intermediate degrees, such as $n=\nu=6$ to $n=\nu=7$, both methods are still in fairly good agreement, and (c) discrepancies on numerical values of some higher-degree Gaunt coefficients are significant; the higher the degree, the more severe the discrepancies. To investigate the accuracy of the calculation of high-degree coefficients, we first tested the numerical values obtained from the $3jm$

formulation by the summation check using Eq. (11), similar to what we had done for our algorithm in the second test. Usually, these values do not satisfactorily fulfil Eq. (11), which indicates that the performance of the $3jm$ formulation is questionable in the case of high degrees. As a second check, we compared the numerical values of a_0, i.e., $a(m, n, \mu, \nu, n+\nu)$, obtained from the $3jm$ formulation with those accurate values evaluated directly from Eq. (23). Table II gives some examples for these particular Gaunt coefficients. This check reveals that the high-degree Gaunt coefficients computed by the $3jm$ formulation are inaccurate. The reliability of the $3jm$ formulation is gradually destroyed as the degree increases. The error comes from the summation over k [see Eq. (3)]. Table III lists the values of all nonzero Gaunt coefficients calculated by both our algorithm and the $3jm$ formulation for an integer group of $(m, n, \mu, \nu) = (2, 12, 3, 15)$. In general, when p is small, the numerical results from both methods still agree, even for high degrees. Similar to the case of increasing degree, the $3jm$ formulation gradually loses its accuracy with increasing p. The reason for this is that the summation (over k) required by the $3jm$ formulation involves delicate cancellations between successive terms that alternate in sign. For high degrees or large values of p, the individual terms in the summation become much larger than their sum, and all accuracy is lost.

TABLE II. Examples for the numerical values of $a(m, n, \mu, \nu, n+\nu)$ obtained by Eq. (23) and by the $3jm$ formulation†

m	n	μ	ν	$a(m,n,\mu,\nu,n+\nu)$	
				Eq. (23)	$3jm$
1	1	−1	1	0.3333333333E+00	0.3333333333E+00
1	2	−1	2	0.3428571429E+00	0.3428571429E+00
1	3	−1	3	0.3246753247E+00	0.3246753247E+00
1	4	−1	4	0.3045843046E+00	0.3045843046E+00
1	5	−1	5	0.2864318344E+00	0.2864318834**2**E+00
1	6	−1	6	0.2706234404E+00	0.2706234**323**E+00
1	7	−1	7	0.2569085117E+00	0.2569084**928**E+00
1	8	−1	8	0.2449469363E+00	0.24494**75523**E+00
1	9	−1	9	0.2344333048E+00	0.23443**97483**E+00
1	10	−1	10	0.2251171504E+00	0.225**3184617**E+00
1	11	−1	11	0.2167981587E+00	0.2**212355063**E+00
1	12	−1	12	0.2093167245E+00	0.2**205655817**E+00
1	13	−1	13	0.2025451116E+00	**−.2678705856E+01**
1	14	−1	14	0.1963803001E+00	**0.5715411956E+03**
1	15	−1	15	0.1907384645E+00	**0.3061141117E+06**
1	16	−1	16	0.1855507769E+00	**0.4108039018E+08**
1	17	−1	17	0.1807602223E+00	**0.1343926421E+11**
1	18	−1	18	0.1763191724E+00	**0.1153973986E+14**
1	19	−1	19	0.1721875249E+00	**−.5749672500E+15**
1	20	−1	20	0.1683312636E+00	**−.6680238706E+18**

† In this table, the highlights (bold style) indicate the discrepancies on the numerical values obtained from Eq. (23) and the $3jm$ formulation.

TABLE III. The numerical values of the Gaunt coefficients $a(2,12,3,15,p)$ obtained by Xu's algorithm and by Cruzan's $3jm$ formulation*†

q^{**}	p	$k^0_{\min}$	$k^0_{\max}$	N^0_k	$k_{\min}$	$k_{\max}$	N_k	$a(2,12,3,15,p) = a(2,12,3,15,27-2q)$	
								Xu	Cruzan
0	27	3	27	25	8	30	23	0.80142−6613E−02	**−.1792613138E+00**
1	25	3	25	23	8	28	21	0.5912933102E−02	0.59**88949904**E−02
2	23	3	23	21	8	26	19	0.6792070512E−02	0.67**82201553**E−02
3	21	3	21	19	8	24	17	0.9061425784E−02	0.9061**981214**E−02
4	19	3	19	17	8	22	15	0.1338922267E−01	0.13389**16655**E−01
5	17	3	17	15	8	20	13	0.2171985247E−01	0.2171985**470**E−01
6	15	3	15	13	8	18	11	0.3890892009E−01	0.3890891**997**E−01
7	13	3	13	11	8	16	9	0.7818971201E−01	0.781897120**2**E−01
8	11	3	11	9	8	14	7	0.1807173136E+00	0.180717313**5**E+00
9	9	3	9	7	8	12	5	0.4952008739E+00	0.495200873**8**E+00
10	7	3	7	5	8	10	3	0.1556202544E+01	0.1556202544E+01
11	5	3	5	3	8	8	1	−.9985632990E+01	−.9985632990E+01

* In the calculation using Cruzan's $3jm$ formulation (Eqs. (2) and (3)), the evaluation of the first $3jm$ coefficient, $\left(\begin{smallmatrix} n & \nu & p \\ 0 & 0 & 0 \end{smallmatrix}\right)$, takes a summation over k from $k^0_{\min}$ to $k^0_{\max}$ for a total of N^0_k terms, and the evaluation of the second $3jm$ coefficient, $\left(\begin{smallmatrix} n & \nu & p \\ m & \mu & -m-\mu \end{smallmatrix}\right)$, takes a summation over k from $k_{\min}$ to $k_{\max}$ for a total of N_k terms.

† In this table, the highlights (bold style) indicate the discrepancies on the numerical values obtained by Xu's algorithm and Cruzan's $3jm$ formulation.

** $q_{\max} = 11$ when $(m,n,\mu,\nu) = (2,12,3,15)$.

9. Conclusions and remarks

We have shown that the algorithm presented in this paper greatly reduces the computing time for the evaluation of the Gaunt coefficients. Furthermore, this algorithm can be applied to both low and high degrees, so that it is applicable to the solution of the multisphere scattering problems where both low- and high-degree coefficients are required. The formulation summarized in §6 has been implemented in a computer code and successfully used in the practical multisphere scattering calculations.

It is worth noting here that the term "Gaunt coefficient" is not used consistently in the literature, and that the closely related Clebsch-Gordan coefficient appears much more frequently. Because of the various definitions adopted by different authors, a systematic comparison of the Gaunt coefficients with the Clebsch-Gordan coefficients is cumbersome. Nevertheless, the integral of the triple associated Legendre functions on the right side of the definition (10) is common to all such coefficients. Thus, simple relations for converting one to the other can be found. In the preceding section, an example of such a conversion has been shown. As mentioned above, the Clebsch-Gordan coefficients are usually expressed in terms of the Winger $3jm$ symbols and are often tabulated for some low degrees in practical applications. The algorithm described in this paper can be analogously applied to the calculation of the Clebsch-Gordan coefficients and will provide substantial savings on the computing time. Because the algorithm is highly efficient, the coefficients needed in the practical applications can be directly computed. Replacing the large table by direct calculation will significantly reduce computer memory usage.

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