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Computation of Clebsch–Gordan and Gaunt Coefficients Using Binomial Coefficients

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Using binomial coefficients the Clebsch–Gordan and Gaunt coefficients were calculated for extremely large quantum numbers. The main advantage of this approach is directly calculating these coefficients, instead of using recursion relations. Accuracy of the results is quite high for quantum numbers l_1 and l_2 up to 100. Despite direct calculation, the CPU times are found comparable with those given in the related literature. © 1995 Academic Press, Inc.

I. INTRODUCTION

Clebsch–Gordan and Gaunt coefficients are of considerable importance in the application of quantum mechanics to the study of physical and chemical properties of atoms, molecules, and solids, and to the other fields of physics. Although, there is not much difficulty in the calculation of these coefficients for small quantum numbers, various difficulties arise for large quantum numbers. Dealing with large quantum numbers is unavoidable in the series expansion formulas for the multicenter integrals over Slater-type orbitals (STOs), which are of special interest to us.

In Refs. [1, 2] recurrence relations are used to avoid factorials in the calculation of the Clebsch–Gordan and Gaunt coefficients for large quantum numbers. However, using recurrence relations makes it impossible to directly get any one of the coefficients. Therefore, calculation of a required coefficient needs calculation of many other coefficients as well.

In this work, for direct calculation of the Clebsch–Gordan and Gaunt coefficients, the analytical expressions derived in Ref. [3] in terms of binomial coefficients were used with some modifications. In addition to that we have also computed the Gaunt coefficients as a product of two Clebsch–Gordan coefficients.

Our study constitutes a beginning for the calculation of multicenter molecular integrals on a computer, based on the method of translation of STOs about a displaced center [4, 5]. In doing so one needs to know the expansion coefficients for the normalized associated Legendre functions [6], for the product of two normalized Legendre functions both with different centers [7], and for the translation of STOs, as well as Clebsch–Gordan and Gaunt coefficients. All of these coefficients are expressed in terms of binomial coefficients [3]. Therefore, binomial coefficients which have very simple recurrence relations can be used as a basis in the calculations of these coefficients. It is well known that molecular *ab initio* calculations require extensive use of computer time and memory. We believe that our method will have important contributions in reducing requirements for computer time and memory.

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II. CLEBSCH–GORDAN COEFFICIENTS

Clebsch–Gordan coefficients $(l_1 l_2 m_1 m_2 | l_1 l_2 L M)$ defined by Eq. (2.9) of Ref. [8] with Condon–Shortley phases can be expressed in terms of binomial coefficients as (see Ref. [3])

$$(l_1 l_2 m_1 m_2 \,|\, l_1 l_2 L M) = \delta_{M,m_1+m_2} \times \left[\frac{(2L+1)^2 F_{l_1+l_2-L}(l_1+l_2+L+1) F_{L+M}(2L)}{(2l_1+1)(2l_2+1) F_{l_1-l_2+L}(l_1+l_2+L+1) F_{l_2-l_1+L}(l_1+l_2+L+1) F_{l_1+m_1}(2l_1) F_{l_2+m_2}(2l_2)} \right]^{1/2} \times \sum_n (-1)^n F_n(l_1+l_2-L) F_{l_2+m_2-n}(L+M) F_{l_1-m_1-n}(L-M), \quad (1)$$

where $F_n(n) = n!/[m!(n-m)!]$ are binomial coefficients and $|l_1 - l_2| \le L \le l_1 + l_2$, $|M| \le L$, and $\max[0, l_2 + m_2 - (L + M), l_1 - m_1 - (L - M)] \le n \le \min[l_1 + l_2 - L, l_2 + m_2, l_1 - m_1]$. Since we use phases according to Ref. [7], our definition of Clebsch–Gordan coefficients has the form in Ref. [9],

$$C^{l_1 l_2 L}_{m_1 m_2 M} = (-1)^{1/2(m_1+|m_1|+m_2+|m_2|+M+|M|)} (l_1 l_2 m_1 m_2 \,|\, l_1 l_2 L M). \quad (2)$$

It is easy to obtain for the Clebsch–Gordan coefficients $C^{l_1 l_2 L}_{m_1 m_2 M}$ the following orthonormality and symmetry relations [3]:

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$$\sum_{m_1,m_2} (-1)^{[m_1+|m_1|+m_2+|m_2|+M+|M|]} C^{l_1 l_2 L}_{m_1 m_2 M} C^{l_1 l_2 L_1}_{m_1 m_2 M_1} = \delta_{LL_1}\,\delta_{MM_1} \quad (3)$$

$$\sum_{L,M} (-1)^{(1/2)(m_1+|m_1|+m_2+|m_2|+m_1'+|m_1'|+m_2'+|m_2'|)+M+|M|} C^{l_1 l_2 L}_{m_1 m_2 M} C^{l_1' l_2' L}_{m_1' m_2' M} \quad (4)$$
$$= \delta_{m_1 m_1'}\,\delta_{m_2 m_2'}$$

$$C^{l_2 l_1 L}_{m_2 m_1 M} = (-1)^{l_1+l_2-L} C^{l_2 l_1 L}_{m_2 m_1 m}$$
$$= (-1)^{l_1+l_2-L} C^{l_1 l_2 L}_{-m_1 -m_2 -M} \quad (5)$$
$$= (-1)^{l_1} \sqrt{(2L+1)/(2l_2+1)}\, C^{l_1 L l_2}_{m_1 -M -m_2}.$$

III. GAUNT COEFFICIENTS

Gaunt coefficients $C^L(l_1 m_1, l_2 m_2)$ defined in Ref. [10] can be expressed in terms of binomial coefficients as in Ref. [3]

$$C^L(l_1 m_1, l_2 m_2)$$
$$= (-1)^{g-(l_2-m_2)+(1/2)(|m_1|+|m_2|+|M|)} \frac{F_{g-l_1}(2g-l_1-l_2)F_L(g)}{(2g+1)F_{2L}(2g)}$$
$$\times \left[\frac{(2l_1+1)(2l_2+1)F_{l_1+m_1}(l_1+l_2+M)F_{l_1+l_2+M}(2L+l_1+l_2+M)}{F_{l_1-m_1}(l_1+l_2-M)F_{L-M}(2L)F_{L+M}(2L+2M)F_{l_2+l_1-M}(2L+l_1+l_2+M)}\right]^{1/2}$$
$$\times \sum_t (-1)^t \frac{F_{L-M-t}(l_2-m_2+L-M-t)F_t(l_1+m_1+t)F_{l_1-m_1-t}(l_1+l_2-L)F_{l_1+l_2-L}(l_1+l_2+M)}{F_{l_1+m_1}(l_1+l_2+M)}, \quad (6)$$

where $g = \frac{1}{2}(l_1 + l_2 + L)$, $M = m_1 - m_2$, $|l_1 - l_2| \le L \le l_1 + l_2$, $|M| \le L$, and $\max[0, L - m_1 - l_2] \le t \le \min[l_1 - |m_1|, L - M, L - m_1 + l_2]$.

The Gaunt coefficients can also be expressed as a product of two Clebsch–Gordan coefficients [11]:

$$C^L(l_1 m_1, l_2 m_2) = \frac{1}{2L+1} \sqrt{(2l_1+1)(2l_2+1)}\, C^{l_1 l_2 L}_{m_1 -m_2 M} C^{l_1 l_2 L}_{000}. \quad (7)$$

The symmetry relations for the Gaunt coefficients are given as

$$C^L(l_1 m_1, l_2 m_2) = \sqrt{(2l_2+1)/(2L+1)}\, C^{l_2}(l_1 m_1, L m_1 - m_2)$$
$$= \sqrt{(2l_1+1)/(2L+1)}\, C^{l_1}(L m_1 - m_2, l_2 - m_2)$$
$$= C^L(l_2 m_2, l_1 m_1). \quad (8)$$

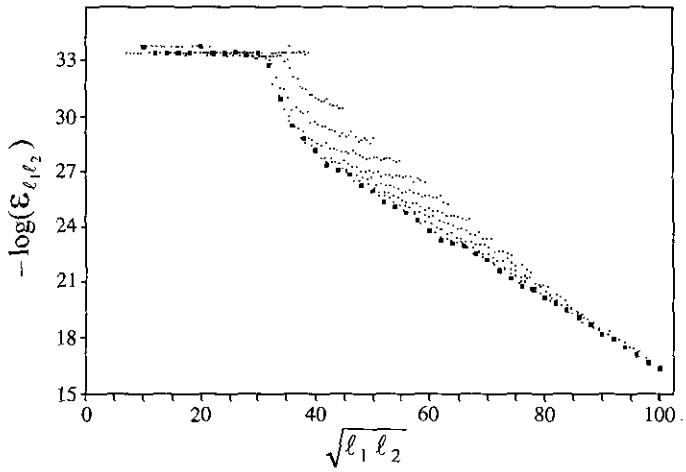

FIG. 1. Plot of $-\log(\varepsilon_{l_1 l_2})$ versus $\sqrt{l_1 l_2}$. Bold points show the situation where $l_1 = l_2$, and faint points show other l_1, l_2 combinations. Note that $-\log(\varepsilon_{l_1 l_2})$ is equivalent to number of correct decimal places.

IV. NUMERICAL RESULTS AND DISCUSSION

Since in the calculation of the Clebsch–Gordan and Gaunt coefficients we use binomial coefficients as a basis it is helpful to keep them in memory of the computer.

During the calculation of the binomial coefficients, recurrence relation

$$F_m(n) = F_m(n-1) + F_{m-1}(n-1) \quad (9)$$

is used to refrain from factorials and to speed up the calculations. Computed binomial coefficients are stored in an array in the memory and in doing so symmetries of the binomial coefficients are used to minimize the memory requirement. Number of the stored binomial coefficients is proportional to $n_{\max}^2/4$. As an example for $n_{\max} = 150$ it takes approximately 0.5 s of CPU time for computation of all the binomial coefficients, and 5476 binomial coefficients are stored in the memory of the computer.

Computer programs are written in FORTRAN 77 on VAX-4000 system. All parts of programs use REAL*16 precision arithmetic. To make the given CPU times comparable we would like to note that one QSQRT evaluation takes approximately 0.4 ms CPU time.

Clebsch–Gordan coefficients were computed from Eqs. (1) and (2) and the accuracy of Clebsch–Gordan coefficients was determined from the orthogonality relations given in Eq. (3). For a given pair of l_1, l_2 all possible m_1, m_2 values were screened and the maximum value of the error

$$\varepsilon_{l_1 l_2} = \left| 1 - \sum_{L,M} \left[C^{l_1 l_2 L}_{m_1 m_2 M} \right]^2 \right| \quad (10)$$

TABLE I

Clebsch–Gordan Coefficients and Their Symmetries for Some Selected Quantum Numbers

Quantum Numbers					Clebsch-Gordan coefficients	Quantum Numbers					Clebsch-Gordan coefficients
L	ℓ_1	m_1	ℓ_2	m_2	and their symmetries	L	ℓ_1	m_1	ℓ_2	m_2	and their symmetries
(9	20	-3	15	2)	-0.20712837720085954207449431722381 8E+00	(34	20	-3	15	2)	-0.36369403442652827464546891615798 9E+00
(9	15	22	0	-3)	-0.20712837720085954207449431722381 8E+00	(34	15	2	20	-3)	-0.36369403442652827464546891615798 9E+00
(15	20	-3	9	1)	-0.20712837720085954207449431722381 8E+00	(15	20	-3	34	1)	-0.36369403442652827464546891615798 9E+00
(9	20	3	15	-2)	-0.20712837720085954207449431722381 8E+00	(34	20	3	15	-2)	-0.36369403442652827464546891615798 9E+00
(40	25	12	35	-17)	-0.10243967888918240170634246636015 3E+00	(60	25	12	35	-17)	0.35895930196826432829957724769857 3E-03
(40	35	-17	25	12)	-0.10243967888918240170634246636015 3E+00	(60	35	-17	25	12)	0.35895930196826432829957724769857 3E-03
(35	25	12	40	5)	-0.10243967888918240170634246636015 3E+00	(35	25	12	60	5)	0.35895930196826432829957724769857 3E-03
(40	25	-12	35	17)	-0.10243967888918240170634246636015 3E+00	(60	25	-12	35	17)	0.35895930196826432829957724769857 3E-03
(49	40	-2	37	1)	-0.12513485268547968017974948130049 2E+00	(77	40	-2	37	1)	0.33827263856136501225193523308617 9E+00
(49	37	1	40	-2)	-0.12513485268547968017974948130049 2E+00	(77	37	1	40	-2)	0.33827263856136501225193523308617 9E+00
(37	40	-2	49	1)	-0.12513485268547968017974948130049 2E+00	(37	40	-2	77	1)	0.33827263856136501225193523308617 9E+00
(49	40	2	37	-1)	-0.12513485268547968017974948130049 2E+00	(77	40	2	37	-1)	0.33827263856136501225193523308617 9E+00
(7	60	3	58	2)	-0.77641434675191276901821525065241 6E-02	(116	60	3	58	2)	-0.22412027861780558947502594755085 7E+00
(7	58	2	60	3)	-0.77641434675191276901821525065241 6E-02	(116	58	2	60	3)	-0.22412027861780558947502594755085 7E+00
(58	60	3	7	-5)	-0.77641434675191276901821525065241 3E-02	(58	60	3	116	-5)	-0.22412027861780558947502594755085 7E+00
(7	60	-3	58	-2)	-0.77641434675191276901821525065241 6E-02	(116	60	-3	58	-2)	-0.22412027861780558947502594755085 7E+00
(6	80	1	77	-3)	0.72445174267338019771914282764110 7E-01	(78	80	1	77	-3)	-0.87205397034066448058687369662229 2E-01
(6	77	-3	80	1)	0.72445174267338019771914282764110 7E-01	(78	77	-3	80	1)	-0.87205397034066448059005926142184 8E-01
(77	80	1	6	2)	0.72445174267338019771914282764110 8E-01	(77	80	1	78	2)	-0.87205397034066448059171563511874 1E-01
(6	80	-1	77	3)	0.72445174267338019771914282764110 7E-01	(78	80	-1	77	3)	-0.87205397034066448059089488589632 6E-01

was determined. For a given l_1, l_2 pair it was observed that the maximum error occurs when $|m_1| \cong |m_2| \cong 0$.

Figure 1 shows a plot of $-\log_{10}(\varepsilon_{l_1 l_2})$ versus $\sqrt{l_1 l_2}$. It is clearly seen from the Fig. 1 that the accuracy is closely related to $\sqrt{l_1 l_2}$ and maximum error occurs for $l_1 = l_2$. Although, the accuracy is higher for $l_1 \neq l_2$, to be on the safe side $l_1 = l_2$ should be taken as the reference. All possible L values were screened for $l_1 \cong l_2$ and $|m_1| \cong |m_2| \cong 0$, where the maximum error occurs, and the accuracy of the Clebsch–Gordan coefficients was also checked by symmetry relations given in Eq. (5). Maximum error occurred in the midrange of L numbers and, as expected, they were an order of magnitude better than those found by orthonormality relations. The Clebsch–Gordan coefficients and their symmetries for some selected quantum numbers are shown in Table I.

Gaunt coefficients are calculated both from the Eq. (6) through the binomial coefficients and from Eq. (7) through the Clebsch–Gordan coefficients. Accuracy of the Gaunt coefficients calculated from Eq. (7) is determined using the symmetry relations given in Eq. (8). We note that the accuracy of the Gaunt coefficients behaves the same as that of the Clebsch–Gordan coefficients.

Gaunt coefficients calculated from Eq. (6) are checked for their accuracy by the symmetry relations given in Eq. (8) and are compared to those obtained from Eq. (7). Accuracy of these Gaunt coefficients was satisfactory for small quantum numbers (l_1, $l_2 \leq 40$), while it was unacceptable for large quantum numbers (l_1, $l_2 \geq 60$). The Gaunt coefficients and their symmetries calculated from both Eq. (6) and Eq. (7) for some selected quantum numbers are shown in Table II.

CPU time required for calculation of only one Clebsch–Gordan or Gaunt coefficient is related to the number of terms of the summation in Eq. (1) or Eq. (6). Table III shows the required CPU times for some selected quantum numbers. It also includes the CPU times for recursive calculations found in the literature. As the authors do not have much experience in computer programming, programs were written quite roughly. We believe that a skilful programmer can considerably reduce these CPU times.

The expression given in Eq. (1) for Clebsch–Gordan coeffi-

TABLE II

Gaunt Coefficients, Calculated from Both Eq. (6) and Eq. (7), for Some Selected Quantum Numbers

Quantum Numbers					Gaunt coefficients	Gaunt coefficients	Number of
L	ℓ_1	m_1	ℓ_2	m_2	computed from Eq.(7)	computed from Eq.(6)	Terms
(35	20	-3	15	2)	0.22831996049136240648383191053241488E+00	0.22831996049136240648383191053241483E+00	1
(31	20	-3	15	2)	0.93333275484180648727646307949475636E-01	0.93333275484180648727646307949469919E-01	5
(15	20	-3	17	-5)	0.71892812332879002898175421943507820E-01	0.71892812332879002898175421943822192E-01	13
(15	20	-3	9	-5)	0.11717778700858182295250895784161305E-01	0.11717778700858182295250895784160806E-01	5
(60	25	12	35	-17)	0.24163144553313471365499107762123419E+00	0.24163144553313471365499107762123438E+00	1
(48	25	12	35	-17)	0.60943321567428860493598105744320768E-01	0.60943321567428860493598105744515016E-01	13
(38	25	12	35	-17)	-0.22935301595927260757197374746587053E-01	-0.22935301595927260757197374746596042E-01	10
(75	40	-2	37	1)	0.11247579572575226261135887302162431E+00	0.11247579572575226261135887302162449E+00	3
(59	40	-2	37	1)	0.41881419529763815637269171732133892E-01	0.41881419529763815637270175392091160E-01	19
(37	40	-2	21	-3)	0.36291809901020190221116604722642449E-01	0.36291809901020190221116599754775377E-01	19
(37	40	-2	5	-3)	0.13869303747693775517032995926234191E+00	0.13869303747693775517032995926234184E+00	3
(118	60	3	58	2)	0.20340851843561319201456541834314557E+00	0.20340851843561319201456541834314564E+00	1
(58	60	3	58	1)	0.19720171333763386799276264116510151E-01	0.19720171333907882495611564193714732E-01	57
(60	38	1	58	-2)	0.43002575255522843899509184748893122E-01	0.43002575255522844056883846443163491E-01	37
(60	2	1	58	-2)	0.20107662497245360032548290534793984E+00	0.20107662497245360032548290534793979E+00	1
(155	80	1	77	-3)	0.10620517180910204513602583910875749E+00	0.10620517180910204513602583910875386E+00	3
(131	80	1	77	-3)	0.13490722345861117500725469942813815E-01	0.13490722345861117749146452295715484E-01	27
(83	80	1	77	-3)	-0.17985243959806236802092417091017870E-01	-0.17980813898293841702895191143202996E-01	75
(5	80	1	77	-3)	0.13523172983645216090536728445612330E+00	0.13523172983645216090536728445612380E+00	2

Also the number of terms of the summation in Eq. (6) are given.

cients is also valid for half-integer quantum numbers and accuracy of the results is the same as that illustrated in Fig. 1.

We believe that errors in the calculations stem from the truncation errors due to the limited accuracy of the computer and cancellation errors arising from the alternating signs in the summations (when two numbers, whose values are very close, are subtracted from each other one loses on a computer as many digits of accuracy as the number of the same digits of the two numbers). In addition, the error tends to increase as the number of terms in the summation increase.

We believe that presented new approach in this work for the calculation of the Clebsch–Gordan and Gaunt coefficients is important for the *ab initio* calculations of atoms and molecules. Following studies related to this work will include calculation of multicenter integrals. The ultimate purpose of these studies is to do molecular *ab initio* calculations using the above-mentioned method of expansion for STOs about a displaced center.

TABLE III

Average CPU Times Used for Computing Various Strings of Clebsch–Gordan and Gaunt Coefficients

Quantum numbers					CPU time per	CPU time per Gaunt coefficient		
L	l_1	m_1	l_2	m_2	C-G coefficient	Eq. (6)	Eq. (7)	Ref. [2][a]
L	15	15	15	15	1.9	2	5	2.1
L	15	0	15	0	2.9	5	6.3	1.3
L	8	−5	10	7	1.8	2.5	5	3.4
L	14	m_1	79	m_2	2.6	3.8	6	3.4
L	35	m_1	35	m_2	3.5	5.5	8.5	3.3
L	71	m_1	79	m_2	5.7	10.2	12.6	3.2
L	51	m_1	99	m_2	4.5	8.1	9.4	3.5

[a] CPU times of Ref. [2] are obtained by running their program on our computer using REAL * 16 arithmetic.

Note. CPU times given are in milliseconds and averaged over the quantum numbers which are not specified.

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