Analytical Evaluation of Two-Center Kinetic Energy Integral for Slater-Type Orbitals Using Guseinov Rotation-Angular Function

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Abstract. A new way of computing kinetic energy integral over Slater type orbitals is proposed. This article is concerned with the construction of the general formulae for the two-center kinetic energy integral using Guseinov rotation-angular function. The analytical formulae of the kinetic energy integral presented in the form of the overlap integral. The final results are expressed through the auxiliary functions which can be evaluated efficiently and accurately. The results of evaluation are play a significant role for the study of electronic structure and electron-nuclei interaction properties of atoms, molecules and solids by Hartree-Fock-Roothaan and correlated theories.

Keywords: kinetic energy, Overlap integrals, Slater type orbital, Guseinov rotation-angular function, auxiliary functions

1. Introduction

It is well known that exact eigen-states of atomic and molecular Hamiltonians satisfy the cusp condition [16] and decrease exponentially at large distances [1].
Consequently, it is not surprising that exponentially decreasing functions (for large arguments), in particular Slater-type functions, could be used successfully as basis functions in atomic calculations. However, an equally successful application of these functions in molecular calculations has so far been prevented by the fact that despite enormous efforts no completely satisfactory method for the evaluation of the notorious multicenter integrals of Slater-type or other exponentially decreasing functions has been found yet. A survey of the older literature on multicenter integrals was given in review papers by Huzinaga [15], Harris and Michels [14] and Browne [4]. More recent references can be found in Ref. [26] and in a review paper by Steinborn [23].

Slater-type functions have the simplest analytical structure of all exponentially decreasing functions. Other commonly occurring functions of that class, for instance, hydrogen eigen-functions, can normally be expressed quite easily as linear combinations of Slater-type functions. This implies that multicenter integrals of other exponentially decreasing functions can be expressed in terms of the basic multicenter integrals over Slater-type functions. Probably, this was the reason why only multicenter integrals of Slater-type functions have been examined thoroughly in the literature whereas the integrals of other exponentially decreasing functions have largely been neglected [28]. Many calculations over the years have been carried out with Slater-type orbitals (STO's), particularly for diatomic molecules. However, it soon became clear that there was a practical problem arising in evaluation of the necessary multicenter integrals over STO's when the orbitals in the integrals are centered on three or four different atoms.

The aim of this report is to evaluate the kinetic energy integral using the relations for overlap integrals in our work [30]. These relations are especially useful for the computation of any overlap and kinetic energy integrals for large quantum numbers contained in the series expansion formulas for molecular integrals. Since the overlap and kinetic energy integrals over STO's are of considerable importance in the evaluation of arbitrary multicenter integrals it is hoped the present work will prove useful in tackling more complicated molecular integrals appearing in the determination of various properties of molecules when the Hartree-Fock-Roothaan approximation is employed and also in the evaluation of the correlation energy when the Hylleraas method is used to describe the multielectron molecules [12].

2. Mathematical Analysis

The two-center kinetic energy integral examined in this work have the following form in which the orbitals are taken to be real [10,19,20].

\[
\frac{1}{2} \nabla^2 \left\{ \phi_a | \phi_b \right\} = \int \chi_{n_a,l_a,m_a} (\zeta_a, r_a, \theta_a, \phi_a) \left( \frac{1}{2} \nabla^2 \right) \chi_{n_b,l_b,m_b} (\zeta_b, r_b, \theta_b, \phi_b) \, dv_a dv_b
\]

The real Slater-Type Orbitals \( \chi_{n,l,m}(\zeta, r \theta \phi) \) are defined by [12]:

\[
\chi_{n,l,m}(\zeta, r \theta \phi) = \sum \text{certain terms}
\]
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\[ \chi_{nlm}(\zeta, r \theta \phi) = \frac{(2 \zeta)^{n+\frac{1}{2}}}{\sqrt{(2n)!}} \cdot e^{-\zeta r} \cdot r^{n-\frac{3}{2}} \cdot S_{lm}(\theta, \phi) \]  \hspace{1cm} (2)

Where \( S_{lm}(\theta, \phi) \) denotes the real spherical harmonic [3].

\[ S_{lm}(\theta, \phi) = P_{l}\left| m \right| (\cos \theta) \cdot \Phi_m(\phi) \]  \hspace{1cm} (3)

Here \( P_{l}\left| m \right| (\cos \theta) \) is the associated Legendre polynomial which has the following form:

\[ P_{l}\left| m \right| (x) = \frac{(-1)^{l-m}}{2^l l!} \frac{d^{l-m}}{dx^{l-m}}[(x^2-1)^l] \]  \hspace{1cm} (4)

Also the \( \Phi_m(\phi) \) is defined by:

\[ \Phi_m(\phi) = \frac{1}{\sqrt{\pi (1+\delta_{m0})}} \begin{cases} \cos |m| \phi & \text{for } m \geq 0 \\ \sin |m| \phi & \text{for } m < 0 \end{cases} \]  \hspace{1cm} (5)

and \( n, l, m \) are the quantum numbers.

It is easy to calculate the effect of the differential operator \( -\frac{1}{2} \nabla^2 \) for the real STO’s \( \chi_{nlm}(\zeta, r \theta \phi) \) or \([n,l,m] \) as the following:

\[ -\frac{1}{2} \nabla^2 [n,l,m] = -\frac{1}{2} \left[ \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \nabla_{\theta,\phi}^2 \right] [n, l, m] \]  \hspace{1cm} (6)

It is well known that:

\[ \nabla_{\theta,\phi}^2 S_{lm}(\theta, \phi) = -l(l+1) S_{lm}(\theta, \phi) \]  \hspace{1cm} (7)

Using (7) in (6) we have:

\[ -\frac{1}{2} \nabla^2 [n,l,m] = -\frac{1}{2} \zeta_b^2 \left[ [n,l,m] - \frac{2}{2n_b - 1} [n_b - 1,l,m] \right] + \frac{4(n_b + l_b)(n_b - l_b - 1)}{(2n_b(2n_b - 3))(2n_b - 2)(2n_b - 3))^\frac{3}{2}} [n_b - 2l_b,m] \]  \hspace{1cm} (8)

Substituting (8) in (1), the kinetic energy integral can be expressed in terms of overlap integral by writing them as:
\[
\left[ (n_a l_a m_a) \mid \frac{-1}{2} \nabla^2 \right] (n_b l_b m_b) = \frac{-1}{2} \zeta^2 b \int \chi_{n_a l_a m_a}(\zeta_a, r_a \theta_a \phi_a) \chi_{n_b l_b m_b}(\zeta_b, r_b \theta_b \phi_b) \, dv_1 \, dv_2 -
\]
\[
2 \left( \frac{2n_b}{2n_b-1} \right)^{\frac{1}{2}} \int \chi_{n_a l_a m_a}(\zeta_a, r_a \theta_a \phi_a) \chi_{n_b l_b m_b}(\zeta_b, r_b \theta_b \phi_b) \, dv_1 \, dv_2 +
\]
\[
\frac{4(n_b + l_b)(n_b - l_b - 1)}{(2n_b(2n_b - 1)(2n_b - 2)(2n_b - 3))^{\frac{3}{2}}} \int \chi_{n_a l_a m_a}(\zeta_a, r_a \theta_a \phi_a) \chi_{n_b l_b m_b}(\zeta_b, r_b \theta_b \phi_b) \, dv_1 \, dv_2 \}
\]
\[
= \frac{-1}{2} \zeta^2 b \left[ \left( (n_a l_a m_a) \mid (n_b l_b m_b) \right] - 2 \left( \frac{2n_b}{2n_b-1} \right)^{\frac{1}{2}} \left( (n_a l_a m_a) \mid (n_b - 1 l_b m_b) \right] +
\]
\[
\frac{4(n_b + l_b)(n_b - l_b - 1)}{(2n_b(2n_b - 1)(2n_b - 2)(2n_b - 3))^{\frac{3}{2}}} \left( (n_a l_a m_a) \mid (n_b - 2 l_b m_b) \right] \}
\]
(9)

Where \([ (n_a l_a m_a) \mid (n_b l_b m_b) ]\), \([ (n_a l_a m_a) \mid (n_b - 1 l_b m_b) ]\) and \([ (n_a l_a m_a) \mid (n_b - 2 l_b m_b) ]\) are the two-center overlap integrals for which a general analytical formulas have been established in our work [30]. Using (15) in Ref. [30] we find, for the two-center kinetic energy integral the following expression:
\[
\left[ (n_a l_a \lambda) \mid \frac{-1}{2} \nabla^2 \right] (n_b l_b \lambda)] = \frac{-1}{2} \zeta^2 b \left( N_{n_a \beta}(\rho, t) \right) \sum_{\alpha=\lambda}^{l_a} \sum_{\beta=\lambda}^{l_b} \sum_{q=0}^{\alpha+\beta} Q^{q}_{N' N}(\rho, t) - 2 \left( \frac{2n_b}{2n_b-1} \right)^{\frac{1}{2}} \cdot
\]
\[
N_{\alpha \beta}(\rho, t) \sum_{\alpha=\lambda}^{l_a} \sum_{\beta=\lambda}^{l_b} \sum_{q=0}^{\alpha+\beta} Q^{q}_{N' N'}(\rho, t) + \frac{4(n_b + l_b)(n_b - l_b - 1)}{[2n_b(2n_b - 1)(2n_b - 2)(2n_b - 3)]^{\frac{3}{2}}} \cdot
\]
\[
N_{\alpha \beta}(\rho, t) \sum_{\alpha=\lambda}^{l_a} \sum_{\beta=\lambda}^{l_b} \sum_{q=0}^{\alpha+\beta} Q^{q}_{N' N'}(\rho, t) \cdot g^{q}_{\alpha \beta}(l_a \lambda, l_b \lambda) \}
\]
(11)

where
\[
N_{\alpha \beta}(\rho, t) = \frac{(1 + t)^{\nu + \frac{1}{2}} (1 - t)^{\nu + \frac{1}{2}} \rho^{\nu + \nu + 1}}{\sqrt{(2n_a)! (2n_b)!}}
\]
(12)

\[
Q^{q}_{N' N}(\rho, t) = \int_{-1}^{1} \int (\mu \nu)^{q} (\mu + \nu)^{N'} (\mu - \nu)^{N} e^{-\rho \mu - \rho \nu} d\mu d\nu
\]
(13)

\[
g^{q}_{\alpha \beta}(l_a \lambda, l_b \lambda) = g^{q}_{\alpha \lambda}(l_a \lambda, l_b \lambda) \cdot F_q(\alpha + \lambda, \beta + \lambda)
\]
(14)

\[
F_m(N, N') = N! N'! \sum_{k=0}^{N'} \frac{(-1)^{N'} k! (m-k')! (N'-k')! (N-(m-k')!)}{(m-k')! (N'-k')! (N-(m-k')!)}
\]
for \(0 \leq m \leq N + N'\), \(N = n_a - \alpha\), \(N' = n_b - \beta\)
(15)
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\[ g_{\alpha \beta}^{(l_a \lambda, l_b \lambda)} = \frac{1}{2^{l_a + l_b + 1}} \left[ \frac{(2l_a + 1)(l_a - \lambda)!}{(l_a + \lambda)!} \frac{(2l_b + 1)(l_b - \lambda)!}{(l_b + \lambda)!} \right]^{\frac{1}{2}} \left[ \frac{(-1)^{l_a} (l_a - \lambda + \frac{1}{2}) \cdot (l_a + \lambda)!}{\frac{1}{2} (l_a - \lambda)!} \right] \left[ \frac{(-1)^{l_b} (l_b - \lambda + \frac{1}{2}) \cdot (l_b + \lambda)!}{\frac{1}{2} (l_b - \lambda)!} \right] \] 

\[ \sum_{j=0}^{l_a} \left( \frac{(-1)^{j} \cdot (l + \alpha + 2\lambda - i)! F_i(\lambda, \lambda)}{\{\frac{1}{2}(\lambda - \alpha)\}! \{\frac{1}{2}(\lambda + \alpha)\}! (\alpha + \lambda - i)!} \right) \] 

and

\[ \rho = \frac{R}{2} (\zeta_a + \zeta_b), \quad t = \frac{(\zeta_a - \zeta_b)}{(\zeta_a + \zeta_b)} \]  

It should be noted that, the some useful recurrence relations for the auxiliary functions \( Q_{N,N'}^{q}(\rho, t) \) and \( F_m(N, N') \) have also been established in appendix of our work \[30\].

Using Guseinov rotation-angular function \[17\], finally we can establish the following general formulae for the two-center kinetic energy integral:

\[ [(n_a l_a m_a) \mid \frac{1}{2} \nabla^2 \mid (n_b l_b m_b)] = \sum_{k=0}^{l_a} T_{l_m, l_a, m_a} (\theta, \phi) [(n_a l_a \lambda)] \frac{1}{2} \nabla^2 [(n_b \lambda \lambda)] = \sum_{k=0}^{l_a} T_{l_m, l_a, m_a} (\theta, \phi) [S_1 + S_2 + S_3] \]  

\( S_1 = -\frac{1}{2} \zeta_b^2 N_{n_a m_a} (\rho, t) \sum_{\alpha = -\lambda}^{\lambda} \sum_{\beta = -\lambda}^{\lambda} Q_{N,N}^{q}(\rho, t) g_{a b}^{q} (l_a \lambda, l_b \lambda) \)  

\( S_2 = \zeta_b^2 \left( \frac{2n_b}{2n_b - 1} \right)^{\frac{1}{2}} N_{n_a m_a - 1} (\rho, t) \sum_{\alpha = -\lambda}^{\lambda} \sum_{\beta = -\lambda}^{\lambda} Q_{N,N}^{q - 1}(\rho, t) g_{a b}^{q} (l_a \lambda, l_b \lambda) \)  

\( S_3 = -2 \zeta_b^2 (n_b + l_b)(n_b - l_b - 1) N_{n_a m_a - 2} (\rho, t) \sum_{\alpha = -\lambda}^{\lambda} \sum_{\beta = -\lambda}^{\lambda} Q_{N,N}^{q - 2}(\rho, t) g_{a b}^{q} (l_a \lambda, l_b \lambda) \)  

\( T_{l,m, l_a, m_a} (\theta, \phi) = \frac{2(\zeta_t^{a+b}{})^{\frac{1}{2}}}{(1 + \delta_{ab}) (l_a + l_b)(l_a + l_b + 1)} \sum_{j=0}^{l_a} \sum_{k=0}^{l_b} (\varepsilon_{m_a, m_b})^{\delta_{j+1} l_a} C_{l_l \lambda, l_m, l_a, l_b}^{\frac{1}{2}} \times \frac{2(\zeta_t^{a+b}{})^{\frac{1}{2}}}{(2l+1)^{\frac{1}{2}}} S_{L MD} (\theta, \phi) \)  

and \( l_- = \min(l_a, l_b) \).

Here the quantities \( C_{l_l \lambda, l_m, l_a, l_b}^{\frac{1}{2}} \) are Clebsch-Gordan coefficients \[13\]:
where the quantities \( F_k(n) \) are determined by:

\[
F_k(n) = \begin{cases} 
\frac{n^k}{k!(n-k)!} & \text{for } 0 \leq k \leq n \\
0 & \text{for } k < 0 \text{ and } k > n
\end{cases}
\]

Here \( \gamma_a = |m_a|, \gamma_b = |m_b|, M_i = \epsilon_{m_a m_b} |\gamma_a + \gamma_b| \) and \( \epsilon_{m_a m_b} = \pm 1 \). The sign of the symbol \( \epsilon_{m_a m_b} \) is determined by the product of the signs \( m_a \) and \( m_b \) (the sign of zero is regarded as positive). The symbol \( \sum^{(2)} \) indicates that the summation is to be performed in steps of two.

Because the importance of the Clebsch-Gordan coefficients and the Gaunt coefficients for the calculation of multicenter integrals over STO's, we have been discussed these auxiliary functions in the appendix of the present article.

### 3. Appendix

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

\[
a(m, n, \mu, \nu, p) = \frac{(2p+1)(p-m-\mu)!}{2(p+m+\mu)!} \int_{-1}^{1} P^m (x) P^\mu (x) P^{m+\mu} (x) dx
\]

Such integrals were first given by Gaunt in 1929 [9] 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 multi-sphere scattering problems when many such integrals need to be evaluated simultaneously.

In the literature there are analytical formulas for the Clebsch-Gordan and Gaunt coefficients in terms of factorials [5,7,25]. Although there is not much difficulty in the calculation of these coefficients for small quantum numbers, various difficulties arise for large quantum numbers, because factorials with extremely large arguments would be needed in the series expansion formulas of multicenter integrals. In Refs. [21,27], recurrence relations are used to avoid factorials for large quantum numbers. However, using recurrence relations makes it impossible to directly get any one of the coefficients since the calculation of a required coefficient needs calculation of many other coefficients as well.

In the derivation of such addition theorems [6,8,22] there occurs a product of two associated Legendre functions, which can be expressed in terms of the linearization expansion.
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\[ P_n^m (\cos \theta) P_p^\nu (\cos \theta) = \sum_{p'=|p'|} a(m, n, \mu, \nu, p) P_{p'}^{m+\nu} (\cos \theta) \]  

(26)

where \( a(m, n, \mu, \nu, p) \) is the so-called Gaunt coefficient [9]. Gaunt coefficients are closely related to the Clebsch-Gordan coefficients [2,18] 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 representation. Clebsch-Gordan coefficients are usually expressed in terms of the Winger 3jm symbols [7,29,31,32]. Cruzan [6] provided a similar expression for the Gaunt coefficient:

\[
a(m, n, \mu, \nu, p) = (-1)^{m+\nu} (2p+1) \left\{ \begin{array}{ccc} n+m & (\nu+\mu)! & (p-m-\mu)! \\ (n-m)! & (\nu-\mu)! & (p+m+\mu)! \end{array} \right\}^{1/2} \left( \begin{array}{ccc} n & \nu & p \\ m & \mu & -m-\mu \end{array} \right) \]  

(27)

where the Winger 3jm symbol is defined by [24]

\[
\left( \begin{array}{ccc} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{array} \right) = \delta_{m_1+m_2+m_3,0} (-j_1-j_2-j_3) \times \left[ \begin{array}{ccc} (j_3+j_1-j_2)! & (j_3-j_1+j_2)! & (j_1+j_2-j_3)! \\ (j_3-j_1+j_2+1)! & (j_1-j_2-j_3)! & (j_2-j_3+j_1)! \\ (j_3-j_1+j_2)! & (j_1-j_2-j_3)! & (j_2-j_3+j_1)! \end{array} \right]^{1/2} \times \sum_k (-1)^{k+j_1+m_2} (j_2+j_3-m_1-k)! (j_1-m_2+k)! \\
(j_3-j_1+j_2-k)! (j_3-m_3-k)! (k+j_1-j_2+m_3)! 
\]  

(28)

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.

\[
C_{j,m_1j,m_2}^{j_1m_1j_2m_2} = (-1)^{j_1-j_2+m_2} \sqrt{2j_3+1} \left( \begin{array}{ccc} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3 \end{array} \right) \]  

(29)

Thus, the Gaunt coefficient can also be computed by:

\[
a(m, n, \mu, \nu, p) = \left\{ \begin{array}{ccc} n+m & (\nu+\mu)! & (p-m-\mu)! \\ (n-m)! & (\nu-\mu)! & (p+m+\mu)! \end{array} \right\}^{1/2} C_{n\nu\theta}^{p\theta} C_{nm\nu}^{pm+\mu} \]  

(30)

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.

Recently, Guseinov derived the analytical formulas for the Clebsch-Gordan and Gaunt coefficients in terms of binomial coefficients [11,13]. For Clebsch-Gordan coefficients:
\[ C^{\ell\ell'}_{m-m'} = \delta_{M,m'M} \left( -1 \right)^{m+m'-m'} \left\{ \left( 2L+1 \right)^2 F_{\ell',-L,M+\ell+L} F_{\ell,1M} \left( 2L+1 \right) \right\}^{1/2} \sum_{t} \left( -1 \right)^{t} F_{t}(l'-L) F_{t-m'-t}(L-M) F_{t,m-t}(L+M) \] (31)

Where
\[
\max [0, l-m-(L-M), l'+m'-(L+M)] \leq t \leq \min [l-m, l'+m', l+l'-L]
\]
and for Gaunt Coefficients:
\[
C^{\ell}_{m-m'} = \delta_{M,m'M} \left( -1 \right)^{m+m'-m'} e^{-\ell-\ell'} \left\{ F_{\ell',-L,M+\ell+L} F_{\ell,1M} \left( 2L+1 \right) \right\}^{1/2} \sum_{t} \left( -1 \right)^{t} F_{t}(l'-L) F_{t-m'-t}(L-M) F_{t,m-t}(L+M) \] (32)

Where
\[
g = (l'+L) \quad \text{and} \quad \max [0, L-m-l'] \leq t \leq \min [l-m, L-M, L-m+l']
\]
Here the quantities \( F_k(n) \) are determined
\[
F_k(n) = \begin{cases} \binom{2L+1}{k} & \text{for } 0 \leq k \leq n \\ 0 & \text{for } k < 0 \text{ and } k > n \end{cases} \] (33)

The summation limits in (31) and (32) follow from the selection rule:
\[
l + l' + L = 2g,
\]
where \( g = 0,1,2,\ldots \) and the properties of coefficients \( F_k(n) \).

The Gaunt coefficients can also be expressed as product of two Clebsch-Gordan coefficients:
\[
C^{\ell}_{m-m'} = \frac{1}{2L+1} \sqrt{(2L+1)(2l'+1)} C^{\ell\ell L}_{m-m'M} C^{\ell\ell L}_{000} \] (34)

The Clebsch-Gordan coefficients which satisfy the selection rule have the following symmetry relations:
\[
C^{\ell\ell L}_{m-m'M} = C^{\ell\ell L}_{m'Mm} \] (35)
\[
C^{\ell\ell L}_{m-m'M} = C^{\ell\ell L}_{m'-m,-M} \] (36)

The selection rule is also satisfied for the Gaunt coefficients which are closely related to the Clebsch-Gordan coefficients. They have the similar to Eqs. (35) and (36) symmetry properties:
\[
C^{\ell}_{m-m'} = C^{\ell}_{l' m', l} \] (37)
\[
C^{\ell}_{m-m'} = C^{\ell}_{l- m, l' - m'} \] (38)
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For non-zero values of Clebsch-Gordan coefficients and Gaunt coefficients, the quantum numbers occurring in (31) and (32) satisfy the following restrictions:

\[ l = 0,1,2,\ldots, \quad -l \leq m \leq l, \quad 0 \leq l' \leq l, \quad 0 \leq m' \leq l' \]  \tag{39}

and

\[ l - l' \leq L \leq l + l' \quad , \quad l + l' + L = \text{even integer} \quad , \quad \lambda \leq L \]  \tag{40}

Where \( \lambda = |m + m'| \) and \( \lambda = |m - m'| \) for Clebsch-Gordan and Gaunt coefficients, respectively. It should be noted that, the coefficients \( C_{m_1m_2,LM}^{l_1l_2} \) have the following orthonormality and symmetry properties [11]:

\[
\sum_{m_1,m_2} (-1)^{m_1+m_2+l} C_{m_1m_2,LM}^{l_1l_2} = \delta_{LL}, \delta_{MM}, \delta_{LM}, \delta_{ML} \quad \tag{41}
\]

\[
\sum_{L,M} (-1)^{l_1+l_2-L} C_{m_1m_2,LM}^{l_1l_2} = \delta_{m_1m_2} \quad \tag{42}
\]

\[
C_{m_1m_2,LM}^{l_1l_2} = (-1)^{l_1+l_2-L} C_{m_1m_2,LM}^{l_1l_2} = (-1)^{l_1+l_2-L} C_{m_1m_2,LM}^{l_1l_2} = (-1)^{l_1} \sqrt{\frac{2L_1+1}{2L+1}} C_{m_1m_2,LM}^{l_1l_2} \quad \tag{43}
\]

Also, the Gaunt coefficients have the following symmetry properties [11]:

\[
C^{l_1}(l_1m_1, l_2m_2) = \sqrt{\frac{2l_2+1}{2L+1}} C^{l_1}(l_1m_1, LM) = \sqrt{\frac{2l_1+1}{2L+1}} C^{l_1}(LM, l_2 - m_2) = C^{l_1}(l_2m_2, l_1m_1) \quad \tag{44}
\]

Summary

A general expansion is derived for two-center kinetic energy integral using Guseinov rotation-angular function. The final results are expressed in the form of a series giving sufficiently accurate values. The proposed algorithm is especially useful for computation of multicenter integrals that arise in the Hartree-Fock-
Roothaan approximation, which plays a significant role for the study of electronic structure.

**References**


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