Süleyman Demirel Üniversitesi Fen Edebiyat Fakültesi Fen Dergisi
Süleyman Demirel University Faculty of Arts and Sciences Journal of Science
2022, 17(2): 438-452
DOI: 10.29233/sdufeffd.1165376
Atıf için / For Citation: S. Akdemir, "Properties of one- and two-center Coulomb integrals over Slater type orbitals", *Süleyman Demirel Üniversitesi Fen Edebiyat Fakültesi Fen Dergisi*, 17(2), 438-452, 2022.

Research Article

Properties of One- and Two-Center Coulomb Integrals over Slater Type Orbitals

Selda AKDEMİR[*1]

[1]*Sinop University, Faculty of Education, Department of Science Education, 57000, Sinop, Turkey*

**corresponding author e-mail: sozcan@sinop.edu.tr*

(Alınış / Received: 22.08.2022, Kabul / Accepted: 13.10.2022, Yayımlanma / Published: 25.11.2022)

Abstract: In this study, two-electron one- and two-center Coulomb integrals with the same and different screening parameters are investigated numerically in the real Slater type orbital (STO) basis using Fourier transform method. In momentum space firstly, for atomic, i.e. one-center, Coulomb integrals are calculated, and analytical expressions are obtained in terms of binomial coefficients. Then, the solutions of the two-center Coulomb integrals are made with the modified Bessel function of second kind and the results are expressed in terms of binomial and Gaunt coefficients, irregular solid harmonics, and finite sum of STOs. A computer program is written in the MATHEMATICA language to determine the accuracy of the analytical expressions that are highly suitable for programming. The numerical results obtained from the program are given in the tables, and it is shown that the results agree with the literature.

Key words: Coulomb integral, Fourier transform method, Slater type atomic orbital, Taylor expansion.

Slater Tipi Orbitaller Bazında Bir- ve İki-Merkezli Coulomb İntegrallerinin Özellikleri

Öz: Bu çalışmada, aynı ve farklı perdeleme sabitlerine sahip iki elektronlu bir- ve iki-merkezli Coulomb integralleri, Fourier dönüşüm yöntemi kullanılarak reel Slater tipi orbitaller (STO) bazında sayısal olarak incelenmiştir. Momentum uzayında ilk olarak atomik, yani tek-merkezli, Coulomb integralleri için hesaplama yapılmış ve analitik ifadeler binom katsayıları cinsinden elde edilmiştir. Daha sonra, iki-merkezli Coulomb integrallerinin çözümleri, ikinci tür modifiye edilmiş Bessel fonksiyonları ile yapılmış ve sonuçlar binom ve Gaunt katsayıları, düzensiz katı harmonikler ve STO'ların sonlu toplamı cinsinden ifade edilmiştir. Programlamaya son derece uygun olan analitik ifadelerin doğruluğunu belirlemek için MATHEMATICA dilinde bir bilgisayar programı yazılmıştır. Programdan elde edilen sayısal sonuçlar tablolarda verilmiş ve sonuçların literatür ile uyumlu olduğu gösterilmiştir.

Anahtar Kelimeler: Coulomb integrali, Fourier dönüşüm metodu, Slater tip atomik orbital, Taylor açılımı.

1. Introduction

Molecular integrals that arise in molecular electronic structure calculations based on the molecular orbital method, molecular orbitals are built from linear combinations of atomic orbitals (LCAO-MO), are an important research area in quantum mechanics. Here it is difficult and time consuming that computation of two-electron integrals containing $1/r_{12}$ factor which describes the Coulomb interaction between the electrons. Therefore, the

further development of the methods used for the calculation of two-electron integrals is unavoidable.

The wave functions of hydrogen atom obtained from the solution of the Schrödinger equation satisfy the cusp condition at the nucleus and exponential decay at large distances from the nucleus [1]. STOs and Gaussian type orbitals (GTOs) are basis functions widely used as atomic orbitals in calculation of molecular integrals. STOs exactly show the behavior of the wave functions near the nuclei and at large distances from them. But the use of STOs is limited due to the difficulty to evaluate efficiently all occurring integrals in a molecular calculation. GTOs do not provide a cusp represents the electron density at the nucleus and decay too quickly. However, molecular integrals can be easily calculated using GTOs. To provide the physical properties, the use of a linear combination of GTOs versus a single STO increases the number of the integrals to be computed over GTOs. As a result, compared to GTOs, STOs have the advantage as they can exhibit the two features of exact wave function. In reference [2], STOs and GTOs are compared and studies using STOs in molecular calculations from past to present are given in detail.

There are many methods of integration used for solving the two-electron molecular integrals. Elliptic coordinate method [3-13] is the transformation of polar coordinates into the elliptical coordinates. Single-center expansion methods [14-25] are based on the translation of the orbitals from the one center to another. Fourier transform method [26-37] evaluates the integrals in momentum space. In the Gaussian expansion method [38, 39], STOs are written as a linear combination of GTOs. Gaussian transform method [40, 41] uses the Laplace transform of the exponential function. The other approaches used in the calculation of molecular integrals are given in references [42-49].

Fourier transform method, primarily suggested by Prosser and Blanchard [50] for one-electron integrals and developed by Geller [26-28] for two-electron integrals, is one of the most important methods used to simplify of the calculation of many-center molecular integrals. Through this method where integrals are transformed into inverse Fourier integrals, two-dimensional integrals in coordinate space with non-separable integration variables can be expressed in one-dimensional integrals in momentum space with easily separable integration variables. A different class of exponentially decreasing basis functions is B functions. Although the B functions, defined in terms of the reduced Bessel functions, have a complicated mathematical structure in coordinate space, their Fourier transforms are exceptional simplicity [31-33].

In this study, using the Fourier transform method, firstly the atomic Coulomb integrals over real STOs has been expressed as finite sums of binomial coefficients. Later for the molecular Coulomb integrals with the same and different screening parameters new expressions have been obtained in terms of Gegenbauer and Gaunt coefficients, irregular solid harmonics, and linear combination of STOs. A computer program in the MATHEMATICA 10.0 software [51] is constructed and the comparisons of numerical results with literature values have been given in Table 1 and Table 2. Atomic units are used throughout this article.

2. Material and Method

2.1 General formulas

As is well known two-electron two-center Coulomb integral includes Coulomb operator that describes the interactions between the charge distributions of each electron. The charge distribution is defined as the product of two atomic orbitals located at the same center. The general formula of two-center Coulomb integral based on STOs is as follows:

$$J^{n_3 l_3 m_3, n_4 l_4 m_4}_{n_1 l_1 m_1, n_2 l_2 m_2}(\varepsilon_a, \varepsilon_{a'}, \varepsilon_b, \varepsilon_{b'}; \mathbf{R}) = \iint \chi^{m_1^*}_{n_1 l_1}(\varepsilon_a, \mathbf{r}_{1a}) \chi^{m_2}_{n_2 l_2}(\varepsilon_{a'}, \mathbf{r}_{1a}) \frac{1}{r_{12}} \chi^{m_3^*}_{n_3 l_3}(\varepsilon_b, \mathbf{r}_{2b}) \chi^{m_4}_{n_4 l_4}(\varepsilon_{b'}, \mathbf{r}_{2b}) d\mathbf{r}_1 d\mathbf{r}_2 \quad (1)$$

We will use the normalized real STOs defined as:

$$\chi^m_{n\,l}(\alpha, \mathbf{r}) = \frac{(2\alpha)^{n+1/2}}{\sqrt{(2n)!}} r^{n-1} e^{-\alpha r} Y^m_l(\theta, \varphi) \quad (2)$$

where *n*, *l*, and *m* are quantum numbers and α is the screening parameter. The principal quantum number *n* is a positive integer. There are also studies using non-integer *n*-STOs in the literature [53, 54]. $Y^m_l(\theta, \varphi)$ is the complex or real spherical harmonic and described as follows

$$Y^m_l(\theta, \varphi) = P^{|m|}_l(cos\theta)\Phi_m(\varphi) \quad (3)$$

in which $P^{|m|}_l(cos\theta)$ is the normalized associated Legendre polynomial [52]. For real spherical harmonics $\Phi_m(\varphi)$ is defined by

$$\Phi_m(\varphi) = \frac{1}{\sqrt{\pi(1+\delta_{m,0})}} \begin{cases} cosm\varphi & \text{for} \quad m \geq 0 \\ sin|m|\varphi & \text{for} \quad m < 0 \end{cases} \quad (4)$$

The product of two real spherical harmonics:

$$Y^{m_1 *}_{l_1}(\theta, \varphi) Y^{m_2}_{l_2}(\theta, \varphi) = \sum_{L=|l_1-l_2|}^{l_1+l_2 (2)} \sum_{M=-L}^{L} \langle l_1 m_1 | l_2 m_2 | LM \rangle A^M_{m_1 m_2} Y^{M*}_L(\theta, \varphi) \quad (5)$$

where $\langle l_1 m_1 | l_2 m_2 | LM \rangle$, so-called generalized Gaunt coefficient and linearized the product of two spherical harmonics, and $A^M_{m_1 m_2}$ are the coefficients obtained with the integration of the product of three real spherical surface harmonics [10]. The symbol $\Sigma^{(2)}$ implies that the summation index *L* proceeds in two steps.

One-center charge distribution which consists of two real STOs centered at the same nuclei can be expressed as a linear combination of STOs using the Equation (5) in reference [55]:

$$\chi_{n_1 l_1}^{m_1 *}(\varepsilon_a, \mathbf{r}_1)\chi_{n_2 l_2}^{m_2}(\varepsilon_{a'}, \mathbf{r}_1) = \sqrt{\frac{2^3\big(2(n_1+n_2-1)\big)!}{(2n_1)!\,(2n_2)!}}\frac{\varepsilon_a^{n_1+1/2}\varepsilon_{a'}^{n_2+1/2}}{(\varepsilon_a+\varepsilon_{a'})^{n_1+n_2-1/2}}$$

$$\sum_{L=|l_1-l_2|}^{l_1+l_2{}^{(2)}}\sum_{M=-L}^{L}\langle l_1 m_1|l_2 m_2|LM\rangle A_{m_1 m_2}^{M}\,\chi_{n_1+n_2-1\,L}^{M}(\varepsilon_a+\varepsilon_{a'}, \mathbf{r}_1) \tag{6}$$

Two-center Coulomb integrals can be written by using the Equation (6) in terms of basic Coulomb integrals as follows:

$$J_{n_1 l_1 m_1, n_2 l_2 m_2}^{n_3 l_3 m_3, n_4 l_4 m_4}(\varepsilon_a, \varepsilon_{a'}, \varepsilon_b, \varepsilon_{b'}; \mathbf{R}) =$$

$$\frac{2^3\,\varepsilon_a^{n_1+1/2}\varepsilon_{a'}^{n_2+1/2}\varepsilon_b^{n_3+1/2}\varepsilon_{b'}^{n_4+1/2}}{(\varepsilon_a+\varepsilon_{a'})^{n_1+n_2-1/2}(\varepsilon_b+\varepsilon_{b'})^{n_3+n_4-1/2}}\sqrt{\frac{\big(2(n_1+n_2-1)\big)!\,\big(2(n_3+n_4-1)\big)!}{(2n_1)!\,(2n_2)!\,(2n_3)!\,(2n_4)!}}$$

$$\sum_{L=|l_1-l_2|}^{l_1+l_2{}^{(2)}}\sum_{M=-L}^{L}\langle l_1 m_1|l_2 m_2|LM\rangle\, A_{m_1 m_2}^{M}\sum_{L'=|l_3-l_4|}^{l_3+l_4{}^{(2)}}\sum_{M'=-L'}^{L'}\langle l_3 m_3|l_4 m_4|L'M'\rangle\, A_{m_3 m_4}^{M'}$$

$$C_{n_1+n_2-1\,L\,M}^{n_3+n_4-1\,L'\,M'}(\varepsilon_a+\varepsilon_{a'}, \varepsilon_b+\varepsilon_{b'}; \mathbf{R}) \tag{7}$$

where the basic Coulomb integrals are defined by:

$$C_{N_1 L_1 M_1}^{N_2 L_2 M_2}(\alpha, \beta; \mathbf{R}) = \iint \chi_{N_1 L_1}^{M_1{}^{*}}(\alpha, \mathbf{r}_1)\frac{1}{r_{12}}\chi_{N_2 L_2}^{M_2}(\beta, \mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2 \tag{8}$$

If the Fourier transform method defined for the two-electron two-center integrals [26-28] is applied to Equation (8), the two-center basic Coulomb integrals are obtained in momentum space as follows [33]:

$$C_{N_1 L_1 M_1}^{N_2 L_2 M_2}(\alpha, \beta; \mathbf{R}) = 4\pi\int\frac{e^{-i\mathbf{R}.\mathbf{p}}}{p^2}U_{N_1 L_1}^{M_1{}^{*}}(\alpha, \mathbf{p})U_{N_2 L_2}^{M_2}(\beta, \mathbf{p})d\mathbf{p} \tag{9}$$

where $U_{N\,L}^{M}(\alpha, \mathbf{p})$ denotes the Fourier transform of STOs.

The Fourier transform of STOs is given in terms of regular solid spherical harmonic defined as $S_l^m(\mathbf{p}) = p^l Y_l^m\big(\theta_p, \varphi_p\big)$ in reference [56]

$$U_{n\,l}^{m}(\alpha, \mathbf{p}) = \frac{2^{n+l+1}\alpha^{n+1/2}}{F_l(n)\sqrt{\pi F_n(2n)(\alpha^2+p^2)^{n+l+2}}}C_{n-l}^{l+1}\left(\frac{\alpha}{\sqrt{\alpha^2+p^2}}\right)S_l^m(-i\mathbf{p}) \tag{10}$$

here $F_l(n)$ are the binomial coefficients and $C_n^{\lambda}(x)$ is Gegenbauer polynomial defined by the following relation [57, 58];

$$C_n^{\lambda}(x) = \sum_{s=0}^{[n/2]} (-1)^s a_s(\lambda, n)(2x)^{n-2s} \tag{11}$$

where

$$\left[\frac{n}{2}\right] = \frac{n}{2} - \frac{1-(-1)^n}{4}$$

$$a_s(\lambda, n) = F_{\lambda-1}(\lambda + n - s - 1)F_s(n-s)$$

The Rayleigh expansion of the plane wave is defined by the well-known relation in terms of spherical Bessel functions $j_l(pR)$ and spherical harmonics

$$e^{\pm i\mathbf{p}.\mathbf{R}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (\pm i)^l j_l(pR) Y_l^{m^*}(\theta_p, \varphi_p) Y_l^m(\theta_R, \varphi_R) \tag{12}$$

2.2 Basic Coulomb integrals in momentum space

2.2.1 One-center basic Coulomb integrals

It is well known that both electrons are centered on the same nuclei in one-center Coulomb integrals, take the name atomic Coulomb integrals, and determined by **R**=0 at Equation (9). In momentum space, atomic Coulomb integrals with the same screening parameters are given by:

$$C_{N_1L_1M_1}^{N_2L_2M_2}(\alpha, \alpha; 0) = 4\pi \int \frac{U_{N_1L_1}^{M_1^*}(\alpha, \mathbf{p})}{p^2} U_{N_2L_2}^{M_2}(\alpha, \mathbf{p}) d\mathbf{p} \tag{13}$$

Substituting Equation (10) into Equation (13), and then by using the orthogonality relation of the spherical harmonics, we write:

$$C_{N_1L_1M_1}^{N_2L_2M_2}(\alpha, \alpha; 0) = \delta_{L_1L_2}\delta_{M_1M_2} \frac{(-1)^{L_1} 2^{2N_1+2N_2+4} \alpha^{2N_1+2N_2-L_1-L_2+1}}{F_{L_1}(N_1)F_{L_2}(N_2)\sqrt{F_{N_1}(2N_1)F_{N_2}(2N_2)}}$$

$$\sum_{s=0}^{\left[\frac{N_1-L_1}{2}\right]} \sum_{r=0}^{\left[\frac{N_2-L_2}{2}\right]} \frac{(-1)^{s+r} a_s(L_1+1, N_1-L_1) a_r(L_2+1, N_2-L_2)}{(2\alpha)^{2s+2r}}$$

$$\int_0^{\infty} \frac{p^{L_1+L_2} dp}{(\alpha^2+p^2)^{N_1+N_2-s-r+2}} \tag{14}$$

When the radial integral is solved easily with the help of the integral tables of reference [57] atomic Coulomb integrals with the same screening parameters are obtained as follows [59]:

$$C_{N_1L_1M_1}^{N_2L_2M_2}(\alpha,\alpha;0)=\delta_{L_1L_2}\delta_{M_1M_2}\frac{(-1)^{L_1}2^{2N_1+2N_2+3}}{F_{L_1}(N_1)F_{L_2}(N_2)\sqrt{F_{N_1}(2N_1)F_{N_2}(2N_2)}\alpha^2}\sum_{s=0}^{\left[\frac{N_1-L_1}{2}\right]}\sum_{r=0}^{\left[\frac{N_2-L_2}{2}\right]}\frac{(-1)^{s+r}a_s(L_1+1,N_1-L_1)a_r(L_2+1,N_2-L_2)}{2^{2s+2r}(N_1+N_2-s-r+1)F_{\frac{L_1+L_2-1}{2}}(N_1+N_2-s-r)} \quad (15)$$

For the atomic Coulomb integrals with the different screening parameters the following radial integral is acquired:

$$C_{N_1L_1M_1}^{N_2L_2M_2}(\alpha,\beta;0)=\delta_{L_1L_2}\delta_{M_1M_2}\frac{(-1)^{L_1}2^{2N_1+2N_2+4}\alpha^{2N_1-L_1+1/2}\beta^{2N_2-L_2+1/2}}{F_{L_1}(N_1)F_{L_2}(N_2)\sqrt{F_{N_1}(2N_1)F_{N_2}(2N_2)}}\sum_{s=0}^{\left[\frac{N_1-L_1}{2}\right]}\sum_{r=0}^{\left[\frac{N_2-L_2}{2}\right]}\frac{(-1)^{s+r}a_s(L_1+1,N_1-L_1)a_r(L_2+1,N_2-L_2)}{(2\alpha)^{2s}(2\beta)^{2r}}\int_0^{\infty}\frac{p^{L_1+L_2}dp}{(\alpha^2+p^2)^{N_1-s+1}(\beta^2+p^2)^{N_2-r+1}} \quad (16)$$

Using the Taylor expansion given by Equation (4.1) of reference [33], we can write the denominator of the integral in terms of simpler functions:

$$C_{N_1L_1M_1}^{N_2L_2M_2}(\alpha,\beta;0)=\delta_{L_1L_2}\delta_{M_1M_2}\frac{(-1)^{L_1}2^{2N_1+2N_2+4}\alpha^{2N_1-L_1+1/2}\beta^{2N_2-L_2+1/2}}{F_{L_1}(N_1)F_{L_2}(N_2)\sqrt{F_{N_1}(2N_1)F_{N_2}(2N_2)}}\sum_{s=0}^{\left[\frac{N_1-L_1}{2}\right]}\sum_{r=0}^{\left[\frac{N_2-L_2}{2}\right]}\frac{(-1)^{s+r}a_s(L_1+1,N_1-L_1)a_r(L_2+1,N_2-L_2)}{(2\alpha)^{2s}(2\beta)^{2r}}\left\{\frac{(-1)^{N_2-r+1}}{(N_2-r)!}\sum_{v_1=0}^{N_1-s}\frac{(N_1+N_2-s-r-v_1)!}{(N_1-s-v_1)!\,(\alpha^2-\beta^2)^{N_1+N_2-s-r-v_1+1}}\int_0^{\infty}\frac{p^{L_1+L_2}dp}{(\alpha^2+p^2)^{v_1+1}}+\frac{(-1)^{N_1-s+1}}{(N_1-s)!}\sum_{v_2=0}^{N_2-r}\frac{(N_1+N_2-s-r-v_2)!}{(N_2-r-v_2)!\,(\beta^2-\alpha^2)^{N_1+N_2-s-r-v_2+1}}\int_0^{\infty}\frac{p^{L_1+L_2}dp}{(\beta^2+p^2)^{v_2+1}}\right\} \quad (17)$$

Finally, the radial integrals in Equation (17) by solving like Equation (14), the atomic Coulomb integral with the different screening parameter is obtained [59]:

$$C_{N_1L_1M_1}^{N_2L_2M_2}(\alpha,\beta;0)=\delta_{L_1L_2}\delta_{M_1M_2}\frac{(-1)^{N_2+L_2-1}2^{2N_1+2N_2+4}\alpha^{2N_1-L_1+1/2}\beta^{2N_2-L_2+1/2}}{(L_1+L_2+1)F_{L_1}(N_1)F_{L_2}(N_2)\sqrt{F_{N_1}(2N_1)F_{N_2}(2N_2)}}$$
$$\sum_{s=0}^{\left[\frac{N_1-L_1}{2}\right]}\sum_{r=0}^{\left[\frac{N_2-L_2}{2}\right]}\frac{(-1)^s a_s(L_1+1,N_1-L_1)a_r(L_2+1,N_2-L_2)}{(2\alpha)^{2s}(2\beta)^{2r}(\alpha^2-\beta^2)^{N_1+N_2-s-r+1}}$$
$$\left\{\alpha^{L_1+L_2-1}\sum_{v_1=0}^{N_1-s}\frac{F_{N_2-r}(N_1+N_2-s-r-v_1)}{F_{\frac{L_1+L_2+1}{2}}(v_1)}\left(1-\frac{\beta^2}{\alpha^2}\right)^{v_1}\right.$$
$$\left.-\beta^{L_1+L_2-1}\sum_{v_2=0}^{N_2-r}\frac{F_{N_1-s}(N_1+N_2-s-r-v_2)}{F_{\frac{L_1+L_2+1}{2}}(v_2)}\left(1-\frac{\alpha^2}{\beta^2}\right)^{v_2}\right\} \tag{18}$$

2.2.2 Two-center basic Coulomb integrals

Two-center Coulomb integrals represent the molecular Coulomb integrals that each one-center charge distribution centered on different nuclei in configuration space. The integral obtained as Equation (9) in momentum space is written for the same screening parameters as follows:

$$C_{N_1L_1M_1}^{N_2L_2M_2}(\alpha,\alpha;\mathbf{R})=4\pi\int\frac{e^{-i\mathbf{R}.\mathbf{p}}}{p^2}U_{N_1L_1}^{M_1{}^*}(\alpha,\mathbf{p})U_{N_2L_2}^{M_2}(\alpha,\mathbf{p})d\mathbf{p} \tag{19}$$

In Equation (9), using the definitions of the FTSTO (Equation (10)), the product of two real spherical harmonics (Equation (5)), and the Rayleigh expansion (Equation (12)), one obtains:

$$C_{N_1L_1M_1}^{N_2L_2M_2}(\alpha,\alpha;\mathbf{R})=\frac{(-1)^{L_2}i^{L_1+L_2}\pi 2^{2N_1+2N_2+6}\alpha^{2N_1+2N_2-L_1-L_2+1}}{F_{L_1}(N_1)F_{L_2}(N_2)\sqrt{F_{N_1}(2N_1)F_{N_2}(2N_2)}}$$
$$\sum_{s=0}^{\left[\frac{N_1-L_1}{2}\right]}\sum_{r=0}^{\left[\frac{N_2-L_2}{2}\right]}\frac{(-1)^{s+r}a_s(L_1+1,N_1-L_1)a_r(L_2+1,N_2-L_2)}{(2\alpha)^{2s+2r}}$$
$$\sum_{l=|L_1-L_2|}^{L_1+L_2}{}^{(2)}\sum_{m=-l}^{l}(-i)^l\langle L_1M_1|L_2M_2|lm\rangle A_{M_1M_2}^m$$
$$Y_l^m(\theta,\varphi)\int_0^\infty\frac{j_l(pR)p^{2L+l+2}dp}{p^2(\alpha^2+p^2)^{N_1+N_2-s-r+2}} \tag{20}$$

here $2L = L_1 + L_2 - l$ is an even positive integer or zero. The series expansion of p^{2L} is given by [33]:

$$p^{2L} = (-1)^L \alpha^{2L} \sum_{t=0}^{L} (-1)^t F_t(L) \frac{(\alpha^2 + p^2)^t}{\alpha^{2t}} \tag{21}$$

To convert the radial integral in Equation (20) simpler, we use Equation (21) for numerator and Taylor expansion given by Equation (4.2) in reference [33] for denominator:

$$C_{N_1 L_1 M_1}^{N_2 L_2 M_2}(\alpha, \alpha; \mathbf{R}) = \frac{(-1)^{L_2} \pi 2^{2N_1 + 2N_2 + 6}}{F_{L_1}(N_1) F_{L_2}(N_2) \sqrt{F_{N_1}(2N_1) F_{N_2}(2N_2)}}$$
$$\sum_{s=0}^{\left[\frac{N_1 - L_1}{2}\right]} \sum_{r=0}^{\left[\frac{N_2 - L_2}{2}\right]} \frac{(-1)^{s+r} a_s(L_1 + 1, N_1 - L_1) a_r(L_2 + 1, N_2 - L_2)}{2^{2s+2r}}$$
$$\sum_{l=|L_1 - L_2|}^{L_1 + L_2}{}^{(2)} \sum_{m=-l}^{l} \langle L_1 M_1 | L_2 M_2 | lm \rangle A_{M_1 M_2}^m Y_l^m(\theta, \varphi) \sum_{t=0}^{L} \frac{(-1)^t F_t(L)}{\alpha^{l+3}}$$
$$\left\{ \int_0^\infty p^l j_l(pR) dp - \sum_{v=0}^{N_1 + N_2 - s - r - t + 1} \alpha^{2v} \int_0^\infty \frac{p^{l+2} j_l(pR) dp}{(\alpha^2 + p^2)^{v+1}} \right\} \tag{22}$$

The first integral in Equation (22) can be proved in terms of irregular solid spherical harmonics defined as $\pounds_l^m(\mathbf{r}) = r^{-l-1} Y_l^m(\theta, \varphi)$ [56],

$$Y_l^m(\theta, \varphi) \int_0^\infty p^l j_l(pR) dp = \frac{\pi}{2} (2l - 1)!! \, \pounds_l^m(\mathbf{R}) \tag{23}$$

Using the integral tables of spherical Bessel functions [57], the second radial integral can be expressed in terms of modified Bessel function of second kind:

$$\int_0^\infty \frac{p^{l+2} j_l(pR) dp}{(\alpha^2 + p^2)^{v+1}} = \sqrt{\pi} \frac{R^{v - 1/2} \alpha^{l - v + 1/2}}{2^{v+1} v!} K_{l - v + 1/2}(\alpha R) \tag{24}$$

Then, this integral with spherical harmonic can be written as a linear combination of STOs when the series expansion of modified Bessel function of second kind is used:

$$Y_l^m(\theta, \varphi) \int_0^\infty \frac{p^{l+2} j_l(pR) dp}{(\alpha^2 + p^2)^{v+1}} = \pi \frac{\alpha^{l - 2v - 1/2}}{2^{2v + 3/2}} \sum_{q=0}^{l-v} g_{v,q}^l \chi_{v-q\, l}^m(\alpha, \mathbf{R}) \tag{25}$$

where

$$g_{v,q}^{l} = \frac{(l-v+q)!\sqrt{(2(v-q))!}}{(l-v-q)!\,v!\,q!} \tag{26}$$

Taking into the account Equations (23) and (25), two-center Coulomb integrals with the same screening parameters take the following form [59]:

$$C_{N_1L_1M_1}^{N_2L_2M_2}(\alpha,\alpha;\mathbf{R}) = \frac{(-1)^{L_2}\pi^2 2^{2N_1+2N_2+5}}{\alpha^2 F_{L_1}(N_1)F_{L_2}(N_2)\sqrt{F_{N_1}(2N_1)F_{N_2}(2N_2)}}$$
$$\sum_{s=0}^{\left[\frac{N_1-L_1}{2}\right]}\sum_{r=0}^{\left[\frac{N_2-L_2}{2}\right]}\frac{(-1)^{s+r}a_s(L_1+1,N_1-L_1)a_r(L_2+1,N_2-L_2)}{2^{2s+2r}}$$
$$\sum_{l=|L_1-L_2|}^{L_1+L_2{}^{(2)}}\sum_{m=-l}^{l}\langle L_1M_1|L_2M_2|lm\rangle A_{M_1M_2}^{m}\sum_{t=0}^{L}(-1)^t F_t(L)$$
$$\left\{(2l-1)!!\,\pounds_l^m(\alpha\mathbf{R}) - \sum_{v=0}^{N_1+N_2-s-r-t+1}\frac{\alpha^{-3/2}}{2^{2v+1/2}}\sum_{q=0}^{l-v}g_{v,q}^{l}\chi_{v-q\,l}^{m}(\alpha,\mathbf{R})\right\} \tag{27}$$

In the analytical evaluation of two-center Coulomb integrals with the different screening parameters the radial integrals written in the following form:

$$C_{N_1L_1M_1}^{N_2L_2M_2}(\alpha,\beta;\mathbf{R}) = \frac{(-1)^{L_2}\pi 2^{2N_1+2N_2+6}\alpha^{2N_1-L_1+1/2}\beta^{2N_2-L_2+1/2}}{F_{L_1}(N_1)F_{L_2}(N_2)\sqrt{F_{N_1}(2N_1)F_{N_2}(2N_2)}}$$
$$\sum_{s=0}^{\left[\frac{N_1-L_1}{2}\right]}\sum_{r=0}^{\left[\frac{N_2-L_2}{2}\right]}\frac{(-1)^{s+r}a_s(L_1+1,N_1-L_1)a_r(L_2+1,N_2-L_2)}{(2\alpha)^{2s}(2\beta)^{2r}}$$
$$\sum_{l=|L_1-L_2|}^{L_1+L_2{}^{(2)}}\sum_{m=-l}^{l}(-1)^L\langle L_1M_1|L_2M_2|lm\rangle A_{M_1M_2}^{m}Y_l^m(\theta,\varphi)$$
$$\int_0^\infty \frac{j_l(pR)p^{2L+l+2}dp}{p^2(\alpha^2+p^2)^{N_1-s+1}(\beta^2+p^2)^{N_2-r+1}} \tag{28}$$

The use of Taylor expansion given by Equation (4.4) in reference [33] allows separating the denominators in Equation (28) as follows:

$$C_{N_1L_1M_1}^{N_2L_2M_2}(\alpha,\beta;\mathbf{R}) = \frac{(-1)^{L_2}\pi 2^{2N_1+2N_2+6}\alpha^{2N_1-L_1+1/2}\beta^{2N_2-L_2+1/2}}{F_{L_1}(N_1)F_{L_2}(N_2)\sqrt{F_{N_1}(2N_1)F_{N_2}(2N_2)}}$$

$$\sum_{s=0}^{\left[\frac{N_1-L_1}{2}\right]}\sum_{r=0}^{\left[\frac{N_2-L_2}{2}\right]}\frac{(-1)^{s+r}a_s(L_1+1,N_1-L_1)a_r(L_2+1,N_2-L_2)}{(2\alpha)^{2s}(2\beta)^{2r}}$$

$$\sum_{l=|L_1-L_2|}^{L_1+L_2}{}^{(2)}\sum_{m=-l}^{l}(-1)^{L}\langle L_1M_1|L_2M_2|lm\rangle A_{M_1M_2}^{m}Y_l^m(\theta,\varphi)$$

$$\left\{\sum_{v_1=0}^{N_1-s}\frac{(-1)^{N_2-r+1}F_{N_2-r}(N_1+N_2-s-r-v_1)}{(\alpha^2-\beta^2)^{N_1+N_2-s-r-v_1+1}}\int_0^{\infty}\frac{j_l(pR)p^{2L+l+2}dp}{p^2(\alpha^2+p^2)^{v_1+1}}\right.$$

$$\left.+\sum_{v_2=0}^{N_2-r}\frac{(-1)^{N_1-s+1}F_{N_1-s}(N_1+N_2-s-r-v_2)}{(\beta^2-\alpha^2)^{N_1+N_2-s-r-v_2+1}}\int_0^{\infty}\frac{j_l(pR)p^{2L+l+2}dp}{p^2(\beta^2+p^2)^{v_2+1}}\right\} \qquad (29)$$

The radial integrals obtained in Equation (29) are the same with the integrals given by Equation (20) derived for the two-center Coulomb integrals with the same screening parameters. Accordingly, applying the same steps used to solve the radial integral in Equation (20) for these integrals, two-center Coulomb integrals with the different screening parameters can be obtained in terms of irregular solid harmonics and linear summation of STOs [59]:

$$C_{N_1L_1M_1}^{N_2L_2M_2}(\alpha,\beta;\mathbf{R}) = \frac{(-1)^{N_2+L_1-1}\pi^2 2^{2N_1+2N_2+5}\alpha^{2N_1-L_1+1/2}\beta^{2N_2-L_2+1/2}}{F_{L_1}(N_1)F_{L_2}(N_2)\sqrt{F_{N_1}(2N_1)F_{N_2}(2N_2)}}$$

$$\sum_{s=0}^{\left[\frac{N_1-L_1}{2}\right]}\sum_{r=0}^{\left[\frac{N_2-L_2}{2}\right]}\frac{(-1)^{s}a_s(L_1+1,N_1-L_1)a_r(L_2+1,N_2-L_2)}{(2\alpha)^{2s}(2\beta)^{2r}(\alpha^2-\beta^2)^{N_1+N_2-s-r+1}}$$

$$\sum_{l=|L_1-L_2|}^{L_1+L_2}{}^{(2)}\sum_{m=-l}^{l}\langle L_1M_1|L_2M_2|lm\rangle A_{M_1M_2}^{m}\sum_{t=0}^{L}(-1)^{t}F_t(L)$$

$$\left\{\alpha^{L_1+L_2-1}\sum_{v_1=0}^{N_1-s}F_{N_2-r}(N_1+N_2-s-r-v_1)(1-\beta^2/\alpha^2)^{v_1}\right.$$

$$\left\{(2l-1)!!\,\pounds_l^m(\alpha\mathbf{R})-\sum_{z_1=0}^{v_1-t}\frac{\alpha^{-3/2}}{2^{2z_1+1/2}}\sum_{q_1=0}^{l-z_1}g_{z_1,q_1}^{l}\chi_{z_1-q_1\,l}^{m}(\alpha,\mathbf{R})\right\}$$

$$\left.-\beta^{L_1+L_2-1}\sum_{v_2=0}^{N_2-r}F_{N_1-s}(N_1+N_2-s-r-v_2)(1-\alpha^2/\beta^2)^{v_2}\right.$$

$$\left\{(2l-1)!!\,\pounds_l^m(\beta\mathbf{R}) - \sum_{z_2=0}^{v_2-t}\frac{\beta^{-3/2}}{2^{2z_2+1/2}}\sum_{q_2=0}^{l-z_2} g_{z_2,q_2}^{l}\,\chi_{z_2-q_2\ l}^{m}(\beta,\mathbf{R})\right\}\Bigg\} \tag{30}$$

3. Results

To order to calculate two-electron Coulomb integrals over real STOs efficiently and accurately an algorithm has been described by using the obtained analytical formulas. The algorithm has been implemented in a computer program written in MATHEMATICA 10.0 programming language. The program has been run for physically significant values of atomic orbital parameters by using Intel(R) Core (TM) i7-6500U CPU @ 2.50 Ghz computer. Numerical results that we obtained for line-up coordinate system have been reported in Table 1 and Table 2 for atomic Coulomb integrals given with 15 decimal digits and two-center molecular Coulomb integrals with 35 decimal digits, respectively. As can be seen from Table 1 and Table 2, all the calculations have been made in range of $1 \leq n \leq 25,\ 0 \leq l \leq 9$ and $-2 \leq m \leq 9$ and for the arbitrary values of screening parameters and internuclear distances. In the tables the first row of the numeric results column shows the numeric values obtained in this study. For the calculations of the atomic Coulomb integral, in Table 1, in the case of same screening Equation (15) and in the case of different screening Equation (18) have been used. In Table 2, where the numerical results of the two-center Coulomb integrals are given, for the same and different screening parameters the expressions of Equation (27) and Equation (30) in terms of the modified Bessel function of second kind have been used.

In the computer program, the modified Bessel function of second kind has been computed with the series expansion given below [57] taking into account the case *n* is negative and positive integer

$$K_{n+1/2}(x) = \sqrt{\frac{\pi}{2x}}\,e^{-x}\sum_{j=0}^{n}\frac{(n+j)!}{j!\,(n-j)!\,(2x)^j} \tag{31}$$

Table 1. The values of one-center Coulomb integrals over STOs using by Equations (15) and (18).

n_1/n_2	l_1/l_2	m_1/m_2	$\varepsilon_a/\varepsilon_{a'}$	n_3/n_4	l_3/l_4	m_3/m_4	$\varepsilon_b/\varepsilon_{b'}$	Numerical results
1/1	0/0	0/0	8.7/8.7	1/1	0/0	0/0	8.7/8.7	5.437500000000000 5.43750 [a]
2/1	0/0	0/0	2.6/8.7	2/1	0/0	0/0	2.6/8.7	1.46328 21330 50426 x 10^{-1} 1.4633 x 10^{-1} [a]
2/2	0/0	0/0	2.6/2.6	2/1	0/0	0/0	2.6/8.7	2.95642 80233 14304 x 10^{-1} 2.9564 x 10^{-1} [a]
2/2	1/0	0/0	2.6/2.6	2/2	1/0	0/0	2.6/2.6	2.08767 36111 11111 x 10^{-1} 2.0877 x 10^{-1} [a]
2/2	1/1	-1/0	2.6/2.6	2/2	1/1	-1/0	2.6/2.6	5.48437 50000 00000 x 10^{-2} 5.484 x 10^{-2} [a]
4/3	3/2	3/-2	3.2/1.7	4/3	3/2	-2/1	1.7/0.7	-1.82643 75834 06783 x 10^{-2} -1.82643 75824 422 x 10^{-2} [b]
10/10	9/9	9/9	1.5/1.22	10/10	9/9	9/9	0.5/0.65	4.50007 13886 75689 x 10^{-2} 4.50007 13886 7520 x 10^{-2} [b]

[a] Reference [60]; [b] Reference [61].

Table 2. Comparative values of two-center Coulomb integrals over STOs in line-up coordinate systems.

n_1/n_2	l_1/l_2	m_1/m_2	$\varepsilon_a/\varepsilon_{a'}$	n_3/n_4	l_3/l_4	m_3/m_4	$\varepsilon_b/\varepsilon_{b'}$	R	Numerical results
1/1	0/0	0/0	0.99/0.99	1/1	0/0	0/0	1.01/1.01	0.01	6.24916 67058 30088 14983 45518 38351 29937 x 10^{-1} 6.24916 67058 30088 14983 45518 38351 29936 x 10^{-1} [a] 6.24916 67058 30088 14983 46 x 10^{-1} [b]
1/1	0/0	0/0	5.2/5.2	2/2	0/0	0/0	4.1/4.1	0.2	1.82289 25537 50662 68097 06249 99472 18106 1.82289 25537 50662 68097 06249 99472 18105 [a] 1.82289 2554 [c]
1/2	0/1	0/1	5.2/4.0	2/2	1/0	-1/0	3.1/4.1	0.2	-2.03568 85382 24252 94658 39569 97218 82383 x 10^{-1} -2.03568 85382 24252 94658 39569 97218 82382 x 10^{-1} [a] -2.03568 8538 x 10^{-1} [c]
2/2	0/0	0/0	0.8/0.9	2/2	0/0	0/0	1.1/1.2	0.2	3.45983 64791 66103 67505 07075 35552 00665 x 10^{-1} 3.45983 64791 66103 67505 07075 3555 x 10^{-1} [d] 3.45983 64791 66104x 10^{-1} [b]
2/2	1/1	0/0	0.8/0.9	2/2	0/0	0/0	1.1/1.2	2.0	3.24756 44802 54982 28658 37023 34107 50971 x 10^{-1} 3.24756 44802 54982 28658 37023 34 x 10^{-1} [d] 3.24756 44802 54982 3 x 10^{-1} [b]
1/10	0/2	0/0	5.2/0.2	5/7	1/0	0/0	0.6/0.5	2.5	-1.20705 70535 94375 77816 23149 97854 51448 x 10^{-18} -1.20705 7054 x 10^{-18} [c]
2/4	1/3	0/-2	3.1/0.2	4/2	2/0	2/0	0.5/4.1	2.5	1. 36325 84822 52802 36788 07621 24881 76923 x 10^{-8} 1. 36325 8482 x 10^{-8} [c]
4/2	3/1	0/0	5.2/4.0	4/4	2/3	2/2	0.5/3.0	2.5	-7. 36773 13766 53888 45151 51235 09992 20224 x 10^{-5} -7. 36773 13766 53888 45151 51235 09992 20224 x 10^{-5} [a] -7. 36773 1377 x 10^{-5} [c]
5/3	0/2	0/0	1.0/3.0	4/4	2/1	1/1	2.0/4.0	8.0	4.88358 08140 37952 76018 31732 66635 47903 x 10^{-5} 4.88358 08140 37952 76018 3173 x 10^{-5} [d] 4.88358 0814 x 10^{-5} [e]
10/10	2/2	0/0	0.2/0.2	5/7	1/0	0/0	0.6/0.5	8.5	-2.25291 88936 55436 05537 04573 40032 86720 x 10^{-4} -2.25291 88936 55436 05537 04573 x 10^{-4} [d] -2.25291 8896 x 10^{-4} [c]
4/1	3/0	0/0	0.8/0.9	3/1	2/0	0/0	1.1/1.2	100	1.32578 24709 36295 45612 88059 75651 53923 x 10^{-10} 1.32578 24709 36295 45612 88059 75651 53922 x 10^{-10} [a] 1.32578 24709 36295 46 x 10^{-10} [b]
25/3	0/0	0/0	1.2/1.2	2/2	0/0	0/0	1.0/1.0	0.22	5.58454 19476 26061 00861 36798 18078 45075 x 10^{-6} 5.58454 19476 260 x 10^{-6} [f]

[a] Reference [49]; [b] Reference [21]; [c] Reference [25]; [d] Reference [44]; [e] Reference [62]; [f] Reference [13].

4. Conclusion and Comment

For evaluating two-electron one- and two-center Coulomb integrals over real STOs analytical formulas have been obtained using Fourier transform method. First, in case **R**=0, the atomic Coulomb integrals have been derived easily in terms of binomial coefficients as given by Equations (15) and (18). In the calculation of two-center molecular Coulomb integrals, we have used some Taylor expansions given by the group of Steinborn in reference [33] to simplify the denominator of the integral structures encountered. The resulting integrals have been expressed in terms of irregular solid spherical harmonics and modified Bessel functions of second kind as given by Equations (23) and (24). Eventually two-center molecular Coulomb integrals have been expressed as finite linear combinations of Gegenbauer coefficients, Gaunt coefficients, irregular solid harmonics and real STOs using the series expansion of modified Bessel functions of second kind.

It has been seen that the program written in the present study gives rise to a highly accurate computation of one- and two-center molecular Coulomb integrals over real STOs. The comparative results given in tables have shown an exact match with the benchmark values of the literature for one- and two-center Coulomb integrals.

Author Statement

Selda Akdemir: Investigation, Resource/Material/Instrument Supply, Conceptualization, Methodology, Software, Validation, Visualization, Review and Editing.

Acknowledgment

As the author of this study, I declare that I do not have any support and thank you statement.

Conflict of Interest

As the author of this study, I declare that I do not have any conflict of interest statement.

Ethics Committee Approval and Informed Consent

As the author of this study, I declare that I do not have any ethics committee approval and/or informed consent statement.

References

[1] T. Kato, "On the eigenfunctions of many-particle systems in quantum mechanics," *Comm. Pure Appl. Math.*, 10 (2), 151-177, 1957.

[2] P. E. Hoggan, M. B. Ruiz, and T. Özdoğan, "Molecular Integrals over Slater-type orbitals. From pioneers to recent progress," in *Quantum Frontiers of Atoms and Molecules*, M. V. Putz, Ed. New York: Nova Publishers Inc., 2010, pp. 63-90.

[3] R. S. Mulliken, C. A. Rieke, D. Orloff, and H. Orloff, "Formulas and numerical tables for overlap integrals," *J. Chem. Phys.*, 17 (12), 1248-1267, 1949.

[4] C. C. J. Roothaan, "A Study of two-center integrals useful in calculations on molecular structure. I," *J. Chem. Phys*., 19 (12), 1445-1458, 1951.

[5] K. Ruedenberg, "A study of two-center integrals useful in calculations on molecular structure. II. The two-center exchange integrals," *J. Chem. Phys.*, 19 (12), 1459-1477, 1951.

[6] C. C. J. Roothaan, "Study of two-center integrals useful in calculations on molecular structure. IV. The auxiliary functions $C_{\alpha\beta}{}^{\gamma\delta\varepsilon}(\rho_a, \rho b)$ for $\alpha \geq 0$," *J. Chem. Phys.*, 24 (5), 947-960, 1956.

[7] K. Ruedenberg, C. C. J. Roothaan, and W. Jaunzemis, "Study of two-center integrals useful in calculations on molecular structure. III. A unified treatment of the hybrid, Coulomb, and one-electron integrals," *J. Chem. Phys.*, 24 (2), 201-220, 1956.

[8] A. C. Wahl, P. E. Cade, and C. C. J. Roothaan, "Study of two-center integrals useful in calculations on molecular structure. V. General methods for diatomic integrals applicable to digital computers," *J. Chem. Phys.*, 41 (9), 2578-2599, 1964.

[9] D. M. Silver and K. Ruedenberg, “Coulomb integrals between Slater-type atomic orbitals,” *J. Chem. Phys.*, 49 (10), 4306-4311, 1968.
[10] I. I. Guseinov, “Analytical evaluation of two-centre Coulomb, hybrid and one electron integrals for Slater type orbitals,” *J. Phys. B*, 3 (11), 1399-1412, 1970.
[11] I. I. Guseinov, “Analytical evaluation of one- and two-center Coulomb and two-center hybrid integrals for Slater-type orbitals,” *J. Chem. Phys.*, 67 (8), 3837-3839, 1977.
[12] J. Yasui and A. Saika, “Unified analytical evaluation of two-center, two-electron integrals over Slater-type orbitals,” *J. Chem. Phys.*, 76 (1), 468-472, 1982.
[13] A. Özmen, A. Karakaş, Ü. Atav, and Y. Yakar, “Computation of two-center Coulomb integrals over Slater-type orbitals using elliptical coordinates,” *Int. J. Quantum Chem.*, 91(1), 13-19, 2003.
[14] M. P. Barnet and C. A. Coulson, “The evaluation of integrals occurring in the theory of molecular structure. Parts I & II,” *Phil. Trans. R. Soc. Lond. A*, 243 (864), 221-249, 1951.
[15] P. O. Löwdin, “Quantum theory of cohesive properties of solids,” *Adv. Phys.*, 5 (17), 1-171, 1956.
[16] F. E. Harris and H. H. Michels, “Multicenter Integrals in Quantum Mechanics. I. Expansion of Slater-Type Orbitals about a New Origin,” *J. Chem. Phys.*, 43 (10), 165-169, 1965.
[17] W. England, “One-Center coulomb, two-center hybrid, and two-center Coulomb integrals over STP functions,” *Int. J. Quantum Chem.*, 6 (3), 509-518, 1972.
[18] R. R. Sharma, “Expansion of a function about a displaced center for multicenter integrals: A general and closed expression for the coefficients in the expansion of a Slater orbital and for overlap integrals,” *Phys. Rev. A*, 13 (2), 517-527, 1976.
[19] H. W. Jones and C. A. Weatherford, “A modified form of Sharma's formula for sto Löwdin alpha functions with recurrence relations for the coefficient matrix,” *Int. J. Quantum Chem. Symp.*, 14 (S12), 483-488, 1978.
[20] H. W. Jones, “Computer-generated formulas for two-center coulomb integrals over Slater–type orbitals,” *Int. J. Quantum Chem.*, 20 (6), 1217-1224, 1981.
[21] H. W. Jones, “Benchmark values for two-center Coulomb integrals over Slater-type orbitals,” *Int. J. Quantum Chem.*, 45 (1), 21-30, 1993.
[22] I. I. Guseinov, “Expansion of Slater-type orbitals about a displaced center and the evaluation of multicenter electron-repulsion integrals,” *Phys Rev A*, 31(5), 2851-2853, 1985.
[23] I. I. Guseinov, “Unified analytical treatment of multicenter multielectron integrals of central and noncentral interaction potentials over Slater orbitals using Ψ^{α}-ETOs,” *J. Chem. Phys.*, 119 (9), 4614-4619, 2003.
[24] J. Fernandez Rico, R. Lopez, and G. Ramirez, “Calculation of integrals with Slater basis from the one-range expansion of the 0*s* function,” *Int. J. Quantum Chem.*, 37 (1), 69-83, 1990.
[25] V. Magnasco and A. Rapallo, “New translation method for STOs and its application to calculation of two-center two-electron integrals,” *Int. J. Quantum Chem.*, 79 (2), 91-100, 2000.
[26] M. Geller, “Two-Electron, one- and two-center Integrals,” *J. Chem. Phys.*, 39 (3), 853-854, 1963.
[27] M. Geller and R. W. Griffith, “Zero-Field splitting, one-and two-center Coulomb-type integrals,” *J. Chem. Phys.*, 40 (8), 2309-2325, 1964.
[28] M. Geller, “Two-Center Coulomb integrals,” *J. Chem. Phys.*, 41 (12), 4006-4007, 1964.
[29] F. E. Harris, “Rapid evaluation of Coulomb integrals,” *J. Chem. Phys.*, 51 (11), 4770-4778, 1969.
[30] H. D. Todd, K. G. Kay, and H. J. Silverstone, “Unified treatment of two-center overlap, Coulomb, and kinetic-energy integrals,” *J. Chem. Phys.*, 53 (10), 3951-3956, 1970.
[31] E. Filter and E. O. Steinborn, “Extremely compact formulas for molecular two-center one-electron integrals and Coulomb integrals over Slater-type atomic orbitals,” *Phys. Rev. A*, 18 (1), 1-11, 1978.
[32] H. P. Trivedi and E. O. Steinborn, “Fourier transform of a two-center product of exponential-type orbitals. Application to one-and two-electron multicenter integrals,” *Phys. Rev. A*, 27 (2), 670-679, 1983.
[33] E. J. Weniger, J. Grotendorst, and E. O. Steinborn, “Unified analytical treatment of overlap, two-center nuclear attraction, and Coulomb integrals of *B* functions via the Fourier-transform method,” *Phys. Rev. A*, 33 (6), 3688-3705, 1986.
[34] J. Grotendorst, E. J. Weniger, and E. O. Steinborn, “Efficient evaluation of infinite-series representations for overlap, two-center nuclear attraction, and Coulomb integrals using nonlinear convergence accelerators,” *Phys. Rev. A*, 33 (6), 3706-3726, 1986.
[35] J. Grotendorst and E. O. Steinborn, “Numerical evaluation of molecular one-and two-electron multicenter integrals with exponential-type orbitals via the Fourier-transform method,” *Phys. Rev. A*, 38 (8), 3857-3876, 1988.
[36] G. Figari, C. Costa, R. Pratolongo, and V. Magnasco, “Two-Centre Coulomb integrals over STOs from analytical evaluation of *k*-integrals by contour integration in the complex plane,” *Chem. Phys. Lett.*, 167 (6), 547-554, 1990.

[37] E. O. Steinborn, H. H. H. Homeier, and E. J. Weniger, "Recent progress on representations for Coulomb integrals of exponential-type orbitals," *J. Mol. Struct.*, 260, 207-221, 1992.
[38] S. F. Boys, G. B. Cook, C. M. Reeves, and I. Shavitt, "Automatic fundamental calculations of molecular structure," *Nature*, 178, 1207-1209, 1956.
[39] J. Fernandez Rico, R. Lopez, A, Aguado, I. Ema, and G. Ramirez, "Reference program for molecular calculations with Slater-type orbitals," *J. Comp. Chem.*, 19 (11), 1284-1293, 1998.
[40] I. Shavitt and M. Karplus, "Gaussian-Transform method for molecular integrals. I. formulation for energy integrals," *J. Chem. Phys.*, 43 (2), 398-414, 1965.
[41] J. Fernandez Rico, R. Lopez, I. Ema, and G. Ramirez, "Efficiency of the algorithms for the calculation of Slater molecular integrals in polyatomic molecules," *J. Comp. Chem.*, 25 (16), 1987-1994, 2004.
[42] L. Berlu, H. Safohi, and P. E. Hoggan, "Fast and accurate evaluation of three-center, two-electron Coulomb, hybrid, and three-center nuclear attraction integrals over Slater-type orbitals using the *SD* transformation," *Int. J. Quantum Chem.*, 99 (4), 221-235, 2004.
[43] H. Safohi and L. Berlu, "The Fourier transform method and the SD approach for the analytical and numerical treatment of multicenter overlap-like quantum similarity integrals," *J. Comp. Phys.*, 216 (1), 19-36, 2006.
[44] S. Gümüş, "On the computation of Two-center Coulomb integrals over Slater type orbitals using the Poisson equation," *Z. Naturforsch A*, 60a, 477-483, 2005.
[45] P. E. Hoggan, "General two-electron exponential type orbital integrals in polyatomics without orbital translations," *Int. J. Quantum Chem.*, 109 (13), 2926-2932, 2009.
[46] P. E. Hoggan, "Four-center Slater-type orbital molecular integrals without orbital translations," *Int. J. Quantum Chem.*, 110 (1), 98-103, 2010.
[47] C. B. Mendl, "Efficient algorithm for two-center Coulomb and exchange integrals of electronic prolate spheroidal orbitals," *J. Comp. Phys.*, 231 (15), 5157-5175, 2012.
[48] M. Lesiuk and R. Moszynski, "Reexamination of the calculation of two-center, two-electron integrals over Slater-type orbitals. I. Coulomb and hybrid integrals," *Phys. Rev. E*, 90 (6), 063318, 2014.
[49] A. Bağcı and P. E. Hoggan, "Benchmark values for molecular two-electron integrals arising from the Dirac equation," *Phys. Rev. E*, 91 (2), 023303, 2015.
[50] F. P. Prosser and C. H. Blanchard, "On the Evaluation of two-center integrals," *J. Chem. Phys.*, 36 (4), 1112-1112, 1962.
[51] S. Wolfram, *Mathematica: A System for Doing Mathematics by Computer*, Addision Wesley, New York, 1998.
[52] G. B. Arfken and H. J. Weber, *Mathematical Methods for Physicists*, Academic Press, London, 2005.
[53] T. Özdoğan and M. Orbay, "Evaluation of two-center overlap and nuclear attraction integrals over slater-type orbitals with integer and noninteger principal quantum numbers," *Int. J. Quantum Chem.*, 87 (1), 15-22, 2002.
[54] A. Bağcı and P. E. Hoggan, "Performance of numerical approximation on the calculation of overlap integrals with noninteger Slater-type orbitals," *Phys. Rev. E*, 89 (5), 053307, 2014.
[55] I. I. Guseinov and B. A. Mamedov, "On the calculation of arbitrary multielectron molecular integrals over Slater-type orbitals using recurrence relations for overlap integrals I. Single-center expansion method," *Int. J. Quantum Chem.*, 78 (3), 146-152, 2000.
[56] E. Öztekin and S. Özcan, "Overlap integrals between irregular solid harmonics and STOs via the Fourier transform methods," *J. Math. Chem.*, 42 (3), 337-351, (2007).
[57] I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Sums, Series and Products*, Academic Press, New York, 2000.
[58] E. Öztekin, S. Özcan, M. Orbay, and M. Yavuz, "Calculation of nuclear-attraction and modified overlap integrals using Gegenbauer coefficients," *Int. J. Quantum Chem.*, 90 (1), 136-143, 2002.
[59] S. A. Kurt, "Bazı atom ve moleküller için moleküler integrallerin hesaplanması," M.S. thesis (Second Thesis Advisor: Selda Akdemir), Dept. Phys., Ondokuz Mayıs Univ., Samsun, Turkey, 2014.
[60] J. A. Pople and D. L. Beveridge, *Approximate Molecular Orbital Theory*, McGraw-Hill, New York, 1970.
[61] I. I. Guseinov, B. A. Mamedov, and A. Rzaeva, "Calculation of molecular integrals over Slater-type orbitals using recurrence relations for overlap integrals and basic one-center Coulomb integrals," *J. Mol. Model.*, 8 (4), 145-149, 2002.
[62] V. Magnasco, M. Casanova, and A. Rapallo, "On the evaluation of two-centre molecular integrals over an STO basis," *Chem. Phys. Lett.*, 289 (1-2), 81-89, (1998).