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Calculation of molecular integrals over Slater-type orbitals using recurrence relations for overlap integrals and basic one-center Coulomb integrals

Abstract The recurrence relations are established for the basic one-center Coulomb integrals over Slater-type orbitals (STOs). These formulae and the recurrence relations for basic overlap integrals are utilized for the calculation of multicenter electron-repulsion integrals. The calculations of multicenter electron-repulsion integrals are performed by the use of translation formulae for STOs obtained from the Lambda and Coulomb Sturmian exponential-type functions (ETFs). It is shown that these integrals show a faster convergence rate in the case of Coulomb Sturmian ETFs. The accuracy of the results is quite high for the quantum numbers of STOs and for the arbitrary values of internuclear distances and screening constants of atomic orbitals.

Keywords Slater-type orbitals · Electron-repulsion integrals · Overlap integrals

Introduction

It is well known that there is general agreement on the high quality of exponential-type functions (ETFs) for describing the electronic structure of molecules. [1] However, difficulties in solving the multicenter molecular integrals have restricted their use to the study of molecular properties. In addition, almost all molecular calculations are done using Gaussian-type orbitals (GTOs). GTOs do not allow important properties of the electronic wavefunction, namely, the cusps at the nuclei [2] and exponential decay at large distances to be represented adequately. [3] For problems in which the long part of the wavefunction or its behavior in the neighborhood of the nuclei is important, it is desirable to use ETOs, which describe the physical situation more accurately than GTOs. Unfortunately, the large body of formulae of the expansion methods of STOs about a displaced center, [4, 5, 6, 7, 8, 9] the Fourier transform methods [10, 11, 12] and the B-function method [13, 14] developed for the evaluation of multicenter molecular integrals over STOs is not quite satisfactory in the numerical aspects of multicenter integrals, especially in the calculation of three- and four-center electron-repulsion integrals of the Hartree–Fock–Roothaan equations for molecules. However, the interest of researchers in the use of ETOs has increased in the last few years (see e.g. [15, 16] and the bibliography quoted in these papers). Single-center expansion methods in spherical harmonics have been applied for the expansion of STOs about a displaced center in most of this work. In [17, 18] a method has been described for obtaining the series expansion formulae for translation of STOs using Lambda and Coulomb Sturmian ETFs that are complete and orthonormal sets of functions. The expansion coefficients for translation of STOs were presented by linear combinations of overlap integrals.

In [19] using the series expansion formula for translation of STOs obtained with the help of Lambda ETFs we presented a study of multicenter electron-repulsion integrals in terms of overlap integrals with the same screening parameters and basic one-center Coulomb integrals determined from analytical relationships. In this work we establish the recurrence relations for basic one-center Coulomb integrals. Here, the calculations of multicenter electron-repulsion integrals are performed by the use of analytical and recurrence relations for basic one-center Coulomb integrals and the series expansion formulae for the translation of STOs obtained in [18] from the Coulomb Sturmian and Lambda ETFs.

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The multicenter electron-repulsion integrals over STOs with respect to the molecular coordinate system examined in the present work have the following form:

$$I_{ac,bd} = \int \chi_{p_1}^* (\zeta_1, \vec{r}_{a1}) \chi_{p'_1} (\zeta'_1, \vec{r}_{c1})$$
$$\frac{1}{r_{21}} \chi_{p_2} (\zeta_2, \vec{r}_{b2}) \chi_{p'_2}^* (\zeta'_2, \vec{r}_{d2}) \, dV_1 dV_2, \tag{1}$$

where $p_i \equiv n_i l_i m_i$, $p'_i \equiv n'_i l'_i m'_i$, $\vec{r}_{gi} = \vec{r}_i - \vec{R}_g$ ($i=1,2$ and $g=a$, b, c, d) and

$$\chi_{nlm} (\zeta, \vec{r}) = (2\zeta)^{n+\frac{1}{2}} [(2n)!]^{-\frac{1}{2}} r^{n-1} e^{-\zeta r} S_{lm} (\theta, \varphi). \tag{2}$$

Here the functions S_{lm} are complex or real spherical harmonics determined by

$$S_{lm}(\theta, \varphi) = P_{l|m|}(\cos\theta) \Phi_m(\varphi), \tag{3}$$

where $P_{l|m|}$ are normalized associated Legendre functions [20] and for complex spherical harmonics

$$\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}; \tag{4}$$

for real spherical harmonics

$$\Phi_m(\varphi) = \frac{1}{\sqrt{\pi(1+\delta_{m0})}} \begin{cases} \cos|m|\varphi & \text{for} \quad m \geq 0 \\ \sin|m|\varphi & \text{for} \quad m < 0 \end{cases}. \tag{5}$$

It should be noted that our definition of phases for the complex spherical harmonics differs from the Condon–Shortley phases [21] by the sign factor. We use phases according to [22] $S_{lm}^*(\theta, \varphi) = S_{l-m}(\theta, \varphi)$.

Expressions in terms of modified basic one-center Coulomb integrals

In order to derive the expressions for Eq. (1) in terms of basic one-center Coulomb integrals, we use Eq. (7) of [23] for the expansion of one- and two-center electron charge density in terms of STOs centered on the nucleus a. Then taking into account the orthogonality relation (13) in [23] we finally obtain for all kinds of multicenter electron-repulsion integrals the following expressions: four-center exchange integrals

$$I_{ac,bd} = \lim_{N \to \infty} \sum_{\mu=1}^{N} \sum_{\nu=0}^{\mu-1} \sum_{\sigma=-\nu}^{\nu} W_{p_1 p'_1 q}^{*N} \left(\zeta_1, \zeta'_1, z; \vec{R}_{ca}, 0\right)$$
$$\lim_{N' \to \infty} \sum_{\mu'=\nu+1}^{N'} W_{p_2 p'_2 q'}^{N'} \left(\zeta_2, \zeta'_2, z'; \vec{R}_{db}, \vec{R}_{ba}\right) \tag{6}$$
$$J_{\mu\nu, \mu'\nu}(z, z'),$$

three-center exchange integrals

$$I_{ac,ad} = I_{ac,bd} \quad \text{for} \quad b \equiv a, \vec{R}_{ba} = 0 \text{ and } \vec{R}_{db} = \vec{R}_{da} \neq 0, \tag{7}$$

two-center exchange integrals

$$I_{ac,ac} = I_{ac,bd} \quad \text{for} \quad b \equiv a, d \equiv c, \vec{R}_{ba} = 0$$
$$\text{and} \quad \vec{R}_{db} = \vec{R}_{ca} \neq 0, \tag{8}$$

three-center hybrid integrals

$$I_{aa,bd} = \sum_{\nu=0}^{\mu-1} \sum_{\sigma=-\nu}^{\nu} W_{p_1 p'_1 q}^* (\zeta_1, \zeta'_1, z)$$
$$\lim_{N' \to \infty} \sum_{\mu'=\nu+1}^{N'} W_{p_2 p'_2 q'}^{N'} \left(\zeta_2, \zeta'_2, z'; \vec{R}_{db}, \vec{R}_{ba}\right) \tag{9}$$
$$J_{\mu\nu, \mu'\nu}(z, z'),$$

two-center hybrid integrals

$$I_{aa,ad} = I_{aa,bd} \quad \text{for} \quad b \equiv a, \vec{R}_{ba} = 0 \text{ and } \vec{R}_{db} = \vec{R}_{da} \neq 0, \tag{10}$$

two-center Coulomb integrals

$$I_{aa,bb} = I_{aa,bd} \quad \text{for} \quad d \equiv b, \vec{R}_{db} = 0 \text{ and } \vec{R}_{ba} \neq 0, \tag{11}$$

one-center Coulomb integrals

$$I_{aa,aa} = \sum_{\nu=0}^{\mu-1} \sum_{\sigma=-\nu}^{\nu} W_{p_1 p'_1 q}^* (\zeta_1, \zeta'_1, z) W_{p_2 p'_2 q'} (\zeta_2, \zeta'_2, z')$$
$$J_{\mu\nu, \mu'\nu}(z, z'), \tag{12}$$

where $q' \equiv \mu'\nu\sigma$, $z = \zeta_1 + \zeta'_1$, $z' = \zeta_2 + \zeta'_2$

In Eqs. (9) and (12), the quantities $W_{nlm, n'l'm', \mu\nu\sigma}(\zeta, \zeta', z) \equiv W_{pp'q}(\zeta, \zeta', z)$ are the expansion coefficients of the electron charge density for the one-center case and are determined by the relation

$$W_{nlm,n'l'm',\mu\nu\sigma} (\zeta, \zeta', z) \equiv W_{nlm,n'l'm',\mu\nu\sigma} (\zeta, \zeta', z; 0, 0) =$$
$$\frac{z\sqrt{z}}{2^\mu} \frac{F_{n'}(\mu)}{n} \left[\frac{2\nu+1}{2} \frac{F_\mu(2\mu)}{F_n(2n)F_{n'}(2n')} \right]^{1/2} \times \tag{13}$$
$$\times (1+t)^{n+\frac{1}{2}} (1-t)^{n'+\frac{1}{2}} C^{\nu|\sigma|} (lm, l'm') A_{mm'}^m \delta_{\mu, n+n'-1},$$

where $t = (\zeta - \zeta')/(\zeta - \zeta')$ and

$$A_{mm'}^\sigma = \begin{cases} \frac{1}{\sqrt{2}} \left(2 - \left| \eta_{mm'}^{m-m'} \right| \right)^{1/2} \\ \delta_{\sigma, \varepsilon|m-m'|} + \frac{1}{\sqrt{2}} \eta_{mm'}^{m+m'} \delta_{\sigma, \varepsilon|m+m'|} \quad \text{for real STOs} \\ \delta_{\sigma, m-m'} \qquad\qquad\qquad\qquad\quad \text{for complex STOs} \end{cases} \tag{14}$$

The quantities $C^{\nu|\sigma|}$ in Eq. (13) are defined by relations $C^{\nu|\sigma|}(lm, l'm') = C^\nu(lm, l'm')$ for $\sigma = m - m'$ and $C^{\nu|\sigma|}(lm, l'm') = C^\nu(lm, l'-m')$ for $\sigma = m + m'$. Here C^ν are the known Gaunt coefficients (see [22] for the exact definition of ε and $\eta_{mm'}^{m\pm m'}$).

The basic one-center Coulomb integrals $J_{\mu\nu, \mu'\nu}(z, z')$ in Eqs. (6), (9) and (12) are determined from the following relations:

$$J_{\mu\nu\sigma, \mu'\nu'\sigma'}(z, z') = \frac{1}{4\pi} \int \frac{1}{r_{21}} \chi_{\mu\nu\sigma}^*(z, \vec{r}_{a1}) \chi_{\mu'\nu'\sigma'}(z', \vec{r}_{a2}) dV_1 dV_2$$
$$= J_{\mu\nu, \mu'\nu}(z, z') \delta_{\nu\nu'} \delta_{\sigma\sigma'} \tag{15}$$

$$J_{\mu\nu, \mu'\nu}(z, z') =$$
$$2^{\mu+\mu'+1} \left[\frac{(2\nu+2)F_{\mu-\nu-1}(\mu+\nu+1)}{(2\nu+1)F_{\mu+\nu+1}(2\mu)F_{\mu'-\nu}(2\mu')F_{\mu'-\nu}(\mu'+\nu)} \right]^{\frac{1}{2}} \frac{\alpha^{\mu'+2}}{zz'\sqrt{\alpha}} P_{\mu\nu, \mu'\nu}(\alpha) \tag{16}$$

$$P_{\mu\nu, \mu'\nu}(\alpha) = \frac{1}{(\mu'-\nu)!} \int_0^\infty \left[1 - e^{-x} \sum_{k=0}^{\mu+\nu} \gamma_k(\mu, \nu) \frac{x^k}{k!} \right]$$
$$x^{\mu'-\nu} e^{-\alpha x} dx, \tag{17}$$

where $\alpha = z'/z$ and

$$\gamma_k(\mu,\nu) =$$
$$\begin{cases} 1 - F_{2\nu+1}(k)/F_{\mu-\nu}(\mu+\nu+1) & \text{for} \quad 0 \le k \le \mu+\nu \\ 0 & \text{for } k < 0 \text{ and } k > \mu+\nu \end{cases} \quad (18)$$

Here the quantity $F_s(n)$ is the binomial coefficient. The basic one-center Coulomb integrals have the following symmetry property:

$$J_{\mu\nu,\mu'\nu}(z,z') = J_{\mu'\nu,\mu\nu}(z',z). \quad (19)$$

As can be seen from Eqs. (6–12), the multicenter electron-repulsion integrals are expressed in terms of the expansion coefficients for the charge density which are the linear combinations of overlap integrals (see Eqs. (9–10) and (14–15) of [23] and the modified basic one-center Coulomb integrals $P_{\mu\nu,\mu'\nu}(\alpha)$.

Analytical and recurrence relations for modified basic one-center Coulomb integrals

In order to obtain the analytical relation for the function $P_{\mu\nu,\mu'\nu}(\alpha)$ we utilize the following formula [20]:

$$\int_0^\infty x^n e^{-px} dx = \frac{n!}{p^{n+1}}. \quad (20)$$

Then we get from Eq. (17)

$$P_{\mu\nu,\mu'\nu}(\alpha) =$$
$$\frac{1}{\alpha^{\mu'-\nu+1}} \left[1 - \sum_{k=0}^{\mu+\nu} \gamma_k(\mu,\nu) F_k(\mu'-\nu+k) \frac{\alpha^{\mu'-\nu+1}}{(1+\alpha)^{\mu'-\nu+k+1}} \right]. \quad (21)$$

For lowering the indices μ' and ν of the function $P_{\mu\nu,\mu'\nu}(\alpha)$, it is easy to establish by partial integration in Eq. (17) the following recurrence relations:

$$P_{\mu\nu,\mu'+1\nu}(\alpha) = \frac{1}{\alpha} P_{\mu\nu,\mu'\nu}(\alpha)$$
$$+ \frac{1}{\alpha} \sum_{k=2\nu}^{\mu+\nu} \frac{F_{2\nu}(k) F_k(\mu'-\nu+k+1)}{F_{\mu-\nu}(\mu+\nu+1)(1+\alpha)^{\mu'-\nu+k+2}} \quad (22)$$

$$P_{\mu\nu+1,\mu'+1\nu+1}(\alpha) =$$
$$P_{\mu\nu,\mu'\nu}(\alpha) + \sum_{k=0}^{\mu+\nu+1} [\gamma_k(\mu,\nu) - \gamma_k(\mu,\nu+1)] \frac{F_k(\mu'-\nu+k)}{(1+\alpha)^{\mu'-\nu+k+1}}. \quad (23)$$

For the derivation of Eqs. (22) and (23) we have taken into account the characteristics of the coefficients $\gamma_k(\mu,\nu)$ determined in Eq. (18). Equations (22) and (23) allow us to express $P_{\mu\nu,\mu'\nu}(\alpha)$ in terms of the functions $P_{\mu0,10}$ for the calculation of which one can use the analytical relation (21) for $\mu'=1\mu'=1$ and $\nu=0$.

It should be noted that using one of the recurrence relations (22) and (23) we can determine the accuracy of computer results for the modified basic one-center Coulomb integrals which are obtained from the other recurrence relation and the analytical formula (21).

Discussion

As can be seen from the formulae of this article, the expansion coefficients for charge density and the modified basic one-center Coulomb integrals occur in the multicenter electron-repulsion integrals over STOs. For

Table 1 The values of multicenter electron-repulsion integrals in molecular coordinate system in a.u. for $N=N'=12$, $\nu=11$, $\sigma=5$, $\theta_{ca}=135°$, $\phi_{ca}=210°$, $\theta_{db}=150°$, $\phi_{db}=45°$, $\theta_{ba}=30°$, $\phi_{ba}=240°$, $\Delta f = f(c{\to}a, d{\to}b, b{\to}a) - f(c{\to}a, b{\to}d, d{\to}a)$

n_1	l_1	m_1	ξ_1	n'_1	l'_1	m'_1	ζ'_1	n_2	l_2	m_2	ξ_2	n'_2	l'_2	m'_2	ζ'_2
4	3	3	3.2	3	2	−2	1.7	4	3	−2	1.7	3	2	1	0.7
10	9	9	1.5	10	9	9	1.22	10	9	9	0.5	10	9	9	0.65
12	11	10	3.5	12	11	10	2.2	12	11	10	5.4	12	11	10	6.5
13	12	12	6.3	13	12	12	3.2	13	12	12	8.5	13	12	12	4.7
2	1	0	4.3	2	1	0	6.3	2	1	0	2.3	2	1	0	8.6
3	2	1	5.4	3	2	1	2.6	2	1	1	7.2	2	1	1	3.8
3	2	2	10.5	3	2	2	5.2	3	2	2	6.7	3	2	2	2.3
4	3	2	7.1	4	3	2	3.5	4	2	2	9.6	4	2	2	3.2
2	1	1	4.1	2	1	1	2.5	2	1	1	6.7	2	1	1	4.2
3	1	1	8.4	3	1	1	4.2	3	1	1	9.6	3	1	1	3.4
3	2	2	10.8	3	2	2	7.4	3	1	1	5.9	3	1	1	8.3
4	3	2	6.1	3	2	2	2.7	4	3	2	7.5	3	2	2	2.8
1	0	0	6.5	1	0	0	3.5	1	0	0	6.5	1	0	0	3.5
2	1	0	8.6	2	1	0	5.3	2	1	0	8.6	2	1	0	5.3
3	2	1	4.8	2	1	1	1.5	3	2	1	4.8	2	1	1	1.5
2	1	1	7.4	2	1	0	3.1	2	1	1	7.4	2	1	0	7.5
2	1	1	6.7	2	1	1	2.3	2	1	1	6.7	2	1	1	4.7
3	2	2	4.6	2	1	1	2.2	3	2	2	4.6	3	2	2	1.4
2	1	0	6.4	2	1	0	6.4	2	1	0	3.2	2	1	0	4.4
2	1	1	4.6	2	1	1	4.6	2	1	1	2.3	2	1	1	6.4
3	2	2	5.4	3	2	2	5.4	2	1	1	1.2	2	1	1	4.6
3	2	1	3.5	3	1	1	3.5	3	2	1	5.1	3	1	1	2.4
2	1	0	4.3	2	0	0	2.5	2	1	0	3.2	2	0	0	1.5
2	1	1	6.4	2	1	1	4.2	2	1	1	7.3	2	1	1	3.1
3	2	1	4.6	3	2	1	2.4	2	1	1	5.7	2	1	1	2.3

Table 2 The values of multi-center electron-repulsion integrals in molecular coordinate system in a.u. for $N=N'=12$, $\nu=11$, $\sigma=5$, $\theta_{ca}=135°$, $\phi_{ca}=210°$, $\theta_{db}=150°$, $\phi_{db}=45°$, $\theta_{ba}=30°$, $\phi_{ba}=240°$, $\Delta f = f(c{\to}a,d{\to}b,b{\to}a)-f(c{\to}a,b{\to}d,d{\to}a)$

Rca	Rdb	Rba	Use of Lambda ETFs: Eqs. (19), (20) in [17]		Use of Coulomb Sturmian ETFs: Eqs. (21), (22) in [17]		
			$c{\to}a,d{\to}b,b{\to}a$	Δf	$c{\to}a,b{\to}d,d{\to}a$	Δf	CPU (ms)
0	0	0	−1.82643758244224E−2	–	–	–	–
0	0	0	4.50007138867520E−2	–	–	–	–
0	0	0	1.08422891092958E−1	–	–	–	–
0	0	0	2.78544950188517E−2	–	–	–	–
0	5	0	6.64519528049128E−2	11	6.64519528049281E−2	12	72.1
0	15	0	3.28353258817532E−2	10	3.28353258817448E−2	11	125.38
0	8.5	0	2.95462005074663E−2	10	2.95462005074222E−2	9	210.5
0	2.8	0	5.55465963805091E−2	9	5.55465963805156E−2	10	290.1
0	0	1.5	1.66040155131987E−2	11	1.66040155126495E−2	12	93.2
0	0	4.1	5.63056481947150E−6	10	5.63056481949391E−6	10	119.21
0	0	3.4	−1.25276489899729E−7	10	−1.25276489899821E−7	12	212.38
0	0	1.3	−8.67419994047523E−1	9	−8.674199940475497E−1	10	386.1
2.5	0.85	0	2.36336133180515E−4	11	2.363361331740410E−4	11	222.5
4.2	2.5	0	6.80464273097439E−7	10	6.804642730986373E−7	11	254.8
1.4	0.8	0	4.97257415780423E−3	8	4.97257415781797E−3	9	304.87
3.1	0.4	0	−1.17760968118471E−3	10	−1.17760968124514E−3	11	174.4
1.3	2.5	0	4.70193483120750E−5	9	4.70193483387439E−5	9	336.9
2.1	1.2	0	−2.07709378149512E−3	8	−2.07709378234201E−3	9	564.6
0	3.1	1.2	−2.29525171973724E−3	10	−2.29525171980067E−3	10	310
0	2.3	1.2	−5.08044628229364E−3	9	−5.08044628216382E−3	10	455.8
0	0.82	2.1	7.47961745441150E−2	8	7.47961745527295E−2	9	659.12
0	1.8	1.1	6.61620909054577E−3	8	6.616209087660916E−3	8	769.5
2.3	3.1	2.1	−6.68381125381913E−4	10	−6.68381123699021E−4	11	253.7
1.2	0.9	1.8	−3.35865148503078E−4	8	−3.35865148381098E−4	9	345.3
0.8	1.1	0.6	1.97152607508997E−2	9	1.97152608399783E−2	9	790.78

Table 3 The values of two-center Coulomb $I_{aa,bb}$, hybrid $I_{aa,ab}$ and exchange $I_{ab,ab}$ integrals in elliptical coordinate system in a.u. for $N=N'=12$, $\nu=11$, $\sigma=5$, $\theta_{ba}=0°$, $\phi_{ba}=0°$, $\Delta f = f(b{\to}a)-f(a{\to}b)$

n_1	l_1	m_1	ξ_1	n'_1	l'_1	m'_1	ζ'_1	n_2	l_2	m_2	ξ_2	n'_2	l'_2	m'_2	ζ'_2	Rba
Coulomb																
1	0	0	5.2	1	0	0	5.2	2	0	0	4.1	2	0	0	4.1	0.2
1	0	0	5.2	2	1	0	3.1	2	0	0	4.1	3	2	0	2.5	0.2
4	3	0	3.5	4	3	0	3.5	3	2	0	2.5	3	2	0	2.5	2.5
4	3	1	2.6	4	3	1	2.6	4	2	2	0.5	4	2	2	0.5	8.5
Hybrid																
1	0	0	5.2	2	1	0	3.1	2	1	1	4	3	2	1	3	0.2
4	3	0	3.5	4	3	0	3.5	4	3	0	3.5	3	2	0	2.5	2.5
2	1	1	4	2	1	1	4	2	1	1	4	3	2	1	1.5	8.5
3	2	−2	1.8	3	2	−2	1.8	4	3	0	3.5	3	2	0	2.5	8.5
Exchange																
1	0	0	5.2	2	0	0	4.1	1	0	0	5.2	2	0	0	4.1	2.5
2	1	0	3.1	3	2	0	2.5	2	1	0	3.1	3	2	0	2.5	2.5
2	1	1	4	3	1	1	1.5	2	1	1	4	3	1	1	1.5	2.5
1	0	0	5.2	7	0	0	0.5	1	0	0	5.2	7	0	0	0.5	0.2

charge-density expansion coefficients the formulae in terms of overlap integrals have recently been established in [23] Therefore, the computer programs written in this work for modified basic one-center Coulomb integrals and presented in [24] for overlap integrals can be used in the calculation of multicenter electron-repulsion integrals.

In [19] we have shown that the convergence of the series with respect to σ is rapid; therefore, we can include only a few terms obtained from the summation over indices σ.

The values of one- and two-center Coulomb, two- and three-center hybrid and two-, three- and four-center ex-change electron-repulsion integrals with respect to the molecular coordinate system for some selected parameters of calculation on a PENTIUM 233 computer (using Turbo Pascal 7.0) are presented in Tables 1 and 2. The results were compared with others obtained with a different procedure. The comparative values obtained in [25] for two-center Coulomb, hybrid and exchange integrals in the elliptical coordinate system are given in Tables 3 and 4. The comparative values for different translations of STOs ($c{\to}a,d{\to}b,b{\to}a$ and $c{\to}a,b{\to}d,d{\to}a$) obtained from the use of Coulomb Sturmian and Lambda ETFs (see Eqs. (18–22) of [18]), the number of correct decimal figures Δf and the CPU time in milliseconds are shown

Table 4 The values of two-center Coulomb $I_{aa,bb}$, hybrid $I_{aa,ab}$ and exchange $I_{ab,ab}$ integrals in elliptical coordinate system in a.u. for $N=N'=12$, $\nu=11$, $\sigma=5$, $\theta_{ba}=0°$, $\phi_{ba}=0°$, $\Delta f=f(b{\to}a)-f(a{\to}b)$

Use of Lambda ETFs: Equations (19), (20) in [17]		Use of Coulomb Sturmian ETFs: [24] Eqs. (21), (22) in [17]			
$b{\to}a$	Δf	$b{\to}a$	Δf	CPU (ms)	
1.82289255375066E–0	11	1.82289255378342E–0	12	2.4	1.822892554E–0
–2.36064302091598E–2	10	–2.36064302093622E–2	11	15.8	–2.360643021E–2
4.55264269053176E–1	10	4.55264269033952E–1	10	25.2	4.552642696E–1
8.75833308718459E–2	9	8.75833306908157E–2	10	67.9	8.758333087E–2
–6.86828291835712E–2	10	–6.86828291821429E–2	11	16.2	–6.868282918E–2
9.54255252019053E–2	9	9.54255252220098E–2	10	34.3	9.542674263E–2
4.24775454962049E–5	10	4.24775470375684E–5	10	26.1	4.083076994E–5
8.80511319007333E–6	9	8.80511319239429E–6	10	69.2	8.805113190E–6
9.94238798394352E–6	11	9.94238798394352E–6	11	31.6	9.438670422E–6
6.87758737484836E–2	10	6.87758737387899E–2	12	53.1	6.877581824E–2
5.37630293164483E–4	9	5.37630291911019E–4	10	64.3	5.377894509E–4
2.08978090446300E–13	16	2.08976163397448E–13	16	23.2	2.065281492E–13

in these tables. As can be seen from the tables, the accuracy and CPU time of computer results for different expansion formulae for translation of STOs obtained by the use of Coulomb Sturmian and Lambda ETFs are satisfactory.

We see from the tables that the multicenter electron-repulsion integrals in the case of Lambda ETFs exhibit a slower convergence rate. Therefore it seems to be recommendable to use in the calculation of multicenter integrals the expansion formulae for translation of STOs obtained from the Coulomb Sturmian ETFs. We notice that the algorithm presented in this paper can be used to calculate any multicenter electron-repulsion integral for arbitrary values of parameters of the STOs.

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