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Numerical Evaluation of Two-Center Overlap Integrals Over Slater-Type Orbitals and Convergence Properties

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Abstract

Motivation. Among the molecular integrals, the two-center overlap integrals play a major role in any accurate molecular structure calculation. They are central to the calculation of multicenter overlap integrals when using the series expansion formulae for Slater type functions about a new center. Consequently, these integrals require an accurate and fast numerical evaluation. Recently, we showed that these integrals are suitable to apply the nonlinear $\overline{D}$ transformation of Sidi, which is shown to be highly efficient in improving convergence of highly oscillatory integrals.

Method. In this work, we present an algorithm for a numerical evaluation of the molecular integrals under consideration over STOs. Convergence properties in the numerical evaluation of these molecular integrals are discussed. It is now shown that the approximation obtained using the nonlinear $\overline{D}$ transformation converges to the exact value of the integral without any constraint.

Results. Numerical results are obtained for two-center overlap integrals over Slater type orbitals with HCN, C_2H_2, BH_3 and CH_4 molecules. Comparisons with results obtained using the ACJU code developed by Hommeier et al. are presented. Numerical results from the litterature were also reproduced using the algorithm described in the present work.

Conclusions. The results obtained in this work illustrate the efficiency of the algorithm based on the nonlinear $\overline{D}$ transformation, which will lead to a highly accurate algorithm for the numerical evaluation of the integrals under consideration.

Keywords. Molecular electronic integrals. Slater type orbitals. B functions. Nonlinear transformations. Convergence accelerators. Numerical integration.

Abbreviations and notations

STO, Slater-type orbital
GTO, Gaussian-type orbital
ETO, exponential-type orbital

1 INTRODUCTION

The numerical evaluation of two-center overlap integrals over exponential type functions is of great importance for any accurate molecular structure calculations. Multicenter molecular integrals can be expressed in terms of the two-center integrals, therefore the accurate and rapid numerical evaluation of these integrals becomes more important in quantum mechanical calculations of the electronic structure of molecules.

STOs [1,2] are chosen for the expansion of atomic orbitals. These functions have a dominating position among ETOs, due to the fact that their analytical expression is very simple. STOs are better

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suited than GTOs to represent electron wave functions near the nucleus and at long range, provided that multicenter integrals using such functions could be computed efficiently.
STOs can be expressed as finite linear combinations of B functions [3,4,5]. The Fourier transforms of these B functions are exceptionally simple [6,7] and well adapted to the Fourier transform method [8,9], which led to analytical expressions for multicenter electronic integrals over B functions. These analytical expressions involve two-dimensional integral representations, which present severe numerical and computation difficulties. The integrand of the inner semi-infinite integral is a very oscillating function due to the presence of spherical Bessel function.

The molecular integrals under consideration are to be evaluated via a numerical quadrature of integral representations in terms of nonphysical integration variables. These integral representations were derived with the help of the Fourier transformation Method.

The semi-infinite integrals can be transformed into infinite series of integrals of alternating sign. These series are slowly convergent and this is why their use is prohibitively long for sufficient accuracy. The epsilon algorithm of Wynn [10] or Levin's u transform [11], accelerate the convergence of infinite series but in the case of the semi-infinite integrals involved in the analytical expressions of molecular integrals, the calculation times for a sufficient accuracy still long. Therefore new numerical integration techniques are required.

Recently [12], we demonstrate that the semi-infinite integrals under consideration are suitable to apply the nonlinear $\overline{D}$ transformation of Sidi [13,14,15]. It is shown that the $\overline{D}$ transformation is much more efficient and rapid compared with the alternative cited above.

In the present work, we disussed the convergence properties of $\overline{D}$ transformation in improving convergence of the smei-infinite integrals occurring in the analytic expression of overlap integrals and we also presented the algorithm for the numerical evaluation of overlap integrals over STOs. We performed calculations with HCN, C_2H_2, BH_3 and CH_4 molecules and we reproduce values from table I in [16]. We also used the ACJU code developed Homeier et al. [17] to perform the same calculations. From the numerical tables, one can easily notice that our numerical results are in a complete agreement with those listed in table I in [16] and with those obtained using the ACJU code. This illustrates clearly that the approach using nonlinear transformations for improving convergence of oscillatory integrals will probably lead to an efficient package for accurate numerical evaluation of all molecular integrals over exponential type functions.

2 Definitions and properties

Slater-type orbital (STOs) are given by [1,2]:

$$\chi_{n,l}^{m}(\zeta,r)=\sqrt{\frac{(2\zeta)^{2n+1}}{(2n)!}}r^{n-1}e^{-\zeta r}Y_{L}^{M}(\theta_r,\varphi_r) \tag{1}$$

where $Y_l^m(\theta_r,\varphi_r)$ stands for the spherical harmonic.

The B function is defined as follows [4,5]:

$$B_{n,l}^{m}(\zeta,r)=\frac{(\zeta r)^{l}}{2^{n+1}(n+1)!}\hat{k}_{n+\frac{1}{2}}(\zeta r)Y_{L}^{M}(\theta_r,\varphi_r) \tag{2}$$

where $\hat{k}_{n+\frac{1}{2}}(\zeta r)$ stands for the reduced Bessel function.

The two-center overlap integral over STOs is defined by:

$$S = \left\langle \chi^{m_1}_{n_1,l_1}(\zeta_1, r_1) \middle| \chi^{m_2}_{n_2,l_2}(\zeta_2, r - R) \right\rangle \tag{3}$$

Using the fact that STFs can be expressed in terms of of B functions, one can express the above integrals in terms of inetgrals over B functions, which are given by:

$$\hat{S} = \left\langle B^{m_1}_{n_1,l_1}(\zeta_1, r_1) \middle| B^{m_2}_{n_2,l_2}(\zeta_2, r - R) \right\rangle \tag{4}$$

The Fourier transform method allowed analytic expressions to be developed for the above integrals over B functions [18]. These analytic expressions involve semi-inifnite highly oscilatory, which are the principal source of the difficulty in the numerical evaluation of the molecular integrals under consideration. These semi-infinite integrals are given by [18]:

$$I = \int_0^\infty \frac{x^{n_x}}{(\zeta_1^2 + x^2)^{k_1} (\zeta_2^2 + x^2)^{k_2}} j_\lambda (vx) \, dx \tag{5}$$

Where n_x, k_1 and k_2 are positive integers. $j_\lambda(vx)$ stands for the spherical Bessel function.

Recently [12], we demonstrate the applicability of the nonlinear $\overline{D}$ transformation of Sidi [13,14]. Numerical results were obtained for two-center overlap integrals over B functions and they were in a complete agreement with results in the litterature [16] and with results obtained using existing codes such as ACJU developed by Hommeier et al [17].

In the present work, we demonstrate by using previous work of Sidi [13,19,20], that the approximation of the above semi-infinite integrals obtained using both the nonlinear $\overline{D}$ transformation converge to the exact value of the semi-infinite integrals without any constraint.

Calculations of these integrals over STFs were also performed and presented, to show that our approach will definitely lead to a highly efficient algorithm for the numerical evaluation of two-center overlap integrals over B functions and over STFs.

3 The nonlinear transformation and convergence properties

The approximation of the semi-infinite integral (5) using $\overline{D}$ is given by:

$$\overline{D}_n^{(2)} = \int_0^{x_l} F(t)\, dt + x_l^2 g(x_l) j'_\lambda (vx_l) \sum_{i=o}^{n-1} \frac{\overline{\beta}_{1,i}}{x_l^i} \tag{6}$$

where $l = 0,1,...,n$ and x_l are the successive positive zeros of the spherical Bessel function. $F(t)$ is the integrand of the semi-infinite integral (5) and $g(x)$ is given by:

$$g(x) = \frac{x^{n_x}}{(\zeta_1^2 + x^2)^{k_1} (\zeta_2^2 + x^2)^{k_2}} \tag{7}$$

Let $\Psi(x)$ be defined by:

$$\Psi(x) = x^2 g(x) j'_\lambda(vx) \tag{8}$$

Let $(\gamma_0, \gamma_1, ..., \gamma_n)$ the first row of the inverse matrix of the linear system given by equation (6). From the fact that the first column of the matrix of the system (6) is the vector $(1,1,...,1)^T$ it follows that:

$$\sum_{i=0}^{n} \gamma_i = 1 \tag{10}$$

In [13], Sidi demonstrated that if:

$$\sum_{i=0}^{n} |\gamma_i| \leq L < \infty \tag{11}$$

then the approximation $\overline{D}_n^{(2)}$ converges to the exact value of the semi-infinite integral without any constraint:

$$\left| I - \overline{D}_n^{(2)} \right| = o(n^{-j}) \tag{12}$$

for any $j > 0$.

In [19], Sidi demonstrated that a necessary and sufficient for $\gamma_i > 0$, $i = 0,1,...,n$, is:

$$\Psi(x_i)\Psi(x_{i+1}) < 0 \tag{13}$$

From the fact that x_i are the leading positive zeros of the spherical Bessel function, it follows that:

$$j'_\lambda(vx_i) j'_\lambda(vx_{i+1}) < 0 \tag{14}$$

Now by using the fact that $x^2 g(x) > 0$, it follows that (13) is satisfied and consequently, the approximation $\overline{D}_n^{(2)}$ converges to the exact value of the semi-inifnite integral without any constraint.

4 RESULTS AND DISCUSSION

The computation of the approximation $\overline{D}_n^{(2)}$ (6), require the computation of the first derivative of the spherical Bessel function. This can be obtained using the following equations:

$$\frac{\lambda}{2\lambda + 1} j_{\lambda-1}(x) - \frac{\lambda - 1}{2\lambda + 1} j_{\lambda+1}(x) = j'_\lambda(x) \tag{15}$$

$$j_{\lambda-1}(x) - \frac{\lambda + 1}{x} j_\lambda(x) = j'_\lambda(x) \tag{16}$$

In our algorithm, we used the following procedure. Note that if x is a zero of the spherical Bessel function of order λ for $\lambda \geq 1$, then equation (16) becomes:

$$j_{\lambda-1}(x) = j'_{\lambda}(x) \tag{17}$$

From the above equation, it follows that it is faster to use equation (17) than equation (15). But in this case, one has to separate the case where $\lambda = 1$, where the use of Cramer's rule is possible since the zeros of $j_0(x) = \frac{\sin(x)}{x}$ are equidistant [13]. In this case, the approximation is given by:

$$\overline{D}_n^{(2)} = \frac{\sum_{i=0}^{n} C_n^i (1+i)^n \left(\int_0^{x_i} F(t)\,dt \right) / \left[x_i^2 g(x_i) \right]}{\sum_{i=0}^{n} C_n^i (1+i)^n / \left[x_i^2 g(x_i) \right]} \tag{18}$$

where x_l are the successive positive zeros of the sine function.

We evaluate two-center overlap integrals over STOs. First, we expressed these integrals over STOs in terms of integrals over B functions, by expressing STOs as finite linear combinations of B functions [21]. Then we used the analytic expression obtained by Weniger et al for the two-center overlap integrals over B functions. These analytic expressions involve the semi-infinite integrals given by equation (5). We notice that these semi-infinite integrals have compact analytic expressions in the case where the scaling parameters are equal [18]. In the case where the scaling parameters are not equal, the semi-infinite integrals are evalauted using the nonlinear $\overline{D}$ transformation (6).

For the computation of the function $F(x)$, we transform the finite integral as follows:

$$\int_0^{x_n} F(t)\,dt = \sum_{l=0}^{n-1} \int_{x_l}^{x_{l+1}} F(t)\,dt \tag{19}$$

For the numerical evaluation of each term of the finite sum in the right hand side of equation (19), we used Gauss-Legendre quadrature of order 48.

The linear system given by equation (6) is solved using the LU decomposition method.

For the numerical evaluation of Gaunt coefficients which occur in the analytic expression of the molecular integrals, we used the subroutine GAUNT.F developed by Weniger [22]. The spherical harmonics $Y_l^m(\theta_r, \varphi_r)$ are computed using the recurrence formulae presented in [22].
We used the ACJU program developed by Homeier et al [17] to evaluate the molecular integrals under consideration. As it can be seen from the numerical tables our numerical results are in a complet agreement with those obtained using ACJU program.

Table (1) contains the values of the screening parameters, which occur in the analytic expression of STOs. Table (2) contains the geometry used for the calculations that we performed for the present work. Table (3) contains values obtained for two-center overlap integrals over STOs with HCN, C_2H_2, BH_3 and CH_4 molecules. The ACJU code was also used to perform the same calculations.

Table (4) contains values obtained for two-center overlap integrals over STOs. In this table, we listed the results obtained using the ACJU code and the results obtained by Talman [16].

As it can be seen from this table our results are in a complete agreement with those obtained using the ACJU code and with the results obtained by Talman [16].

The abbreviations $2p_z$ and $2p_{+1}$ refer to orbitals defined with the quantum numbers: n=2, l=1, m=0 and n=2, l=1, m=1 respectively. Numbers in parentheses represent powers of 10.

All the calculations were performed on a PC-Workstation Intel Xeon Processor 2.4GHz.

5 CONCLUSION

Analytic expressions for the two-center overlap integrals over STOs are obtained by expressing these STOs in terms of the so-called B functions and then by applying the Fourier transform method. These analytic expressions turned out very difficult to evaluate to because of the presence of highly semi-infinite integrals involving spherical Bessel functions.

It was shown that these semi-infinite integrals are suitable to apply the nonlinear $\overline{D}$ method, which consists on transforming the semi-infinite integrals involving Bessel functions into asymptotic expansions in inverse powers of x as $x \to \infty$. These asymptotic expansions are transformed into sets of linear equations. The approximations of semi-infinite integrals are obtained by solving these linear systems and it is shown that the approximations obtained using $\overline{D}$ transformation converge to the exact values of the semi-infinite integrals.

The numerical results show that the approach described in this work yields values for these integrals to a high pre-determined accuracy and in a complete agreement with values from the litterature.

These results confirm that this $\overline{D}$ transformation represents another most significant advance on the road to routine precise and rapid evaluation of these molecular electronic integrals.

5 Numerical tables

Table 1 Exponents of STOs for a series of orbitals

Orbitals	B	C	N	H
1s	4.649767	5.636105	6.621925	1.00000
2s	1.076139	1.346562	1.612481	
2p	1.226030	1.581274	1.929475	

Table 2 The geometry used for the molecular calculations

Molecules	**Geometry**	**Cartesian Coordinates**
C_2H_2	Linear H-C = a = 2.002 a.u. C-C = b = 2.281 a.u.	H^1(0.0, 0.0, -a-b/2) C^1(0.0, 0.0, -b/2) C^2(0.0, 0.0, b/2) H^2(0.0, 0.0, a+b/2)
BH_3	Equilateral Triangle, Planar B-H = a = 2.250 a.u. b = 3.897 a.u.	B (0.0, 0.0, 0.0) H^1(0.0, 0.0, a) H^2(b/2, 0.0, -a/2) H^3(-b/2, 0.0, -a/2)
CH_4	Regular Tetrahedron C-H = a = 2.0665 a.u. b = 1.1931 a.u.	C (0.0, 0.0, 0.0) H^1(b, b, b) H^2(b,-b, -b) H^3(-b,b, -b) H^4(-b,-b, b)
HCN	Linear H-C = a = 2.000 a.u. C-N = b = 2.187 a.u.	H(0.0, 0.0, -a) C(0.0, 0.0, 0.0) N(0.0, 0.0, b)

Table 3 Values obtained for the two-center overlap integrals over STOs

Molecules	**Integrales**	**Values** $\overline{D}$	**Values** ACJU
C_2H_2	$<1s^{C1} \mid 1s^{C2}>$	0.17999067797259(-03)	0.179990672868803(-03)
	$<2s^{C1} \mid 1s^{C2}>$	0.75773470045080(-01)	0.757734700451693(-01)
	$<2p_z^{C1} \mid 1s^{C2}>$	0.11347210396549(+00)	0.113472103965470(+00)
	$<2p_z^{C1} \mid 2p_z^{C2}>$	-.28034732991369(+00)	-0.280347329913672(+00)
	$<2p_{+1}^{C1} \mid 2p_z^{C2}>$	0.35111604505883(+00)	0.351116045058850(+00)
BH_3	$<1s^{B} \mid 1s^{H1}>$	0.84488384216158(-01)	0.844883842160902(-01)
	$<2s^{B} \mid 1s^{H1}>$	0.61417323135024(+00)	0.614173231350241(+00)
	$<2p_z^{B} \mid 1s^{H1}>$	0.54664981962486(+00)	0.546649819624870(+00)
	$<1s^{H1} \mid 1s^{H2}>$	0.20218404614891(+00)	0.202184046148936(+00)
CH_4	$<1s^{C} \mid 1s^{H1}>$	0.75634817563177(-01	0.756348175631746(-01)
	$<2s^{C} \mid 1s^{H1}>$	0.62274411537583(+00)	0.622744115375811(+00)
	$<2p_z^{C} \mid 1s^{H1}>$	0.47623357260361(+00)	0.274991804720407(+00)
	$<1s^{H1} \mid 1s^{H2}>$	0.27969702358746(+00)	0.279697023587438(+00)
HCN	$<1s^{N} \mid 1s^{c}>$	0.12627258447390(-03)	0.126272578207178(-03)
	$<2s^{N} \mid 1s^{c}>$	0.73192433120423(-01)	0.731924331205254(-01)
	$<2p_z^{N} \mid 1s^{c}>$	-.99048113986006(-01)	-0.991971925002319(-01)

Table 4 Values obtained for two-center overlap integrals over STOs. The two-centers are separated by unit distance in the z direction. Results are computed in double precision. Numbers in parenthesis represent powers of 10.

n_1	l_1	m_1	ξ_1	n_2	l_2	m_2	ξ_2	**Values** $^{\overline{D}}$	**Values** $^{\text{ACJU}}$	**Values** [16]
1	0	0	0.1	1	0	0	0.1	.998337272657	.99833728456	.9983372846
1	0	0	1.0	1	0	0	0.1	.187051615915	.18705161626	.1870516163
1	0	0	5.0	1	0	0	0.1	.201680371415(-1)	.20168086523(-1)	.2016803717(-1)
1	0	0	1.0	1	0	0	1.0	.858385362733	.85838536273	.8583853627
1	0	0	5.0	1	0	0	1.0	.239940017735	.23994001773	.2399400177
1	0	0	5.0	1	0	0	5.0	.965772403202(-1)	.96577240320(-1)	.9657724032(-1)
8	0	0	1.0	8	0	0	1.0	.989015721319	.98901572133	.98901572133
8	0	0	5.0	8	0	0	1.0	.107437341700(-1)	.10743703415(-1)	.1074373417(-1)
8	0	0	5.0	8	0	0	5.0	.785230850122	.78523085000	.7852308500
5	4	0	1.0	5	4	0	0.1	.219794514202(-2)	.22132767718(-2)	.2213276772(-2)
5	4	4	1.0	5	4	4	0.1	.225942860190(-2)	.22596477308(-2)	.2259647731(-2)
5	4	0	5.0	5	4	0	0.1	.664469344963(-6)	.66675704065(-6)	.6667585746(-6)
5	4	4	5.0	5	4	4	0.1	.729423185992(-6)	.72945439326(-6)	.7294559035(-6)
5	4	0	1.0	5	4	0	1.0	.768617010819	.76861701556	.7686170156
5	4	4	1.0	5	4	4	1.0	.955778746226	.95577874629	.9557787463
5	4	0	5.0	5	4	0	1.0	.900262308903(-2)	.90026230924(-2)	.9002623092(-2)
5	4	4	5.0	5	4	4	1.0	.318003745747(-1)	.31800374574(-1)	.3180037457(-1)
5	4	0	5.0	5	4	0	5.0	-.138257011551	-.13825701155	-.1382570116
5	4	4	5.0	5	4	4	5.0	.356825986845	.35682598684	.3568259868

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Biographies

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Second Author is assistant professor of mathematics at Faculté Saint Jean, Univ. of Alberta. After a PhD devoted mainly to study numerical algorithms geared towards an efficient evaluation of molecular integrals over Slater Type Orbitals (STOs), he developed a software package based on STOs for molecular structure determination. He then spent few years at Florida A&M University as a postdoctoral fellow during which he collaborated with Pr. H.W. Jones and Pr. C.A. Weatherford on various problems including multicenter integrals over STOs, electron/molecule scattering and molecules subjected to strong magnetic fields. At Ottawa Univ., the author collaborated with Pr. D.M. Bishop on a non-linear optics related problem the result of which was a technique allowing one to visualize the overall molecular polarizability and hyper-polarizability as a "sum" of "elementary" contributions from the functional groups of the molecule.