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Calculation of One- and Two-Center Overlap Like Quantum Similarity Integrals over $\psi^{(\alpha)}$ Exponential Type Functions

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ABSTRACT

One- and two-center overlap like quantum similarity integrals over $\psi^{(\alpha)}$ functions are evaluated using the one-center expansion method. These integrals are expressed through expansion coefficients and usual two-center overlap integrals. The expressions derived in this work have no restrictions for the values of orbital parameters, quantum numbers and internuclear distances. Since these integrals of $\psi^{(\alpha)}$ functions are calculated for the first time, the comparison is made with literature values obtained from Slater type functions. The computation results are in good agreement with literature values. The algorithm presented in this study could be useful when exponential type functions are employed in quantum similarity measures of atomic and molecular systems.

Keywords: $\psi^{(\alpha)}$ function, Expansion theorem, Overlap-like quantum similarity integral, Exponential type function

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Introduction

Quantum similarity measure (QSM) was firstly introduced in early 1980s as a quantitative comparison tool between molecules via their electron density functions [1]. Nowadays, QSM has a wide range of application area in quantitative structure-activity/property relationship (QSAR and QSPR) problems. The main idea of the QSM concept is that molecular electron density distribution can be used as a descriptor to compare molecular structures. Further details and extensive bibliography can be found in refs. [2-6]. The QSM is also extended to atomic [7] and nuclear [8] systems to analyze periodicity of the properties of them.

Electron density is used as information carrier of the system in QSM approach. Hence, description of the electron density is important subject to obtain reliable results. In most of the ab initio methods, density is defined by means of one-particle wave functions of investigated system and therefore used basis functions have significance. Gaussian type functions are the most popular basis functions and the first choice in QSM calculations due to their computational simplicity. Molecular electronic densities are modeled by spherical Gaussians with the help of atomic shell approximation [9, 10]. However, it is well known that the electronic wave function of atomic or molecular systems can be better represented with exponential type functions (ETFs) [11]. For this reason, the simplest form of ETFs called Slater type functions (STFs) were tested in atomic QSM studies. Larger electron charge concentration was obtained near the nuclei with STFs, and this led to better description of atomic overlap self-similarities [12]. Molecular overlap-like quantum similarity (OLQS) integrals of STFs were also investigated by using one-center two-range expansion [13] and Fourier transform [14-17] methods. The accuracy in Fourier transform method was improved through the convergence acceleration techniques such as epsilon algorithm of Wynn [14], nonlinear $\bar{D}$ transformation [15, 16] and nonlinear $S\bar{D}$ transformation [17].

In the present work, we use $\psi^{(\alpha)}$ functions [18, 19] as basis function to express electron density in molecular QSM calculations. These functions collect a large class of ETFs. Each value of the α parameter in the range $-\infty < \alpha < 3$ corresponds to a different complete orthonormal set of ETFs. For instance, Coulomb-Sturmian and Lambda functions can be obtained from $\psi^{(\alpha)}$ functions for $\alpha = 1$ and $\alpha = 0$ cases, respectively. The $\psi^{(\alpha)}$ functions play a significant role in different topics of atomic and molecular physics such as electronic structure studies, momentum and four-dimensional space representations of ETFs, and molecular integral solutions of STFs [20]. The aim of this study is to perform one- and two-center OLQS integrals of $\boldsymbol{\psi}^{(\alpha)}$ functions. This can be considered as a first step for the usage of these functions in QSMs.

General Definitions and Properties

$\psi^{(\alpha)}$ Complete Orthonormal Sets of Exponential Type Functions

In this study, we have used standard definition of $\psi^{(\alpha)}$ ETFs for integer values of α parameter $(\alpha = 2, 1, 0, -1, \dots)$ given by [18]:

$$\psi^{(\alpha)}_{nlm}(\zeta,\vec{r}) = N^{\alpha}_{nl}(\zeta)(2\zeta r)^{l} e^{-\zeta r} L^{2l+2-\alpha}_{n+l+1-\alpha}(2\zeta r) S_{lm}(\theta,\varphi)\,, \qquad (1)$$

where ζ and $S_{lm}(\theta,\varphi)$ stand for orbital parameter and real spherical harmonics, respectively. Here $N_{nl}^{\alpha}(\zeta)$ and $L_q^p(x)$ refer to the normalization constant and generalized Laguerre polynomials, respectively, and they are given by

$$N_{nl}^{\alpha}(\zeta)=(-1)^{\alpha}\left(\frac{(2\zeta)^3(n-l-1)!}{(2n)^{\alpha}((n+l+1-\alpha)!)^3}\right)^{1/2} \tag{2}$$

$$L_q^p(x)=\sum_{i=0}^{q-p}\gamma_{qi}^p x^i \ ,\ \gamma_{qi}^p=\frac{(-1)^{p+i}(q!)^2}{i!(p+i)!(q-p-i)!}\ . \tag{3}$$

Orthonormality condition satisfied with the weight function $(n/\zeta r)^{\alpha}$:

$$\int \psi_{nlm}^{(\alpha)*}(\zeta,\vec{r})\left(\frac{n}{\zeta r}\right)^{\alpha}\psi_{n'l'm'}^{(\alpha)}(\zeta,\vec{r})dV=\delta_{nn'}\delta_{ll'}\delta_{mm'}\ . \tag{4}$$

The products of the $\psi^{(\alpha)}$ functions at the same center can be expressed by linear combinations with the help of expansion theorem of them [21]:

$$\psi_{nlm}^{(\alpha)}(\zeta,\vec{r})\psi_{n'l'm'}^{(\alpha)}(\zeta',\vec{r})=\frac{(2z)^{3/2}}{\sqrt{4\pi}}\sum_{N=1}^{n+n'-1}\sum_{L=0}^{N-1}\sum_{M=-L}^{L}B_{nlm,n'l'm'}^{\alpha NLM}(\zeta,\zeta')\psi_{NLM}^{(\alpha)}(z,\vec{r})\ , \tag{5}$$

where $z=\zeta+\zeta'$. The analytical expression of $B_{nlm,n'l'm'}^{\alpha NLM}$ coefficients is given in ref. [21].

STFs defined by

$$\chi_{nlm}(\zeta,\vec{r})=\left((2\zeta)^{2n+1}/(2n)!\right)^{1/2}r^{n-1}e^{-\zeta r}S_{lm}(\theta,\varphi) \tag{6}$$

are written as finite linear combinations of $\psi^{(\alpha)}$ functions [18]:

$$\chi_{nlm}(\zeta,\vec{r})=\sum_{n'=l+1}^{n}\bar{\omega}_{nn'}^{\alpha l}\psi_{n'lm}^{(\alpha)}(\zeta,\vec{r})\ , \tag{7}$$

see ref. [18] for the definition of $\bar{\omega}_{nn'}^{\alpha l}$ coefficients. Using eq. (7), molecular integrals of STFs can be obtained as finite linear combinations of integrals with $\psi^{(\alpha)}$ functions.

Molecular Overlap-like Quantum Similarity Integrals

The QSMs of molecules A and B require multicenter integrals involving molecular electron density functions $\rho_A(\vec{r})$ and $\rho_B(\vec{r})$, and a positive definite operator $\Omega(\vec{r}_1,\vec{r}_2)$ as below:

$$Z_{AB}=\int\int\rho_A(\vec{r}_1)\Omega(\vec{r}_1,\vec{r}_2)\rho_B(\vec{r}_2)d\vec{r}_1 d\vec{r}_2\ . \tag{8}$$

Various QSMs can be defined by selecting different Hermitian bielectronic operators [2-6]. The most common and simple choose of mentioned operator is Dirac's delta function, $\Omega(\vec{r}_1,\vec{r}_2)=\delta(\vec{r}_1-\vec{r}_2)$, and then similarity integral in eq. (8) transforms into overlap-like QSM:

$$Z_{AB}=\int\int\rho_A(\vec{r})\rho_B(\vec{r})d\vec{r}\ . \tag{9}$$

If compared molecules are the same, the self-similarity measure is obtained as

$$Z_{AA}=\int\int\rho_A(\vec{r})^2\,d\vec{r}\ . \tag{10}$$

Z_{AA} is also used in general definition of the similarity indices called "Carbo index" [1]:

$$C_{AB}=\frac{Z_{AB}}{\sqrt{Z_{AA}Z_{BB}}}\ . \tag{11}$$

The Carbo index transforms QSM into a number in the interval (0,1] and allows the quantitative comparison of quantum systems. When C_{AB} approaches 1, the compared systems can be considered as more similar. The exact unity value is only achieved in the case of A=B.

In the Hartree-Fock-Roothaan or other linear combination of atomic orbitals (LCAO) based ab initio methods, the electron density of the molecular systems is expanded with appropriate basis functions and QSM integral in eq. (9) becomes a molecular integral up to four centers. The general form of OLQS integrals can be written as below:

$$Z_{1234}^{abcd}=\int\int\phi_1^*(\vec{r}_a)\phi_2(\vec{r}_b)\phi_3^*(\vec{r}_c)\phi_4(\vec{r}_d)d\vec{r}\ . \tag{12}$$

Here $\phi_i(\vec{r}_x)$ represents the basis function centered at atom "x" with quantum numbers n_i, l_i and m_i. In this work, we have used $\psi^{(\alpha)}$ basis functions and calculated one- and two-center integrals.

One-Center Overlap-Like Quantum Similarity Integrals

One-center, atomic, OLQS integrals over $\psi^{(\alpha)}$ functions are given by using eq. (12) in the case of a=b=c=d:

$$Z_{1234}^{aaaa}=\int\int\psi_{n_1l_1m_1}^{(\alpha)}(\zeta_1,\vec{r})\psi_{n_2l_2m_2}^{(\alpha)}(\zeta_2,\vec{r})\psi_{n_3l_3m_3}^{(\alpha)}(\zeta_3,\vec{r})\psi_{n_4l_4m_4}^{(\alpha)}(\zeta_4,\vec{r})d\vec{r}\ . \tag{13}$$

Using expansion formula in eq. (5), orthonormality of the spherical harmonics and auxiliary radial integrals [22]

$$\int_0^\infty x^n e^{-qx} dx = \frac{n!}{q^{n+1}} \tag{14}$$

one can express the one-center integrals as follow:

$$\begin{aligned} Z_{1234}^{aaaa} = & \sum_{N,N',L,M} N_{NL}^{\alpha}(\zeta_1+\zeta_2) N_{N'L}^{\alpha}(\zeta_3+\zeta_4) B_{n_1l_1m_1,n_2l_2m_2}^{\alpha NLM}(\zeta_1,\zeta_2) B_{n_3l_3m_3,n_4l_4m_4}^{\alpha N'LM}(\zeta_3,\zeta_4) \\ & \times \sum_{i,i'} \gamma_{Qi}^{P} \gamma_{Q'i'}^{P} \frac{2^{2L+i+i'+1}(2L+i+i'+2)!}{\pi(\zeta_1+\zeta_2+\zeta_3+\zeta_4)^{2L+i+i'+3}} (\zeta_1+\zeta_2)^{L+i+(3/2)} (\zeta_3+\zeta_4)^{L+i'+(3/2)}, \end{aligned} \tag{15}$$

where $1 \le N \le n_1+n_2-1$, $1 \le N' \le n_3+n_4-1$, $\max(|l_1-l_2|, |l_3-l_4|) \le L \le \min(l_1+l_2, l_3+l_4)$, $-L \le M \le L$, $0 \le i \le N-L-1$, $0 \le i' \le N'-L-1$, $Q = N+L+1-\alpha$, $Q' = N'+L+1-\alpha$ and $P = 2L+2-\alpha$.

Two-Center Overlap-Like Quantum Similarity Integrals

Two-center integrals are divided into two groups according to the number of basis functions found in the same atom.

- Two-center integrals of the first kind:

$$Z_{123\_4}^{aaa\_b} = \iint \psi_{n_1l_1m_1}^{(\alpha)}(\zeta_1,\vec{r}_a) \psi_{n_2l_2m_2}^{(\alpha)}(\zeta_2,\vec{r}_a) \psi_{n_3l_3m_3}^{(\alpha)}(\zeta_3,\vec{r}_a) \psi_{n_4l_4m_4}^{(\alpha)}(\zeta_4,\vec{r}_b) d\vec{r}\,. \tag{16}$$

- Two-center integrals of the second kind:

$$Z_{12\_34}^{aa\_bb} = \iint \psi_{n_1l_1m_1}^{(\alpha)}(\zeta_1,\vec{r}_a) \psi_{n_2l_2m_2}^{(\alpha)}(\zeta_2,\vec{r}_a) \psi_{n_3l_3m_3}^{(\alpha)}(\zeta_3,\vec{r}_b) \psi_{n_4l_4m_4}^{(\alpha)}(\zeta_4,\vec{r}_b) d\vec{r}\,. \tag{17}$$

Now by using eq. (5), we can express two-center OLQS integrals in terms of usual overlap integrals as follow:

- Two-center integrals of the first kind:

$$\begin{aligned} Z_{123\_4}^{aaa\_b} = & 2(\zeta_1+\zeta_2)^{3/2}(\zeta_3+\zeta_4)^{3/2}(\pi)^{-1} \sum_{N,L,M,N',L',M'} B_{n_1l_1m_1,n_2l_2m_2}^{\alpha NLM}(\zeta_1,\zeta_2) B_{NLM,n_3l_3m_3}^{\alpha N'L'M'}(\zeta_1+\zeta_2,\zeta_3) \\ & \times S_{N'L'M',n_4l_4m_4}^{\alpha}(\zeta_1+\zeta_2+\zeta_3,\zeta_4;\vec{R}_{ab}), \end{aligned} \tag{18}$$

where $1 \le N \le n_1+n_2-1$, $|l_1-l_2| \le L \le l_1+l_2$, $-L \le M \le L$, $1 \le N' \le N+n_3-1$, $|L-l_3| \le L' \le L+l_3$ and $-L' \le M' \le L'$.

- Two-center integrals of the second kind:

$$\begin{aligned} Z_{12\_34}^{aa\_bb} = & 2(\zeta_1+\zeta_2)^{3/2}(\zeta_3+\zeta_4)^{3/2}(\pi)^{-1} \sum_{N,L,M,N',L',M'} B_{n_1l_1m_1,n_2l_2m_2}^{\alpha NLM}(\zeta_1,\zeta_2) B_{n_3l_3m_3,n_4l_4m_4}^{\alpha N'L'M'}(\zeta_3,\zeta_4) \\ & \times S_{NLM,N'L'M'}^{\alpha}(\zeta_1+\zeta_2,\zeta_3+\zeta_4;\vec{R}_{ab}), \end{aligned} \tag{19}$$

where $1 \le N \le n_1+n_2-1$, $|l_1-l_2| \le L \le l_1+l_2$, $-L \le M \le L$, $1 \le N' \le n_3+n_4-1$, $|l_3-l_4| \le L' \le l_3+l_4$ and $-L' \le M' \le L'$.

In the above equations (18) and (19), S^{α} stand for two-center overlap integrals over $\psi^{(\alpha)}$ functions which are given by the following expression:

$$S_{nlm,n'l'm'}^{\alpha}(\zeta,\zeta';\vec{R}_{ab}) = \int \psi_{nlm}^{(\alpha)*}(\zeta,\vec{r}_a) \psi_{n'l'm'}^{(\alpha)}(\zeta',\vec{r}_b) dV\,, \tag{20}$$

where $\vec{R}_{ab} = \vec{r}_a - \vec{r}_b$. With the help of Fourier transform method, analytic expressions of S^{α} were developed for $\zeta = \zeta'$ case in ref. [21]. The more general solutions for $\zeta = \zeta'$ or $\zeta \neq \zeta'$ were derived by using ellipsoidal coordinates [23].

All two-center OLQS integrals involving other combinations of functions can be expressed by eqs. (18) and (19) using symmetry properties. It should be noted that we have used real spherical harmonics in $\psi^{(\alpha)}$ functions for simplicity. If complex spherical harmonics are used in basis functions, symmetry properties of them must be considered according to eq. (12).

Numerical Results and Discussion

The algorithm for evaluating one- and two-center OLQS integrals over $\psi^{(\alpha)}$ functions was described. For this purpose, we have used one-center expansion of functions. For two-center cases, OLQS integrals are expressed in terms of the standard two-center overlap integrals which can be calculated accurately and efficiently [21, 23]. The algorithm was implemented in a computer program written in Mathematica 12 software that capable to perform calculations with a high pre-determined accuracy.

Since there is not any calculation about OLQS integrals over $\psi^{(\alpha)}$ functions up to now, we have used STF results found in the literature to support the reliability of our procedures. We present numerical results for one- and two-center OLQS integrals over STFs obtained from those with $\psi^{(\alpha)}$ functions using eq. (7). Table 1 contains orbital parameters of STFs used for the calculations. In table 2, we listed values of one-center, atomic, OLQS integrals. Numerical results for two-center OLQS integrals of the first and second kind are given in tables 3 and 4, respectively. The numbers in parentheses in the tables show powers of 10. All values are given in atomic units. As can be seen from tables 2-4, our results for OLQS integrals are in good agreement with literature values [13, 16]. Accurate calculations of expansion coefficients and two-center overlap integrals of $\psi^{(\alpha)}$ functions, and integral transformations from $\psi^{(\alpha)}$ functions to STFs are performed efficiently.

The accuracy of molecular quantum similarity measurements and the quantum similarity index are highly dependent on the description of the electron density of systems. Effective one-electron basis functions must be employed to construct reliable electron density. Asymptotic properties of the electronic wave functions are well represented by $\psi^{(\alpha)}$ functions. Therefore, the use of these functions in molecular similarity calculations were proposed in this work. We demonstrate that the algorithm constructed in this study could be useful when ETFs containing Laguerre functions are employed in the QSM of atoms and diatomic molecular systems. The expressions derived for one- and two-center OLQS integrals have no restrictions for the values of orbital parameters, quantum numbers and internuclear distances. Application of presented procedure to molecular systems using specific ETFs such as Coulomb - Sturmian or Hydrogen-like functions, and evaluation of remaining three- and four-center integrals can be considered as the next step of this work.

Table 1. Orbital parameters of Slater type functions

Orbitals	Carbon	Nitrogen
1s	5.6727	6.6651
2s	1.6083	1.9237
$2p_z$ (2z)	1.5679	1.9170

Table 2. One-center integrals over Slater type functions. *

Integrals	Carbon	Nitrogen
$Z^{aaaa}_{1s1s1s1s}$	7.263 226 539 889	11.780 945 572 070
	7.263 226 534	11.780 945 572
$Z^{aaaa}_{1s1s1s2s}$	0.296 453 696 849	0.499 679 084 708
	0.296 453 696	0.499 679 084
$Z^{aaaa}_{1s1s2s2s}$	0.030 556 227 264	0.053 124 445 791
	0.030 556 227	0.053 124 445
$Z^{aaaa}_{1s2s2s2s}$	0.010 478 691 378	0.018 493 682 096
	0.010 478 691	0.018 493 682
$Z^{aaaa}_{2s2s2s2s}$	0.025 863 146 042	0.044 258 042 479
	0.025 863 146	0.044 258 042
$Z^{aaaa}_{1s1s2z2z}$	0.027 665 504 721	0.052 409 841 641
	0.027 665 504	0.052 409 841
$Z^{aaaa}_{2z2z2z2z}$	0.043 132 809 946	0.078 834 988 765
	0.043 132 809	0.078 834 988

* The values in the first line were calculated in this work using eqs. (7) and (15). The values in the second line were taken from ref. [13].

Table 3. Two-center integrals of the first kind $Z^{aaa\_b}_{123\_4}$ over Slater type functions. a and b denote carbon and nitrogen atoms, respectively. a = (0, 0, 0) and b = (0, 0, z_b).

Integrals	z_b	Eqs. (7) and (18)	Ref. [16]
$Z^{aaa\_b}_{1s1s1s\_1s}$	0.5	0.858 425 675 390 877(0)	0.858 425 675 391(0)
	1.0	0.347 537 588 662 945(-1)	0.347 537 588 663(-1)
	1.5	0.129 121 127 852 282(-2)	0.129 121 127 852(-2)
	2.0	0.469 994 519 132 161(-4)	0.469 994 519 132(-4)
$Z^{aaa\_b}_{1s1s2s\_2s}$	0.5	0.501 691 891 383 981(-1)	0.501 691 891 384(-1)
	1.0	0.390 207 911 608 111(-1)	0.390 207 911 608(-1)
	1.5	0.230 014 520 893 589(-1)	0.230 014 520 894(-1)
	2.0	0.119 332 536 416 542(-1)	0.119 332 536 417(-1)
$Z^{aaa\_b}_{1s1s2s\_2z}$	0.5	-0.737 349 020 140 985(-1)	-0.737 349 020 141(-1)
	1.0	-0.646 924 813 965 509(-1)	-0.646 924 813 966(-1)
	1.5	-0.391 558 341 502 100(-1)	-0.391 558 341 502(-1)
	2.0	-0.205 470 626 696 680(-1)	-0.205 470 626 697(-1)

Table 4. Two-center integrals of the second kind $Z^{aa\_bb}_{12\_34}$ over Slater type functions. a and b denote carbon and nitrogen atoms, respectively. a = (0, 0, 0) and b = (0, 0, z_b).

Integrals	z_b	Eqs. (7) and (19)	Ref. [16]
$Z^{aa\_bb}_{1s1s\_1s1s}$	0.5	0.392 518 041 234 902(0)	0.392 518 041 235(0)
	1.0	0.287 291 441 055 918(-2)	0.287 291 441 056(-2)
	1.5	0.142 141 502 024 259(-4)	0.142 141 502 024(-4)
	2.0	0.600 438 755 929 345(-7)	0.600 438 755 929(-7)
$Z^{aa\_bb}_{1s2s\_1s2s}$	0.5	0.185 319 053 139 597(-1)	0.185 319 053 140(-1)
	1.0	0.266 806 719 446 299(-2)	0.266 806 719 446(-2)
	1.5	0.206 888 508 259 901(-3)	0.206 888 508 260(-3)
	2.0	0.115 769 691 748 916(-4)	0.115 769 691 749(-4)
$Z^{aa\_bb}_{1s2s\_1s2z}$	0.5	-0.159 539 790 120 835(-1)	-0.159 539 790 121(-1)
	1.0	-0.324 008 018 849 674(-2)	-0.324 008 018 850(-2)
	1.5	-0.280 545 795 502 279(-3)	-0.280 545 795 502(-3)
	2.0	-0.165 259 528 950 509(-4)	-0.165 259 528 951(-4)

Conflicts of interest

There are no conflicts of interest in this work.

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