Evaluation of Multicenter Multielectron Integrals Using One-range Addition Theorems in Terms of STOs for STOs and Coulomb-Yukawa Like Correlated Interaction Potentials with Integer and Noninteger Indices

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Using one-range addition theorems for Slater type orbitals (STOs) and Coulomb-Yukawa like correlated interaction potentials (CIPs) introduced by the author, the series expansion formulae are derived for the multicenter multielectron integrals. The expansion coefficients occurring in these relations are presented through the overlap integrals of two STOs. The convergence of series expansion relations is tested by calculating concrete cases. The accuracy of the results is quite high for quantum number, screening constants and location of orbitals. The final results are especially useful in the calculation of multielectron properties for atoms and molecules when Hartree-Fock-Roothaan (HFR) and explicitly correlated methods are employed.

Key Words: One-range addition theorems, Slater type orbitals, Coulomb-Yukawa like correlated interaction potentials, Multicenter multielectron integrals

Introduction

Quantum theory of electronic structure for atoms and molecules requires the more accurate solutions of Schrödinger equation. For improving the solutions, one can use more accurate wave functions that include electron correlation by means of Hylleraas correlated wave function (Hy) and configuration interaction (CI) approaches.[1-6] We notice that the CI expansions converge much more slowly than Hy-method expansions. The Hy method first developed by James and Collidge[7] has been used for determination of the ground state energy of H_2 molecule[8,9] and is still valid for two- and three-electron atomic and molecular systems (see, e.g., Refs.[10-12] and references quoted therein). A drawback in the Hy-type expansions, however, is the complexity of the calculation of multicenter multielectron integrals. There exist other correlational approaches like explicitly correlated Gaussians or the R12 methods, of which the applicability in practical calculations (see Ref.[13] and references quoted therein) has already been proven.

The principal tools of above-mentioned explicitly correlated methods are the two-range additional theorems the best known example of which is the Laplace expansion. The two-range addition theorems can lead to nontrivial technical problems in applications. The use of one-range addition theorems would be highly desirable since they are capable to simplify subsequent integrations in multicenter integrals substantially. The one-range addition theorems established in our published papers using complete orthonormal sets of Ψ^{α}-exponential type orbitals (Ψ^{α}- *ETOs*)[14] could be utilized for the calculation of arbitrary multicenter multielectron integrals occurring in the explicitly correlated theories. In Ref.[15], we presented a particular method for obtaining the one-range addition theorems for STOs and CIPs of integer and noninteger indices using complete orthonormal sets of Ψ^{α} - *ETOs* (see also Ref.[16] Using these one-range addition theorems, the general formulas can be established for the multicenter t-electron integrals which arise in the study of electronic structure of N-electron atomic and molecular systems ($1 \le t \le N$).

Evaluation of Multicenter Multielectron Integrals

According to a theorem for matrix elements of a general t-electron operator, the required matrix elements between N-dimensional determinantal wave functions are sums of matrix elements over t-dimensional basic determinantal wave functions.[17,18] These matrix elements, therefore, the matrix elements between N-dimensional determinantal wave functions of atomic and molecular systems can be expressed through the following 2t-center basic integrals of STOs and Coulomb-Yukawa like CIPs with integer and noninteger indices:

$$I^{ac,bd,gh,\ldots,ef}_{p_1^* p_1'^*, p_2^* p_2'^*, p_3^* p_3'^*, \ldots, p_t^* p_t'^*; q^*}(\zeta_1 \zeta_1', \zeta_2 \zeta_2', \zeta_3 \zeta_3', \ldots, \zeta_t \zeta_t'; \xi^*)$$
$$= \int \chi^*_{p_1^*}(\zeta_1, \vec{r}_{a1}) \chi_{p_1'^*}(\zeta_1', \vec{r}_{c1}) \chi_{p_2^*}(\zeta_2, \vec{r}_{b2}) \chi^*_{p_2'^*}(\zeta_2', \vec{r}_{d2}) \chi_{p_3^*}(\zeta_3, \vec{r}_{g3})$$
$$\times \chi^*_{p_3'^*}(\zeta_3', \vec{r}_{h3}) \cdots \chi_{p_t^*}(\zeta_t, \vec{r}_{et}) \chi^*_{p_t'^*}(\zeta_t', \vec{r}_{ft})$$
$$\times O_{q^*}(\xi^*, \vec{r}_{123\ldots t}) dv_1 dv_2 dv_3 \ldots dv_t, \quad (1)$$

where $1 \le t \le N$, $p_i^* = n_i^* l_i m_i$, $p_i'^* = n_i'^* l_i' m_i'$, $q^* = \mu^* \nu \sigma$ and

$$O_{q^*}(\xi^*, \vec{r}_{123\ldots t}) = f_{q^*}(\xi^*, \vec{r}_{21}) f_{q^*}(\xi^*, \vec{r}_{31}) f_{q^*}(\xi^*, \vec{r}_{41}) \ldots f_{q^*}(\xi^*, \vec{r}_{t1})$$
$$\times f_{q^*}(\xi^*, \vec{r}_{32}) f_{q^*}(\xi^*, \vec{r}_{42}) \ldots f_{q^*}(\xi^*, \vec{r}_{t2})$$
$$\times f_{q^*}(\xi^*, \vec{r}_{43}) \ldots f_{q^*}(\xi^*, \vec{r}_{t3}) \times \ldots \times f_{q^*}(\xi^*, \vec{r}_{tt-1}). \quad (2)$$

In Ref.,[19] we have established the general formulae for

integral (1) using one-range addition theorems in terms of Ψ^{α}-*ETOs* for STOs and Coulomb-Yukawa like CIPs. The aim of this work is with the help of one-range addition theorems in terms of STOs for STOs and Coulomb-Yukawa like CIPs, and the expansion formulae for the integer and noninteger n STO charge densities presented in previous papers[15,16] to evaluate the multicenter multielectron integrals defined by Eq.(1).

For the evaluation of integral (1) we first utilize the following relations for the noninteger μ CIPs in terms of integer μ CIPs and their symmetrical one-range addition theorems:[15]

$$f_{q^*}(\xi^*,\vec{r}_{21}) = \lim_{M\to\infty}\sum_{\mu=\nu+1}^{M} Q^{\alpha M}_{\mu^*\nu,\mu^*\nu}(\tau^*) f_q(\xi,\vec{r}_{21}) \tag{3}$$

$$f_q(\xi,\vec{r}_{21}) = 4\pi \lim_{\substack{N\to\infty\\ N'\to\infty}} \sum_{\mu'=1}^{N}\sum_{\nu'=0}^{\mu'-1}\sum_{\sigma'=-\nu'}^{\nu'} \sum_{u=1}^{N+N'-\alpha+1}\sum_{\upsilon=0}^{u-1}\sum_{s=-\upsilon}^{\upsilon} L^{\alpha k}_{qq'}(\xi\xi',NN')\chi_{q'}(\xi',\vec{r}_{a1})\chi^*_k(\xi',\vec{r}_{a2}), \tag{4}$$

where $q\equiv\mu\nu\sigma$, $q'\equiv\mu'\nu'\sigma'$, $k\equiv u\upsilon s$ and

$$L^{\alpha k}_{qq'}(\xi\xi',NN') = \frac{2^{3/2}}{\sqrt{4\pi}(2\xi')^{\mu+\frac{1}{2}}} B^{\alpha k}_{qq'}(\xi\xi',NN'). \tag{5}$$

Then, the integral (1) can be expressed through the 2t-center basic integrals of noninteger n STOs and Coulomb-Yukawa like CIPs with integer indices:

$$\begin{aligned} &I^{ac,bd,gh,\ldots,ef}_{p_1^*p_1'^*,p_2^*p_2'^*,p_3^*p_3'^*,\ldots,p_t^*p_t'^*;q}(\zeta_1\zeta_1',\zeta_2\zeta_2',\zeta_3\zeta_3',\ldots,\zeta_t\zeta_t';\xi)\\ &= \int \chi^*_{p_1^*}(\zeta_1,\vec{r}_{a1})\chi_{p_1'^*}(\zeta_1',\vec{r}_{c1})\chi_{p_2^*}(\zeta_2,\vec{r}_{b2})\chi^*_{p_2'^*}(\zeta_2',\vec{r}_{d2})\\ &\times \chi_{p_3^*}(\zeta_3,\vec{r}_{g3})\chi^*_{p_3'^*}(\zeta_3',\vec{r}_{h3})\cdots\chi_{p_t^*}(\zeta_t,\vec{r}_{et})\chi^*_{p_t'^*}(\zeta_t',\vec{r}_{ft})\\ &\times O_q(\xi,\vec{r}_{123\ldots t})d\nu_1 d\nu_2 d\nu_3\ldots d\nu_t. \end{aligned} \tag{6}$$

Using Eq.(4) in Eq.(6), we obtain finally for the multicenter multielectron integrals the following series expansion relations:

$$\begin{aligned} &I^{ac,bd,gh,\ldots,ef}_{p_1^*p_1'^*,p_2^*p_2'^*,p_3^*p_3'^*,\ldots,p_t^*p_t'^*;q}(\zeta_1\zeta_1',\zeta_2\zeta_2',\zeta_3\zeta_3',\ldots,\zeta_t\zeta_t';\xi)\\ &= \lim_{\substack{N\to\infty\\ N'\to\infty}}\sum_{q'}\sum_{k}\Big[L^{\alpha k_{21}}_{qq'_{21}}(\xi\xi',N_{21}N'_{21})\,L^{\alpha k_{31}}_{qq'_{31}}(\xi\xi',N_{31}N'_{31})\\ &\times L^{\alpha k_{41}}_{qq'_{41}}(\xi\xi',N_{41}N'_{41})\ldots L^{\alpha k_{t1}}_{qq'_{t1}}(\xi\xi',N_{t1}N'_{t1})\,L^{\alpha k_{32}}_{qq'_{32}}(\xi\xi',N_{32}N'_{32})\\ &\times L^{\alpha k_{42}}_{qq'_{42}}(\xi\xi',N_{42}N'_{42})\ldots L^{\alpha k_{t2}}_{qq'_{t2}}(\xi\xi',N_{t2}N'_{t2})\,L^{\alpha k_{43}}_{qq'_{43}}(\xi\xi',N_{43}N'_{43})\\ &\times \ldots L^{\alpha k_{t3}}_{qq'_{t3}}(\xi\xi',N_{t3}N'_{t3})\times\ldots\times L^{\alpha k_{tt-1}}_{qq'_{tt-1}}(\xi\xi',N_{tt-1}N'_{tt-1})\Big]\\ &\times S^{acaaa\ldots a}_{p_1^*p_1'^*q'_{21}q'_{31}q'_{41}\ldots q'_{t1}}(\zeta_1\zeta_1'\ \xi'\xi'\xi'\ldots\xi')\\ &\times S^{bdaa\ldots a}_{p_2^*p_2'^*q'_{32}q'_{42}\ldots q'_{t2}k_{21}}(\zeta_2\zeta_2'\ \xi'\xi'\ldots\xi'\xi')\\ &\times S^{gha\ldots aaa}_{p_3^*p_3'^*q'_{43}\ldots q'_{t3}k_{31}k_{32}}(\zeta_3\zeta_3'\ \xi'\ldots\xi'\xi'\xi')\\ &\times \ldots S^{efaaa\ldots a}_{p_t^*p_t'^*k_{t1}k_{t2}k_{t3}\ldots k_{tt-1}}(\zeta_t\zeta_t'\ \xi'\xi'\xi'\ldots\xi'), \end{aligned} \tag{7}$$

where $\alpha = 1, 0, -1, -2, \ldots$ and

$$\begin{aligned} N &\equiv N_{21},N_{31},N_{41},\ldots,N_{t1};N_{32},N_{42},\ldots,N_{t2};N_{43},\ldots,N_{t3};\ldots;N_{tt-1}\\ N' &\equiv N'_{21},N'_{31},N'_{41},\ldots,N'_{t1};N'_{32},N'_{42},\ldots,N'_{t2};N'_{43},\ldots,N'_{t3};\ldots;N'_{tt-1} \end{aligned} \tag{8}$$

$$\begin{aligned} q' &\equiv q'_{21},q'_{31},q'_{41},\ldots,q'_{t1};q'_{32},q'_{42},\ldots,q'_{t2};q'_{43},\ldots,q'_{t3};\ldots;q'_{tt-1}\\ k &\equiv k_{21},k_{31},k_{41},\ldots,k_{t1};k_{32},k_{42},\ldots,k_{t2};k_{43},\ldots,k_{t3};\ldots;k_{tt-1}. \end{aligned} \tag{9}$$

The quantities S occurring in Eq.(7) are the one ($g=h=a$) -, two ($g=a, h\neq a$ or $g\neq a, h=a$) - and three ($g\neq a, h\neq a$) - center overlap integrals of t+1 STOs. They are defined as

$$\begin{aligned} &S^{ghaa\ldots a}_{p^*p'^*q_1q_2\ldots q_{t-1}}(\zeta\zeta'\xi\xi\ldots\xi)\\ &= (4\pi)^{\frac{t-1}{2}}\int \chi^*_{p^*}(\zeta,\vec{r}_{g1})\chi_{p'^*}(\zeta',\vec{r}_{h1})\chi_{q_1}(\xi,\vec{r}_{a1})\chi_{q_2}(\xi,\vec{r}_{a1})\\ &\times\ldots\chi_{q_{t-1}}(\xi,\vec{r}_{a1})d\nu_1. \end{aligned} \tag{10}$$

The first few special cases of multicenter multielectron integrals obtained from Eq.(7) are determined by

for t = 2

$$\begin{aligned} &I^{ac,bd}_{p_1^*p_1'^*,p_2^*p_2'^*;q}(\zeta_1\zeta_1',\zeta_2\zeta_2';\xi)\\ &= \lim_{\substack{N\to\infty\\ N'\to\infty}}\sum_{q'}\sum_{k} L^{\alpha k}_{qq'}(\xi\xi',NN')S^{aca}_{p_1^*p_1'^*q'}(\zeta_1\zeta_1'\ \xi')S^{bda\,*}_{p_2^*p_2'^*k}(\zeta_2\zeta_2'\ \xi') \end{aligned} \tag{11a}$$

$$\begin{aligned} &S^{gha}_{p^*p'^*q}(\zeta\zeta'\xi)\\ &= \sqrt{4\pi}\int \chi^*_{p^*}(\zeta,\vec{r}_{g1})\chi_{p'^*}(\zeta',\vec{r}_{h1})\chi_q(\xi,\vec{r}_{a1})d\nu_1, \end{aligned} \tag{11b}$$

for t = 3

$$\begin{aligned} &I^{ac,bd,gh}_{p_1^*p_1'^*,p_2^*p_2'^*,p_3^*p_3'^*;q}(\zeta_1\zeta_1',\zeta_2\zeta_2',\zeta_3\zeta_3';\xi)\\ &= \lim_{\substack{N\to\infty\\ N'\to\infty}}\sum_{q'}\sum_{k} L^{\alpha k_{21}}_{qq'_{21}}(\xi\xi',N_{21}N'_{21})L^{\alpha k_{31}}_{qq'_{31}}(\xi\xi',N_{31}N'_{31})\\ &\times L^{\alpha k_{32}}_{qq'_{32}}(\xi\xi',N_{32}N'_{32})\,S^{bdaa}_{p_2^*p_2'^*q'_{32}k_{21}}(\zeta_2\zeta_2'\ \xi'\xi')\\ &\times S^{bdaa}_{p_2^*p_2'^*q'_{32}k_{21}}(\zeta_2\zeta_2'\ \xi'\xi')S^{ghaa}_{p_3^*p_3'^*k_{31}k_{32}}(\zeta_3\zeta_3'\ \xi'\xi') \end{aligned} \tag{12a}$$

$$\begin{aligned} &S^{ghaa}_{p^*p'^*q_1q_2}(\zeta\zeta',\xi\xi)\\ &= 4\pi\int \chi^*_{p^*}(\zeta,\vec{r}_{g1})\chi_{p'^*}(\zeta',\vec{r}_{h1})\chi_{q_1}(\xi,\vec{r}_{a1})\chi^*_{q_2}(\xi,\vec{r}_{a1})d\nu_1. \end{aligned} \tag{12b}$$

Carrying through calculations analogous to those for the multielectron case, it is easy to derive for the one- electron multicenter integrals of Coulomb-Yukawa like CIPs the following relations:

$$\begin{aligned} &I^{ac,g}_{p_1^*p_1'^*;q}(\zeta_1\zeta_1';\xi)\\ &= \sqrt{4\pi}\lim_{\substack{N\to\infty\\ N'\to\infty}}\sum_{q'}\sum_{k} L^{\alpha k}_{qq'}(\xi\xi',NN')S^{aca}_{p_1^*p_1'^*q'}(\zeta_1\zeta_1'\xi)\chi^*_k(\xi',\vec{r}_{ga}) \end{aligned} \tag{13a}$$

Table 1. Comparison of methods of computing three-center integrals with STOs and Coulomb-Yukawa like CIPs for $N' = 15$

n_1	l_1	m_1	ξ_1	n'_1	l'_1	m'_1	ξ'_1	μ	ν	σ	ξ	R_{ac}	θ_{ac}	φ_{ac}	R_{ab}	θ_{ab}	φ_{ab}	Eq.(13a)	
																		$\alpha = 0$	$\alpha = 1$
1	0	0	8.2	1	0	0	4.3	1	0	0	2.4	0.2	120	126	0.4	60	90	3.705369622E-01	3.705478488E-01
1.5	0	0	3.4	1.7	0	0	2.3	0	0	0	2.1	0.3	126	108	0.5	90	108	3.291990691E-01	3.291984692E-01
2	1	0	9.8	2	1	0	6.4	2	1	0	5.2	0.3	180	144	0.08	45	135	-1.534697999E-02	-1.534443530E-02
2.5	1	0	6.3	2.7	1	0	1.2	1.5	0	0	4.2	0.17	70	144	0.21	100	126	5.155671059E-03	5.155975858E-03
2.1	1	0	9.3	2.1	1	0	4.5	0.2	0	0	5.3	0.1	126	108	0.4	126	90	1.100592954E-01	1.100546661E-01
2	1	1	10.9	2	1	1	8.4	1	0	0	2.5	0.8	18	162	1.1	90	180	1.217857344E-03	1.217869659E-03

Table 2. Convergence of the series expansion relation for three-center integral $I^{ac,b}_{210,210,200}(9.2,3.8,1.2)$ as a function of summation limit L for $R_{ac} = 0.14$, $\theta_{ac} = 18^o$, $\varphi_{ac} = 162^o$, $R_{ab} = 0.24$, $\theta_{ab} = 135^o$, $\varphi_{ab} = 225^o$ and $N' = 15$

L	α = 0
1	1.31001409200918E-01
2	1.31001410175056E-01
3	1.31001409878574E-01
4	1.31001409544016E-01
5	1.31001409580279E-01
6	1.31001409581107E-01
7	1.31001409581031E-01
8	1.31001409581032E-01
9	1.31001409581032E-01
10	1.31001409581032E-01
11	1.31001409581032E-01
12	1.31001409581032E-01
13	1.31001409581032E-01
14	1.31001409581032E-01

Table 3. Convergence of the series expansion relation for three-center integral $I^{ac,b}_{210,210,200}(9.2,3.8,1.2)$ as a function of summation limit M for $R_{ac} = 0.14$, $\theta_{ac} = 18^o$, $\varphi_{ac} = 162^o$, $R_{ab} = 0.24$, $\theta_{ab} = 135^o$, $\varphi_{ab} = 225^o$ and $N' = 15$, $L = 14$

M	α = 0
1	1.31001409581032E-01
2	1.31001409581032E-01
3	1.31001409581032E-01
4	1.31001409581032E-01
5	1.31001409581032E-01
6	1.31001409581032E-01
7	1.31001409581032E-01
8	1.31001409581032E-01
9	1.31001409581032E-01
10	1.31001409581032E-01
11	1.31001409581032E-01
12	1.31001409581032E-01
13	1.31001409581032E-01
14	1.31001409581032E-01

$$S^{aca}_{p^*p'^*q}(\zeta\zeta'\xi) = \sqrt{4\pi}\int \chi^*_{p^*}(\zeta,\vec{r}_{a1})\chi_{p'^*}(\zeta',\vec{r}_{c1})\chi_q(\xi,\vec{r}_{a1})dv_1, \quad (13b)$$

where $g = a, b, c, \ldots$

By the use of unsymmetrical one-range addition theorems for STOs in the charge density expansion approximation (see Refs.[15, 16, 20]) and the expansion relations for one-center product of STOs,[21] the multicenter overlap integrals (10) can be reduced to the two-center overlap integrals of two STOs:

$$S_{pp'}(z,z';\vec{R}_{ab}) = \int \chi^*_p(z,\vec{r}_a)\chi_{p'}(z',\vec{r}_b)dv. \quad (14)$$

For the calculation of two-center overlap integrals, Eq.(14), the efficient computer programs especially useful for large quantum number are available in our group.[22] Therefore by using the computer programs for the overlap integrals one can calculate the multicenter multielectron integrals of STOs and Coulomb-Yukawa like CIPs with integer and noninteger indices that arise in the study of atomic and molecular multielectron properties when the HFR and correlated interaction potentials approximations are employed.

Thus, we have established a large number of different (α = 1, 0, -1, -2, …) sets of series expansion formulae for the arbitrary multicenter multielectron integrals which can be chosen properly according to the nature of the electronic structure problems of atomic and molecular systems under consideration. This is rather important because the choice of the series expansion relation set for the multicenter multielectron integrals will determine the rate of convergence of the using series expansions

Table 4. Convergence of the series expansion relation for three-center integral $I^{ac,b}_{210,210,200}(9.2,3.8,1.2)$ as a function of summation limit N' for $R_{ac} = 0.14$, $\theta_{ac} = 18^o$, $\varphi_{ac} = 162^o$, $R_{ab} = 0.24$, $\theta_{ab} = 135^o$, $\varphi_{ab} = 225^o$

N'	α = 0
11	1.28071141096E-01
12	1.31483647851E-01
13	1.30953982079E-01
14	1.31003528062E-01
15	1.31001409581E-01

Numerical Results and Discussion

As an example of application of one-range addition theo-

rems, the calculations are performed for the nuclear attraction integrals determined by Eq. (13a). For this purpose, the computer programs presented in Ref.[22] for overlap integrals are used. The results of calculations in atomic units are given in Tables 1, 2, 3 and 4.

The convergence properties of the series expansion relation for three-center nuclear attraction integral $I^{ac,b}_{210,210,200}$ (9.2, 3.8, 1.2) for $\alpha = 0$ are shown in Tables 2, 3 and 4. The partial summations in Eq. (13a) corresponding to progressively increasing upper summation limits are denoted by N, L and M. As can be seen from Tables 2 and 3 that the Eq. (13a) displays the most rapid convergence to the numerical results with twelve digits stable as a functions of summation limits L and M. The convergence of the series with respect to L and M is rapid. So, in the summations over indices ν' and σ', one can include only a few terms. As can be seen from Table 3 that the accuracy of computer calculations obtained in the present algorithm is satisfactory for $N' = 15$. We see from Table 1 that the calculated three-center nuclear attraction integrals with the arbitrary values of parameters of Coulomb-Yukawa like CIPs show a good rate agreement for $\alpha = 0$ and $\alpha = 1$. The greater accuracy is attainable by the use of more terms in the series expansion formula (13a).

As is clear from our tests that the analytical formulas presented in this study are useful tool for exact evaluation of the multicenter integrals of Coulomb-Yukawa like CIPs for the arbitrary values of quantum numbers, orbital parameters and internuclear distances.

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