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LETTER

Comment on "Analytical evaluation for two-center nuclear attraction integrals over Slater type orbitals by using Fourier transform method" by S. Özcan and E. Öztekin (J. Math. Chem. DOI 10.1007/s10910-008-9398-z)

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Abstract S. Özcan and E. Öztekin, (J. Math. Chem. doi:10.1007/s10910-008-9398-z) published formulas for evaluating the two-center nuclear attraction integrals over Slater type orbitals. It is shown that the analytical relations for these integrals through the expansion coefficients of the electron charge density for the one-center case and the overlap integrals presented in Sect. 3 of this work can easily be derived by means of a simple algebra from the formulas published in our papers (I.I. Guseinov, J Mol Struct (Theochem) 417:117, 1997; J Math Chem 42:415, 2007 and B.A. Mamedov, Chin J Chem 22:545, 2004). It should be noted that the formulas of overlap integrals presented by E. Öztekin et al., in previous paper (E. Öztekin, M. Yavuz, Ş. Atalay, J Mol Struct (Theochem) 544:69, 2001) for the calculation of two-center nuclear attraction integrals also are obtained from our papers (see Comment: I.I. Guseinov, J Mol Struct (Theochem) 638:235, 2003).

Keywords Slater type orbital · Nuclear attraction integral · Overlap integral

1 Introduction

The evaluation of two-center nuclear attraction integrals over Slater type orbitals (STOs) is of fundamental importance in the study of molecular systems. These integrals arise not only in their own right, but are also central to the calculation of the multicenter electron-repulsion and three-center nuclear-attraction integrals based on the translation formulas given by the present author for the expansion of STOs about a new center. It should be noted that the two-center nuclear attraction integrals of types $\langle a|\,(1/r_a)\,|b\rangle$ and $\langle a|\,(1/r_b)\,|b\rangle$ can be expressed through the overlap integrals [1].

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Recently, Özcan and Öztekin [2] published the formulas for the two-center nuclear attraction integrals of $\langle a|\,(1/r_b)\,|a'\rangle$ type. In this Comment we demonstrate that the relations for this type of nuclear attraction integrals presented in Sect. 3 of Ref. [2] can easily be derived from the formulas published in our papers.

2 Theory

The two-center nuclear attraction integrals of $\langle a|\,(1/r_b)\,|a'\rangle$ type are defined by [1]

$$I_{nlm,n'l'm'}\left(\zeta,\zeta',\vec{R}\right)=\int \chi^*_{nlm}\left(\zeta,\vec{r}_a\right)\chi_{n'l'm'}\left(\zeta',\vec{r}_a\right)\frac{1}{r_b}dV, \tag{1}$$

where $\vec{R}\equiv\vec{R}_{ab}=\vec{r}_a-\vec{r}_b$ and

$$\chi_{nlm}\left(\zeta,\vec{r}\right)=R_n(\zeta,r)Y_{lm}(\theta,\varphi) \tag{2}$$

$$R_n(\zeta,r)=(2\zeta)^{n+\frac{1}{2}}\left[(2n)!\right]^{-\frac{1}{2}}r^{n-1}e^{-\zeta r}. \tag{3}$$

Here, n is integer principal quantum number and $Y_{lm}(\theta,\varphi)$ is the complex spherical harmonics.

Taking into account the relation for one-center charge distribution determined by [3,4]

$$\chi^*_{nlm}\left(\zeta,\vec{r}\right)\chi_{n'l'm'}\left(\zeta',\vec{r}\right)=\frac{1}{\sqrt{4\pi}}\sum_{\nu=|l-l'|}^{l+l'}{}^{(2)}\sum_{\sigma=-\nu}^{\nu}W_{nlm,n'l'm',\mu\nu\sigma}(\zeta,\zeta',z)\chi^*_{\mu\nu\sigma}(z,\vec{r}) \tag{4}$$

it is easy to show that the integral (1) can be expressed through the two-center basic nuclear attraction integrals $J_{nlm}(\zeta,\vec{R})$:

$$I_{nlm,n'l'm'}(\zeta,\zeta',\vec{R})=\sum_{\nu=|l-l'|}^{l+l'}{}^{(2)}\sum_{\sigma=-\nu}^{\nu}W_{nlm,n'l'm',\mu\nu\sigma}(\zeta,\zeta',z)J_{\mu\nu\sigma}(z,\vec{R}), \tag{5}$$

where $z=\zeta+\zeta'$, $\mu=n+n'-1$, $t=(\zeta-\zeta')/(\zeta+\zeta')$ and

$$W_{nlm,n'l'm',\mu\nu\sigma}\left(\zeta,\zeta',z\right)=\frac{z^{3/2}}{2^{\mu}}\left[\frac{2\nu+1}{2}\frac{(2\mu)!}{(2n)!\,(2n')!}\right]^{1/2}\times(1+t)^{n+\frac{1}{2}}(1-t)^{n'+\frac{1}{2}}C^{\nu}\left(lm,l'm'\right)\delta_{\sigma,m-m'} \tag{6}$$

$$J_{nlm}(\zeta,\vec{R})=\frac{1}{\sqrt{4\pi}}\int\chi^*_{nlm}(\zeta,\vec{r}_a)\frac{1}{r_b}dV. \tag{7}$$

Table 1 The comparative formulas for the two-center nuclear attraction integrals

This work		Ref. [2]	
$I_{nlm,n'l'm'}\left(\zeta,\zeta',\vec{R}\right)=\int\chi^*_{nlm}(\zeta,\vec{r}_a)\frac{1}{r_b}\chi_{n'l'm'}\left(\zeta',\vec{r}_a\right)dV$	(1)	$A^{n_2l_2m_2}_{n_1l_1m_1}\left(\alpha,\beta;\vec{R}\right)=\int\left[\chi^{m_1}_{n_1l_1}(\alpha,\vec{r})\right]^*\frac{1}{\left\lvert\vec{r}-\vec{R}\right\rvert}\chi^{m_2}_{n_2l_2}(\beta,\vec{r})\,d\vec{r}$	(14)
$\chi^*_{nlm}(\zeta,\vec{r})\,\chi_{n'l'm'}\left(\zeta',\vec{r}\right)=\frac{1}{\sqrt{4\pi}}\sum_{\nu=\lvert l-l'\rvert}^{l+l'}{}^{(2)}\sum_{\sigma=-\nu}^{\nu}W_{nlm,n'l'm',\mu\nu\sigma}(\zeta,\zeta',z)\chi^*_{\mu\nu\sigma}(z,\vec{r})$	(4)	$\left[\chi^{m_1}_{n_1l_1}(\alpha,\vec{r})\right]^*\chi^{m_2}_{n_2l_2}(\beta,\vec{r})=\sqrt{2^3\frac{(2(n_1+n_2-1))!}{(2n_1)!(2n_2)!}\frac{\alpha^{n_1+1/2}\beta^{n_2+1/2}}{(\alpha+\beta)^{n_1+n_2-1/2}}}\times\sum_{l=l_{\min}}^{l_{\max}}{}^{(2)}\langle l_2m_2\lvert\, l_1m_1\,\rvert lm_2-m_1\rangle\,\chi^{m_2-m_1}_{n_1+n_2-1,l}(\alpha+\beta,\vec{r})$	(15)
$W_{nlm,n'l'm',\mu\nu\sigma}\left(\zeta,\zeta',z\right)=\frac{z^{3/2}}{2^{\mu}}\left[\frac{2\nu+1}{2}\frac{(2\mu)!}{(2n)!(2n')!}\right]^{1/2}\times(1+t)^{n+\frac{1}{2}}(1-t)^{n'+\frac{1}{2}}C^{\nu}\left(lm,l'm'\right)\delta_{\sigma,m-m'}$	(6)		
$\mu=n+n'-1,\ z=\zeta+\zeta',\ t=(\zeta-\zeta')/(\zeta+\zeta'),\ 1+t=\frac{2\zeta}{\zeta+\zeta'},\ 1-t=\frac{2\zeta'}{\zeta+\zeta'}$			
$I_{nlm,n'l'm'}(\zeta,\zeta',\vec{R})=\sum_{\nu=\lvert l-l'\rvert}^{l+l'}{}^{(2)}\sum_{\sigma=-\nu}^{\nu}W_{nlm,n'l'm',\mu\nu\sigma}(\zeta,\zeta',z)J_{\mu\nu\sigma}(z,\vec{R})$	(5)	$A^{n_2l_2m_2}_{n_1l_1m_1}\left(\alpha,\beta;\vec{R}\right)=\sqrt{2^3\frac{(2(n_1+n_2-1))!}{(2n_1)!(2n_2)!}\frac{\alpha^{n_1+1/2}\beta^{n_2+1/2}}{(\alpha+\beta)^{n_1+n_2-1/2}}}\times\sum_{l=l_{\min}}^{l_{\max}}{}^{(2)}\langle l_2m_2\lvert\, l_1m_1\,\rvert lm_2-m_1\rangle A^{m_2-m_1}_{n_1+n_2-1,l}\left(\alpha+\beta,\vec{R}\right)=\sqrt{16\pi\frac{(2(n_1+n_2-1))!}{(2n_1)!(2n_2)!}\frac{\alpha^{n_1+1/2}\beta^{n_2+1/2}}{(\alpha+\beta)^{n_1+n_2-1/2}}}\sum_{l=l_{\min}}^{l_{\max}}{}^{(2)}\langle l_2m_2\lvert\, l_1m_1\,\rvert lm_2-m_1\rangle$	(16)
$J_{nlm}(\zeta,\vec{R})=\lim_{\zeta'\to 0}\frac{1}{(2\zeta')^{1/2}}S_{nlm,000}(\zeta,\zeta',\vec{R})$	(9)	$\times\lim_{\varepsilon\to 0}\left\{\frac{1}{\sqrt{\varepsilon}}S^{n_1+n_2-1lm_2-m_1}_{000}\left(\varepsilon,(\alpha+\beta);\vec{R}\right)\right\}$	(17)
$J_{nlm}(\zeta,\vec{R})=\frac{1}{\sqrt{4\pi}}\int\chi^*_{nlm}(\zeta,\vec{r}_a)\frac{1}{r_b}dV$	(7)	$A^{m}_{nl}\left(\alpha;\vec{R}\right)=\int\frac{\chi^{m}_{nl}(\alpha,\vec{r})}{\left\lvert\vec{r}-\vec{R}\right\rvert}d\vec{r}$	(18)
$S_{nlm,000}\left(\zeta,\zeta',\vec{R}\right)=\int\chi^*_{nlm}(\zeta,\vec{r}_a)\chi_{000}\left(\zeta',\vec{r}_b\right)dV$	(10)	$S^{Nlm}_{000}\left(a,b,\vec{R}\right)=\int\left[\chi^0_{00}\left(a,\vec{r}-\vec{R}\right)\right]^*\chi^{m}_{Nl}(b,\vec{r})\,d\vec{r}$	(19)

The basic nuclear attraction integrals can be expressed through the two-center overlap integrals (see, e.g., Ref. [5]):

$$J_{nlm}(\zeta, \vec{R}) = \frac{1}{\sqrt{4\pi}} \lim_{\zeta' \to 0} \frac{\sqrt{4\pi}}{(2\zeta')^{1/2}} \int \chi^*_{nlm}(\zeta, \vec{r}_a) \chi_{000}\left(\zeta', \vec{r}_b\right) dV \tag{8}$$

$$= \lim_{\zeta' \to 0} \frac{1}{(2\zeta')^{1/2}} S_{nlm,000}(\zeta, \zeta', \vec{R}), \tag{9}$$

where

$$S_{nlm,000}\left(\zeta, \zeta', \vec{R}\right) = \int \chi^*_{nlm}(\zeta, \vec{r}_a) \chi_{000}\left(\zeta', \vec{r}_b\right) dV. \tag{10}$$

As can be seen from Table 1 that the published in Sect. 3 of Ref. [2] formulas (14–19) can easily be obtained from Eqs. 1–10 by application of a simple algebra. In Comment [6] we have also shown that the presented in [7] by E. Öztekin et al. formulas for the overlap integrals, through of which two-center nuclear attraction integrals are expressed, are obtained from the formulas presented in our paper [8]. Thus, the formulas for the two-center nuclear attraction and overlap integrals presented in Refs. [2] and [7] by E. Öztekin et al., respectively, can easily be obtained from our papers by changing the summation indices or by means of a simple algebra.

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