Journal of Mathematical Chemistry Vol. 36, No. 2, June 2004 (© 2004)

Analytical evaluation of multicenter multielectron integrals of central and noncentral interaction potentials over Slater orbitals using overlap integrals and auxiliary functions

I.I. Guseinov

Department of Physics, Faculty of Arts and Sciences, Onsekiz Mart University, Çanakkale, Turkey
E-mail: iguseinov@cheerful.com

Received 16 December 2003; revised 12 March 2004

Using expansion formulas for central and noncentral interaction potentials (CIPs and NCIPs, respectively) in terms of Slater type orbitals (STOs) obtained by the author (I.I. Guseinov, J. Mol. Model., in press), the multicenter multielectron integrals of arbitrary interaction potentials (AIPs) are expressed through the products of overlap integrals with the same screening parameters and new auxiliary functions. For auxiliary functions, the analytic and recurrence relations are derived. The relationships obtained for multicenter multielectron integrals of AIDs are valid for the arbitrary quantum numbers, screening parameters and location of orbitals.

KEY WORDS: overlap integrals, multicenter multielectron integrals, central and noncentral potentials, auxiliary functions

AMS subject classification: 81-08, 81V55, 81V45

1. Introduction

It is well known that the multicenter multielectron integrals are of fundamental importance in the study of multielectron properties for atoms and molecules when the Hylleraas approach in Hartree–Fock theory is employed [1]. However, the difficulties in calculation of these integrals have restricted the application of Hylleraas approximation in quantum chemistry. In the literature there is renewed interest in developing efficient methods for the calculation of multicenter multielectron integrals over Slater type orbitals (STOs) (see, e.g., [2–5] and references quoted therein). Older work are reviewed in [6, 7]. It should be noted that the preexisting formulas for the evaluation of multicenter multielectron integrals of interaction potentials do not generally apply to arbitrary Central and noncentral interaction potentials (CIPs and NCIPs respectively).

0259-9791/04/0600-0083/0

In [8], by the use of complete orthonormal sets of Ψ^{α}-ETOs [9] we presented a particular method for obtaining the addition theorems for STOs and Arbitary interaction potentials (AIPs) which has been utilized for the evaluation of multicenter multielectron integrals of CIPs and NCIPs in terms of two-center overlap integrals with the same screening parameters. The aim of this work is to establish the series expansion formulas for multicenter multielectron integrals through the overlap integrals and auxiliary functions using the expansion formulas for AIPs derived in [8].

2. Expressions in terms of two-center overlap integrals and auxiliary functions

The multicenter multielectron integrals of t-electron operator over normalized STOs arising in calculations on atoms and molecules with N-electrons $(2 \leqslant t \leqslant N)$ in molecular coordinate system are defined by [8]

$$\begin{aligned} I^{ac,bd,gh,\ldots,ef}_{p_1p_1',p_2p_2',p_3p_3',\ldots,p_tp_t';\tau} = \int & \chi^*_{p_1}(\zeta_1,\vec{r}_{a1})\chi_{p_1'}(\zeta_1',\vec{r}_{c1})\chi_{p_2}(\zeta_2,\vec{r}_{b2})\chi^*_{p_2'}(\zeta_2',\vec{r}_{d2}) \\ & \times \chi_{p_3}(\zeta_3,\vec{r}_{g3})\chi^*_{p_3'}(\zeta_3',\vec{r}_{h3})\cdots\chi_{p_t}(\zeta_t,\vec{r}_{et}) \\ & \times \chi^*_{p_t'}(\zeta_t',\vec{r}_{ft})O_{\tau}(\eta,\vec{r}_{123\ldots t})\mathrm{d}v_1\mathrm{d}v_2\mathrm{d}v_3\cdots\mathrm{d}v_t, \end{aligned} \tag{1}$$

where $p_i \equiv n_i l_i m_i$, $p_i' \equiv n_i' l_i' m_i'$, $\tau \equiv u\upsilon s$ and

$$\begin{aligned} O_{\tau}(\eta,\vec{r}_{12\cdots t}) = & f_{\tau}(\eta,\vec{r}_{21})f_{\tau}(\eta,\vec{r}_{31})f_{\tau}(\eta,\vec{r}_{41})\cdots \\ & \times f_{\tau}(\eta,\vec{r}_{t-11})f_{\tau}(\eta,\vec{r}_{t1})f_{\tau}(\eta,\vec{r}_{32})f_{\tau}(\eta,\vec{r}_{42}) \\ & \times\cdots f_{\tau}(\eta,\vec{r}_{t-12})f_{\tau}(\eta,\vec{r}_{t2})\cdots f_{\tau}(\eta,\vec{r}_{t-1t-2}) \\ & \times f_{\tau}(\eta,\vec{r}_{tt-2})f_{\tau}(\eta,\vec{r}_{tt-1}), \end{aligned} \tag{2}$$

$$\chi_{nlm}(\zeta,\vec{r}) = R_n(\zeta,r)S_{lm}(\theta,\varphi), \tag{3}$$

$$R_n(\zeta,r) = (2\zeta)^{n+1/2}[(2n)!]^{-1/2}\, r^{n-1}\mathrm{e}^{-\zeta r}. \tag{4}$$

In order to evaluate the integral (1) we utilize the following expansion formulas: for one-center expansion of AIPs in terms of STOs

$$f_{u\upsilon s}(\eta,\vec{r}) = f_u(\eta,r)\left(\frac{4\pi}{2\nu+1}\right)S_{lm}(\theta,\phi) \tag{5}$$

$$= (4\pi)^{1/2}\lim_{k\to\infty}\sum_{k=\upsilon+1}^{K} B^{\alpha K}_{u\upsilon,k\upsilon}(\eta,\eta')\chi_{k\upsilon s}(\eta',\vec{r}) \tag{6}$$

for expansion of AIPs through the product of STOs (addition theorems)

$$f_{u\upsilon s}(\eta,\vec{r}_{21}) = f_u(\eta,r_{21})\left(\frac{4\pi}{2\upsilon+1}\right)^{1/2} S_{\upsilon s}(\theta_{21},\varphi_{21}) \tag{7}$$

$$= \frac{4\pi}{\eta' 3/2}\lim_{\substack{K\to\infty\\ N\to\infty}} \sum_{k=\upsilon+1}^{K}\sum_{\mu=1}^{N}\sum_{\nu=0}^{\mu-1}\sum_{\sigma=-\nu}^{\nu}\sum_{\mu'=1}^{N+k-\alpha+1}\sum_{\nu'=0}^{\mu'-1}\sum_{\sigma'=-\nu'}^{\nu'} Y^{\alpha KN,\mu'\nu'\sigma'}_{ku\upsilon s,\mu\nu\sigma} \times(\eta,\eta')\chi_{\mu\nu\sigma}\left(\eta',\vec{r}_{a1}\right)\chi^{*}_{\mu'\nu'\sigma'}\left(\eta',\vec{r}_{a2}\right) \tag{8}$$

for expansion of electron charge densities in terms of STOs

$$\chi_p(\zeta,\vec{r}_g)\chi^{*}_{p'}(\zeta',\vec{r}_h) = \frac{1}{\sqrt{4\pi}}\lim_{N\to\infty}\sum_{\mu=1}^{N}\sum_{\nu=0}^{\mu-1}\sum_{\sigma=-\nu}^{\nu} W^{\alpha N}_{pp'q}(\zeta,\zeta',z;\vec{R}_{hg},\vec{R}_{ga})\chi_q(z,\vec{r}_a), \tag{9}$$

where $\alpha = 1, 0, -1, -2, \ldots, p \equiv nlm,\ \ p' \equiv n'l'm',\ \ \tau \equiv \mu\nu\sigma,\ \ z = \zeta + \zeta'$ and

$$B^{\alpha K}_{u\upsilon,k\upsilon}(\eta,\eta') = \left(\frac{1}{2\upsilon+1}\right)^{1/2}\begin{cases} \frac{\sqrt{(2u)!}}{(2\eta)^{u+1/2}}\delta_{ku}\delta_{\eta'\eta} & \text{for } u \geqslant 0, \quad (10)\\ \sum\limits_{\mu=\upsilon+1}^{K}\Omega^{\alpha\upsilon}_{k\mu}(K)P^{\alpha}_{u\mu}(\eta,\eta') & \text{for } u < 0, \quad (11)\end{cases}$$

$$P^{\alpha}_{u\mu}(\eta,\eta') = \int_0^{\infty} f_u(\eta,r)R_{\mu-\alpha}(\eta',r)r^2\mathrm{d}r, \tag{12}$$

$$Y^{\alpha KN,\mu'\nu'\sigma'}_{ku\upsilon s,\mu\nu\sigma}(\eta,\eta') = (-1)^{\nu'} Z^{\alpha N,\mu'\nu'\sigma'}_{k\upsilon s,\mu\nu\sigma} B^{\alpha K}_{u\upsilon,k\upsilon}(\eta,\eta'), \tag{13}$$

$$Z^{\alpha N,\mu'\nu\sigma'}_{k\upsilon s,\mu\nu\sigma} = \sum_{\mu'=\nu+1}^{N}\Omega^{\alpha\nu}_{\mu\mu'}(N)g^{\alpha\mu'\nu'\sigma'}_{k\upsilon s,\mu'-\alpha\nu\sigma}. \tag{14}$$

See [10] and [11] the exact definition of the coefficients $W^{\alpha N}$, $\Omega^{\alpha\nu}$ and $g^{\alpha\mu'\nu'\sigma'}$, respectively. Here, the quantities $Z^{\alpha N}$ are the expansion coefficients of addition theorems for STOs established in [8]. It should be noted that the values of integral (12) are determined by the arbitrary radial pats of interaction potentials and STOs.

Now we can move on to the evaluation of multicenter integrals (equation (1)). For this purpose, we use the expansion theorems (6) and (8) for AIPs which were derived with help of complete orthonormal sets of Ψ^{α}-ETOs introduced in [9]. Then we obtain:

$$I^{ac,bd,gh\ldots,ef}_{p_1p_1',p_2p_2',p_3p_3',\ldots,p_tp_t';\tau} = \frac{1}{(\eta'\sqrt{\eta'})^{t(t-1)-1}} \lim_{\substack{K\to\infty\\ N\to\infty}} \sum_{k}^{K}\sum_{qq'}^{N} (Y^{\alpha K_{31}N_{31}q'_{31}}_{k_{31}\tau q_{31}}(\eta,\eta')Y^{\alpha K_{41}N_{41}q'_{41}}_{k_{41}\tau q_{41}}$$
$$\times(\eta,\eta')\cdots Y^{\alpha K_{t-11}N_{t-11}q'_{t-11}}_{k_{t-11}\tau q_{t-11}}(\eta,\eta')Y^{\alpha K_{t1}N_{t1}q'_{t1}}_{k_{t1}\tau q_{t1}}(\eta,\eta'))$$
$$\times(Y^{\alpha K_{32}N_{32}q'_{32}}_{k_{32}\tau q_{32}}(\eta,\eta')Y^{\alpha K_{42}N_{42}q'_{42}}_{k_{42}\tau q_{42}}(\eta,\eta')\cdots$$
$$\times Y^{\alpha K_{t2}N_{t2}q'_{t2}}_{k_{t2}\tau q_{t2}}(\eta,\eta'))(Y^{\alpha K_{43}N_{43}q'_{43}}_{k_{43}\tau q_{43}}(\eta,\eta')\cdots Y^{\alpha K_{t3}N_{t3}q'_{t3}}_{k_{t3}\tau q_{t3}}(\eta,\eta'))\cdots$$
$$\times(Y^{\alpha K_{tt-1}N_{tt-1}q'_{tt-1}}_{k_{tt-1}\tau q_{tt-1}}(\eta,\eta'))J^{aaa\ldots aac,aaa\ldots abd}_{p_1q_{31}q_{41}\ldots q_{t-11}q_{t1}p'_1,\tau,q_{32}q_{42}q_{52}\ldots q_{t2}p_2p'_2}$$
$$\times S^{aaa\ldots agh}_{q'_{31}q'_{32}q_{43}\ldots q_{t3}p_3p'_3}\cdots S^{aaa\ldots aef}_{q'_{t1}q'_{t2}q'_{t3}\ldots q'_{tt-1}p_tp'_t}, \tag{15}$$

where

$$K \equiv [(K_{31}K_{41}\ldots K_{t1}),(K_{32}K_{42}\ldots K_{t2}),\ldots,(K_{t-1t-2}K_{tt-2}),(K_{tt-1})],$$
$$k \equiv [(k_{31}k_{41}\ldots k_{t1}),(k_{32}k_{42}\ldots k_{t2}),\ldots,(k_{t-1t-2}k_{tt-2}),(k_{tt-1})],$$
$$N \equiv [(N_{31}N_{41}\ldots N_{t1}),(N_{32}N_{42}\ldots N_{t2}),\ldots,(N_{t-1t-2}N_{tt-2}),(N_{tt-1})],$$
$$q \equiv [(q_{31}q_{41}\ldots q_{t1}),(q_{32}q_{42}\ldots q_{t2}),\ldots,(q_{t-1t-2}q_{tt-2}),(q_{tt-1})],$$
$$q' \equiv [(q'_{31}q'_{41}\ldots q'_{t1}),(q'_{32}q'_{42}\ldots q'_{t2}),\ldots,(q'_{t-1t-2}q'_{tt-2}),(q'_{tt-1})],$$

$$\upsilon+1 \leqslant k_{ij} \leqslant K_{ij},\quad q_{ij} \equiv \mu_{ij}\nu_{ij}\sigma_{ij},\quad 1 \leqslant \mu_{ij} \leqslant N_{ij},\quad 0 \leqslant \nu_{ij}\mu_{ij}-1, -\nu_{ij} \leqslant \sigma_{ij} \leqslant \nu_{ij},$$
$$q'_{ij} \equiv \mu'_{ij}\nu'_{ij}\sigma'_{ij}, 1 \leqslant \mu'_{ij} \leqslant N_{ij}+k_{ij}-\alpha+1, 0 \leqslant \nu'_{ij} \leqslant \mu'_{ij}-1,\ -\nu'_{ij} \leqslant \sigma'_{ij} \leqslant \nu'_{ij},$$

$g^{\alpha\mu'_{ij}\nu'_{ij}\sigma'_{ij}}_{\tau k_{ij}\upsilon s,\mu_{ij}\nu_{ij}\sigma_{ij}} \equiv 0$ for $\mu'_{ij} > \mu_{ij}+k_{ij}+1$ and the quantities J and S are defined by

$$J^{aaa\ldots aac,aaa\ldots abd}_{p_1q_{31}q_{41}\ldots q_{t-11}q_{t1}p'_1,\tau,q_{32}q_{42}q_{52}\ldots q_{t2}p_2p'_2} = (\sqrt{4\pi})^{2t-4}\int\int \chi^*_{p_1}(\zeta_1,\vec{r}_{a1})\chi_{q_{31}}(\eta',\vec{r}_{a1})$$
$$\times\chi_{q_{41}}(\eta',\vec{r}_{a1})\cdots\chi_{q_{t-11}}(\eta',\vec{r}_{a1})\chi_{q_{t1}}(\eta',\vec{r}_{a1})$$
$$\times\chi_{p'_1}(\zeta'_1,\vec{r}_{c1})f_\tau(\eta',\vec{r}_{12})\chi_{q_{32}}(\eta',\vec{r}_{a2})\chi_{q_{42}}(\eta',\vec{r}_{a2})$$
$$\times\chi_{q_{52}}(\eta',\vec{r}_{a2})\cdots\chi_{q_{t2}}(\eta',\vec{r}_{a2})\chi_{p_2}(\zeta_2,\vec{r}_{b2})$$
$$\times\chi^*_{p'_2}(\zeta'_2,\vec{r}_{d2})dv_1dv_2 \tag{16}$$

$$S^{aaa\ldots agh}_{q'_{31}q'_{32}q_{43}\ldots q_{t3}p_3p'_3} = (\sqrt{4\pi})^{t-1}\int \chi^*_{q'_{31}}(\eta',\vec{r}_{a3})\chi^*_{q'_{32}}(\eta',\vec{r}_{a3})\chi_{q_{43}}(\eta',\vec{r}_{a3})\cdots$$
$$\times\chi_{q_{t3}}(\eta',\vec{r}_{a3})\chi_{p_3}(\zeta_3,\vec{r}_{g3})\chi^*_{p'_3}(\zeta'_3,\vec{r}_{h3})\,\mathrm{d}v_3 \qquad (17.3)$$

$$\vdots$$

$$S^{aaa\ldots aef}_{q'_{t1}q'_{t2}q_{t3}\ldots q'_{tt-1}p_tp'_t} = (\sqrt{4\pi})^{t-1}\int \chi^*_{q'_{t1}}(\eta',\vec{r}_{at})\chi^*_{q'_{t2}}(\eta',\vec{r}_{at})\chi_{q'_{t3}}(\eta',\vec{r}_{at})\cdots\chi^*_{q'_{tt-1}}$$
$$\times(\eta',\vec{r}_{at})\chi_{p_t}(\zeta_t,\vec{r}_{et})\chi^*_{p'_t}(\zeta'_t,\vec{r}_{ft})\mathrm{d}v_t \qquad (17.t)$$

The analytical relationships for one-electron integrals (equations (17.3)–(17.t)) in terms of two-center overlap integrals with the same screening parameters have been obtained in [8]. With the evaluation of two-electron integrals (equation (16)) we use the charge density expansion formula (9) and equations (27) and (28) of [8]. Then, the integrals (16) can be expressed through the following basic two-electron one-center integrals of AIPs:

$$Q^{q'}_{q\tau}(z\eta z') = \frac{1}{4\pi}\int\int \chi^*_q(z,\vec{r}_{a1})f_\tau(\eta,\vec{r}_{21})\chi_{q'}(z',\vec{r}_{a2})\mathrm{d}V_1\mathrm{d}V_2, \qquad (18)$$

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

For the derivation of expression for the integral (18) we take into account equation (6) for the one-center expression of AIPs in terms of STOs. Then we obtain:

$$Q^{q'}_{q\tau}(z\eta z) = \lim_{K\to\infty}\sum_{k=\upsilon+1}^{K} B^{\alpha K}_{u\upsilon,k\upsilon}(\eta,\eta')S^{\mu'\nu'\sigma'}_{\mu\nu\sigma,k\upsilon s}(z,\eta',z'), \qquad (19)$$

where $\eta' = \eta$ for $u \geqslant 0$ and $\eta' = z$ for $u < 0$ and

$$S^{\mu'\nu'\sigma'}_{\mu\nu\sigma,k\upsilon s}(z,\eta',z') = \frac{1}{\sqrt{4\pi}}\int S_{\mu\nu\sigma,k\upsilon s}(z,\eta';\vec{r}_{a2})\chi_{\mu'\nu'\sigma'}(z',\vec{r}_{a2})\,\mathrm{d}V_2. \qquad (20)$$

Here, the quantity $S_{\mu\nu\sigma,k\upsilon s}$ is the overlap integral defined by

$$S_{\mu\nu\sigma,k\upsilon s}(z,\eta';\vec{r}_{a2}) = \int \chi^*_{\mu\nu\sigma}(z,\vec{r}_{a1})\chi_{k\upsilon s}(\eta',\vec{r}_{21})\mathrm{d}V_1 \qquad (21)$$

In order to evaluate the integral (20) we utilize equations (5) and (17) of [12] for the rotation of two-center overlap integrals:

$$S^{\mu'\nu'\sigma'}_{\mu\nu\sigma,k\upsilon s}(z,\eta',z') = \sum_{\lambda=0}^{\min(\nu,\upsilon)} T^{\lambda,\nu'\sigma'}_{\nu\sigma,\upsilon s}R^{\mu'}_{\mu\nu\lambda,k\upsilon\lambda}(z,\eta',z') \qquad (22)$$

where

$$T^{\lambda,\nu'\sigma'}_{\nu\sigma,\upsilon s} = \frac{1}{\sqrt{4\pi}} \oint T^{\lambda^*}_{\nu\sigma,\upsilon s}(\theta,\varphi) S_{\nu'\sigma'}(\theta,\varphi)\, \mathrm{d}\Omega$$

$$= \frac{2}{(1+\delta_{\lambda 0})(2\nu'+1)^{1/2}} C^{\nu\upsilon\nu'}_{\lambda,-\lambda,0}$$

$$\times \begin{cases} C^{\nu\upsilon\nu'}_{\sigma,-s,\sigma-s}\delta_{\sigma',\sigma-s} & \text{for complex } SH \qquad (23a) \\ [(1+\delta_{\sigma 0})(1+\delta_{s0})]^{-1/2} \sum\limits_{i=-1}^{1}{}^{(2)} (\delta_{\sigma 0})^{\delta_{i,\varepsilon\sigma s}} & \\ \quad \times C^{\nu\upsilon\nu'}_{i\gamma,æ,i\gamma+æ}[(1+\delta_{\sigma' 0})/2]^{1/2}\delta_{\sigma'_i\sigma'} & \text{for real } SH \qquad (23b) \end{cases}$$

and

$$R^{\mu'}_{\mu\nu\lambda,k\upsilon\lambda}(z,\eta',z') = \int_0^\infty S_{\mu\nu\lambda,k\upsilon\lambda}(z,\eta';r) R_{\mu'}(z',r) r^2\, \mathrm{d}r$$

$$= \frac{2^{\mu'+2}}{(z+\eta')^{3/2}} \frac{(1+t)^{\mu+1/2}(1-t)^{k+1/2}(b-1)^{\mu'+1/2}}{[(2\mu)!(2k)!(2\mu')!]^{1/2}}$$

$$\times \sum_{\alpha=-\lambda}^{\nu} \sum_{\beta=\lambda}^{\upsilon} \sum_{q=0}^{\alpha+\beta} g^q_{\alpha\beta}(\nu\lambda,\upsilon\lambda)$$

$$\times \sum_{m=0}^{\mu-\alpha+k-\beta} F_m(\mu-\alpha,k-\beta)(\mu-\alpha+k-\beta+q-m)!$$

$$\times \sum_{j=0}^{\mu-\alpha+k-\beta+q-m} \frac{1}{j!} B^{j+\alpha+\beta-q+m+\mu'+1}_{q+j}(t,b). \qquad (24)$$

Here $\gamma = |\sigma|$, $æ = |s|$, $\sigma'_i = \varepsilon_{\sigma s}\,|i\gamma + æ|$. The symbol $\sum^{(2)}$ indicates that the summation is to be performed in steps of two. For $\gamma = æ$ and $\varepsilon_{\sigma s} = -1$ terms with a negative value of index $i (i = -1)$ contained in (23b) should be equated to zero. The relationships for Clebsh-Gordan coefficients through the binomial coefficients are given in [13]. The quantities $B^n_k(t,b)$ are the auxiliary functions defined by

$$B^n_k(t,b) = \int_0^\infty B_k(tx) x^n \mathrm{e}^{-bx}\, \mathrm{d}x, \qquad (25)$$

where $t = \frac{z-\eta'}{z+\eta'}$, $b = 1 + \frac{2z'}{z+\eta'}$ and

$$B_k(tx) = \int_{-1}^{1} \nu^k \mathrm{e}^{-tx\nu}\, \mathrm{d}\nu, \tag{26}$$

For $t = 0$ ($\eta' = z$ and $b = 1 + z'/z$) we should use the relation:

$$B_k^n(0, b) = \frac{1 + (-1)^k}{k+1} \frac{n!}{b^{n+1}}. \tag{27}$$

The auxiliary functions $B_k^n(t, b)$ have the following symmetry property:

$$B_k^n(-t, b) = (-1)^k B_k^n(t, b). \tag{28}$$

As can be seen from the formulas obtained in this study, the multicenter multielectron integrals of AIPs are expressed through the auxiliary functions B_k^n.

3. Expressions for auxiliary functions

In order to derive the analytical and recurrence relations for auxiliary functions B_k^n we use equation (25) for $t \neq 0$ in the form:

$$B_k^n(t, b) = \frac{1}{t^{n+1}} B_k^n(p), \tag{29}$$

where $p = b/t$ and

$$B_k^n(p) = B_k^n(1, p) = \int_0^{\infty} B_k(x) x^n \mathrm{e}^{-px}\, \mathrm{d}x. \tag{30}$$

By the use of well known analytical and recurrence relations for the auxiliary functions $B_k(x)$ (see [14,15]) it is easy to establish for $B_k^n(p)$ the following expressions: analytical relations

$$B_k^n(p) = \begin{cases} \sum\limits_{m=0}^{k} \frac{k!(n-k+m-1)!}{m!} \left[\frac{(-1)^m}{(p-1)^{n-k+m}} - \frac{1}{(p+1)^{n-k+m}} \right] & \text{for } n > k, \quad (31a) \\ \left\{ n! F_n(k) (-p)^{k-n} \ln \frac{p+1}{p-1} \right. & \\ \left. \quad + \sum\limits_{\substack{m=0 \\ m \neq n}}^{k} \frac{F_m(k)}{m-n} (-p)^{k-m} [(p+1)^{m-n} - (p-1)^{m-n}] \right\} & \text{for } n \leqslant k, \quad (31b) \end{cases}$$

recurrence relations

$$B_{k+1}^{n+1}(p) = (k+1)B_k^n(p) + n!\left[\frac{(-1)^{k+1}}{(p-1)^{n+1}} - \frac{1}{(p+1)^{n+1}}\right], \tag{32}$$

$$B_{k+1}^{0}(p) = -pB_k^0(p) + \frac{1+(-1)^k}{k+1}. \tag{33}$$

Using these recurrence relations, the auxiliary functions $B_k^n(p)$ can be calculated from the functions $B_0^n(p)$ determined by

$$B_0^n(p) = \begin{cases} \ln\frac{p+1}{p-1}, & \text{for } n = 0, \quad (34a) \\ (n-1)!\left[\frac{1}{(p-1)^n} - \frac{1}{(p+1)^n}\right] & \text{for } n > 0. \quad (34b) \end{cases}$$

The auxiliary functions $B_k^n(t,b)$ can also be calculated from the following series expansion:

$$B_k^n(t,b) = \frac{n!}{b^{n+1}} \sum_{m=0}^{\infty} \frac{1+(-1)^{k+m}}{k+m+1} F_m(n+m)(-t/b)^m, \tag{35}$$

where $\left|\frac{t}{b}\right| = \frac{|z-\eta'|}{z+\eta'+2z'} < 1$. For the derivation of equation (35) we have taken into account the relation

$$\mathrm{e}^{-x} = \sum_{k=0}^{\infty} \frac{(-x)^k}{k!}, \tag{36}$$

As can be seen from the formulas of this work obtained by the use of complete orthonormal sets of $\Psi^1, \Psi^0, \Psi^{-1}, \Psi^{-2}, \cdots$, ETOs, the evaluation of two-electron multicenter multielectron integrals of central and noncentral interaction potentials is reduced to the calculation of two-center overlap integrals and auxiliary functions. These formulas are correct for arbitrary values of screening parameter ($\eta \geqslant 0$). Thus, with the aid of the different relationships that have been obtained in this study for $\alpha = 1, 0, -1, -2, \cdots$, one can calculate the multielectron multicenter integrals of screened and nonscreened interaction potentials over STOs.

References

[1] J.C. Slater, *Quantum Theory of Atomic Structure*, Vol. 2 (McGraw-Hill, New York, 1960).
[2] A. Lüchow and H. Kleindienst, Int. J. Quantum Chem. 45 (1993) 445.
[3] F.W. King and J. Chem. Phys. 99 (1993) 3622.
[4] I. Porras and F.W. King, Phys. Rev. A 49 (1994) 1637.
[5] J.S. Sims and S.A. Hagstrom, Int. J. Quantum Chem. 90 (2002) 1600.
[6] W. Kolos and C.C.J. Roothaan, Rev. Mod. Phys. 32 (1960) 205.
[7] W. Kolos and L. Wolniewicz, J. Chem. Phys. 41 (1964) 3663.
[8] I.I. Guseinov, J. Mol. Model. (2003) on line DOI 10.1007/s00894-003-0134-0.

[9] I.I. Guseinov, Int. J. Quantum Chem. 90 (2002) 114.
[10] I.I. Guseinov, Int. J. Quantum Chem. 90 (2002) 980.
[11] I.I. Guseinov, J. Mol. Model. (2003) on line DOI 10.1007/s00894-002-0109-6.
[12] I.I. Guseinov, Phys. Rev. A 32 (1985) 1834.
[13] I.I. Guseinov, J. Mol. Struct. (Theochem) 336 (1995) 17.
[14] C. Zerner and V. Guillemin, Phys. Rev. 34 (1929) 999.
[15] R.S. Mulliken, C.A. Rieke, D. Orloff and H. Orloff, J. Chem. Phys. 17 (1949) 1248.