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Use of Cartesian coordinates in evaluation of multicenter multielectron integrals over Slater type orbitals and their derivatives

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Using addition theorems for interaction potentials and Slater type orbitals (STOs) obtained by the author, and the Cartesian expressions through the binomial coefficients for complex and real regular solid spherical harmonics (RSSH) and their derivatives presented in this study, the series expansion formulas for multicenter multielectron integrals of arbitrary Coulomb and Yukawa like central and noncentral interaction potentials and their first and second derivatives in Cartesian coordinates were established. These relations are useful for the study of electronic structure and electron-nuclei interaction properties of atoms, molecules, and solids by Hartree–Fock–Roothaan and correlated theories. The formulas obtained are valid for arbitrary principal quantum numbers, screening constants and locations of STOs.

KEY WORDS: slater type orbitals, addition theorems, regular solid spherical harmonics, multicenter multielectron integrals

1. Introduction

It is well known that the multicenter integrals are of fundamental importance in the study of electronic structure and a whole series of electron-nuclei interaction properties of atomic and molecular systems by the Hartree–Fock and correlated methods. These integrals are evaluated by the use of two types of orbitals: Gaussian-type orbitals (GTOs) and Slater type orbitals (STOs). The GTOs do not allow sufficiently representing important properties of the electronic wave function, namely, the cusps at the nuclei [1] and exponential decay at large distances [2]. For problems in which the long part of the wave function or its behavior in the neighborhood of the nuclei is important, it is desirable to use STOs, which describe the physical situation more accurately than GTOs. On the other hand a comparison of STOs and GTOs basis of various size showed that a GTOs basis needs about twice the size of a STOs basis to obtain comparable accuracy [3, 4]. Thus, in these areas, and if relatively small basis sets are

necessary, for Hartree–Fock electronic structure calculations, GTOs should by replaced by STOs which are more physical basis functions. However, the difficulties in the calculation of multicenter integrals has restricted the use of STOs in molecular quantum mechanics.

In recent years, the interest in the use of STOs for molecular calculations has been renewed (see, e.g., [5, 6] and references quoted therein). The central problem for these efforts is the calculation of multicenter integrals with such basis sets.

It is well known that the addition theorems for operators, atomic orbitals, and their derivatives are of fundamental importance in the calculation of multicenter integrals of STOs. In practice, two types of addition theorems occur in the literature [7]. Two-range addition theorems can be derived by expanding the quantity of interest in terms of spherical harmonics. There is a long history starting with [8–15] of systematic attempts to obtain accurate and fast evaluations of multicenter integrals using two-range addition theorems (see, e.g., [6] and references quoted therein). Unfortunately, they were not entirely successful.

The one-range addition theorems, which are usually obtained by considering an expansion over complete orthonormal sets of functions, are amongst the most promising approaches that were proposed to solve the multicenter integrals problem [16–24]. Two kinds of such functions into atomic and molecular calculations were introduced in [25–27] using a standard convention for the generalized Laguerre polynomials which is normally used in special function theory [28]. In a recent article [29] we established a large number of different complete orthonormal sets of Ψ^{α} -ETOs ($\alpha = 1, 0, -1, -2, \ldots$) by the use of non-standard conventions:

$$\Psi^{\alpha}_{nlm}(\zeta, \vec{r}) = (-1)^{\alpha} \left[\frac{2l+1}{4\pi} \frac{(2\zeta)^{2l+3}(q-p)!}{(2n)^{\alpha}(q!)^3} \right]^{1/2} e^{-\zeta r} L^{p}_{q}(2\zeta r) T_{lm}(x, y, z), \quad (1)$$

where $p = 2l + 2 - \alpha$ and $q = n + l + 1 - \alpha$. The non-standard generalized Laguerre polynomials $L^{p}_{q}(x)$, regular solid spherical harmonics $T_{lm}(x, y, z)$ and surface spherical harmonics $S_{lm}(\theta, \phi)$ occurring in equation (1) are determined by the relations

$$L^{p}_{q}(x) = \sum_{i=0}^{q-p} \beta^{p}_{qi} x^{i}, \quad (2)$$

$$T_{lm}(x, y, z) = \left(\frac{4\pi}{2l+1} \right)^{1/2} r^{l} S_{lm}(\theta, \phi), \quad (3)$$

$$S_{lm}(\theta, \phi) = P_{l|m|}(cos\theta) \Phi_{m}(\phi), \quad (4)$$

where

$$\beta_{qi}^{p} = (-1)^{p+i}(q-i)!F_i(q)F_{p+i}(q), \tag{5}$$

$$F_i(q) = \begin{cases} q!/[i!(q-i)!] & \text{for } 0 \leqslant i \leqslant q, \\ 0 & \text{for } i \prec 0 \text{ and } i \succ q. \end{cases} \tag{6}$$

Here, $P_{l|m|}(\cos\theta)$ are normalized associated Legendre functions. For complex spherical harmonics ($S_{lm} \equiv Y_{lm}$)

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \tag{7}$$

and for real spherical harmonics

$$\Phi_m(\phi) = \frac{1}{\sqrt{\pi(1+\delta_{m0})}} \begin{cases} \cos|m|\,\phi & \text{for} \quad m \geqslant 0, \\ \sin|m|\,\phi & \text{for} \quad m < 0. \end{cases} \tag{8}$$

Non-standard conventions for the generalized Laguerre polynomials, equation(2), were discussed in [30]. In our previous works [31–41], with the help of complete orthonormal sets of Ψ^{α}-ETOs obtained by utilizing a non-standard convention, one-range addition theorems and expansion formulas for multicenter multielectron integrals, and their derivatives in spherical coordinates have been established. The purpose of this paper is to express these expansion formulas through the Cartesian coordinates. The similar formulas can also be derived using the following relation for complete orthonormal sets of Ψ^{α}-ETOs in standard conventions:

$$\Psi_{nlm}^{\alpha}(\zeta,\vec{r}) = \left[\frac{2l+1}{4\pi}\frac{(2\zeta)^{2l+3}(q-p)!}{(2n)^{\alpha}q!}\right]^{1/2} e^{-\zeta r}\mathcal{L}_{q-p}^{p}(2\zeta\, r)T_{lm}(X,Y,Z), \tag{9}$$

where the standard generalized Laguerre polynomials are determined by

$$\mathcal{L}_{q-p}^{p}(x) = \frac{(-1)^p}{q!}L_q^p(x) = \frac{(-1)^{\alpha}}{q!}L_q^p(x). \tag{10}$$

We notice that the Ψ^{α}-ETOs, equations (1) and (9), are represented as finite linear combinations of normalized STOs [29]:

$$\Psi_{nlm}^{\alpha}(\zeta,\vec{r}) = \sum_{n'=l+1}^{n} \omega_{nn'}^{\alpha\, l}\chi_{n'lm}(\zeta,\vec{r}), \tag{11}$$

where

$$\begin{aligned}\chi_{nlm}(\zeta,\vec{r}) &= \chi_{nlm}(\zeta;x,y,z) \\ &= (2\zeta)^{n+1/2}\left[\frac{4\pi}{2l+1}(2n)!\right]^{-1/2} r^{n-l-1}e^{-\zeta r}T_{lm}(x,y,z),\end{aligned} \tag{12}$$

As can be seen from the formulas of Refs. 31–41, all of the addition theorems, multicenter multielectron integrals and their derivatives are expressed in terms of RSSH in spherical coordinates. In section 2 the relationships for RSSH in Cartesian coordinates are derived.

2. Cartesian expressions for RSSH and their derivatives

In order to derive Cartesian expressions of RSSH, equation (3), through the binomial coefficients, we take into account equation(12) of Ref. [42] for normalized associated Legendre functions in the following form:

$$P_{l\lambda}(cos\theta) = (sin\theta)^{\lambda} \sum_{k=0}^{E\left(\frac{l-\lambda}{2}\right)} \left(\frac{2l+1}{2}\right)^{1/2} B_{l\lambda}^{k} (cos\theta)^{l-\lambda-2k}, \tag{13}$$

$$B_{l\lambda}^{k} = \frac{(-1)^k F_k(\lambda+k) F_{l-k}(2l-2k) F_{l-\lambda-2k}(l-k)}{2^l [F_\lambda(l) F_\lambda(l+\lambda)]^{1/2}}. \tag{14}$$

Here, $\lambda = |m|$ and $F_k(n)$ are the binomial coefficients determined by equation (6). Then, finally, we obtain:

$$T_{lm}(x, y, z) = \sum_{k=0}^{E\left(\frac{l-\lambda}{2}\right)} B_{l\lambda}^{k} z^{l-\lambda-2k} r^{2k} \times \begin{cases} (x + i\varepsilon_m y)^{\lambda} & \text{for complex RSSH,} \quad (15) \\ (2-\delta_{m0})^{1/2} \sum_{\sigma} (-1)^{(\sigma-1+\delta_{m\lambda})} F_\sigma(\lambda) x^{\lambda-\sigma} y^{\sigma} & \text{for real RSSH.} \quad (16) \end{cases}$$

where $\sigma = 0, 2, \ldots, [\lambda-(1-(-1)^{\lambda})/2]$ for $m \geqslant 0$, $\sigma = 1, 3, \ldots, [\lambda-(1+(-1)^{\lambda})/2]$ for $m < 0$ and

$$\varepsilon_m = \begin{cases} 1 & \text{for } m \geqslant 0, \\ -1 & \text{for } m < 0. \end{cases} \tag{17}$$

Using the well-known characteristics of associated Legendre functions and surface spherical harmonics (see, e.g., [43, 44]) it is easy to show that the first and second derivatives of the functions $T_{lm}(x, y, z)$ with respect to Cartesian coordinates can be expressed in terms of $T_{l-1m'}(x, y, z)$ and $T_{l-2m'}(x, y, z)$, respectively:

$$\frac{\partial T_{lm}}{\partial x_i} = \sum_{m'=-(l-1)}^{l-1} a_{lm,m'}^{i} T_{l-1m'}, \tag{18}$$

$$\frac{\partial^2 T_{lm}}{\partial x_i \partial x_j} = \sum_{m'=-(l-2)}^{l-2} a_{lm,m'}^{ij} T_{l-2m'}, \tag{19}$$

where $x_1 = x, x_{-1} = y, x_0 = z (i, j = 1, -1, 0)$, $a_{lm,m'}^{i} \equiv 0 for, l = 0, a_{lm,m'}^{ij} \equiv 0$ for $l = 0, 1$ and

$$a_{lm,m'}^{ij} = a_{lm,m'}^{ji} = \sum_{m''=-(l-1)}^{l-1} a_{lm,m''}^{i} a_{l-1m'',m'}^{j}, \tag{20}$$

For complex RSSH

$$\begin{aligned} a_{lm,m'}^{1} = \frac{1}{2}(-1)^{(\lambda-m+\lambda'-m')/2} \{ & -[(l-m)(l-m-1)]^{1/2} \delta_{m',m+1} \\ & + [(l+m)(l+m-1)]^{1/2} \delta_{m',m-1} \}, \end{aligned} \tag{21}$$

$$\begin{aligned} a_{lm,m'}^{-1} = \frac{i}{2}(-1)^{(\lambda-m+\lambda'-m')} \{ & [(l-m)(l-m-1)]^{1/2} \delta_{m',m+1} \\ & + [(l+m)(l+m-1)]^{1/2} \delta_{m',m-1} \}, \end{aligned} \tag{22}$$

$$a_{lm,m'}^{0} = [(l+m)(l-m)]^{1/2} \delta_{m'm}, \tag{23}$$

where $\lambda = |m|, \lambda' = |m'|$ and for real RSSH

$$\begin{aligned} a_{lm,m'}^{1} = -\frac{\varepsilon_m}{2} \{ & [(1+\delta_{m0})(1-\delta_{m,-1})(l-m)(l-m-1)]^{1/2} \delta_{m',m+1} \\ & - [(1-\delta_{m0})(1+\delta_{m1})(l+m)(l+m-1)]^{1/2} \delta_{m',m-1} \}, \end{aligned} \tag{24}$$

$$\begin{aligned} a_{lm,m'}^{-1} = -\frac{\varepsilon_m}{2} \{ & [(1+\delta_{m0})(1+\delta_{m,-1})(l-m)(l-m-1)]^{1/2} \delta_{m',-m-1} \\ & + [(1-\delta_{m0})(1-\delta_{m1})(l+m)(l+m-1)]^{1/2} \delta_{m',-m+1} \}, \end{aligned} \tag{25}$$

$$a_{lm,m'}^{0} = [(l+m)(l-m)]^{1/2} \delta_{m'm}. \tag{26}$$

It is easy to show that the Cartesian expressions (15) and (16) for RSSH satisfy the Laplace equation:

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) T_{lm}(x, y, z) = \sum_{i=-1}^{1} \frac{\partial^2}{\partial x_i^2} T_{lm}(x, y, z) = 0. \tag{27}$$

Thus, we have established the desired Cartesian expressions for RSSH and their derivatives in terms of binomial coefficients.

3. Evaluation of multicenter multielectron integrals in Cartesian coordinates

In [32–41], using the addition theorems for STOs and arbitrary Coulomb ($\eta = 0$) and Yukawa ($\eta > 0$) like potentials defined by

$$f_{uvs}(\eta, \vec{r}) = r^{u-v-1} e^{-\eta r} T_{vs}(x, y, z) \tag{28}$$

the general formulas in terms of two-center overlap integrals with the same screening constants were established for the multicenter t-electron integrals (see [32])

$$\begin{aligned} & I^{ac,bd,gh,\ldots,ef}_{p_1 p_1', p_2 p_2', p_3 p_3', \ldots, p_t p_t'; \tau}(\zeta_1\zeta_1', \zeta_2\zeta_2', \zeta_3\zeta_3', \ldots, \zeta_t\zeta_t'; \eta) \\ & = \int \chi^*_{p_1}(\zeta_1, \vec{r}_{a1}) \chi_{p_1'}(\zeta_1', \vec{r}_{c1}) \chi_{p_2}(\zeta_2, \vec{r}_{b2}) \overset{(}{\chi}_{p_2'}(\zeta_2', \vec{r}_{d2}) \chi_{p_3}(\zeta_3, \vec{r}_{g3}) \overset{(}{\chi}_{p_3'}(\zeta_3', \vec{r}_{h3}) \ldots \\ & \quad \times \chi_{p_t}(\zeta_t, \vec{r}_{et}) \overset{(}{\chi}_{p_t'}(\zeta_t', \vec{r}_{ft}) O_\tau(\eta, \vec{r}_{1,2,3,\ldots,t}) \mathrm{d}v_1 \mathrm{d}v_2 \mathrm{d}v_3 \ldots \mathrm{d}v_t \end{aligned} \tag{29}$$

that arise in the solution of the N-electron atomic and molecular problem ($2 \leqslant t \leqslant N$)when Hartree–Fock–Roothaan and correlated approximations are employed. Here, $2 \leqslant t \leqslant N$, $p_i \equiv n_i l_i m_i$, $p_i' \equiv n_i' l_i' m_i'$, $\tau \equiv uvs$ and $\hat{O}_\tau(\eta, \vec{r}_{1,2,3,\ldots,t})$ is the t-electron operator.

The two-center overlap integrals occurring in series expansion formulas for multicenter multielectron integrals are determined solely from the linear combinations of STOs, equation (12), depending on radius vector of nuclei [31]:

$$\begin{aligned} S_{nlm,n'l'm'}(\zeta, \vec{R}) &= \int \chi^*_{nlm}(\zeta, \vec{r}_a) \chi_{n'l'm'}(\zeta, \vec{r}_b) \mathrm{d}v \\ &= \frac{1}{\zeta^{3/2}} \sum_{N=1}^{n+n'+1} \sum_{L=0}^{N-1} \sum_{M=-L}^{L} g^{\alpha NLM}_{nlm,n'l'm'} \chi^*_{NLM}(\zeta, \vec{R}), \end{aligned} \tag{30}$$

where $\vec{R} = \vec{R}(XYZ) = \vec{R}_b(X_b Y_b Z_b) - \vec{R}_a(X_a Y_a Z_a)$, and $\alpha = 1, 0, -1, -2, \ldots$ (see [31]) for the exact definition of coefficients $g^{\alpha NLM}_{nlm,n'l'm'}$.

Now we are able to obtain the derivatives of overlap integrals with respect to Cartesian coordinates of the nucleus a. Using equations (16) and (17) of Ref. 33 one gets the following relations:

$$\begin{aligned} S^i_{nlm,n'l'm'}(\zeta, \vec{R}) = \frac{\partial}{\partial X^i} S_{nlm,n'l'm'}(\zeta, \vec{R}) = 2\zeta \Bigg\{ & \eta^{11}_{nl} \sum_{\sigma=-(l-1)}^{l-1} a^i_{lm,\sigma} S_{n-1l-1\sigma,n'l'm'}(\zeta, \vec{R}) \\ & - \frac{X^i}{R} \left[(n-l-1) \eta^{10}_{nl} S_{n-1lm,n'l'm'}(\zeta, \vec{R}) - \frac{1}{2} S_{nlm,n'l'm'}(\zeta, \vec{R}) \right] \Bigg\} \end{aligned} \tag{31}$$

$$
\begin{aligned}
S^{ij}_{nlm,n'l'm'}(\zeta,\vec{R}) &= \frac{\partial^2}{\partial X^i \partial X^j} S_{nlm,n'l'm'}(\zeta,\vec{R}) \\
&= (2\zeta)^2 \Bigg\{ \eta^{22}_{nl} \sum_{\sigma=-(l-2)}^{l-2} a^{ij}_{lm,\sigma} S_{n-2l-2\sigma,n'l'm'}(\zeta,\vec{R}) \\
&\quad - \sum_{\sigma=-(l-1)}^{l-1} \left[a^{i}_{lm,\sigma} \left(\frac{X^j}{R}\right) + a^{j}_{lm,\sigma} \left(\frac{X^i}{R}\right) \right] \\
&\quad \left[(n-l-1)\eta^{21}_{nl} S_{n-2l-1\sigma,n'l'm'}(\zeta,\vec{R}) - \frac{1}{2}\eta^{11}_{nl} S_{n-1l-1\sigma,n'l'm'}(\zeta,\vec{R}) \right] \\
&\quad + \left(\frac{X^i}{R}\right)\left(\frac{X^j}{R}\right) \Big[(n-l-1)(n-l-3)\eta^{20}_{nl} S_{n-2lm,n'l'm'}(\zeta,\vec{R}) \\
&\quad - \frac{1}{2}(2n-2l-3)\eta^{10}_{nl} S_{n-1lm,n'l'm'}(\zeta,\vec{R}) + \frac{1}{4} S_{nlm,n'l'm'}(\zeta,\vec{R}) \Big] \\
&\quad + \delta_{ij} \left[(n-l-1)\eta^{20}_{nl} S_{n-2lm,n'l'm'}(\zeta,\vec{R}) - \frac{1}{2}\eta^{10}_{nl} S_{n-1lm,n'l'm'}(\zeta,\vec{R}) \right] \Bigg\}.
\end{aligned}
\tag{32}
$$

As can be seen from equations (30–32) and equations (24) and (25) of Ref. 33, all the two-center overlap integrals and the arbitrary multicenter multielectron integrals, and their derivatives are expressed through the STOs determined by equation (12) with the help of RSSH in Cartesian coordinates of nuclei. The convergence and numerical stability of series occurring in these integrals have been tested in previous papers (see, e.g., [36, 45, 46] and references to our works quoted therein). Work is in progress for the calculation of multicenter multielectron integrals of integer and noninteger n STOs, and their derivatives appearing in the Hartree–Fock–Roothaan and correlated theories based on the formulas presented in this article.

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