One-Range Addition Theorems for Yukawa-Like Central and Noncentral Interaction Potentials and Their Derivatives

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Using addition theorems for Slater-type orbitals, obtained by the author with the help of complete orthonormal sets of Ψ^{α}-Exponential type orbitals ($\alpha = 1, 0, -1, -2, \ldots$), the one-range addition theorems for arbitrary Yukawa-like central and noncentral interaction potentials and their first and second derivatives are established. The addition theorems derived for the interaction potentials and the Slater orbitals are especially useful for machine computations of arbitrary multielectron multicenter integrals that arise in the Hartree–Fock–Roothaan approximation, and also in the Hylleraas-correlated wave-function method, which play a significant role in the theory and applications to quantum mechanics of atoms, molecules, and solids. The obtained relationships are valid for arbitrary nonzero screening constants of the potentials.

In the vast majority of all atomic and molecular electronic-structure calculations, it is often necessary to transform operators and Slater-type orbitals (STOs) that depend upon the coordinates of two particles, in such a way that the coordinates of the pertaining particles appear in a computationally more convenient form. In most cases this requires a separation of the variables, which can be accomplished with the help of the so-called addition theorems. Two fundamentally different types of addition theorems occur in the literature. The addition theorems of the first type all have the typical two-range form of the Laplace expansion of the Coulomb potential,

$$\frac{1}{r_{21}} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{2l+1} \frac{r_<^l}{r_>^{l+1}} S_{lm}^{*}(\theta_2, \varphi_2) S_{lm}(\theta_1, \varphi_1), \tag{1}$$

where $r_< = \min(r_1, r_2)$ and $r_> = \max(r_1, r_2)$. Here, the complex or real spherical harmonics, S_{lm}, are determined by the relation

$$S_{lm}(\theta, \phi) = P_{l|m|}(\cos\theta)\Phi_m(\phi), \tag{2}$$

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

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{im\varphi}, \tag{3}$$

and for real spherical harmonics

$$\Phi_m(\phi) = \frac{1}{\sqrt{\pi(1+\delta_{m0})}} \begin{cases} \cos|m|\phi & \text{for } m \geq 0 \\ \sin|m|\phi & \text{for } m < 0. \end{cases} \tag{4}$$

It should be noted that our definition of the phases for complex spherical harmonics ($Y_{lm}^{*} = Y_{l-m}$) differs from the Condon–Shortley phases[1] by a sign factor $(-1)^m$. This addition theorem can be derived as shown in Refs. 2, 3 via rearrangements of a 3-dimensional Taylor expansion.

Then, there is a second class of addition theorems that can be constructed by expanding a function located at a center a in terms of a complete orthonormal set located at a center b. In such an addition theorem, the expansion coefficients are the overlap integrals. Consequently, such an addition theorem has a one-range form that further simplifies integrations. If the complete orthonormal set occurring in the one-range addition theorem consists of exponentially decaying functions, then its elements can usually be expanded by finite linear combinations of STOs. Consequently, the expansion coefficients can be expressed in terms of overlap integrals over STOs. The earliest approaches with exponentially decaying functions consisted of using relatively complicated one-range addition theorems of STOs to separate the integration variables from those related to the geometry of the molecule.[4–21] The great progress made in both applied mathematics and computer science has led a number of researchers to focus their efforts on elaborating new approaches directed to computing the multicenter integrals over STOs. Unfortunately, they also were not entirely successful. To our knowledge, many authors (see Refs. 22–26 and references therein) have addressed this problem, and although many improvements have been made in the past few years by the use of computers, an efficient general program for calculating multicenter integrals over STOs is not yet available. We have had considerable success in using the one-range addition theorems of STOs to evaluate multicenter molecular integrals. In previous work,[27] by using complete orthonormal sets of Ψ^{α}-Exponential type orbitals all (Ψ^{α}-ETOs), of the multicenter multielectron integrals of the central and noncentral interaction potentials were calculated by using the following one-range addition theorems for spherically symmetric (for $\upsilon = 0$) and spherically nonsymmetric (for $\upsilon \neq 0$) STOs:[27]

$$\chi_{uvs}(\eta, \vec{r}_{21}) = \frac{\sqrt{4\pi}}{\eta^{3/2}} \lim_{N\to\infty} \sum_{\mu=1}^{N} \sum_{\nu=0}^{\mu-1} \sum_{\sigma=-\nu}^{\nu} \sum_{\mu'=1}^{N+u-\alpha+1} \sum_{\nu'=0}^{\mu'-1} \sum_{\sigma'=-\nu'}^{\nu'} \times Y_{uvs,\mu\nu\sigma}^{\alpha N,\mu'\nu'\sigma'} \chi_{\mu\nu\sigma}(\eta, \vec{r}_1)$$

$$\times \chi_{\mu'\nu'\sigma'}^{*}(\eta, \vec{r}_2) \begin{cases} \delta_{\nu'\nu}\delta_{\sigma'\sigma} & \text{for } \upsilon = 0 \quad \text{(5a)} \\ 1 & \text{for } \upsilon \neq 0, \quad \text{(5b)} \end{cases}$$

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where η is the screening constant ($\eta > 0$), $u \geq 0$, $v = 0, 1, 2, \ldots, -v \leq s \leq v$, and $\alpha = 1, 0, -1, -2, \ldots$. It should be noted that the coefficients $Y^{\alpha N,\mu' v\sigma}_{u00,\mu v\sigma}$ in Eq. 5a do not depend upon the indices σ:

$$Y^{\alpha N,\mu' v\sigma}_{u00,\mu v\sigma} \equiv Y^{\alpha N,\mu' v}_{u0,\mu v} = (-1)^{v} \sum_{\mu^*=v+1}^{N} \Omega^{\alpha v}_{\mu\mu^*}(N) g^{\alpha\mu' v}_{u00,\mu^*-\alpha v}, \quad (6)$$

where $g^{\alpha\mu' v}_{u00,\mu^*-\alpha v} \equiv g^{\alpha\mu' v\sigma}_{u00,\mu^*-\alpha v\sigma}$ (see Eqs. 60 and 62 of Ref. 28).

The purpose of this work is to use the addition theorems for STOs, in order to obtain one-range addition theorems for arbitrary Yukawa-like central and noncentral interaction potentials (CIPs and NCIPs) and their derivatives, which arise in solving atomic and molecular multielectron problems when Hartree–Fock–Roothaan and Hylleraas approximations are employed.

Addition Theorems for Potentials

The interaction potentials used in this work are defined as

$$f_{uvs}(\eta, \vec{r}) = f_u(\eta, r)\left(\frac{4\pi}{2v+1}\right)^{1/2} S_{vs}(\theta, \varphi), \quad (7)$$

where $u \geq 0$ and $\eta > 0$. The coefficient η in Eq. 7 is a parameter characterizing the screening of the nuclear field by the electrons. The radial part of the potential is the screened central potential,

$$f_u(\eta, r) = f_{u00}(\eta, r) = r^{u-1} \mathrm{e}^{-\eta r}. \quad (8)$$

In order to establish addition theorems for CIPs and NCIPs, we express the STOs containing in Eqs. 5a and 5b through the potentials

$$\chi_{uvs}(\eta, \vec{r}) = \frac{(2\eta)^{u+1/2}}{\sqrt{(2u)!}} \left(\frac{2v+1}{4\pi}\right)^{1/2} f_{uvs}(\eta, \vec{r}). \quad (9)$$

Then, it is easy to establish for CIPs ($v = 0$) and NCIPs ($v \neq 0$) the following one-range addition theorems:

$$f_{uvs}(\eta, \vec{r}_{21}) = \lim_{N\to\infty} \sum_{\mu=1}^{N} \sum_{\nu=0}^{\mu-1} \sum_{\sigma=-\nu}^{\nu} \sum_{\mu'=1}^{N+u-\alpha+1} \sum_{\nu'=0}^{\mu'-1} \sum_{\sigma'=-\nu'}^{\nu'} \times D^{\alpha N,\mu'\nu'\sigma'}_{uvs,\mu\nu\sigma} (2\eta)^{\mu+\mu'-u-1} f_{\mu\nu\sigma}(\eta, \vec{r}_1) f^{*}_{\mu'\nu'\sigma'}(\eta, \vec{r}_2) \quad (10)$$

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

$$D^{\alpha N,\mu'\nu'\sigma'}_{uvs,\mu\nu\sigma} = 2\left[\frac{2(2\nu+1)(2\nu'+1)(2u)!}{(2v+1)(2\mu)!(2\mu')!}\right]^{1/2} \times Y^{\alpha N,\mu'\nu'\sigma'}_{uvs,\mu\nu\sigma} \begin{cases} \delta_{\nu' v}\delta_{\sigma'\sigma} & \text{for } v = 0 \\ 1 & \text{for } v \neq 0. \end{cases} \quad (11)$$

We can now move on to derive one-range addition theorems for the derivatives of potentials.

Addition Theorems for Derivatives of Potentials

As can be seen from Eq. 10, the derivatives of potentials with respect to Cartesian coordinates of second electron are defined as

$$f^{i}_{uvs}(\eta, \vec{r}_{21}) = \frac{\partial}{\partial x^i_2} f_{uvs}(\eta, \vec{r}_{21}) = \lim_{N\to\infty} \sum_{\mu=1}^{N} \sum_{\nu=0}^{\mu-1} \sum_{\sigma=-\nu}^{\nu} \sum_{\mu'=1}^{N+u-\alpha+1} \sum_{\nu'=0}^{\mu'-1} \sum_{\sigma'=-\nu'}^{\nu'} \times D^{\alpha N,\mu'\nu'\sigma'}_{uvs,\mu\nu\sigma} (2\eta)^{\mu+\mu'-u-1} f_{\mu\nu\sigma}(\eta, \vec{r}_1) f^{i*}_{\mu'\nu'\sigma'}(\eta, \vec{r}_2), \quad (12)$$

$$f^{ij}_{uvs}(\eta, \vec{r}_{21}) = \frac{\partial^2}{\partial x^i_2 \partial x^j_2} f_{uvs}(\eta, \vec{r}_{21}) = \lim_{N\to\infty} \sum_{\mu=1}^{N} \sum_{\nu=0}^{\mu-1} \sum_{\sigma=-\nu}^{\nu} \sum_{\mu'=1}^{N+u-\alpha+1} \sum_{\nu'=0}^{\mu'-1} \sum_{\sigma'=-\nu'}^{\nu'} \times D^{\alpha N,\mu'\nu'\sigma'}_{uvs,\mu\nu\sigma} (2\eta)^{\mu+\mu'-u-1} f_{\mu\nu\sigma}(\eta, \vec{r}_1) f^{ij*}_{\mu'\nu'\sigma'}(\eta, \vec{r}_2), \quad (13)$$

where $i, j = 1, -1, 0$, $x^1_2 = x_2$, $x^{-1}_2 = y_2$, $x^0_2 = z_2$ and

$$f^{i}_{\mu'\nu'\sigma'}(\eta, \vec{r}_2) = \frac{\partial}{\partial x^i_2} f_{\mu'\nu'\sigma'}(\eta, \vec{r}_2), \quad (14)$$

$$f^{ij}_{\mu'\nu'\sigma'}(\eta, \vec{r}_2) = \frac{\partial^2}{\partial x^i_2 \partial x^j_2} f_{\mu'\nu'\sigma'}(\eta, \vec{r}_2). \quad (15)$$

In order to obtain relations for derivatives 14 and 15, we use the relation for a potential in the following form:

$$f_{\mu\nu\sigma}(\eta, \vec{r}) = M_{\nu\sigma}(x, y, z) R(r), \quad (16)$$

where $r = (x^2 + y^2 + z^2)^{1/2}$ and

$$M_{\nu\sigma}(x, y, z) = r^{\nu} \bar{S}_{\nu\sigma}(\theta, \varphi),$$
$$\bar{S}_{\nu\sigma}(\theta, \varphi) = \left(\frac{4\pi}{2\nu+1}\right)^{1/2} S_{\nu\sigma}(\theta, \varphi), \quad (17)$$
$$R(r) = r^{\mu-\nu-1} \mathrm{e}^{-\eta r}. \quad (18)$$

The derivatives of a product of functions $M_{\nu\sigma}(x, y, z)$ and $R(r)$ with respect to the Cartesian coordinates can be determined from the formulas

$$\frac{\partial(M_{\nu\sigma}R)}{\partial x^i} = \frac{\partial M_{\nu\sigma}}{\partial x^i} R + M_{\nu\sigma} x^i \left(\frac{1}{r}\frac{\partial R}{\partial r}\right), \quad (19)$$

$$\frac{\partial^2(M_{\nu\sigma}R)}{\partial x^i \partial x^j} = \frac{\partial^2 M_{\nu\sigma}}{\partial x^i \partial x^j} R + \frac{\partial M_{\nu\sigma}}{\partial x^i} x^j \left(\frac{1}{r}\frac{\partial R}{\partial r}\right) + \frac{\partial M_{\nu\sigma}}{\partial x^j} x^i \left(\frac{1}{r}\frac{\partial R}{\partial r}\right) + M_{\nu\sigma}\left[\delta_{ij}\left(\frac{1}{r}\frac{\partial R}{\partial r}\right) + x^i x^j \frac{1}{r}\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial R}{\partial r}\right)\right], \quad (20)$$

where

$$\frac{\partial M_{\nu\sigma}}{\partial x^i} = \sum_{\sigma'=-(\nu-1)}^{\nu-1} a^{i}_{\nu\sigma,\sigma'} M_{\nu-1\sigma'}, \quad (21)$$

$$\frac{\partial^2 M_{\nu\sigma}}{\partial x^i \partial x^j} = \sum_{\sigma'=-(\nu-2)}^{\nu-2} a^{ij}_{\nu\sigma,\sigma'} M_{\nu-2\sigma'} \quad (22)$$

and

$$\frac{1}{r}\frac{\partial R}{\partial r} = [(\mu - \nu - 1) r^{\mu-\nu-3} - \eta r^{\mu-\nu-2}] \mathrm{e}^{-\eta r}, \quad (23)$$

$$\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial R}{\partial r}\right) = [(\mu-\nu-1)(\mu-\nu-3) r^{\mu-\nu-5} - \eta(2\mu - 2\nu - 3) r^{\mu-\nu-4} + \eta^2 r^{\mu-\nu-3}] \mathrm{e}^{-\eta r}. \quad (24)$$

Here, $a^{i}_{\nu\sigma,\sigma'} \equiv 0$ for $\nu = 0$, $a^{ij}_{\nu\sigma,\sigma'} \equiv 0$ for $\nu = 0, 1$ and

$$a^{1}_{\nu\sigma,\sigma'} = -\frac{\varepsilon_\sigma}{2}\{[(1+\delta_{\sigma 0})(1-\delta_{\sigma,-1})(\nu-\sigma)(\nu-\sigma-1)]^{1/2}\delta_{\sigma',\sigma+1} - [(1-\delta_{\sigma 0})(1+\delta_{\sigma 1})(\nu+\sigma)(\nu+\sigma-1)]^{1/2}\delta_{\sigma',\sigma-1}\}, \quad (25)$$

$$a^{-1}_{\nu\sigma,\sigma'} = -\frac{\varepsilon_\sigma}{2}\{[(1+\delta_{\sigma0})(1+\delta_{\sigma,-1})(\nu-\sigma)(\nu-\sigma-1)]^{1/2}\delta_{\sigma',-\sigma-1} + [(1-\delta_{\sigma0})(1-\delta_{\sigma1})(\nu+\sigma)(\nu+\sigma-1)]^{1/2}\delta_{\sigma',-\sigma+1}\}, \quad (26)$$

$$a^{0}_{\nu\sigma,\sigma'} = [(\nu+\sigma)(\nu-\sigma)]^{1/2}\delta_{\sigma'\sigma} \quad \text{for} \quad \nu \geq 1, \quad (27)$$

$$a^{ij}_{\nu\sigma,\sigma'} = a^{ij}_{\nu\sigma,\sigma'} = \sum_{\sigma^*=-(\nu-1)}^{\nu-1} a^{j}_{\nu\sigma,\sigma^*} a^{i}_{\nu-1\sigma^*,\sigma'} \quad \text{for} \quad \nu \geq 2, \quad (28)$$

where $\varepsilon_\sigma = \pm 1$. The sign of the symbol ε_σ is determined by the sign of σ, i.e., $\varepsilon_\sigma = +1$ for $\sigma \geq 0$ and $\varepsilon_\sigma = -1$ for $\sigma < 0$.

Taking into account Eqs. 16–24 in 14 and 15, we finally find for the derivatives in terms of CIPs (for $\nu = \sigma = 0$) and NCIPs (for $\nu \neq 0$, $-\nu \leq \sigma \leq \nu$) the following relationships:

$$f^{i}_{\mu\nu\sigma}(\eta,\vec{r}) = \sum_{\sigma'=-(\nu-1)}^{\nu-1} a^{i}_{\nu\sigma,\sigma'} f_{u-1\nu-1\sigma'}(\eta,\vec{r}) + \frac{x^i}{r}[(\mu-\nu-1)f_{\mu-1\nu\sigma}(\eta,\vec{r}) - \eta f_{\mu\nu\sigma}(\eta,\vec{r})], \quad (29)$$

$$\begin{aligned} f^{ij}_{\mu\nu\sigma}(\eta,\vec{r}) &= \sum_{\sigma'=-(\nu-2)}^{\nu-2} a^{ij}_{\nu\sigma,\sigma'} f_{u-2\nu-2\sigma'}(\eta,\vec{r}) \\ &+ \sum_{\sigma'=-(\nu-1)}^{\nu-1}\left[a^{i}_{\nu\sigma,\sigma'}\left(\frac{x^j}{r}\right) + a^{j}_{\nu\sigma,\sigma'}\left(\frac{x^i}{r}\right)\right] \\ &\times [(\mu-\nu-1)f_{\mu-2\nu-1\sigma'}(\eta,\vec{r}) - \eta f_{\mu-1\nu-1\sigma'}(\eta,\vec{r})] \\ &+ (\mu-\nu-1)\left[\delta_{ij} + (\mu-\nu-3)\left(\frac{x^i}{r}\right)\left(\frac{x^j}{r}\right)\right] \\ &\times f_{\mu-2\nu\sigma}(\eta,\vec{r}) - \eta\left[\delta_{ij} + (2\mu-2\nu-3)\left(\frac{x^i}{r}\right)\left(\frac{x^j}{r}\right)\right] \\ &\times f_{\mu-1\nu\sigma}(\eta,\vec{r}) + \eta^2\left(\frac{x^i}{r}\right)\left(\frac{x^j}{r}\right) f_{\mu\nu\sigma}(\eta,\vec{r}) \\ &- \begin{cases} \frac{4\pi}{3}\delta_{ij}\delta(\vec{r}) & \text{for } \mu = 0 \quad (\nu = \sigma = 0) \quad (30a) \\ 0 & \text{for } \mu \geq 1, \quad (30b) \end{cases} \end{aligned}$$

where $\delta(\vec{r})$ is the Dirac delta function.

The Yukawa-like central interaction potential and its derivatives are obtained from Eqs. 16, 29, and 30a for $\mu = \nu = \sigma = 0$:

$$f_{000}(\eta, r) = \frac{e^{-\eta r}}{r}, \quad (31)$$

$$f^{i}_{000}(\eta,\vec{r}) = \frac{x^i}{r^3}(1+\eta r)e^{-\eta r}, \quad (32)$$

$$f^{ij}_{000}(\eta,\vec{r}) = \left[\frac{1}{r^5}(3x^i x^j - \delta_{ij}r^2)(1+\eta r) + \frac{\eta^2}{r^3}x^i x^j\right] \times e^{-\eta r} - \frac{4\pi}{3}\delta_{ij}\delta(\vec{r}). \quad (33)$$

This potential, Eq. 31, satisfies the modified Helmholtz equation,[29]

$$\begin{aligned} f^{11}_{000}(\eta,\vec{r}) + f^{-1-1}_{000}(\eta,\vec{r}) + f^{00}_{000}(\eta,\vec{r}) &= \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) f_{000}(\eta, r) \\ &= \eta^2 f_{000}(\eta, r) - 4\pi\delta(\vec{r}). \end{aligned} \quad (34)$$

Using Eqs. 31–33 for $\eta = 0$ and $\eta \neq 0$ with the help of Ψ^α-ETOs, we recently established series expansion formulas for the multicenter electronic attraction, electric field and electric field gradient integrals of the nonscreened and Yukawa-like screened Coulomb potentials in terms of the new central and noncentral interaction potentials.[30,31]

Numerical Results and Discussion

On the basis of the formulae presented in this work for one-range addition theorems of Yukawa-like central and noncentral interaction potentials and their derivatives, the multicenter electronic attraction (EA), electric field (EF), and electric field gradient (EFG) integrals over STOs were calculated. The results of the calculations on a Pentium III 800 MHz (using Turbo Pascal language) for the three-center EF and EFG integrals,

$$U^{i,abc}_{uvs,nlm,n^*l'm'}(\eta,\zeta,\zeta') = \int f^{i}_{uvs}(\eta,\vec{r}_{a1})\chi_{nlm}(\zeta,\vec{r}_{b1})\chi^*_{n'l'm'}(\zeta',\vec{r}_{c1})dV_1, \quad (35)$$

$$U^{ij,abc}_{uvs,nlm,n^*l'm'}(\eta,\zeta,\zeta') = \int f^{ij}_{uvs}(\eta,\vec{r}_{a1})\chi_{nlm}(\zeta,\vec{r}_{b1})\chi^*_{n'l'm'}(\zeta',\vec{r}_{c1})dV_1, \quad (36)$$

are given in Table 1. Here, the first and second derivatives of the potentials were determined from Eqs. 12 and 13 for $\vec{r}_{21} = \vec{r}_{a1}$. The comparative values obtained from Eqs. 35 and 36 with the expansion of Ψ^0 and Ψ^{-1}-ETOs are shown in this table. As can be seen from the table, the accuracy of the computer results obtained from the different complete orthonormal sets of Ψ^α-ETOs is satisfactory.

Table 1. The Values of Three-Center EF and EFG Integrals in Molecular Coordinate System for $u = v = s = 0$ and $N = 12$ (in a.u.)

n	l	m	ζ	n'	l'	m'	ζ'	η	i	j	Eqs. 35 and 36 for $N = 12$	
											$\alpha = 0$	$\alpha = 1$
1	0	0	4.3	1	0	0	2.1	0.2	−1		−2.6644222237E−04	−2.6644073433E−04
2	1	0	3.4	2	1	0	4.2	0.6	0		2.1512437031E−03	2.1512299076E−03
2	1	0	5.3	1	0	0	6.4	1.2	1		9.4193594682E−05	9.4194660268E−05
2	1	1	3.4	1	0	0	1.5	0.3	−1	0	3.0470674815E−03	3.0472558972E−03
1	0	0	6.3	1	0	0	4.1	1.5	1	−1	2.0919958866E−01	2.0919936098E−01

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