# Use of self-friction polynomials in standard convention and auxiliary functions for construction of One-Range addition theorems for noninteger slater type orbitals

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Using $\mathcal{L}^{(p_l*)}$-self-friction polynomials ($\mathcal{L}^{(p_l^*)}$-SFPs), complete orthonormal sets of $\psi^{(p_l^*)}$-SF exponential type orbitals ( $\psi^{(p_l^*)}$-SFETOs) in standard convention and $Q^q$-integer auxiliary functions ($Q^q$-IAFs) introduced by the author, the combined one- and two-center one-range addition theorems for $\chi$-noninteger Slater type orbitals ($\chi$-NISTOs) are established, where $p_l^* = 2l + 2 - \alpha^*$ and $\alpha^*$ is SF quantum number. As an application, the one-center atomic nuclear attraction integrals of $\chi$-NISTOs and $V$-noninteger Coulombic potential ($V$-NICPs) are calculated. The obtained formulas can be useful especially in the electronic structure calculations of atoms, molecules and solids.

*Keywords:* Addition theorems; standard convention; exponential type orbitals; self-friction quantum number.

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## 1. Introduction

It is well known that the addition theorems can be constructed by expanding a function located at a center $b$ in terms of a complete orthonormal set located at a center $a$ [1,2]. In a previous paper [3], with the help of $\mathcal{L}^{(p_l^*)}$-SFPs, the one-range addition theorems for $\chi$-NISTOs have been suggested. It is shown in Ref. 4 that, for disappearing SF properties, the $\mathcal{L}^{(p_l^*)}$-SFPs are reduced to the $\mathcal{L}^p$-associated Laguerre polynomials ( $\mathcal{L}^p$-ALPs) arising in nonstandard convention for the Schrodinger's bound-state hydrogen-like eigenfunctions and, therefore, become the noncomplete. Since the $\mathcal{L}^p$-ALPs are not complete sets, some convergence difficulties occur especially in series expansions. Accordingly, it is desirable to use the $\mathcal{L}^{(p_l^*)}$-SFPs and $\psi^{(p_l^*)}$-SFETOs that are a large class (for $-\infty < \alpha^* < 3$) of complete and orthogonal functions.

The purpose of this work is to obtain the one-range addition theorems for $\chi$-NISTOs by the use of $\mathcal{L}^{(p_l*)}$-SFPs, complete orthonormal sets of $\psi^{(p_l^*)}$-SFETOs and $Q^q$-IAFs, where $\alpha*$ is the integer (for $\alpha^* = \alpha$, $\infty < \alpha \leq 2$) and noninteger (for $\alpha* \neq \alpha$, $-\infty < \alpha^* < 3$) SF quantum number. We note that the suggested approach is based on the use of SF polynomials in standard convention introduced in our previous works (see [5] and references therein to our papers on standard convention).

## 2. Definition and basic formulas

The complete orthonormal sets of $\psi^{(p_l*)}$-SFETOs, $\mathcal{L}^{(p_l*)}$-SFPs, $\chi$-NISTOs and $Q^q$-IAFs used in this work are defined as

$$\psi_{nlm}^{(p_l^*)}(\zeta,\vec{r}) = R_{nl}^{(p_l^*)}(\zeta,r)S_{lm}(\theta,\phi) \tag{1}$$

$$R_{nl}^{(p_l^*)}(\zeta,r) = (2\zeta)^{\frac{3}{2}}R_{nl}^{(p_l^*)}(t) = (2\zeta)^{\frac{3}{2}}e^{-t/2}L_{nl}^{(p_l^*)}(t) \tag{2}$$

$$\begin{aligned} L_{nl}^{(p_l^*)}(t) &= \frac{\Gamma(q_n^*+1)}{(n-(l+1))!\Gamma(p_l^*+1)} \\ &\times F_1(-[n-(l+1)];p_l^*+1,t) \\ &= \frac{\Gamma(q_n^*+1)}{(n-(l+1))!}\sum_{n'=l+1}^{n}\tilde{a}_{nn'}^{(p_l^*)l}t^{n'-(l+1)} \end{aligned} \tag{3}$$

$$\chi_{u*vs}(\beta,\vec{r}) = R_{u^*}(\beta,r)S_{vs}(\theta,\phi) \tag{4}$$

$$R_{u^*}(\beta,r) = (2\beta)^{u^*+\frac{1}{2}}[\Gamma(2u^*+1)]^{-\frac{1}{2}}r^{u^*-1}e^{-\beta r} \tag{5}$$

$$\begin{aligned} Q_{NN'}^{q}(\rho,\tau) &= \int_{1}^{\infty}\int_{-1}^{1}(\mu\nu)^q(\mu+\nu)^{N'} \\ &\times(\mu-\nu)^{N'}e^{-\rho\mu-\rho\tau\nu}d\mu d\nu \end{aligned} \tag{6}$$

where $t = 2\zeta r$, $p_l^* = 2l + 2 - \alpha^*$, $q_n^* = n + l + 1 - \alpha^*$ and $S_{lm} = (\theta, \phi)$ are the complex or real spherical harmonics. Our definition of phases [6] for the complex spherical harmonics ($Y_{lm}^* = Y_{l-m}$) differs from the Condon-Shortly phases [7] by the sign factor $(-1)^m$. The quantities $\tilde{a}_{nn'}^{(p_l^*)l}$ occurring in Eq. (3) are expressed through the Gamma functions and Pochhammer symbols [8],

$$\tilde{a}_{nn'}^{(p_l^*)l} = \frac{(-[n-(l+1)])_{n'-(l+1)}}{\Gamma(p_l^*+1)(p_l^*+1)_{n'-(l+1)}[n'-(l+1)]!} \tag{7}$$

Using Eqs. (2) and (3) in (1), the $\psi^{(p_l^*)}$-SFETOs can be expressed through the $\chi$-integer STOs ($\chi$-ISTOs),

$$\psi_{nlm}^{(p_l^*)l}(\zeta,\vec{r}) = \sum_{n'=1}^{n-l}\tilde{\Delta}_{nn'}^{(p_l^*)l}\chi_{n'lm}(\varsigma,\vec{r}), \tag{8}$$

where

$$\tilde{\Delta}_{nn'}^{(p_l^*)l} = \frac{\Gamma(q_n^*+1)}{(n-(l+1))!}\sqrt{(2n')!}\;\tilde{a}_{nn'+l}^{(p_l^*)l}. \tag{9}$$

The $\mathcal{L}^{(p_l^*)}$- SFPs and $\psi^{(p_l^*)}$- SFETOs satisfy the following orthogonality relations:

$$\int_0^\infty e^{-t} t^{p_l^*} L_{nl}^{(p_l^*)} L_{n'l}^{(p_l^*)}(t)dt = \frac{\Gamma(q_n^*+1)}{(n-(l+1))!}\delta_{nn'} \quad (10)$$

$$\int \bar{\psi}_{nlm}^{(p_l^*)^*}(\zeta,\vec{r})\psi_{n'l'm'}^{(p_l^*)}(\zeta,\vec{r})d^3\vec{r} = \delta_{nn'}\delta_{ll'}\delta_{mm'}, \quad (11)$$

where

$$\bar{\psi}_{nlm}^{(p_l^*)^*}(\zeta,\vec{r}) = \frac{(n-(l+1))!}{\Gamma(q_n^*+1)}\frac{1}{(2\zeta r)^{2-p_l^*}}\psi_{nlm}^{(p_l^*)}(\zeta,\vec{r})$$

$$= \bar{R}_{nl}^{(p_l^*)}(\zeta,r)S_{lm}(\theta,\phi) \quad (12)$$

$$\bar{R}_{nl}^{(p_l^*)}(\zeta,r) = \frac{(n-(l+1))!}{\Gamma(q_n^*+1)}\frac{1}{(2\zeta r)^{2-p_l^*}}R_{nl}^{(p_l^*)}(\zeta,r). \quad (13)$$

## 3. Combined one- and two-center one-range addition theorems for $\chi$-NISTOs

To obtain the combined one-range addition theorems presented in this article we use for $\chi$-NISTOs the following the series expansion relation in terms of complete sets of $\psi^{(p_l^*)}$-SFETOs:

$$\chi_{k*}(\beta,\vec{r}_b) = \sum_{\mu=1}^{\infty}\sum_{\nu=0}^{\mu-1}\sum_{\sigma=-\nu}^{\nu}\Delta_{qk^*}^{(p_\nu^*)\nu\sigma,\upsilon s}$$

$$\times(\xi,\beta;\vec{R}_{ab})\psi_q^{(p_\upsilon^*}(\xi,\vec{r}_a), \quad (14)$$

where $k^* = u^*\upsilon s$, $q = \mu\nu\sigma$, $0<\beta<\infty$, $0<\xi<\infty$, $\vec{R}_{ab} = \vec{R}_b - \vec{R}_a$ and

$$\Delta_{\mu u^*}^{(p_\nu^*)\nu\sigma,\upsilon s}(\xi,\beta;\vec{R}_{ab}) = \int \bar{\psi}_q^{(p_\nu^*)}(\xi,\vec{r}_a)\chi_{k^*}(\beta,\vec{r}_b)d^3\vec{r}$$

$$= \frac{(\mu-(\nu+1))!}{\Gamma(q_n^*+1)}\int \frac{1}{(2\zeta r)^{2-p_\nu^*}}\psi_q^{(p_\nu^*)^*}$$

$$\times(\xi,\vec{r}_a)\chi_{k^*}(\beta,\vec{r}_b)d^3\vec{r}. \quad (15)$$

Using (8) in Eq. (14) we obtain for the two-center one-range addition theorems of $\chi$-NISTOs the following expression:

$$\chi_{k^*}(\beta,\vec{r}_b) = \sum_{\mu=1}^{\infty}\sum_{\nu=0}^{\mu-1}\sum_{\sigma=-\nu}^{\nu}\sum_{u=1}^{\nu-\nu}\tilde{W}_{\mu u,u^*}^{(p_\nu^*)\nu\sigma,\upsilon s}$$

$$\times(\xi,\beta;\vec{R}_{ab})\chi_k(\xi,\vec{r}_a), \quad (16)$$

where $k = u\nu\sigma$ and

$$\tilde{W}_{\mu u,u^*}^{(p_\nu^*)\nu\sigma,\upsilon s}(\xi,\beta;\vec{R}_{ab})$$

$$= \tilde{\Delta}_{\mu u}^{(p_\nu^*)\nu}\Delta_{\mu u^*}^{(p_\nu^*)\nu\sigma,\upsilon s}(\xi,\beta;\vec{R}_{ab}). \quad (17)$$

Now we evaluate the integral (15) which is defined in the molecular coordinate system. For this purpose, we move on to the lined-up coordinate systems. Then, using method set out in a previous paper [6], it is easy to find the relations

$$\Delta_{\mu u^*}^{(p_\nu^*)\nu\sigma,\upsilon s}(\xi,\beta;\vec{R}_{ab}) = \sum_{\lambda=0}^{\min(\nu,\upsilon)}\sum_{L=|\nu-\upsilon|}^{\nu+\upsilon}T_{\nu\sigma,\upsilon s}^{\lambda L^*}\Delta_{\mu u^*}^{(p_\nu^*)\nu\lambda,\upsilon\lambda}$$

$$\times(\xi,\beta;R_{ab})S_{LM}^*(\Theta_{ab},\Phi_{ab}) \quad (18)$$

$$\Delta_{\mu u^*}^{(p_\nu^*)\nu\lambda,\upsilon\lambda}(\xi,\beta;R) = \frac{(\mu-(\nu+1))!}{\Gamma(q_\mu^*+1)}$$

$$\times\int \frac{1}{(2\zeta r)^{2-p_\nu^*}}\psi_{\mu\nu\lambda}^{(p_\nu^*)^*}(\xi,\vec{r}_a)\chi_{u^*\upsilon\lambda}(\beta,\vec{r}_b)d^3\vec{r} \quad (19)$$

where $M = -\sigma + s$ and $R = R_a b$. Here, $T_{\nu\sigma,\upsilon s}^{\lambda L}(\Theta_{ab},\Phi_{ab})$ and $\Delta_{\mu u^*}^{(p_\nu^*)\nu\lambda,\upsilon\lambda}(\xi,\beta;R)$ are the rotation coefficients [9] and the expansion coefficients in lined-up coordinate systems, respectively,

$$\Delta_{\mu u^*}^{(p_\nu^*)\nu\lambda,\upsilon\lambda}(\xi,\beta;R) = \frac{(\mu-(\nu+1))!}{\Gamma(q_\mu^*+1)}\sum_{k=1}^{\mu-\nu}\tilde{\Delta}_{\mu k}^{(p_\nu^*)\nu}$$

$$\times\frac{(1+\tau)^{p_\nu^*+k-\frac{3}{2}}(1-\tau)^{u^*+\frac{1}{2}}}{\sqrt{(2k)!\Gamma(2u^*+1)}}$$

$$\times\sum_{\gamma=-\lambda}^{\nu}\sum_{\omega=\lambda}^{\upsilon}\sum_{q=0}^{\gamma+\omega}g_{\gamma\omega}^q(\nu\lambda,\upsilon\lambda)\rho^{\gamma+\omega+1}$$

$$\times[\rho^{N^*+N'^*}Q_{N^*+N'^*}^q(\rho,\tau)], \quad (20)$$

where $N^* = p_\nu^*+k-\gamma-2$, $N'^* = u^*-\omega$, $\rho = (R/2)(\xi+\beta)$, $\tau = \xi-\beta/\xi+\beta$ and

$$[\rho^{N^*+N'^*}Q_{N^*+N'^*}^q(\rho,\tau)] = \int_1^\infty\int_{-1}^1(\mu'\nu')^q$$

$$\times[\rho(\mu'n+\nu')]^{N^*}[\rho((\mu'n+\nu')]^{N^*}e^{-\rho\mu'-\rho\tau\nu'}d\mu'd\nu'$$

$$= \int_1^\infty\int_{-1}^1(\mu'\nu')^q[\rho(\mu'+\nu')]^{n+\eta^*}$$

$$\times[\rho(\mu'-\nu')]^{n'+\eta'*}e^{-\rho\mu'-\rho\tau\nu'}d\mu'd\nu' \quad (21)$$

are the auxiliary functions with noninteger indices. Here, $N^* = n+\eta^*$, $0<\eta^*<1$, $N'^* = n'+\eta'^*$, $0<\eta'^*<1$; the indices $n$ and $n'$ are the integral parts of $N^*$ and $N'^*$, respectively.

For the evaluation of auxiliary functions (21), we use the series expansion of $x^{\eta^*}$ derived with the help of $\mathcal{L}^{(p_l^*)}$-SFPs,

$$x^{\eta^*} = \sum_{u=\nu+1}^{\infty}\sum_{k=\upsilon+1}^{u}\tilde{Y}_{uk,\eta^*}^{(p_\nu^*)\nu}x^k \quad (22)$$

$$\tilde{Y}_{uk,\eta^*}^{(p_\nu^*)\nu} = \tilde{a}_{uk}^{(p_l^*)\nu}\frac{\Gamma(u-\eta^*)\Gamma(\eta^*-\alpha^*+\upsilon+2))}{[u-(\upsilon+1)]!\Gamma(\upsilon+1-\eta^*)}, \quad (23)$$

where $x = \rho(\mu' \pm \nu')$. Using Eq. (22) in (21), the quantities $[\rho^{N^*+N'^*} Q^q_{N^*+N'^*}(\rho,\tau)]$ are expressed through the $Q^q$-IAFs,

$$\rho^{N^*+N'^*} Q^q_{N^*+N'^*}(\rho,\tau) = \sum_{u=\nu+1}^{\infty}\sum_{k=\upsilon+1}^{u} \tilde{Y}^{(p^*_\nu)\nu}_{uk,\eta^*} \times \sum_{u'=\nu'+1}^{\infty}\sum_{k'=\upsilon'+1}^{u'} \tilde{Y}^{(p'^*_\nu)\nu'}_{u'k',\eta'^*} \rho^{N+N'} Q^q_{NN'}(\rho,\tau), \tag{24}$$

$$Q^q_{NN'}(\rho,\tau) = \int_1^\infty \int_{-1}^1 (\mu'\nu')^q \times (\mu'+\nu')^N (\mu'-\nu')^{N'} e^{-\rho\mu'-\rho\tau\nu'} d\mu' d\nu' \tag{25}$$

where $N = k + n$ and $N' = k' + n'$. The properties of $Q^q_{NN'}$ are described in the previous papers [6,10]. Using Eq. (20) in (17), it is easy to show that the expansion coefficients $\tilde{W}^{(p^*_\nu)\nu\sigma,\upsilon s}_{\mu u,u^*}(\xi,\beta;\vec{R}_{ab})$ occurring in (16) for the one-range addition theorems of $\chi$-NISTOs are defined as for $R_{ab} \neq 0$

$$\tilde{W}^{(p^*_\nu)\nu\sigma,\upsilon s}_{\mu u,u^*}(\xi,\beta;\vec{R}_{ab}) = \tilde{\Delta}^{(p^*_\nu)\nu}_{\mu u} \times \sum_{\lambda=0}^{\min(\nu,\upsilon)} \sum_{L=|\nu-\upsilon|}^{\nu+\upsilon} T^{\lambda L^*}_{\nu\sigma,\upsilon s} \Delta^{(p^*_\nu)\nu\lambda,\upsilon\lambda}_{\mu u^*} \times (\xi,\beta;R_{ab}) S^*_{LM}(\Theta_{ab},\Phi_{ab}), \tag{26}$$

for $R_{ab} = 0$

$$\tilde{W}^{(p^*_\nu)\nu\sigma,\upsilon s}_{\mu u,u^*}(\xi,\beta) = \tilde{W}^{(p^*_\nu)\nu\sigma,\upsilon s}_{\mu u,u^*}(\xi,\beta;0) = \delta_{\nu\upsilon}\delta_{\sigma s}\tilde{W}^{(p^*_\nu)\nu\sigma,\upsilon s}_{\mu u,u^*}(\xi,\beta) \tag{27}$$

where

$$\tilde{W}^{(p^*_\nu)\nu}_{\mu u,u^*}(\xi,\beta) = \tilde{\Delta}^{(p^*_\nu)\nu}_{\mu u} \Delta^{(p^*_\nu)\nu}_{\mu u^*}(\xi,\beta) \tag{28}$$

$$\Delta^{(p^*_\nu)\nu}_{\mu u^*}(\xi,\beta) = \frac{(\mu-(\upsilon+1)!)}{\Gamma(q^*_\mu+1)} \times \int_0^\infty (2\xi r)^{p^*_\upsilon-2} R^{P^*_\upsilon}_{\mu\upsilon}(\xi,r) R_{u^*}(\beta,r) r^2 dr$$
$$= \frac{(\mu-(\nu+1))!}{\Gamma(q^*_\mu+1)} \sum_{k=1}^{\mu-\upsilon} \tilde{\Delta}^{(p^*_\upsilon)\upsilon}_{\mu k} \frac{\Gamma(k+p^*_\upsilon+u^*-1)}{\sqrt{(2k)!\Gamma(2u^*+1)}} \times \left(\frac{2\xi}{\xi+\beta}\right)^{k+p^*_\upsilon-3/2} \left(\frac{2\beta}{\xi+\beta}\right)^{u^*+1/2}. \tag{29}$$

As can be seen from Eqs. (26) and (27), the one-center addition theorems are the special cases of the two-center one-range addition theorems of $\chi$-NISTOs,

$$\chi^*_k(\beta,\vec{r}) = \sum_{\mu=\upsilon+1}^{\infty}\sum_{u=\upsilon+1}^{\mu} \tilde{W}^{(p^*_\nu)\nu}_{\mu u,u^*}(\xi,\beta)\chi_k(\xi,\vec{r}), \tag{30}$$

where $k^* = u^*\upsilon s$, $k = u\upsilon s$ and

$$\tilde{W}^{(p^*_\nu)\nu}_{\mu u,u^*}(\xi,\beta) = \begin{cases} \tilde{\Delta}^{(p^*_\nu)\nu}_{\mu u} \sum_{k=1}^{\mu-\upsilon} \tilde{\Delta}^{(p^*_\nu)\nu}_{\mu k} \frac{(\mu-(\upsilon+1))!\Gamma(k+p^*_\upsilon+u^*-1)}{\Gamma(q^*_\mu+1)\sqrt{(2k)!\Gamma(2u^*+1)}} \left(\frac{2\xi}{\xi+\beta}\right)^{k+p^*_\upsilon-3/2} \left(\frac{2\beta}{\xi+\beta}\right)^{u^*+1/2} & \text{for} \quad \xi \neq \beta \quad (31) \\ = \frac{\Gamma(q^*_\mu+1)}{(\mu-(\upsilon+1))!} \left(\frac{(2u)!}{\Gamma(2u^*+1)}\right)^{\frac{1}{2}} \tilde{a}^{(\alpha^*)\upsilon}_{\mu u+\upsilon} \sum_{k=1}^{\mu-\upsilon} \tilde{a}^{(\alpha^*)\upsilon}_{\mu k+\upsilon}\Gamma(k+p^*_\upsilon+u^*-1) & \text{for} \quad \xi = \beta \quad (32) \end{cases}$$

Accordingly, by the use of $Q^q$-IAFs, complete sets of $\psi^{(p^*_l)}$-SFETOs and $\mathcal{L}^{(p^*_l)}$-SFPs, we have derived a large number ($-\infty < \alpha \leq 2$ and $\infty < \alpha \leq 3$) of the unified one- and two-center one-range addition theorems for the $\chi$-NISTOs.

## 4. Application

As an application of one-range addition theorems (16) we calculate the atomic nuclear attraction integrals of $\chi$-NISTOs and $V$-NICPs defined as

$$I^{q^*}_{p^*p'^*}(\varsigma,\varsigma') = \int \chi^*_{p^*}(\varsigma,\vec{r})\chi'^*_{p}(\varsigma,\vec{r}) V^{q^*}(\vec{r}) d^3\vec{r}, \tag{33}$$

where $p^* = n^*lm$, $p'^* = n'^*l'm'$, $q^* = \mu^*\nu\sigma$, $\mu^* \geq 0$ and

$$V^{\mu^*\nu\sigma}(\vec{r}) = V^{\mu^*}(r) S_{\nu\sigma}(\theta,\phi) \tag{34}$$

$$V^{\mu^*}(r) = \frac{1}{r^{1-\mu^*}} \tag{35}$$

It is easy to show that

$$I^{q^*}_{p^*p'^*}(\varsigma,\varsigma') = C^{\nu|\sigma|}(lm,l'm') A^\sigma_{mm'} I_{n^*n'^*}(\varsigma,\varsigma') \tag{36}$$

$$I^{n^*n'^*}_{\mu^*} = \int_0^\infty R_{n^*}(\varsigma,r) R_{n'^*}(\varsigma',r) V^{\mu^*}(r) r^2 dr, \tag{37}$$

where $C^{\nu|\sigma|}(lm,l'm')$ and $A^\sigma_{mm'}$ are the generalized Gaunt and Kronecker's $\delta$ coefficients, respectively [6].

The analytical expression for integral (37) is determined as follows:

$$I^{\mu^*}_{n^*n'^*}(\varsigma,\varsigma') = \left[\frac{\Gamma(2N^*+1)}{\Gamma(2n^*+1)\Gamma(2n'^*+1)}\right]^{1/2} \times \frac{\tau^{3/2}}{2^{N^*+1/2}} (1+t)^{n^*+1/2} (1-t)^{n'^*+1/2} I^{\mu^*}_{N^*}(\tau) \tag{38}$$

TABLE I. Numerical values of atomic nuclear attraction integrals of $\chi$-NISTOs and $V$-NICPs calculated by analytical and series expansion relations (in a.u.).

| $\mu^*$ | $n^*$ | $n'^*$ | $\zeta$ | $\zeta'$ | Eq. (38) | $\alpha^*$ | Eq. (43) $N=60$ | Eq. (43) $N=80$ |
|---|---|---|---|---|---|---|---|---|
| 0.9 | 6.3 | 4.9 | 7.0397 | 2.2886 | 0.3141510287 | 1 | 0.3141509034 | 0.3141510230 |
| | | | | | | 0 | 0.3141510925 | 0.3141510200 |
| | | | | | | -1 | 0.3141510309 | 0.3141510326 |
| | | | | | | -1.8 | 0.3141510045 | 0.3141510303 |
| | | | | | | -2 | 0.3141510059 | 0.3141510292 |
| | | | | | | -2.3 | 0.3141510125 | 0.3141510278 |
| | | | | | | -2.8 | 0.3141510297 | 0.3141510266 |

$$I_{N^*}^{\mu^*}(\tau) = \int_0^\infty R_{N^*}(\tau,r)V^{\mu^*}(r)r^2dr = \frac{\Gamma(N^*+\mu^*+1)2^{N^*+1/2}}{[\Gamma(2N^*+1)]^{1/2}\tau^{\mu^*+1/2}}, \tag{39}$$

where $N^* = n^* + n'^* - 1$, $\tau = \zeta + \zeta'$, $t = \zeta - \zeta'/\zeta + \zeta'$. The Eqs. (38) and (39) describe the analytical approach of nuclear attraction integrals of $\chi$-NISTOs and $V$-NICPs.

To establish the series expansion relations, we use Eq. (22) for the SF power series of radial part of the $\chi$-NISTOs occurring in Eq. (39),

$$R_{N^*}(\tau,r) = \sum_{k=l+1}^{\infty}\sum_{\eta=l+1}^{k} \tilde{Y}_{k\eta,\eta^*}^{(p_l^*)l} \times \left[\frac{(2(N+\eta))!}{\Gamma(2N^*+1)}\right]^{1/2} R_{N+\eta}(\tau,r), \tag{40}$$

where $N^* = N + \eta^*$, $0 < \eta^* < 1$ and $N$ is the integer part of $N^*$. Then, we obtain:

$$I_{N^*}^{\mu^*}(\tau) = \sum_{k=l+1}^{\infty}\sum_{\eta=l+1}^{k} \tilde{Y}_{k\eta,\eta^*}^{(p_l^*)l} \times \left[\frac{(2(N+\eta))!}{\Gamma(2N^*+1)}\right]^{1/2} J_{N+\eta}^{\mu^*} \tag{41}$$

$$J_n^{\mu^*} = \int_0^\infty R_n(\tau,r)V^{\mu^*}(r)r^2dr = \frac{\Gamma(n+\mu^*+1)2^{n+1/2}}{[(2n)!]^{1/2}\tau^{\mu^*1/2}} \tag{42}$$

where $n = N + \eta$. The substitution (41) into Eq. (38) gives the following series expansion relations:

$$I_{n^*n'^*}^{\mu^*}(\zeta,\zeta') = N_{n^*n'^*}(t)\sum_{k=l+1}^{\infty}\sum_{\eta=l+1}^{k} \tilde{Y}_{k\eta,\eta^*}^{(p_l^*)l} \times \left[\frac{\Gamma(\mu^*+N+\eta+1)}{\sqrt{(2N+1)!}2^{N^*-(N+\eta)}\tau^{\mu^*-1}}\right]^{1/2} \tag{43}$$

where

$$N_{n^*n'^*}(t) = \frac{(1+t)^{n^*+1/2}(1-t)^{n'^*+1/2}}{[\Gamma(2n^*+1)\Gamma(2n'^*+1)]^{1/2}} \tag{44}$$

Thus, we have derived the analytical and series expansion formulas for the atomic nuclear attraction integrals of $\chi$-NISTOs and $V$-NICPs using one-center one-range addition theorems established with the help of $\psi^{(p_l^*)}$-SFETOs and $\mathcal{L}^{(p_l^*)}$-SFPs in standard convention.

The convergence properties of nuclear attraction integrals of $\chi$-NISTOs and $V$-NICPs have been tested. The results of calculations for some values of parameters are shown in Table I. The quantities $N$ in this table are the number of terms over summation indices $k$. As can be seen from this table, the convergence of series for $\chi$-NISTOs and $V$-NICPs is guaranteed for all the values of parameters of $\chi$-NISTOs and $V$-NICPs.

## 5. Conclusion

In this work, with the help of $\mathcal{L}^{(p_l^*)}$-SFPs and $\psi^{(p_l^*)}$-SFETOs, the combined one- and two-center one-range addition theorems for $\chi$-NISTOs in terms of $Q^q$-IAFs auxiliary functions are obtained. The presented series expansion formulas can be used in a study of different problems arising in the quantum chemistry. They can be especially useful tools in the electronic structure calculations when $\chi$-NISTOs are used as basis functions. The suggested one-range addition theorems will also be of interest for the broader multidisciplinary areas, which span over fields as diverse as physics, chemistry, biology, astrophysics and mathematics. It should be noted that the origin of the obtained one-range addition theorems presented in this work is the quantum forces which are analog of the self-frictional forces introduced by Lorentz in classical electrodynamics [11-13].

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