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Translations of Fields Represented by Spherical-Harmonic Expansions for Molecular Calculations

III. Translations of Reduced Bessel Functions, Slater-Type s-Orbitals, and Other Functions

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Addition theorems are derived for reduced Bessel functions $r^{N+1}k_N(\beta r)$, where k_N is a modified spherical Bessel function, and for functions $r^{-N}b_N(\beta r)$ with b_N being a spherical Bessel, Neumann, or Hankel function. Furthermore, addition theorems are derived for the logarithm, the Gaussian function, and the function $(r\cos\theta)^N$, i.e. powers of the scalar product $(\boldsymbol{e}_z \cdot \boldsymbol{r})$. With the help of the addition theorem of reduced Bessel functions one obtains a one-center expansion of Slater-type s-orbitals, which can be compared with Barnett and Coulson's zeta function expansion. This yields a closed form expression of the zeta function.

The given addition theorems for the functions considered, which in fact describe translations of these functions, are expansions in which the radial and angular dependencies are separated. The angular dependencies are expressed by spherical harmonics, as it is most appropriate for physical applications. For the derivations of the addition theorems use is made of the concept of generating functions for Gegenbauer polynomials. It turns out that the coefficients $T_{l,k}^N$ of the one-center expansion of r^N, which was given in the preceding paper, play a dominant role in all the expansions considered. Possible fields of applications of the theorems are scattering theory, the calculation of stationary states and other problems in molecular theory.

Key words: Bessel functions, Slater-type s-orbitals, addition theorems of ~ – Zeta function – Gegenbauer polynomials, spherical harmonics, expansions in ~

1. Introduction

Difficulties encountered in evaluating quantum mechanical matrix elements can often be surmounted only by using expansions of the operators or orbitals which occur, provided such expansions exist.

In the present article certain new expansion theorems are derived for reduced Bessel functions $r^{N+1}k_N(\beta r)$ and for functions $r^{-N}j_N(\beta r)$, where j_N is a spherical and k_N is a modified spherical Bessel function. Furthermore, expansion theorems are given for scalar Slater-type orbitals $r^N e^{-\beta r}$, for the Gaussian function $\exp[-(kr)^2]$, for the logarithm $\log(kr)$, and for powers of $(r \cdot \cos\theta)$ given by $(\boldsymbol{e}_z \cdot \boldsymbol{r})^N$. These functions are of great physical interest because they are contained in many different quantum mechanical operators and wave functions. They are also needed in a wide variety of physical problems as, for instance, the theory of interatomic interactions and scattering theory.

The expansion theorems presented have the form of addition theorems with explicitly given coefficients suitable for practical applications. In the expansions the angular dependencies are separated from the radial ones and expressed by surface spherical harmonics. These expansions in spherical harmonics represent translations of fields defined by the functions considered.

The derivations and results given in the present article are based on the treatments given in the two preceding papers of this series [1, 2], hereafter referred to as I and II, respectively.

2. Expansions of Gegenbauer Polynomials in Terms of Legendre Polynomials

In the following some addition theorems will be discussed that can be expressed by expansions in spherical harmonics, but which originally are connected with expansions in Gegenbauer polynomials.

The generating function for the Gegenbauer polynomials $C_k^\lambda(\zeta)$ with $\zeta = \cos\omega$ is given by the expansion of $(r')^{-\lambda}$ according to

$$(r_<^2 + r_>^2 - 2r_< r_> \zeta)^{-\lambda/2} = r_>^{-\lambda} \sum_{k=0}^{\infty} C_k^{\lambda/2}(\zeta)(r_</r_>)^k , \tag{2.1a}$$

$$\boldsymbol{r}' = \boldsymbol{r} - \boldsymbol{R}, \quad r_< = \mathrm{Min}(r, R), \quad r_> = \mathrm{Max}(r, R), \tag{2.1b}$$

which is a generalization of Eq. (I.3.16), because $C_k^{1/2} = P_k$. In the present paper, the power λ of the potential $1/r'$ may be restricted to integer values N. A comparison of Eq. (2.1) with Eq. (II.3.19) yields immediately

$$C_k^{N/2}(\zeta) = \sum_{l=[0,1]}^{k}{}^{(2)} (2l+1) T_{l,k}^{-N} P_l(\zeta) , \tag{2.2}$$

if the summations over l and k in Eq. (II.3.19) are interchanged according to Eq. (II.3.7). Because of the orthogonality of the Legendre polynomials due to

$$\int_{-1}^{1} d\zeta P_k(\zeta) P_l(\zeta) = [(2l+1)/2]^{-1} \delta_{k,l} , \tag{2.3}$$

it holds that

$$\int_{-1}^{1} d\zeta P_l(\zeta) C_k^{N/2}(\zeta) = 2T_{l,k}^{-N} . \tag{2.4}$$

Hence, the coefficients of the expansion of Gegenbauer polynomials in terms of Legendre polynomials are represented by the $T_{l,k}^{-N}$. These coefficients are also given by Rainville [3] in a different form. The degrees and the parity behavior of the polynomials P_l and $C_k^{N/2}$ determine the limits of the indices k and l as discussed in Section 3 of II.

The relation Eq. (2.1) is in fact a formula for the translation of the function $r^{-\lambda}$ which is represented by an expansion in terms of Gegenbauer polynomials. With the help of Eq. (2.2) this representation can be changed into one which is given by an expansion in a series of Legendre polynomials.

For some functions different from $(r')^{-\lambda}$, which may also be called generating functions for the C_k^ν, there exist expansions in terms of Gegenbauer polynomials with explicitly known coefficients. With the help of Eq. (2.2), these expansions can be transformed into series of functions of $r_<$ and $r_>$ multiplied with Legendre polynomials which contain the angular dependence, as is desirable for physical applications. The main advantage of an expansion in terms of Legendre polynomials is based on the fact that due to the addition theorem given in Eq. (I.3.19) the variables $\boldsymbol{r}_<$ and $\boldsymbol{r}_>$ are completely separated in each term of the series. This is actually a criterion for an addition theorem, as has been discussed in connection with Eq. (I.3.15). However, the so-called addition theorem of the Gegenbauer polynomials [4], which corresponds to Eq. (I.3.19), does not allow the separation of the variables $\boldsymbol{r}_<$ and $\boldsymbol{r}_>$ completely. Therefore, by transforming Gegenbauer polynomials to Legendre polynomials within a given expansion for a certain function, it is possible to derive real addition theorems as they are needed for applications.

3. Translations of Reduced Bessel Functions

Shavitt [5] emphasized the physical importance of the functions $(\beta r)^\lambda K_\lambda(\beta r)$, which he called reduced Bessel functions, where K_λ defines the second solution of the modified Bessel differential equation [6, 7] and $\lambda > 0$, $\beta > 0$. The parameter β should not be confused with the function β_q^p defined by Eq. (II.3.6a). These reduced Bessel functions are regular at the origin and decrease exponentially as $r \to \infty$. For $\lambda = N + (1/2)$, N being a positive integer, they can be represented by modified spherical Bessel functions k_N with $x = (\beta r)$ according to

$$x^{N+1} k_N(x) = (2/\pi)^{1/2} x^{N+(1/2)} K_{N+(1/2)}(x) . \tag{3.1}$$

Putting $x^{N+1} k_N(x) = \hat{k}_{N+(1/2)}(x)$, these functions can be represented by [5, 8]

$$\hat{k}_{N-(1/2)}(x) = e^{-x} \sum_{q=1}^{N} \frac{(2N-q-1)!}{(q-1)!(2N-2q)!!} x^{q-1} . \tag{3.2}$$

Because these functions are polynomials multiplied by $\exp(-x)$, Shavitt discussed the possibility of using them as the radial part of a generalized type of orbital in atomic and molecular calculations.

In the following a formula for the translation of reduced Bessel functions will be derived which may prove helpful for practical applications.

Gegenbauer's addition theorem [9, 10] allows one to express the function $(\beta r')^\nu K_{-\nu}(\beta r')$ by an infinite series such that each term of the expansion essentially consists of a product $I_{\nu+n}(\beta r_<) \cdot K_{\nu+n}(\beta r_>)$ and a Gegenbauer polynomial depending on $\zeta = \cos\omega$, whereby:

$$r' = |\boldsymbol{r}_> - \boldsymbol{r}_<| = (r_<^2 + r_>^2 - 2r_< r_> \cos\omega)^{1/2} . \tag{3.3}$$

The function I_ν is the first solution of the modified Bessel equation [7]. Using $K_\nu(x) = K_{-\nu}(x)$ and expanding the Gegenbauer polynomials in terms of Legendre polynomials according to Eq. (2.2), one arrives at a new expansion in which the angular variables are completely separated. The addition theorem for the reduced

Bessel functions has the form

$$\hat{k}_{N-(1/2)}(\beta r') = 4\pi(-1)^N[(2N-1)!!]^{-1}(\beta r_<\beta r_>)^{N-(1/2)}$$
$$\cdot \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=l}^{l+2N}{}^{(2)} (2n-2N+1) T_{l,n}^{2N-1} I_{n-N+(1/2)}(\beta r_<)$$
$$\cdot K_{n-N+(1/2)}(\beta r_>) Y_l^{m*}(\boldsymbol{r}_</r_<) Y_l^m(\boldsymbol{r}_>/r_>) . \quad (3.4)$$

4. Translations of Slater-Type *s*-Orbitals

The addition theorem for reduced Bessel functions given by Eq. (3.4) is closely connected with the translation formula for Slater-type *s*-orbitals, which is usually written as

$$(r')^{N-1} e^{-\beta r'} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} (r_< r_>)^{-1/2} \zeta_{N,l}(\beta; r, R) Y_l^{m*}(\boldsymbol{r}_</r_<) \cdot Y_l^m(\boldsymbol{r}_>/r_>) , \quad (4.1)$$

where the zeta-function $\zeta_{N,l}$ was introduced by Barnett and Coulson [11, 12].

It is possible to invert the relationship Eq. (3.2), yielding the result

$$x^{N-1} e^{-x} = \sum_p \frac{(-1)^{N-p} N!}{(2p-N)!(2N-2p)!!} \hat{k}_{p-(1/2)}(x) . \quad (4.2a)$$

The summation index p runs in steps of one from Min p to Max $p=N$ with

$$\text{Min}\, p = \begin{cases} N/2 & \text{for } N \text{ even} . \\ (N+1)/2 & \text{for } N \text{ odd} . \end{cases} \quad (4.2b)$$

This identity can be shown to hold by performing a complete induction with respect to N, using the well known recursion formula for Bessel functions [7], which for the reduced Bessel functions reads

$$x^2 \hat{k}_{\nu-(1/2)}(x) = \hat{k}_{\nu+(3/2)}(x) - (2\nu-1)\hat{k}_{\nu+(1/2)}(x) . \quad (4.3)$$

The addition theorem Eq. (3.4) can be applied to each term of the expansion Eq. (4.2a). If the result is compared with the expansion Eq. (4.1), one obtains the zeta function in closed form by the following finite series

$$\zeta_{N,l}(\beta; r, R) = \beta^{-N} \sum_p \sum_n{}^{(2)} \frac{(-1)^N N!(2n-2p+1)}{(2p-1)!!(2p-N)!(2N-2p)!!} T_{l,n}^{2p-1}$$
$$\cdot (\beta r_<)^p (\beta r_>)^p I_{n-p+(1/2)}(\beta r_<) K_{n-p+(1/2)}(\beta r_>) . \quad (4.4)$$

Again, the summation index p runs in steps of one from Min p defined by Eq. (4.2b) to Max $p=N$, whereas the summation index n runs in steps of two between the limits $l \leqq n \leqq l+2p$.

Barnett and Coulson [11, 12] gave recurrence formulas for computing zeta functions of higher indices N and l, respectively, by starting from $\zeta_{0,l}$ and $\zeta_{N,0}$. Silverstone [13] showed that it is possible to construct the zeta function $\zeta_{N,l}$ by successive differentiation, which if done would lead to a less compact formula, containing products of I and K functions of *different* order.

5. Addition Theorems Involving Spherical Bessel Functions

If Gegenbauer's addition theorem [9, 10] is applied to the function $(kr')^{-\nu}J_\nu(kr')$, each term of the expansion consists of a product $J_{\nu+n}(kr_<)J_{\nu+n}(kr_>)$ and a Gegenbauer polynomial depending on $\zeta=\cos\omega$. The function $J_\nu(kr')$ is the Bessel function of the first kind [7]. If again Eq. (2.2) is used to expand the Gegenbauer polynomials in terms of Legendre polynomials, one obtains the following new expansion in spherical harmonics.

For the spherical Bessel functions $b_l(x)$, which are of physical interest, the addition theorem is given by

$$(\beta r')^{-L}b_L(\beta r')=4\pi(2L-1)!!(\beta r_<)^{-L}(\beta r_>)^{-L}$$
$$\cdot\sum_{l=0}^{\infty}\sum_{n=l}^{\infty}{}^{(2)}\sum_{m=-l}^{l}(2L+2n+1)T_{l,n}^{-2L-1}j_{L+n}(\beta r_<)b_{L+n}(\beta r_>)$$
$$\cdot Y_l^{m*}(\boldsymbol{r}_</r_<)Y_l^m(\boldsymbol{r}_>/r_>)\,. \tag{5.1}$$

Here, $b_l(x)$ with real x stands for spherical Bessel, Neumann, or Hankel functions defined by Eqs. (5.2a)–(5.2d):

$$j_l(x)=(\pi/2x)^{1/2}J_{l+(1/2)}(x)\,, \tag{5.2a}$$
$$n_l(x)=(-1)^{l+1}(\pi/2x)^{1/2}J_{-l-(1/2)}(x)\,, \tag{5.2b}$$
$$h_l^{(1)}(x)=j_l(x)+in_l(x)\,, \tag{5.2c}$$
$$h_l^{(2)}(x)=j_l(x)-in_l(x)\,. \tag{5.2d}$$

The modified spherical Bessel functions are defined by

$$i_l(x)=i^{-l}j_l(ix)\,, \tag{5.2e}$$
$$k_l(x)=-i^{-l}h_l^{(1)}(ix)\,. \tag{5.2f}$$

The modified spherical Bessel function i_l should not be confused with the imaginary unit i.

The addition theorem for $(\beta r')^{-L}k_L(\beta r')$ is obtained from Eq. (5.1) if b_λ is replaced by k_λ and j_{L+n} is substituted by i_{L+n}. The addition theorem for $(\beta r')^{-L}i_L(\beta r')$ is obtained from Eq. (5.1) if b_λ is replaced by i_λ, whereas j_{L+n} is replaced by $(-1)^n i_{L+n}$. In this relationship $r_<$ and $r_>$ may be interchanged.

Except for the case $L=0$ [14], these addition theorems do not seem to have been given before.

6. Addition Theorems for the Logarithm and the Gaussian Function

The logarithm is the generating function for C_n^0 according to

$$\log(kr')=\log(kr_>)-(1/2)\sum_{n=1}^{\infty}C_n^0(\zeta)(r_</r_>)^n \tag{6.1}$$

with $C_0^0(\zeta)=1$, whereas $C_k^0(\cos\omega)=(2/k)\cos(k\omega)$ for $k\neq 0$ [4, 15]. A comparison of the known expansion [16] of $\cos(k\omega)$ in terms of $P_l(\zeta)$ with Eq. (2.2) for $N=0$

yields

$$T^0_{l,k} = -2\beta^k_l \gamma^{k-3}_l, \quad l+k \neq 0, \tag{6.1a}$$

$$T^0_{0,0} = 1, \quad (-1)!! = 1, \quad (-3)!! = -1. \tag{6.1b}$$

With these coefficients, one obtains with the help of Eq. (2.2) the relationship

$$\log(kr')^\lambda = \log(kr_>)^\lambda - (\lambda/2) \sum_{l=0}^{\infty} \sum_{k=l}^{\infty}{}^{(2)} \sum_{m=-l}^{l} (1-\delta_{k,0}) \cdot 4\pi T^0_{l,k}(r_</r_>)^k Y^{m*}_l(\boldsymbol{r}_</r_<) Y^m_l(\boldsymbol{r}_>/r_>). \tag{6.2}$$

The Gaussian function is easy to handle in molecular integrals, mainly because the product of two Gaussians having different centers is itself a Gaussian centered between the original ones [17]. However, the translation of a Gaussian represented by an expansion in spherical harmonics is given by the following more complicated formula, which holds for any v which is a natural number or half an odd integer:

$$e^{-(kr')^2} = \Gamma(v) e^{-(kr_<)^2-(kr_>)^2} \sum_{l=0}^{\infty} \sum_{n=l}^{\infty}{}^{(2)} \sum_{m=-l}^{l} 4\pi(v+n) \cdot T^{-2v}_{l,n}(k^2 r_< r_>)^{-v} I_{v+n}(2k^2 r_< r_>) Y^{m*}_l(\boldsymbol{r}_</r_<) Y^m_l(\boldsymbol{r}_>/r_>). \tag{6.3}$$

This relationship is obtained from Gegenbauer's [18] or Sonine's [19] expansion of $z^\lambda e^{\zeta z}$ in a series of the Neumann type by application of the formula Eq. (2.2). In Eq. (6.3), $I_\mu(z)$ is the modified Bessel function, and $\Gamma(v)$ is the gamma function [20]. Because the variables $\boldsymbol{r}_<$ and $\boldsymbol{r}_>$ are not separated completely in Eq. (6.3), this relation is not an exact addition theorem in the sense of Eq. (I.3.15). It has some flexibility, however, because v can be chosen as required for practical purposes.

Because $C^{1/2}_l = P_l$, Rayleigh's plane wave expansion is a special case of Gegenbauer's plane wave expansion. In the same sense, the expansion Eq. (6.3) for $v = 1/2$ is a special case of the general expansion Eq. (6.3).

7. Translations of Powers of the Scalar Product $(\boldsymbol{e}_z \cdot \boldsymbol{r})$

The function $(\boldsymbol{e}_z \cdot \boldsymbol{r})^N$, where $\boldsymbol{e}_z$ is the unit vector coinciding with the z-axis, is not a scalar function but exhibits an angular dependence. In order to describe a translation of this function, one needs expansions of $(\boldsymbol{e}_z \cdot \boldsymbol{r}')^N$, which are difficult to obtain due to the transformational behavior of non-scalar functions. Therefore, until now the expansions can be given only for translations along the z-axis and for certain regions in space.

Starting from an expansion of $(R - r\cos\omega)^N$ in Gegenbauer polynomials [21], one obtains for $N = -1, -2, -3, \ldots$, if $\boldsymbol{r}_>$ coincides with the z-axis, the formula

$$(r'\cos\theta')^N = (-1)^N(-2N-3)!![(-N-1)!]^{-1} r^N_< \cdot \sum_{l=0}^{\infty} \sum_{k=l}^{\infty}{}^{(2)} (2l+1)(2k-2N-1) T^{2N+1}_{l,k} \cdot \mathcal{Q}_{-N+k-1}(r_>/r_<) P_l(\cos\omega). \tag{7.1}$$

For powers $N=1,2,3,\ldots$, one obtains, if $\boldsymbol{R}$ coincides with the z-axis, the following expansion which holds for $R<r\cos\omega$:

$$(r'\cos\theta')^N = N![4(2N-1)!!]^{-1} r^N \sum_{l=0}^{\infty} \sum_{k=l}^{\infty}{}^{(2)} (2l+1) \cdot (2k-2N-1) T_{l,k}^{2N+1} P_{-N+k-1}(-R/r) P_l(\cos\omega). \tag{7.2}$$

The $\mathcal{Q}_\nu^\mu$ are Legendre functions of the second kind [22]. Those of the first kind [23] obey $P_\nu^\mu(\zeta)=P_{-\nu-1}^\mu(\zeta)$. Equation (7.1) corresponds to case B, Eq. (7.2) corresponds to case A as discussed in Section 3 of I. One case is missing for each formula. A generalization of the formulas to translations in arbitrary directions is not immediately possible because $(\boldsymbol{e}_z \cdot \boldsymbol{r})^N$ does not transform under rotations like a spherical harmonic. These problems and the transformational behavior of non-scalar functions will be dealt with in a subsequent investigation.

8. Summary

For application in physics it is of greatest advantage to have expansions in terms of spherical harmonics instead of other functions. Sometimes, expansions in Gegenbauer polynomials are known. With the help of Eq. (2.2), an expansion of a function in terms of Gegenbauer polynomials can be transformed into an expansion of the same function in a series of Legendre polynomials. If these are expressed by spherical harmonics, use can be made of orthogonality relations and other theorems established in the theory of angular momentum. Therefore, the relationship Eq. (2.2) is useful for the construction of expansions in spherical harmonics which are especially needed in the theory of molecular integrals and intermolecular interactions.

In the present paper translation formulas are derived for the following functions: The expansion theorem for reduced Bessel functions is given by Eq. (3.4), whereas the addition theorem for the related functions $r^{-L} b_L(\beta r)$ is given by Eq. (5.1). The translation formula for scalar Slater-type orbitals $r^N \cdot e^{-\beta r}$ is given by Eqs. (4.1) and (4.4). The relationships Eqs. (6.3), (6.2), (7.1), and (7.2) represent the expansion theorems for the functions $\exp[-(kr)^2]$, $\log(kr)$, and $(\boldsymbol{e}_z \cdot \boldsymbol{r})^N$, respectively.

These expansions, which can be used in many different problems, are particularly useful in quantum mechanical computations. Molecular calculations often require that an atomic orbital be expressed as an expansion in spherical harmonics about a center which is displaced from the orbital's origin. The relevant methods to solve this problem have been reported by Löwdin [24]. Naturally, the main interest was in the translation of Slater-type atomic orbitals which was elaborated by Coolidge [25], Landshoff [26], Löwdin [24, 27], and Barnett and Coulson [11, 12], especially for scalar (s-type) functions. A related problem is the translation of the functions $r^{-L} b_L(\beta r)$ and the translation of reduced Bessel functions, which, as was suggested by Shavitt [5], may be used as the radial part of a generalized type of orbital. It turns out that the expansion theorems for these functions allow the derivation of the explicit form of Barnett-Coulson's zeta function, as given by Eq. (4.4).

Computational aspects arising with the translation of non-scalar Slater-type functions have been considered by Harris and Michels [28]. In view of the remaining difficulties with Slater-type atomic orbitals, use of Gaussian-type orbitals is frequently favored. Although molecular integrals over Gaussian-type orbitals are rather simple, the formula Eq. (6.3) shows that translations of scalar Gaussian functions result in complicated expressions, too. For the special case $\nu = 1/2$, this formula was already given by Sack [14], who also gave expansions in spherical harmonics of the logarithm and spherical Bessel functions of zero order: $j_0(\beta r)$, $n_0(\beta r), \ldots$, which are special cases ($L=0$) of Eq. (5.1). These special addition theorems were rederived by Rafiqullah [29] with the help of a double Bessel transformation.

As expansions in spherical harmonics are most appropriate for the treatment of three-dimensional problems, expansions in terms of $\cos(l\omega)$ may be useful for two-dimensional problems, ω being the angle between $\boldsymbol{r}_<$ and $\boldsymbol{r}_>$. Therefore, Ashour [30] derived expansions of the functions considered by Sack [14] in terms of $\cos(l\omega)$, applying Sack's method which was discussed in I. Because the considered functions are generating functions for the Gegenbauer polynomials C_k^λ, these results can be obtained in a more straightforward way by expressing the $C_k(\cos\omega)$ by the well-known Fourier expansion [31, 32] in terms of $\cos(l\omega)$. Moreover, this makes it possible to derive expansions in terms of $\cos(l\omega)$ for all functions considered in the present article.

So far expansion theorems for scalar functions have been dealt with. The only non-scalar function considered was $(r\cos\theta)^N$, which is no longer invariant under rotations of the coordinate system. The results presented allow the derivation of addition theorems of further non-scalar functions, which will be given in subsequent notes.

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Note Added in Proof. Some research workers elaborated general expressions for Barnett-Coulson's zeta function in order to evaluate molecular integrals. Christoffersen and Ruedenberg [33] arrived at explicit expressions for zeta functions in terms of powers, exponentials, and modified Bessel functions of the first kind using very intricate numerical coefficients. In unpublished work Power and Pitzer [34] used general formulas for computing $\zeta_{N,l}$ in terms of modified Bessel functions, I and K.

It may be advantageous that the explicit expansion for $\zeta_{N,l}$ as given by Eq. (4.4) contains only products of modified Bessel functions I and K of *equal* order. Therefore, the zeta function may be expressed as a finite combination of Barnett and Coulson's functions $\gamma_n(\beta; r, R) = I_{n+(1/2)}(\beta r_<)\ K_{n+(1/2)}(\beta r_>)$. General formulas for the translation of non-scalar Slater-type orbitals [35], which also yield closed-form expressions for Harris and Michels' V-function [28], will be given in forthcoming articles.

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