A new perspective for evaluation of relativistic atomic and molecular integrals.

I. Evaluation of the electron repulsion integrals

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The electron repulsion integrals over the Slater-type orbitals with non–integer principal quantum numbers are considered. These integrals are useful in both non–relativistic and relativistic calculations of many–electron systems. They involve hyper–geometric functions. Due to the non–trivial structure of infinite series that are used to define them, the hyper–geometric functions are practically difficult to compute. Convergence of the series are strictly depends on the values of parameters. Computational issues such as cancellation or round–off error emerge. Relationships free from hyper–geometric functions for expectation values of Coulomb potential \( \langle r^{-1} \rangle \) are derived. These relationships are new and show that the complication coming from two–range nature of Laplace expansion for the Coulomb potential is removed. These integrals also form an initial condition for expectation of a potential with arbitrary power. The electron repulsion integrals are expressed by two finite series of power functions. The methodology given here for evaluation of electron repulsion integrals are adapted to multi–center integrals.

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I. INTRODUCTION

Analytical relationships for the electron repulsion integrals are derived using a series representation for the Coulomb interaction via the Laplace expansion and spherical harmonics addition theorem. Finally, the angular parts are separated. They are represented by Clebsch–Gordan coefficients. The problem is reduced to a solution of two–dimensional radial integral. If Slater–type orbitals with non–integer principal quantum numbers are considered as a basis then, the radial integrals are expressed in terms of incomplete gamma functions \([1, 2]\) or Gauss’s hyper–geometric functions \([2]\). For both cases, incomplete gamma or hyper–geometric functions the convergence should be investigated in well–defined domain. Any representation (recurrence relationship, continued fraction, series expansion formula or asymptotic method) of these special functions depending on the parameters constructs a different domain of convergence \([3–8]\).

The present paper recomposes the evaluation of electron repulsion integrals and free the resulting formulas form special functions or any infinite series representation. Another meaning of such procedure is new relationships for the special functions arising in the atomic and molecular calculations. This work is organized as follows, In the Section II the procedure for the evaluation of electron repulsion integrals is revisited. The next Section III starts with evaluation of radial integrals. The derived new relationships and their mathematical nature are given in this section. The advantages of using the formulas presented in this study in both atomic and molecular calculations are discussed in the last the Section IV.

The Schrödinger–like differential equation solution has recently been generalized to non–integer values of quantum numbers by one of the author \([9]\). The solution is characterized depending to pre–determined sequence of quantum numbers. The Slater–type orbitals take form according to this solution. There exist four variants of the Slater–type orbitals with non–integer principal quantum numbers. They are obtained by simplification of the Laguerre polynomials to highest power of \( r \). In this work, the most common variant of the STOs is considered. The relationships obtained here for this type of STOs are available to be used for any other variant. The considered variant of STOs are given as,

\[
\chi_{n\ell m}(\vec{r}, \zeta) = R_n(\zeta, r) S_{\ell m}(\theta, \varphi) = N_n(\zeta) r^{n-1} e^{-\zeta r} S_{\ell m}(\theta, \varphi), \tag{1}
\]

here, \( n \in \mathbb{R}, \zeta, \zeta > 0 \) is the orbital parameters,

\[
N_n(\zeta) = \frac{(2\zeta)^{n+1/2}}{\sqrt{\Gamma(2n+1)}} \tag{2}
\]
II. REVISITING THE ELECTRON REPULSION INTEGRALS

One–center electron repulsion integrals over STOs are given as [11],

\[ J_{p_1, r_1', p_2, r_2'} (\zeta_1, \zeta_1', \zeta_2, \zeta_2') = \int \chi_{p_1}^* (r_1) \chi_{p_1'} (r_1) \frac{1}{r_{12}} \chi_{p_2} (r_2) \chi_{p_2'} (r_2') dV_1 dV_2, \]

(3)

with

\[ \chi_{p, n, l, m} (\zeta, r) = \chi_{n, l, m} (\zeta, r). \]

(4)

\[ \chi_{p_1'} (r_1) = \chi_{n_1', l_1', m_1'} (\zeta_1, r_1). \]

(5)

Taking into account the expansion for the spherical harmonics with the same center,

\[ R_n (\zeta, r) S_{lm} (\theta_1, \varphi_1) R_{n'} (\zeta', r) S_{l'm'}^{*} (\theta_1, \varphi_1) = \int \frac{2L+1}{4\pi} C^{LM} |(lm, l'm') \times A_{nm}^{M} S_{LM}^* (\theta_1, \varphi_1) \]

(6)

and Laplace expansion for Coulomb interaction,

\[ \frac{1}{r_{12}} = \sum_{LM} \left( \frac{4\pi}{2L+1} \right) \frac{r_{12}^{L}}{r_{12}^{L}} S_{LM} (\theta_1, \varphi_1) S_{LM}^* (\theta_2, \varphi_2), \]

(7)

the electron repulsion integrals finally are expressed as follows,

\[ J_{n_1, l_1, m_1, n_2, l_2, m_2} (\zeta_1, \zeta_1', \zeta_2, \zeta_2') = \sum_{LM} C^{LM} |(l_1, m_1, l_1', m_1') C^{LM} |(l_2, m_2, l_2', m_2') \]

\[ \times A_{n_1 m_1}^{M} A_{n_2 m_2}^{M} R_{n_1, n_1', n_2, n_2'} (\zeta_1, \zeta_1', \zeta_2, \zeta_2'). \]

(8)

Here,

\[ \text{Max} (|l_1 - l_1'|, |l_2 - l_2'|) \leq L \leq \text{Min} (l_1 + l_1', l_2 + l_2'), \]

\[ -L \leq m \leq L. \]

Please see [12, 13], for Gaunt \( C^{LM} | \) and \( A_{nm}^{M} | \) coefficients that arise from product of two spherical harmonics. The remaining radial integrals \( R_{n}^{L} \) are defined as [14],

\[ R_{n_1, n_1', n_2, n_2'} (\zeta_1, \zeta_1', \zeta_2, \zeta_2') = \int_{0}^{\infty} \int_{0}^{\infty} r_{1}^{n_1 + n_1'} e^{-(\zeta_1 + \zeta_1') r_{1}} \frac{r_{1}^{L}}{r_{1}^{L}} \]

\[ \times r_{2}^{n_2 + n_2'} e^{-(\zeta_2 + \zeta_2') r_{2}} dr_{1} dr_{2}. \]

(9)

So far obtained analytical expressions for the radial integrals given in the Eq. (9) were in terms of incomplete gamma functions or Gauss’s hyper–geometric functions. The method of solution for the Eq. (9) is detailed here as it is important for our discussion in the next section on how it can be used for molecular integrals. Explicit form of the Eq. (9) is written as,

\[ R_{n_1, n_1', n_2, n_2'} (\zeta_1, \zeta_1', \zeta_2, \zeta_2') = \int_{0}^{\infty} \left\{ \int_{0}^{r_2} r_{1}^{n_1 + n_1'} e^{-(\zeta_1 + \zeta_1') r_{1}} \frac{r_{1}^{L}}{r_{1}^{L}} dr_{1} \right. \]

\[ + \int_{r_2}^{\infty} r_{1}^{n_1 + n_1'} e^{-(\zeta_1 + \zeta_1') r_{1}} \frac{r_{1}^{L}}{r_{1}^{L}} dr_{1} \}

\[ \times r_{2}^{n_2 + n_2'} e^{-(\zeta_2 + \zeta_2') r_{2}} dr_{2}. \]

(10)

By applying rule of definite integral to the first term and changing the variable as \( x = r_1/r_2 \), the following expression is obtained,

\[ R_{n_1, n_1', n_2, n_2'} (\zeta_1, \zeta_1', \zeta_2, \zeta_2') = \frac{\Gamma (n_1 + n_1' + L + 1)}{(\zeta_1 + \zeta_1')^{n_1 + n_1' + L + 1}} \int_{0}^{\infty} r_{2}^{n_2 + n_2'} e^{-(\zeta_2 + \zeta_2') r_{2}} dr_{2} \]

\[ - \int_{0}^{\infty} \left[ A_{n_1 + n_1' + L} ((\zeta_1 + \zeta_1') r_{2}) \right. \]

\[ - A_{n_1 + n_1' + L - 1} ((\zeta_1 + \zeta_1') r_{2}) \]

\[ \times r_{2}^{n_2 + n_2'} e^{-(\zeta_2 + \zeta_2') r_{2}} dr_{2}. \]

(11)

where,

\[ A_{n} (p) = p^{-n-1} \Gamma [n + 1, p]. \]

(12)

This form of integrals are used to represent the electron repulsion integrals in terms of both incomplete gamma functions or hyper–geometric functions. Inserting the Eq. (12) into the Eq. (11), after a slightly manipulation we have,

\[ R_{n_1, n_1', n_2, n_2'} (\zeta_1, \zeta_1', \zeta_2, \zeta_2') = \frac{1}{\Gamma (n_1 + n_1' + L + 1)} \int_{0}^{\infty} \gamma \left[ n_1 + n_1' + L + 1, (\zeta_1 + \zeta_1') r_{2} \right] \]

\[ + \int_{0}^{\infty} \Gamma \left[ n_1 + n_1' + L - 1, (\zeta_1 + \zeta_1') r_{2} \right] \]

\[ \times r_{2}^{n_2 + n_2'} e^{-(\zeta_2 + \zeta_2') r_{2}} dr_{2}. \]

(13)

\[ \Gamma [n, x], \gamma [n, x] \] are the upper and lower incomplete gamma functions. Note that the first and second terms in the Eq. (13) represents the integrals given the Eq. (10) over the ranges \( r_1 \in [0, r_2], r_1 \in [r_2, \infty], \) respectively.
By using the following relationships between incomplete gamma functions and hyper-geometric functions [15]:

$$\frac{1}{a^n} \int_0^\infty x^{m-1} e^{-bx} \Gamma [n, ax] dx = \frac{\Gamma (m+n)}{m (a+b)^{m+n}} F_1 \left[ 1, m+n, m+1; \frac{b}{a+b} \right]$$

$$\frac{1}{a^n} \int_0^\infty x^{m-1} e^{-bx} \gamma [n, ax] dx = \frac{\Gamma (m+n)}{n (a+b)^{m+n}} F_1 \left[ 1, m+n, n+1; \frac{a}{a+b} \right]$$

The electron repulsion integrals take the form that [16],

$$R_{n_1, n_2, \cdots, n_n}^{L} (\zeta_1, \zeta_2, \cdots, \zeta_n) = \frac{\Gamma (n + n_1 + n_2 + n_3 + 1)}{(\zeta_1 + \zeta_2 + \cdots + \zeta_n + n_1 + n_2 + n_3 + 1)} \left\{ \begin{array}{c} 1 \\ n_1 + n_2 + L + 1 \end{array} \right\} \times 2 F_1 \left[ 1, n_1 + n_2 + n_3 + 1, n_1 + n_2 + L + 2, \frac{\zeta_1 + \zeta_2}{\zeta_1 + \zeta_2 + 1} \right]$$

III. NEW RELATIONSHIPS FOR THE ELECTRON REPULSION INTEGRALS

By replacing the $n_1 + n_2$ with $n$, $n_2 + n_3$ with $n'$ and $\zeta_1 + \zeta_2$ with $\zeta'$, the Eq. (16) has a simpler form as,

$$R_{n, n'}^{L} (\zeta, \zeta') = \frac{\Gamma (n + n' + 1)}{(\zeta + \zeta')^{n+n'}} \left\{ \begin{array}{c} 1 \\ n + L + 1 \end{array} \right\} \times 2 F_1 \left[ 1, n + n' + 1, n + L + 2, \frac{\zeta}{\zeta + \zeta'} \right]$$

For the hyper-geometric functions arising in the Eq. (17) we obtain,

$$F_{nm}^{L} (\zeta, \zeta') = 2 F_1 \left[ 1, n + n' + 1, n + L + 2; \frac{\zeta}{\zeta + \zeta'} \right]$$

$$= f_{nm}^{L} 2 F_1 \left[ 1, n + n' + 1, n' - L + 1; \frac{\zeta}{\zeta + \zeta'} \right] - g_{nm}^{L} (\zeta, \zeta')$$

$$f_{nm}^{L} = \frac{\pi \csc \left[ \left( -n' + L \right) \pi \right] (n + L + 1)}{(n' - L + 1)}$$

$$g_{nm}^{L} (\zeta, \zeta') = f_{nm}^{L} \frac{\Gamma (n' - L + 1) \Gamma (n + L + 1)}{(n + n' + 1)} \times \left( \frac{\zeta}{\zeta + \zeta'} \right)^{-n-L-1} \left( \frac{\zeta'}{\zeta + \zeta'} \right)^{n' + L}$$

If the second term in the Eq. (17) is considered then, $f_{nm}^{L} \rightarrow f_{nm}^{L}$, $g_{nm}^{L} (\zeta, \zeta') \rightarrow g_{nm}^{L} (\zeta', \zeta)$. Two types of expressions for electron repulsion integrals are derived from the Eq. (20). The recurrence relationships given below for each expression leads to either increasing $n - L + 1$ and $n - L + 1$ to $n + L + 2$ and $n' + L + 2$, or decreasing $n + L + 2$ and $n' + L + 2$ to $n - L + 1$ and $n' - L + 1$, respectively.

$$2 F_1 [1, b, c; z] = \frac{1}{(b - c + 2)^2} 2 F_1 [1, b, c + 2; z]$$

$$+ \left( \frac{1}{z} \right) \sum_{k=1}^{m} \frac{(1 - c)_k}{(b - c + 1)_k} \left( \frac{z - 1}{z} \right)^{k-1}$$
\[2F_1 \left[ 1, b, c; m; z \right] = \frac{(b - c + 1)_m}{(1 - c)_m} \left( \frac{z}{1} \right)^m \]
\[\times 2F_1 \left[ 1, b, c; z \right] - \frac{1}{z - 1} \left( \frac{1}{z} \right) \sum_{k=1}^{m} \frac{(b - c + 1 + k)_m}{(1 - c + k)_m} \left( \frac{z - 1}{z} \right)^{k-1}. \tag{24} \]

Finally, we obtain four different types of expressions for electron repulsion integrals. Two of them for hyper–geometric functions involve \( n + L + 2 \), \( n' + L + 2 \) and other two of them for \( n - L + 1 \), \( n' - L + 1 \):

For electron repulsion integrals with hyper–geometric functions involve \( n + L + 2 \) and \( n' + L + 2 \),

\[R_{n,n'}^L (\zeta, \zeta') = \frac{\Gamma (n + n' + 1)}{(\zeta + \zeta')^{n+n'}} \frac{1}{n' + L + 1} \]
\[\times 2F_1 \left[ 1, n + n' + 1, n' + L + 2; \frac{\zeta'}{\zeta + \zeta'} \right] g_{n'n'}^L (\zeta, \zeta')
- \Gamma (n + n' + 1) \frac{1}{(\zeta + \zeta')^{n+n'}} \frac{1}{n' + L + 1} \]
\[\times \left\{ g_{n'n'}^L (\zeta', \zeta) + l_{n'n'}^L (\zeta, \zeta') \right\}. \tag{25} \]

Notice that, \( R_{n,n'}^L (\zeta, \zeta') = R_{n,n'}^L (\zeta', \zeta) \).

For electron repulsion integrals with hyper–geometric functions involve \( n - L + 1 \), \( n' - L + 1 \),

\[R_{n,n'}^L (\zeta, \zeta') = \frac{\Gamma (n + n' + 1)}{(\zeta + \zeta')^{n+n'}} \frac{1}{n' + L + 1} \]
\[\times 2F_1 \left[ 1, n + n' + 1, n' + L + 2; \frac{\zeta}{\zeta + \zeta'} \right] h_{n'n'}^L (\zeta', \zeta)
- \Gamma (n + n' + 1) \frac{1}{(\zeta + \zeta')^{n+n'}} \frac{1}{n' + L + 1} \]
\[\times \left\{ h_{n'n'}^L (\zeta', \zeta) + l_{n'n'}^L (\zeta, \zeta') \right\}. \tag{26} \]

The four relationships obtained for electron repulsion integrals are still involve hyper–geometric functions although this time only one. Reducing the number of hyper–geometric functions decreases the CPU time. On the other hand the Eqs. (25, 26) and (27, 28) are linearly independent. The each coupled equations represent a linear system with two equations and same solution given in the Eq. (17).

Finally the hyper–geometric functions arising in the electron repulsion integrals are completed eliminated or in other words, they are obtained in terms of finite power series by the solution of following simple system of equation:

\[\begin{align*}
x X - z_1 & = X + Y, \\
y Y - z_2 & = X + Y, \tag{31} \end{align*} \]

where,

\[\begin{align*}
X & = -z_1 - y z_1 - z_2, \tag{32} \\
Y & = -z_1 + z_2 - x z_2. \tag{33} \end{align*} \]
Considering the coupled Eqs (26, 27) and using the Eq. (31) into the Eq. (17) we have,

\[ R = X + Y = \frac{x z_2 + y z_1}{x y - x - y}, \quad (34) \]

where, \( R \equiv R_{n n'} (\zeta, \zeta') \) and

\[ x \equiv h^{L}_{n n'} (\zeta, \zeta') \quad \text{and} \quad y \equiv l^{L}_{n n'} (\zeta, \zeta') \quad (35) \]

\[ z_1 \equiv \Gamma (n + n' + 1) \frac{1}{(\zeta + \zeta')^{n + n' + 1}} \frac{1}{n + L + 1} \times \left\{ g^{L}_{n n'} (\zeta, \zeta') + l^{L}_{n n'} (\zeta, \zeta') \right\}, \quad (36) \]

\[ z_2 \equiv \Gamma (n + n' + 1) \frac{1}{(\zeta + \zeta')^{n + n' + 1}} \frac{1}{n' + L + 1} \times \left\{ l^{L}_{n n'} (\zeta', \zeta) + g^{L}_{n n'} (\zeta', \zeta) \right\}. \quad (37) \]

### IV. DISCUSSIONS. EXTENDING THE SOLUTION TO MORE DIFFICULT PROBLEMS

In this section we consider the Laplace expansions for arbitrary powers \( r^\mu \), \( \mu = -1, -2, -3, \ldots \) and their applications in solution of the Dirac equation for many–electron systems. We also consider extension of the solution given in the previous section to relativistic molecular integrals.

#### A. On the integrals involve Laplace expansion for arbitrary power \( r^\mu \)

The differential equation corresponding to radial part of Laplace expansion for arbitrary power and its solution given as [17],

\[ \frac{\partial R^L_\mu}{\partial r_2} + 2 \frac{\partial R^L_\mu}{\partial r_2} - L (L + 1) \frac{R^L_\mu}{r_2^2} = \frac{\partial R^L_\mu}{\partial r_1} + \frac{2 \partial R^L_\mu}{\partial r_2} - L (L + 1) \frac{R^L_\mu}{r_2^2}, \quad (38) \]

\[ R^L_\mu (r_1, r_2) = \frac{(-\frac{1}{2} \mu)_L}{(\frac{1}{2} L)} r_1^{-\mu} (r_2^{-L}) \times _2 F_1 \left[ a, b, L + \frac{3}{2} ; \frac{r_2^2}{r_2^2} \right], \quad (39) \]

here, if \( \mu = -1, -3, -5, \ldots \), then \( a = -\frac{1}{2} - \frac{1}{2} \mu \) and \( b = L - \frac{1}{2} \mu \). If \( \mu = -2, -4, -6, \ldots \), then \( a = L - \frac{1}{2} \mu \) and \( b = -\frac{1}{2} \mu \). For both cases \( a \in \mathbb{N} \) and \( b - c \in \mathbb{N} \).

The radial integrals for \( R^L_\mu \)

\[ \mu R^L_{n_1 n_2 n_3 n_4} (\zeta_1, \zeta_1', \zeta_2, \zeta_2') = \int_0^\infty \int_0^\infty r_1^{n_1 + n_3} e^{-(\zeta_1 + \zeta_1') r_1} R^L_\mu (r_1, r_2) \times r_2^{n_2 + n_4} e^{-(\zeta_2 + \zeta_2') r_2} dr_1 dr_2. \quad (40) \]

The recurrence relationships given for \( R^L_\mu \) [17] are useful to represent the Eq. (40) in terms of standard electron repulsion integrals;

\[ (4 + 2 \mu + 2 (2 L - 2 - \mu) \frac{R^L_{n_1 n_2 n_3 n_4}}{r_2^2} + (\mu + 2)^2 r_2^2 R^L_\mu + 2 (\mu + 2)^2 r_2^2 R^L_\mu - 2 - \mu (\mu + 2) 2 r_1 r_2 R^L_C + \mu (\mu + 2) r_2^2 R^L_\mu - 2, \quad (41) \]

therefore,

\[ (4 + 2 \mu + 2 (2 L - 2 - \mu) \frac{R^L_{n_1 n_2 n_3 n_4}}{r_2^2} + 2 (\mu + 2)^2 r_2^2 R^L_\mu + 2 (\mu + 2)^2 r_2^2 R^L_\mu - 2 - \mu (\mu + 2) 2 r_1 r_2 R^L_C + \mu (\mu + 2) r_2^2 R^L_\mu - 2, \quad (42) \]

where, \( -1 R^L_{n_1 n_2 n_3 n_4} = R^L_{n_1 n_2 n_3 n_4} \). In [17] recurrence relationships over \( L \) and \( \mu, L \) were also derived. They were considered useful due to existence of hyper–geometric functions. Here, the basic electron repulsion integrals are free from special functions or infinite series representation.

The Breit interaction is the lower order correction to electron–electron Coulomb interaction [18].

\[ H_{ij} = H_{ij}^G + H_{ij}^{ret} = -\frac{\alpha_i \alpha_j}{r_{ij}} + \frac{1}{2} \left\{ \frac{\alpha_i \alpha_j}{r_{ij}} - \left( \frac{\tilde{r}_{ij} \alpha_i}{r_{ij}} \right) \left( \frac{\tilde{r}_{ij} \alpha_j}{r_{ij}} \right) \right\}, \quad (43) \]

here, \( \alpha_i \) are the Dirac matrices. The first term, represents the un–retarded interaction between two Dirac currents and it includes spin–spin, spin–other–orbit and spin–spin interactions. The second term accounts for retardation effects [19, 20]. A computer program code to calculate the Breit interaction was given in [21, 22] via the tensor form representation. The most of resulting radial integrals were directly expressed by electrostatic interaction \( -1 R^L_C \) by simply adding a correction which is a constant. The integrals come from the spin–spin,
spin–other–orbit were given as [21],

\[ N^L_{n_1,n_2,n_3} (\zeta_1, \zeta_2, \zeta_3) \]
\[ = \int_0^\infty \int_0^\infty r_1^{n_1+n_1'} e^{-(\zeta_1+\zeta_1')} r_1 \left( \frac{r_1^{L+3}}{r_1^{L+3}} \right) \]
\[ \times e (r_1 - r_2) r_2^{n_2+n_2'} e^{-(\zeta_2+\zeta_2')} r_2^2 dr_1 dr_2, \]
\[ \text{(44)} \]

\[ V^L_{n_1,n_2,n_3} (\zeta_1, \zeta_2, \zeta_3) \]
\[ = \int_0^\infty \int_0^\infty r_1^{n_1} e^{-\zeta_1} r_1 \left( \frac{\partial}{\partial r_1} r_1^{n_1'} e^{-\zeta_1'} r_1 \right) \left( \frac{r_1^{L+3}}{r_1^{L+3}} \right) \]
\[ \times r_2^{n_2+n_2'} e^{-(\zeta_2+\zeta_2')} r_2^2 dr_1 dr_2, \]
\[ \text{(45)} \]

where,

\[ e (x) = \begin{cases} 
1 & x > 1 \\
0 & x \leq 1.
\end{cases} \]
\[ \text{(46)} \]

The Eqs. (44, 45) can also be represented in terms of electrostatic interaction via the Eq. (42).

**B. On the two–center integrals**

The Eq. (13) for two center case is expressed in prolate spheroidal coordinates. The resulting auxiliary functions have similar symmetry with right–hand side of the Eqs. (14, 15) but in two–dimensions. They are given as [23] (please see also references therein),

\[ \begin{align*}
\left\{ \begin{array}{c}
P_{n_2,n_3}^{n_1,n_4} (p_{12}) \\
Q_{n_2,n_3}^{n_1,n_4} (p_{12})
\end{array} \right\} \\
= \frac{p_{12}^{-n_1}}{(n_4-n_1)_n} \int_0^1 \int_{-1}^1 (\xi \nu)^{n_2} (\xi - \nu)^n d\xi d\nu,
\end{align*} \]
\[ \text{(47)} \]

The Eqs. (14, 15) are expressed in terms of Gauss’s hyper–geometric functions. Finite series representations for the Eq. (47) as given in previous section for electron repulsion integrals may be possible but only if corresponding special functions are found. The relationships given in the Eqs. (14, 15) are obtained by series representation of lower incomplete gamma functions,

\[ \gamma [n, x] = x^n \Gamma (n) e^{-x} \sum_{k=0}^\infty \frac{x^k}{\Gamma (n+k+1)}. \]
\[ \text{(48)} \]

and, the following integrals of elementary functions,

\[ \int_0^\infty x^n e^{-\zeta x} dx = \Gamma (n+1) \zeta^{-n-1}. \]
\[ \text{(49)} \]

The expression for integrals involve the upper incomplete gamma functions (Eq. (15)) is then, derived by using the recurrence relationships for hyper–geometric functions,

\[ _2F_1 [a, b, c; z] = \frac{\Gamma (c) \Gamma (a+b-c)}{\Gamma (a) \Gamma (b)} (1-z)^{c-a-b} \]
\[ \times _2F_1 [c-a, c-b, c-a-b+1; 1-z] \]
\[ + \frac{\Gamma (c) \Gamma (c-a-b)}{\Gamma (c-a) \Gamma (c-b)} _2F_1 [a, b, a+b+1; 1-z]. \]
\[ \text{(50)} \]

Implementing a similar routine to Eq. (47) requires convergent series representation for power series such as, \((x+a)^n\), \(n \in \mathbb{N}\), for both \(|x/a| < 1\) and \(|x/a| > 1\). The following binomial expansion satisfies this requirements,

\[ (x \pm a)^{[n]+\epsilon} = (\pm 1)^{\delta_\epsilon} \lim_{N \to \infty} \sum_{k=0}^{[n]+N} (\pm 1)^k \]
\[ \frac{\Gamma ([n] + \epsilon + 1)}{\Gamma (k - \delta_N + \epsilon + 1) \Gamma ([n] - k + \delta_N + 1)} x^{k - \delta_N + \epsilon} a^{[n] + \delta_N - k}, \]
\[ \text{(51)} \]

\[ \delta_N = \begin{cases} 
N & |x/a| > 1 \\
\epsilon & |x/a| < 1
\end{cases} \]
\[ \text{(52)} \]

\(\delta_\epsilon = \epsilon\) for \(x-a < 0\) and \(\delta_\epsilon = [n]\) for \(x-a > 0\).

The problem about the conditional existence of binomial expansion can be eliminated by writing the Eq. (47) in a two–range form depending on domain for \(\nu\) as \(-1 \leq \nu \leq 0\) and \(0 \leq \nu \leq 1\) and using the following expressions,

\[ (\xi + \nu)^2 = (\xi - \nu)^2 + 4 (\xi \nu), \]
\[ \text{(53)} \]

for \(-1 \leq \nu \leq 0\) and,

\[ (\xi - \nu)^2 = (\xi + \nu)^2 - 4 (\xi \nu), \]
\[ \text{(54)} \]

for \(0 \leq \nu \leq 1\).

Finally, as corresponding special functions for the Eq. (47) we expect to have another special functions such as Appell functions but we remain this task for next paper of our series.

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