Analytic evaluation of some three- and four- electron atomic integrals involving s STO’s and exponential correlation with unlinked \( r_{ij} \)’s

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Abstract

The method of evaluation outlined in a previous work has been utilized here to evaluate certain other three- electron and four- electron atomic integrals involving s Slater-type orbitals and exponential correlation with unlinked \( r_{ij} \)’s. Limiting expressions for various such integrals have been derived, which has not been done earlier. Closed-form expressions for \(< r_{12}r_{13}/r_{14} >, < r_{12}r_{34}/r_{23} >, < r_{12}r_{23}/r_{34} >, < r_{12}r_{13}/r_{34} >\) and \(< r_{12}r_{34}/r_{13} >\) have been obtained.

Keywords: exponentially correlated integrals, Hy-CI calculations, three- and four- electron systems.

1. Introduction

It is well accepted that the details of the way in which electrons mutually correlate their motion in a many-electron system are to be included in order to obtain very accurate wave functions and energies for the system by employing quantum mechanical calculations in the framework of the Rayleigh - Ritz variational procedure [1]. The two standard methods which include these electron- electron correlations are (i) the configuration - interaction (CI) method and (ii) the Hylleraas (Hy) method. In the CI method, the trial function is represented as a linear combination of a large number of antisymmetrized products of one- electron functions, each product referring to one particular configuration of the system. This method is easy to apply to any system, in principle, for calculations. However, it is plagued with the weakness of extremely slow convergence. On the other hand, the Hy method, in which the interelectronic separation coordinates are included explicitly in variational basis functions, as was first proposed by Hylleraas [2, 3], gives quick convergence in energy compared to the CI method. This method is regarded as the most powerful method among the existing theoretical approaches to produce results of high accuracy [4]. It has been quite successful in obtaining highly accurate energy for two-electron systems [5, 6]. However, the number of interelectronic separation coordinates involved in the trial function for an N-electron atom is \( N(N-1)/2 \), and hence the evaluation of the corresponding generating integrals in the Hy method becomes more and more difficult for systems with increasing N. As far as the knowledge of the author goes, the application of the Hy method for variational calculations is limited upto only four - electron systems till date [7].

As regards the application of the Hy method to three-electron atomic systems, James and Coolidge [8] were the first to attempt to compute the energy for the ground state of Li atom. They were successful in expressing the so called triangle integral (with integrand involving all the three interelectronic separation coordinates) in terms of auxiliary
functions A, V and W, which are themselves of one-, two-, and three-dimensional integrals, respectively. For knowledge about progressive development of various numerical methods of evaluation, with greater accuracy, of three-electron correlated integrals over atomic Slater-type orbitals (STO’s) [9], the reader is advised to go through the review article by King [10], the paper by Pelzl and King [11] and references therein, as well as the paper by Yan and Drake [12]. However, analytic expressions have been reported by Frolov and Smith [13] for the functions A, V and W. In all reports cited above in this paragraph, no exponential correlation has been considered.

In an alternative approach, employing Fourier transform method, Fromm and Hill [14] could succeed for the first time in obtaining a closed-form expression for the triangle integral involving exponential correlation. The expression reported by them [14] does not involve the auxiliary functions A, V and W. Subsequently, five more reports of analytic evaluation of the triangle integral with certain comments and modifications were published by different authors [15 - 19]. Employing the Hylleraas basis set with and/or without exponential correlation, many investigations relating to various properties of the three-electron atomic system have been reported [20-23] by Pachucki and Puchalski and coworkers. Making use of results in [14, 24], formulas for the recursive generation of many other three-electron exponentially correlated integrals have been reported by Harris [25].

For the accurate determination of wave functions and energies for atomic systems with more than three electrons by avoiding computational difficulty met in the Hy method, an alternative procedure was systematically developed in early seventies by Sims and Hagstrom [26, 27] by introducing explicitly interelectronic separation coordinates into a CI wave function with certain restrictions. In this method, known as the Hylleraas - configuration - interaction (Hy-CI) method, each term in the expansion of the proposed CI function was restricted to contain explicitly only one two-electron correlation factor of the form $r_{ij}^p$, with $p$ restricted to the value 0, 1 and 2. Of course, with $p = 0$, one gets the original CI wave function. To include electron-electron correlations in this manner in the wave function expansion had been first proposed by James and Coolidge [8], and was later employed by others [28-31]. The Hy-CI method was employed for the first time by Sims and Hagstrom [26, 27] for the study of the ground state of the beryllium atom by taking a 107 - configuration wave function. An auxiliary function X, which is itself a four-dimensional integral, was introduced by them in addition to the auxiliary functions A, V and W introduced in [8]. Also, a computational scheme was reported by them for the accurate calculation of the auxiliary function X in terms of A, V and W functions. The Hy-CI method was further utilized successfully to investigate the ground state and some excited states of Li atom [32-34], the ground state of Li$^-$ ion [35], the ground state of neon atom [36], and the ground state of neutral helium and He-like ions [37]. Several low-lying states in Li atom and Be$^+$ ion have been investigated by Ruiz et al. [38] recently employing the Hy-CI analysis. The most accurate result available using this approach for the ground state of Be atom and its isoelectronic sequence yields energies accurate to better than one microhartree[39,40]. Sims and Hagstrom, in a series of papers [41-43], have discussed thoroughly certain mathematical and computational science issues in high precision calculation of the three-electron triangle integral, three-electron kinetic energy and four-electron integrals which arise while employing Hy-CI method of variation. Some three-electron and four-electron integrals have been evaluated by Ruiz [44,45] by integration over the coordinates of one electron and calculated to a high degree of accuracy. Same method of evaluation was employed by Ruiz[46,47] to calculate the two-electron kinetic energy and the three-electron kinetic energy. Frolov et al. [48] have investigated bound state spectra and properties of the doublet states in Li
atom and some Li-like ions employing Hy-CI and CI methods. The basic four-electron atomic correlated integral with integrand involving all the six electron-electron separation coordinates was reduced to a sum of several auxiliary functions X (denoted as $W_4$) [49-51], and later reevaluated by King [52] to increase the effectiveness in computation and reported closed-form expressions for some integrals as special cases. Analytical expressions for the auxiliary functions $A$, $V$, $W$ and $X$ (renoted as $A_1$, $A_2$, $A_3$ and $A_4$, respectively) along with their highly accurate values have been reported in [53, 54]. A computationally efficient and numerically stable method was reported in [4,55] for the highly accurate calculation of auxiliary functions $W$ and $X$ (denoted as $W_3$ and $W_4$). All the papers cited above in this paragraph do not involve exponential correlation. Further, it is observed that the trial wave function expansion has been chosen to consist of a large number of terms even in the Hy and the Hy-CI variation methods. For example, in the latest investigation for the ground state of Be atom by Hy method a 200 term Hylleraas wave function was taken in [7]; for the investigation of the ground state of Be atom and its isoelectronic sequence by Hy-CI method, about 40000 terms were considered in [39,40].

It is expected that with the involvement of exponential correlation in the Hy and the Hy-CI methods, the convergence will be quicker even with less number of terms, though the evaluation of respective integrals will be relatively difficult. Accordingly, one speaks of the Extended-Hylleraas-configuration-interaction (E-Hy-CI) method [56] in which each configuration in the CI wave function expansion is restricted to contain at best one correlation factor of the form $r_{ij}^\nu \exp(-\lambda_{ij} r_{ij})$. Thus closed-form expressions have been reported by the author [57] for certain three- and four-electron atomic integrals which involve exponential correlation and s STO’s with $r_{ij}$’s having unlinked indices; also, three different five-electron atomic integrals of this category have been evaluated in closed-form and reported in [58]. Analytical expressions for some such three- and four-electron atomic integrals have been recently reported by King [59], wherein stability issues for obtaining correct numerical values from analytic formulas were discussed. Certain such three- and four-electron atomic integrals, but involving nonspherically symmetric STO’s also evaluated and reported by Wang at al. [56]. There are several earlier reports relating to evaluation of correlated atomic integrals involving exponential correlation [60-64] and without exponential correlation [30,65-68].

The plan of this paper is as follows. In section 2, the key integral to be utilized several times in the paper has been evaluated in closed-form. Certain two-electron atomic integrals have been evaluated in section 3. Three equivalent three-electron atomic integrals represented by two-vortex diagrams have been evaluated in closed-form in section 4. In section 5.1, analytic expressions for four equivalent four-electron atomic integrals represented by three-vortex diagrams, as well as for $<r_{12}r_{13}/r_{14}>$ have been derived. Closed-form expressions for eight different four-electron atomic integrals represented by open square diagrams as well as for $<r_{12}r_{34}/r_{23}>$, $<r_{12}r_{23}/r_{34}>$, $<r_{12}r_{24}/r_{13}>$, and $<r_{12}r_{34}/r_{13}>$, have been obtained in section 5.2. Limiting expressions have also been derived for various integrals. Concluding remarks are given in section 6.

2. Evaluation of the key integral

In the previous paper [57], hereinafter referred as paper I, a simple method was outlined for obtaining closed-form expressions for some two-, three-, and four-electron atomic integrals involving spherically symmetric STO’s and exponential correlation,
with the restriction that the inter-electron separation coordinates with unlinked indices only are present in the integrand. This successful analytic evaluation is consistent with the conjecture 'A' put forward by Bonham [63]. The key to this successful evaluation lies in deriving a closed-form expression for the following integral $J$ defined by

$$J(\lambda_t, \lambda_{st}, r_s) = \int d\vec{r}_t (r_{t \cdot r_{st}})^{-1} \exp(-\lambda_t r_t - \lambda_{st} r_{st}),$$

where $\vec{r}_s$ and $\vec{r}_t$, respectively, are the position vectors of the $s^{th}$ and the $t^{th}$ electrons with respect to the nucleus assumed to be infinitely heavy and situated at the origin of the coordinate system chosen. Here $r_{st} = r_{ts} = |\vec{r}_s - \vec{r}_t|$ is the distance between the $s^{th}$ and the $t^{th}$ electrons, and $\lambda_t$ and $\lambda_{st}$ are the exponential parameters. Obviously, $\lambda_{st} = \lambda_{ts}$.

To evaluate the integral in equation(1), the following Fourier representation

$$\frac{\exp(-\lambda_{st} r_{st})}{r_{st}} = \frac{1}{2\pi^2} \int d\vec{K} \frac{\exp[i\vec{K} \cdot (\vec{r}_s - \vec{r}_t)]}{\vec{K}^2 + \lambda_{st}^2}$$

is employed on the right hand side, then the orders of integration are interchanged and the integration over $\vec{r}_t$ is performed. Subsequently, the integral over the Fourier transform variable $\vec{K}$ is evaluated by making use of the inverse Fourier transform to get

$$J(\lambda_t, \lambda_{st}, r_s) = \frac{4\pi}{\lambda_t^2 - \lambda_{st}^2} \frac{\exp(-\lambda_{st} r_s) - \exp(-\lambda_t r_s)}{r_s}.$$

If $\lambda_{st} \to \lambda_t$, then L’Hospital’s rule for $0/0$ can be employed on the right hand side expression in equation(3) to obtain

$$J(\lambda_t, \lambda_t, r_s) = \frac{2\pi}{\lambda_t} \exp(-\lambda_t r_s).$$

3. Evaluation of two-electron atomic integrals

3.1 The general integral

The general two-electron atomic integral involving s STO’s and exponential correlation, denoted by $I_2$, is given by

$$I_2(i, j, k; \lambda_1, \lambda_2, \lambda_{12}) = \int d\vec{r}_1 d\vec{r}_2 d\vec{r}_{12} r_{12}^k \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_{12} r_{12}),$$

where the integers $i, j, k$ are each $\geq -1$, and the exponential parameters $\lambda_1, \lambda_2$ and $\lambda_{12}$ are such that $\lambda_1 + \lambda_2, \lambda_1 + \lambda_{12}$ and $\lambda_2 + \lambda_{12}$ are positive, although there are no such restrictions on these parameters individually [62]. The graphical representation [63] of the integral in equation(5) is just a straight line connecting the electron positions 1 and 2, indicating that the integrand involves only one inter-electron coordinate $r_{12}$ which takes into account correlation. equation(5) can be written as
Making use of equations (1) and (3) in equation (7) above, it can be recast as
\[ I_2(i, j; \lambda_1, \lambda_2, \lambda_{12}) = \left(-\frac{\partial}{\partial \lambda_1}\right)^{i+1} \left(-\frac{\partial}{\partial \lambda_2}\right)^{j+1} \left(-\frac{\partial}{\partial \lambda_{12}}\right)^{k+1} \times I_2(-1, -1, -1; \lambda_1, \lambda_2, \lambda_{12}), \]
where \( I_2(-1, -1, -1; \lambda_1, \lambda_2, \lambda_{12}) \), in which \( i = j = k = -1 \), is termed as the corresponding generating integral and is denoted, in short, by \( I^g_2(\lambda_1, \lambda_2, \lambda_{12}) \), the superscript ‘g’ signifying the generating integral. Clearly we have
\[ I^g_2(\lambda_1, \lambda_2, \lambda_{12}) = \int \frac{d\mathbf{r}_1}{r_1} \frac{d\mathbf{r}_2}{r_2} \frac{d\lambda}{\lambda_{12}} \cdot \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_{12} r_{12}). \]  
Making use of equations (1) and (3) in equation (7) above, it can be recast as
\[ I^g_2(\lambda_1, \lambda_2, \lambda_{12}) = \int \frac{d\mathbf{r}_1}{r_1} \frac{d\mathbf{r}_2}{r_2} \frac{d\lambda}{\lambda_{12}} \cdot \exp(-\lambda_1 r_1) J(\lambda_2, \lambda_{12}, r_1), \]
and evaluated analytically to obtain the following closed form expression:
\[ I^g_2(\lambda_1, \lambda_2, \lambda_{12}) = 16\pi^2[(\lambda_1 + \lambda_2)(\lambda_1 + \lambda_{12})(\lambda_2 + \lambda_{12})]^{-1}. \]

The above expression is exactly in agreement with the one obtained by Calais and Lowdin [61] by employing perimetric coordinates, first introduced by Coolidge and James [69]. The result in equation (9) can be used in equation (6) to obtain closed - form expressions for a sequence of integrals given by equation (5) by the method of parametric differentiation. The expressions obtained in this manner for certain three such integrals are given here only for the purpose of record:
\[ I_2(-1, -1, 0; \lambda_1, \lambda_2, \lambda_{12}) = 16\pi^2(\lambda_1 + \lambda_2 + 2\lambda_{12})[(\lambda_1 + \lambda_2)(\lambda_1 + \lambda_{12})^2(\lambda_2 + \lambda_{12})^2]^{-1}, \]
\[ I_2(0, 0, -1; \lambda_1, \lambda_2, \lambda_{12}) = 32\pi^2[(\lambda_1 + \lambda_2 + \lambda_{12})^2 + \lambda_1 \lambda_2][(\lambda_1 + \lambda_2)^3(\lambda_1 + \lambda_{12})^2(\lambda_2 + \lambda_{12})^2]^{-1}, \]
\[ I_2(0, 0, 0; \lambda_1, \lambda_2, \lambda_{12}) = 64\pi^2[\lambda_1 \lambda_2 \lambda_{12} + (\lambda_1 + \lambda_2 + \lambda_{12})^3][(\lambda_1 + \lambda_2)(\lambda_1 + \lambda_{12})(\lambda_2 + \lambda_{12})]^{-3}. \]

It is observed that the right hand side expressions in equations (10-12) are symmetric with interchange of \( \lambda_1 \) and \( \lambda_2 \), as expected.

### 3.2 Some other two-electron integrals

It is worth mentioning here four other nonsingular two-electron integrals of interest which do not come under the general category of integrals defined in equation (5), but are useful for the evaluation of certain relativistic corrections. These are: (i) \( I_2(-1, -1, -2; \lambda_1, \lambda_2, \lambda_{12}) \), (ii) \( I_2(-1, -2, -1; \lambda_1, \lambda_2, \lambda_{12}) \), (iii) \( I_2(-2, -1, -1; \lambda_1, \lambda_2, \lambda_{12}) \) and (iv) \( I_2(-2, -2, -1; \lambda_1, \lambda_2, \lambda_{12}) \).

**Evaluation of integrals in (i) - (iii)**
Integrals in (i) -(iii) are evaluated by the method of integration with respect to parameters $\lambda_1, \lambda_2$ and $\lambda_1$, respectively, and using the expression in equation(9). For example, to evaluate the integral in (i), one makes use of the following observation:

$$\frac{\partial}{\partial \lambda_2} I_2(-1, -1, -2; \lambda_1, \lambda_2, \lambda_{12}) = -I_2'(\lambda_1, \lambda_2, \lambda_{12}).$$

(13)

Inserting equation(9) in equation(13) and then integrating both sides with respect to the parameter $\lambda_{12}$ in the range $\lambda_{12}$ to $\infty$, and noting that $I_2(-1, -1, -2; \lambda_1, \lambda_2, \lambda_{12}) \to 0$ as $\lambda_{12} \to \infty$, the following closed-form expression is obtained:

$$I_2(-1, -1, -2; \lambda_1, \lambda_2, \lambda_{12}) = \frac{16\pi^2}{\lambda_2^2 - \lambda_1^2} \ln \left(\frac{\lambda_2 + \lambda_{12}}{\lambda_1 + \lambda_{12}}\right),$$

(14)

which is in conformity with equation(9) of the report of Puchalski and Pachucki [22]. If $\lambda_{12} \to 0$ on both sides of the above equation, it simplifies to

$$I_2(-1, -1, -2; \lambda_1, \lambda_2, 0) = 16\pi^2(\lambda_2^2 - \lambda_1^2)^{-1}\ln(\lambda_2/\lambda_1),$$

(15)

which is identical with equation(15) of the paper reported by Roberts [65], but evaluated in a different approach. It is worth mentioning here that the integral in equation(15) above has also been evaluated by us independently by using Hylleraas coordinates [3] to get the right hand side expression exactly, as reported in paper I.

If the parameter $\lambda_2 \to \lambda_1$ in the integral in (i), then the following closed-form expression is obtained, as a special case, by employing L’Hospital’s rule for $0/0$ on the right hand side expression in equation(14):

$$I_2(-1, -1, -2; \lambda_1, \lambda_1, \lambda_{12}) = 8\pi^2[\lambda_1(\lambda_1 + \lambda_{12})]^{-1}.$$  

(16)

If, further, $\lambda_1 = \lambda_2 = \lambda_{12} = \delta$, then

$$I_2(-1, -1, -2; \delta, \delta, \delta) = (2\pi/\delta)^2.$$  

(17)

The integral in (ii) is evaluated in the same manner as in (i) to obtain the following closed-form expression:

$$I_2(-1, -2, -1; \lambda_1, \lambda_2, \lambda_{12}) = \frac{16\pi^2}{\lambda_1^2 - \lambda_2^2} \ln \left(\frac{\lambda_1 + \lambda_2}{\lambda_2 + \lambda_{12}}\right).$$

(18)

In yet another method, the same integral can be evaluated by making use of equation(3) and the standard integral [70]

$$\int_0^\infty \frac{dx}{x} [\exp(-ax) - \exp(-bx)] = \ln(b/a)$$

(19)

to establish equation(18), as was done in paper I. If $\lambda_{12} \to \lambda_1$, then employing L’Hospital’s rule for $0/0$ on the right hand side expression in equation(18), one gets

$$I_2(-1, -2, -1; \lambda_1, \lambda_2, \lambda_1) = 8\pi^2[\lambda_1(\lambda_1 + \lambda_2)]^{-1}.$$  

(20)

If, further, $\lambda_1 = \lambda_2 = \lambda_{12} = \delta$, then one obtains

$$I_2(-1, -2, -1; \delta, \delta, \delta) = (2\pi/\delta)^2.$$  

(21)

Closed-form expression in equations(20) and (21) can also be obtained directly by carrying out integrations employing equations(1) and (4).
Following exactly the same two different methods of evaluation employed for the integral in (ii), it is easy to obtain the following closed-form expression for the integral in (iii):

\[ I_2(-2, -1, -1; \lambda_1, \lambda_2, \lambda_{12}) = \frac{16\pi^2}{\lambda_2^2 - \lambda_{12}^2} \ln \left( \frac{\lambda_1 + \lambda_2}{\lambda_1 + \lambda_{12}} \right), \]  

(22)

which is in conformity with equation (12) of the paper of Harris et al.\[62\]. As pointed out earlier, equation (22) can also be obtained from equation (18) by interchanging \( \lambda_1 \leftrightarrow \lambda_2 \). Similarly, the following equations are established:

\[ I_2(-2, -1, -1; \lambda_1, \lambda_2, \lambda_{12}) = 16 \pi^2 \left[ \frac{1}{\lambda_2} \right]^2 \ln \left( \frac{\lambda_1 + \lambda_2}{\lambda_1 + \lambda_{12}} \right), \]  

(23)

\[ I_2(-2, -1, -1; \delta, \delta, \delta) = (2\pi/\delta)^2. \]  

(24)

Evaluation of integral in (iv)

The expression for the integral in (iv) can be obtained by substituting \( \alpha = \lambda_1, \beta = \lambda_2 \) and \( \gamma = \lambda_{12} \) in the general expression reported in \[62\]

\[ I_2(-2, -2, -1; \alpha, \beta, \gamma) = \frac{8\pi^2}{\gamma} Q(\alpha, \beta, \gamma), \]  

(25)

where

\[ Q(\alpha, \beta, \gamma) = \frac{1}{2} \ln^2 \left( \frac{\alpha + \gamma}{\beta + \gamma} \right) + \text{dilog} \left( \frac{\alpha + \beta}{\beta + \gamma} \right) + \text{dilog} \left( \frac{\alpha + \beta}{\alpha + \gamma} \right) + \frac{\pi^2}{6}. \]  

(26)

Here the dilogarithm function, denoted as \( \text{dilog}(x) \), is defined by

\[ \text{dilog}(x) = \int_1^x \frac{\ln t}{1-t} dt = \sum_{n=1}^{\infty} \frac{(1-x)^n}{n^2}, \]  

(27)

with the properties that the series is convergent for \( |x - 1| \leq 1 \) and

\[ \frac{d}{dx} \text{dilog}(x) = \frac{\ln x}{1-x}. \]  

(28)

It is observed that the right hand side of equation (25) is symmetric with respect to interchange \( (\alpha \leftrightarrow \beta) \), as expected. It had been shown \[62\] that \( Q(\alpha, \beta, \gamma) \to 0 \) as \( \gamma \to 0 \), so that the right hand side expression in equation (25) assumes \( 0/0 \) form. Hence, in the limit \( \gamma \to 0 \), L'Hospital's rule for \( 0/0 \) was applied to obtain, as a special case,

\[ I_2(-2, -2, -1; \alpha, \beta, 0) = \frac{16\pi^2}{\alpha} \ln \left( \frac{\alpha + \beta}{\beta} \right) + \frac{16\pi^2}{\beta} \ln \left( \frac{\alpha + \beta}{\alpha} \right). \]  

(29)

The above integral has also been evaluated independently in a different approach to establish equation (29) as pointed out in paper I. Further, if \( \alpha = \beta = \gamma = \delta \), then \( Q(\delta, \delta, \delta) = \pi^2/6 \), since \( \ln(1) = \text{dilog}(1) = 0 \), and hence

\[ I_2(-2, -2, -1; \delta, \delta, \delta) = (4/3)(\pi^4/\delta). \]  

(30)

4. Evaluation of three-electron atomic integrals

4.1 Integrals with unlinked indices
There are three equivalent general three-electron integrals involving s STO’s and exponential correlation, which are graphically represented by three equivalent two-vortex diagrams indicating the presence of only two of the three inter-electron separations of the type \( r_{st} \) and \( r_{su}, s \neq t \neq u = 1, 2, 3 \), each line emanating from a common electron site ‘s’ in one such integral. These are denoted as (i)\( I_{31} \), (ii)\( I_{32} \) and (iii) \( I_{33} \).

**Definition and evaluation of \( I_{31}, I_{32} \) and \( I_{33} \)**

(i) The first integral denoted by \( I_{31} \) is defined as

\[
I_{31}(i, j, k; l, m; \lambda_1, \lambda_2, \lambda_3; \lambda_{12}, \lambda_{13}) = \int d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 r_1^i r_2^j r_3^k r_{12}^l r_{13}^m \times \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_{12} r_{12} - \lambda_{13} r_{13}).
\]

Here \( i, j, k, l \) and \( m \) are integers, each \( \geq -1 \) and the values of the exponential parameters \( \lambda_1, \lambda_2, \lambda_3, \lambda_{12} \) and \( \lambda_{13} \) should be such that the integral converges. The above integral can be written as

\[
I_{31}(i, j, k; l, m; \lambda_1, \lambda_2, \lambda_3; \lambda_{12}, \lambda_{13}) = \left(-\frac{\partial}{\partial \lambda_1}\right)^{i+1} \left(-\frac{\partial}{\partial \lambda_2}\right)^{j+1} \left(-\frac{\partial}{\partial \lambda_3}\right)^{k+1} \left(-\frac{\partial}{\partial \lambda_{12}}\right)^{l+1} \left(-\frac{\partial}{\partial \lambda_{13}}\right)^{m+1} \times I_{31}(-1, -1, -1, -1, \lambda_1, \lambda_2, \lambda_3; \lambda_{12}, \lambda_{13}),
\]

where the corresponding generating integral, in which \( i = j = k = l = m = -1 \), is

\[
I_{31}(-1, -1, -1, -1, \lambda_1, \lambda_2, \lambda_3; \lambda_{12}, \lambda_{13}) = \int d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 (r_1 r_2 r_3 r_{12} r_{13})^{-1} \times \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_{12} r_{12} - \lambda_{13} r_{13}).
\]

It is denoted, in short, by \( I_{31}^g(\lambda_1, \lambda_2, \lambda_3; \lambda_{12}, \lambda_{13}) \) and expressed as

\[
I_{31}^g = \int d\vec{r}_1 r_1^{-1} \exp(-\lambda_1 r_1) J(\lambda_2, \lambda_1, r_1) J(\lambda_3, \lambda_{13}, r_1),
\]

where the \( J \)’s are the integrals defined in equation(1) with their closed-form expressions given by equation(3). Substituting the respective closed-form expressions for the \( J \)’s in equation(34), the angular integration over the variable \( \vec{r}_1 \) is performed easily employing spherical polar coordinates. Then the standard integral given in equation(19) is employed to obtain the following closed-form expression for the generating integral \( I_{31}^g \) :

\[
I_{31}^g = \frac{64\pi^3}{(\lambda_2^2 - \lambda_1^2)(\lambda_3^2 - \lambda_{12}^2)} \ln \left[ \frac{(\lambda_1 + \lambda_3 + \lambda_{12})(\lambda_1 + \lambda_2 + \lambda_{13})}{(\lambda_1 + \lambda_{12} + \lambda_{13})(\lambda_1 + \lambda_2 + \lambda_3)} \right].
\]

**Limiting expressions for \( I_{31}^g \)**

If \( \lambda_{12} = \lambda_{13} = 0 \), then

\[
I_{31}^g(\lambda_1, \lambda_2, \lambda_3; 0, 0) = \frac{64\pi^3}{\lambda_2^2 \lambda_3^2} \ln \left[ \frac{(\lambda_1 + \lambda_3)(\lambda_1 + \lambda_2)}{\lambda_1(\lambda_1 + \lambda_2 + \lambda_3)} \right].
\]

If, further, the exponential parameters \( \lambda_1 = \lambda_2 = \lambda_3 = \delta \), then

\[
I_{31}^g(\delta, \delta, \delta; 0, 0) = 64\pi^3 \ln(4/3) \delta^{-4}.
\]
Also it is observed in equation (35) that if either \( \lambda_{12} \to \lambda_2 \) or \( \lambda_{13} \to \lambda_3 \) or \( \lambda_{12} \to \lambda_2 \) and \( \lambda_{13} \to \lambda_3 \) simultaneously, the right hand side expression assumes 0/0 form, and hence limiting expression can be obtained by applying L’Hospital’s rule for 0/0. Thus, if \( \lambda_{12} \to \lambda_2 \) alone, one gets

\[
I_{31}^g(\lambda_1, \lambda_2, \lambda_3; \lambda_2, \lambda_{13}) = \frac{32\pi^3}{\lambda_2(\lambda_2^2 - \lambda_2^2)} \left[ \frac{1}{\lambda_1 + \lambda_2 + \lambda_{13}} - \frac{1}{\lambda_1 + \lambda_2 + \lambda_3} \right].
\]

Similarly, if \( \lambda_{13} \to \lambda_3 \) alone, one obtains

\[
I_{31}^g(\lambda_1, \lambda_2, \lambda_3; \lambda_2, \lambda_{13}) = \frac{32\pi^3}{\lambda_3(\lambda_2^2 - \lambda_2^2)} \left[ \frac{1}{\lambda_1 + \lambda_2 + \lambda_{13}} - \frac{1}{\lambda_1 + \lambda_2 + \lambda_3} \right].
\]

In case \( \lambda_{12} \to \lambda_1 \) and \( \lambda_{13} \to \lambda_3 \) simultaneously, then the result is

\[
I_{31}^g(\lambda_1, \lambda_2, \lambda_3; \lambda_2, \lambda_{13}) = 16\pi^3[\lambda_2\lambda_3(\lambda_1 + \lambda_2 + \lambda_3)^2]^{-1}.
\]

Also, if each one of all the five exponential parameters (\( \lambda \)’s) is equal to \( \delta \), then

\[
I_{31}^g(\delta, \delta, \delta; \delta, \delta) = (16/9)\pi^3\delta^{-4}.
\]

It is worth mentioning here that equations (36-41) can also be directly established starting from equation (33) and replacing the \( J \)'s in the integrand in equation (34) as per equation (3) and / or equation (4) as desired in the limits \( \lambda_{12} \to \lambda_2 \) and / or \( \lambda_{13} \to \lambda_3 \), and then carrying out the integration. This statement has actually been verified by obtaining the expressions in equations (36-41).

Closed-form expressions for a sequence of integrals given by equation (31) can be obtained for various values of \( i, j, k, l \) and \( m \) by parametric differentiation method employing equations (32) and (35). Thus, all the six entries in the fifth column of table 1 of the paper of Harris et al.[68] are reproduced by differentiating first both sides of equation (35) with respect to suitable parameters and then setting \( \lambda_{12} = \lambda_{13} = 0 \) in the final expression. As an example, to reproduce the sixth entry, the following integral is considered:

\[
(64\pi^3)^{-1} I_{31}(-1, -1, -1; 1; \lambda_1, \lambda_2, \lambda_3; \lambda_{12}, \lambda_{13}) = \frac{1}{64\pi^3} \frac{\partial^2}{\partial \lambda_{12}^2} \frac{\partial^2}{\partial \lambda_{13}^2} I_{31}^g(\lambda_1, \lambda_2, \lambda_3; \lambda_{12}, \lambda_{13}).
\]

The above differentiations are performed on the right hand side expression in equation (35) and then in the final expression \( \lambda_{12} = \lambda_{13} = 0 \) substituted. The resulting expression comes out to be exactly identical with the sixth entry.

Also the expression on the right hand side of equation (36) is in conformity with the fourth entry. Proceeding in a similar manner, the other four entries are exactly reproduced.

(ii) The second three-electron integral denoted by \( I_{32} \) is defined as

\[
I_{32}(i, j, k; l, m; \lambda_1, \lambda_2, \lambda_3; \lambda_{21}, \lambda_{23}) = \int \int \int \int \int \int d^3r_1 d^3r_2 d^3r_3 d^3r_1' d^3r_2' d^3r_3' \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_{21} r_{21} - \lambda_{23} r_{23})
\]

\[
\times \exp(-\lambda_1 r_1' - \lambda_2 r_2' - \lambda_3 r_3' - \lambda_{21} r_{21}' - \lambda_{23} r_{23}').
\]
The corresponding generating integral, analogous with definitions in equations (31-33), is given by

$$I_{32}^g(\lambda_1, \lambda_2, \lambda_3; \lambda_{21}, \lambda_{23}) = \int d\tau_1 d\tau_2 d\tau_3 (r_1 r_2 r_3 r_{21} r_{23})^{-1} \times \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_{21} r_{23} - \lambda_{23} r_{23}).$$

(44)

It is observed that if a change (1 \rightleftharpoons 2) is performed in equation (33), and noting that $r_{12} = r_{21}$ and $\lambda_{12} = \lambda_{21}$, equation (44) is obtained. Accordingly, the following closed-form expression for the integral in equation (44) is obtained from the right hand side expression in equation (35) by inspection:

$$I_{32}^g = \frac{64\pi^3}{(\lambda_1^2 - \lambda_{12}^2)(\lambda_3^2 - \lambda_{23}^2)} \ln \left[ \frac{(\lambda_2 + \lambda_3 + \lambda_{12})(\lambda_1 + \lambda_2 + \lambda_{23})}{(\lambda_2 + \lambda_{12} + \lambda_{23})(\lambda_1 + \lambda_2 + \lambda_3)} \right].$$

(45)

This expression was also reported earlier in paper I. The integral given in equation (5) and its closed-form expression given in equation (9) in the paper of Bonham[63] are exactly reproduced by suitable parametric differentiations of both sides of equation (45). Also various limiting expressions of the generating integral $I_{32}^g$ above can be obtained following the procedure adopted for deriving equations (36-41) relating to $I_{31}^g$.

(iii) The third three-electron integral denoted by $I_{33}$ is defined as

$$I_{33}(i, j, k; l, m; \lambda_1, \lambda_2, \lambda_3; \lambda_{13}, \lambda_{23}) = \int d\tau_1 d\tau_2 d\tau_3 (r_{12} r_{13} r_{23})^{i} \times \exp(-\lambda_i r_i - \lambda_j r_j - \lambda_k r_k - \lambda_{13} r_{13} - \lambda_{23} r_{23}).$$

(46)

The corresponding generating integral is given by

$$I_{33}^g(\lambda_1, \lambda_2, \lambda_3; \lambda_{13}, \lambda_{23}) = \int d\tau_1 d\tau_2 d\tau_3 (r_1 r_2 r_3 r_{13} r_{23})^{-1} \times \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_{13} r_{13} - \lambda_{23} r_{23}).$$

(47)

It is observed that, if we make either a change (2 \rightleftharpoons 3) in equation (44) or a change (3 \rightleftharpoons 1) in equation (33), we get equation (47). Hence, by inspection, the following closed-form expression for $I_{33}^g$ is obtained either from equation (45) by performing a change (2 \rightleftharpoons 3) or from equation (35) by making a change (3 \rightleftharpoons 1):

$$I_{33}^g = \frac{64\pi^3}{(\lambda_2^2 - \lambda_{23}^2)(\lambda_3^2 - \lambda_{13}^2)} \ln \left[ \frac{(\lambda_1 + \lambda_3 + \lambda_{12})(\lambda_3 + \lambda_2 + \lambda_{13})}{(\lambda_3 + \lambda_{23} + \lambda_{13})(\lambda_1 + \lambda_2 + \lambda_3)} \right].$$

(48)

Various limiting expressions for the above generating integral can be obtained as outlined in the case of other two generating integrals.

4.2 Integral with linked indices

The only other three-electron integral which is graphically represented by a triangle, hence known as the triangle integral, indicates the involvements of all the three inter-electron separation coordinates with linked indices in the integrand. It does not come under the category of integrals mentioned in section 2.1 above.

For the development of various numerical and analytical methods of evaluation, with greater accuracy, of the triangle integral, it is advisable to go through the second and
the third paragraph in the introduction.

5. Evaluation of four-electron integrals with unlinked indices

Four-electron integrals with exponential correlation involving only three inter-electron separation coordinates with unlinked indices are divided into two different categories on the basis of their graphical representation: the first category corresponds to three-vortex diagrams and the second to open squares.

5.1 Integrals represented by three-vortex diagrams

There are four equivalent general four-electron integrals with exponential correlation, each one of which is graphically represented by a three-vortex diagram indicating that the integrand involves explicitly only three inter-electron separation coordinates (of the type $r_{st}, r_{su}$ and $r_{sv}, s \neq t \neq u \neq v = 1, 2, 3, 4$, each line emanating from a common electron site 's') with unlinked indices out of the total six inter-electron separation coordinates of a four-electron atom. These are denoted here as (i) $I_{41}$, (ii) $I_{42}$, (iii) $I_{43}$ and (iv) $I_{44}$, and defined by

$$I_{41}(i, j, k, l; m, n, p; \lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{13}, \lambda_{14})$$

$$= \int d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 r_1^{i}r_2^{j}r_3^{k}r_4^{l}r_{12}^{m}r_{13}^{n}r_{14}^{p}$$

$$\times \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_4 r_4 - \lambda_{12} r_{12} - \lambda_{13} r_{13} - \lambda_{14} r_{14}),$$

$$I_{42}(i, j, k, l; m, n, p; \lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{21}, \lambda_{23}, \lambda_{24})$$

$$= \int d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 r_1^{i}r_2^{j}r_3^{k}r_4^{l}r_{21}^{m}r_{23}^{n}r_{24}^{p}$$

$$\times \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_4 r_4 - \lambda_{21} r_{21} - \lambda_{23} r_{23} - \lambda_{24} r_{24}),$$

with similar definitions for the integrals $I_{43}$ and $I_{44}$. Here $i, j, k, l, m, n$ and $p$ are the integers, each $\geq -1$, and the values of the exponential parameters ($\lambda$'s) should be such that the integral converges. Each one of these integrals can be expressed in terms of the corresponding generating integrals in which ($i = j = k = l = m = n = p = -1$) by the method of parametric differentiation. For example,

$$I_{41}(i, j, k, l; m, n, p; \lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{13}, \lambda_{14})$$

$$= \left( -\frac{\partial}{\partial \lambda_1} \right)^{i+1} \left( -\frac{\partial}{\partial \lambda_2} \right)^{j+1} \left( -\frac{\partial}{\partial \lambda_3} \right)^{k+1} \left( -\frac{\partial}{\partial \lambda_4} \right)^{l+1}$$

$$\times I_{41}(-1, -1, -1, -1, -1, -1, -1, -1, -1, -1, \lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{13}, \lambda_{14}).$$

The respective generating integral is given by

$$I_{41}(-1, -1, -1, -1, -1, -1, -1, -1, -1, \lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{13}, \lambda_{14})$$

$$= \int d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 (r_1 r_2 r_3 r_4 r_{12} r_{13} r_{14})^{-1}$$

$$\times \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_4 r_4 - \lambda_{12} r_{12} - \lambda_{13} r_{13} - \lambda_{14} r_{14}),$$

and is denoted, in short, by $I_{41}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{13}, \lambda_{14})$. Similarly from equation (50) we can express the generating integral as
\[ I^g_{42}(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{21}, \lambda_{23}, \lambda_{24}) = \int dr_1^2 dr_2^2 dr_3^2 (r_1 r_2 r_3 r_4 r_{21} r_{23} r_{24})^{-1} \times \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_4 r_4 - \lambda_{21} r_{21} - \lambda_{23} r_{23} - \lambda_{24} r_{24}). \] (53)

The other two generating integrals corresponding to integrals \( I_{43} \) and \( I_{44} \) are, respectively, given by

\[ I^g_{43}(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{31}, \lambda_{32}, \lambda_{34}) = \int dr_1^2 dr_2^2 dr_3^2 (r_1 r_2 r_3 r_{31} r_{32} r_{34})^{-1} \times \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_4 r_4 - \lambda_{31} r_{31} - \lambda_{32} r_{32} - \lambda_{34} r_{34}), \] (54)

and

\[ I^g_{44}(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{41}, \lambda_{42}, \lambda_{43}) = \int dr_1^2 dr_2^2 dr_3^2 dr_4^2 (r_1 r_2 r_3 r_4 r_{41} r_{42} r_{43})^{-1} \times \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_4 r_4 - \lambda_{41} r_{41} - \lambda_{42} r_{42} - \lambda_{43} r_{43}). \] (55)

It is easy to observe that if any one of the generating integrals given by equations (52-55) is evaluated analytically, the closed-form expressions for the other three can be written by inspection, keeping in mind that \( r_{ij} = r_{ji} \) and \( \lambda_{ij} = \lambda_{ji} \). Hence expression for all the general four-electron integrals \( I_{41}, I_{42}, I_{43} \) and \( I_{44} \) can be obtained by parametric differentiation method as mentioned in equation (51).

### 5.1 (a) Evaluation of the generating integral \( I^g_{42} \)

Closed-form expression for the generating integral \( I^g_{42} \) as defined in equation (53) has already been reported in paper I. Only few steps will be repeated here before giving the final expression with the intention to obtain several limiting expressions for \( I^g_{42} \) which were not reported earlier. The integral given by equation (53) can be recast as

\[ I^g_{42}(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{23}, \lambda_{24}) = \int dr_2^2 \exp(-\lambda_2 r_2) \times J(\lambda_3, \lambda_{23}, r_2)J(\lambda_4, \lambda_{24}, r_2)J(\lambda_1, \lambda_{12}, r_2), \] (56)

where the \( J \)'s are the integrals defined in equation (1). Substituting proper closed-form expression for the \( J \)'s from equation (3) in equation (56) and doing the angular integration, \( I^g_{42} \) is reduced to the following one-dimensional form:

\[ I^g_{42} = \int_0^\infty dr_2 r_2^{-2} f(r_2), \] (57)

where the function \( A \) is given by

\[ A = 256\pi^4[(\lambda_1^2 - \lambda_{12}^2)(\lambda_3^2 - \lambda_{23}^2)(\lambda_4^2 - \lambda_{24}^2)]^{-1}, \] (58)

and the function \( f(r_2) \) is a sum of eight terms of the form \( \exp(-\beta_i r_2), i = 1, 2, 3, 4, \ldots, 8 \). Each \( \beta_i \) is a sum of four different \( \lambda \)'s out of the seven \( \lambda \)'s in equation (56), and the expressions for all the \( \beta_i \)'s are different.

It can be shown that all three functions \( f(r_2), f'(r_2) \) and \( f''(r_2) \) tend to zero as \( r_2 \) tends to zero. Here \( f'(r_2) \) and \( f''(r_2) \) represent the first order and the second order
derivatives, respectively. Also by employing L'Hospital's rule for 0/0, it is easy to prove that \( \frac{f(r_2)}{r_2^3} \to 0, \frac{f'(r_2)}{r_2} \to 0 \) and \( \frac{f''(r_2)}{r_2} \to 0 \) as \( r_2 \to 0 \). Integrating by parts, and then making use of equation(19), the integral in equation(57) is evaluated to obtain the following closed-form expression:

\[
I_{42}^g = AL, \tag{59}
\]

where the function \( A \) is given by equation(58) and the function \( L \) by

\[
L(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{23}, \lambda_{24}) = \sum_{i=1}^{8} L_i, \tag{60}
\]

with

\[
L_1 = (\lambda_2 + \lambda_{12} + \lambda_{23}) \ln \left[ \frac{\lambda_2 + \lambda_{12} + \lambda_{23} + \lambda_{24}}{\lambda_2 + \lambda_{12} + \lambda_{23}} \right],
\]

\[
L_2 = (\lambda_2 + \lambda_{12} + \lambda_3) \ln \left[ \frac{\lambda_2 + \lambda_{12} + \lambda_3 + \lambda_4}{\lambda_2 + \lambda_{12} + \lambda_3 + \lambda_{24}} \right],
\]

\[
L_3 = (\lambda_1 + \lambda_2 + \lambda_{23}) \ln \left[ \frac{\lambda_1 + \lambda_2 + \lambda_{23} + \lambda_{24}}{\lambda_1 + \lambda_2 + \lambda_{23} + \lambda_{24}} \right],
\]

\[
L_4 = (\lambda_1 + \lambda_2 + \lambda_3) \ln \left[ \frac{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_{24}}{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4} \right],
\]

\[
L_5 = \lambda_{24} \ln \left[ \frac{\lambda_2 + \lambda_{12} + \lambda_{23} + \lambda_{24}}{\lambda_2 + \lambda_{12} + \lambda_{23}} \right],
\]

\[
L_6 = \lambda_{24} \ln \left[ \frac{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_{24}}{\lambda_1 + \lambda_2 + \lambda_{23} + \lambda_{24}} \right],
\]

\[
L_7 = \lambda_4 \ln \left[ \frac{\lambda_2 + \lambda_3 + \lambda_4 + \lambda_{12}}{\lambda_2 + \lambda_4 + \lambda_{12} + \lambda_{23}} \right],
\]

\[
L_8 = \lambda_4 \ln \left[ \frac{\lambda_1 + \lambda_2 + \lambda_4 + \lambda_{23}}{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4} \right].
\]

It is worth mentioning here that an alternative expression with larger symmetry than the one reported in paper I, and now given by equation(59) above, for \( I_{42}^g \), has been reported very recently by King [59]. However, by minor manipulations, it is easily shown that the above expression becomes exactly identical with that given by equation(35) in [59], and hence, all the following discussions are made relating to the expression given by equation(59).

**Limiting expressions for \( I_{42}^g \)**

If, as a special case, \( \lambda_{12} = \lambda_{23} = \lambda_{24} = 0 \), then, after some manipulations equation(59) simplifies to

\[
I_{42}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; 0, 0, 0, 0) = 256\pi^4(\lambda_1\lambda_2\lambda_4)^{-2}[\lambda_2\ln \lambda_2 - (\lambda_2 + \lambda_1)\ln(\lambda_2 + \lambda_1) - (\lambda_2 + \lambda_3)\ln(\lambda_2 + \lambda_3) - (\lambda_2 + \lambda_4)\ln(\lambda_2 + \lambda_4) + (\lambda_2 + \lambda_3 + \lambda_4)\ln(\lambda_2 + \lambda_3 + \lambda_4)
\]

\[
+ (\lambda_2 + \lambda_1 + \lambda_4)\ln(\lambda_2 + \lambda_1 + \lambda_4) + (\lambda_2 + \lambda_1 + \lambda_3)\ln(\lambda_2 + \lambda_1 + \lambda_3)
\]

\[
- (\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4)\ln(\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4)]. \tag{61}
\]

It is worth pointing out here that a closed-form expression for the integral on the left hand side of equation(61) was obtained by King [52] directly, by employing expansion
formula of Sack [71] and of Perkins [72] for \( r_{ij}^o \). The corresponding expression contains a minor typographical error which is corrected by changing the signs before the fourth and the fifth terms within the curly brackets on the right hand side of equation(44) of the reported paper [52], which has been pointed out very recently in [59]. Incorporating these minor corrections, it is easy to show that the corrected expression becomes identical with the one given on the right hand side of equation(61) obtained, as a special case, from the generating integral \( I_{42}^g \) defined in equation(53) and evaluated and reported earlier in paper I.

By differentiating both side of equation(59) with respect to \( \lambda_2 \), a closed-form expression for the integral \( I_{42}(-1, 0, -1, -1; -1, -1, -1, -1; \lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{23}, \lambda_{24}) \), as a special case, is obtained which is exactly identical with the right hand side expression in equation(62) of the recent paper [59], wherein the integral has been evaluated directly. Then substituting \( \lambda_{12} = \lambda_{23} = \lambda_{24} = 0 \) in that expression the following integral is evaluated:

\[
I_{42}^g(-1, 0, -1, -1; -1, -1, -1; \lambda_1, \lambda_2, \lambda_3, \lambda_4; 0, 0, 0) = \frac{128\pi^4}{\lambda_1(\lambda_1^2 - \lambda_{12}^2)(\lambda_3^2 - \lambda_{23}^2)} \ln \left[ \frac{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4}{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4} \right],
\]

which is in conformity with equation(16) of the report of Roberts [65] who had evaluated the integral by expanding \((r_{12}r_{23}r_{24})^{-1}\) in spherical harmonics. Also it is easy to establish equation(62) by differentiating both sides of equation(61) with respect to \( \lambda_2 \). Further, if \( \lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = \delta \), then equation(61) becomes

\[
I_{42}^g(\delta, \delta, \delta, \delta; 0, 0, 0) = 256\pi^4\delta^{-6}(9\ln3 - 14\ln2) \quad (63)
\]

and equation(62) becomes

\[
I_{42}(-1, 0, -1, -1; -1, -1, -1; \delta, \delta, \delta, \delta; 0, 0, 0) = 256\pi^4\delta^{-6}(5\ln2 - 3\ln3). \quad (64)
\]

The expressions obtained in equations(62-64) here have also been reported in [52].

It is observed in equation(60) that if \( \lambda_{12} \rightarrow \lambda_1 \), then \( L \rightarrow 0 \). Similarly if \( \lambda_{23} \rightarrow \lambda_3 \), then also \( L \rightarrow 0 \). So also \( L \rightarrow 0 \) if \( \lambda_{24} \rightarrow \lambda_4 \). In such cases the right hand side expression in equation(59) assumes \( 0/0 \) form. Hence, finite expression for \( I_{42}^g \) in various limiting cases can be obtained by applying L'Hospital's rule for \( 0/0 \).

Thus if \( \lambda_{12} \rightarrow \lambda_1 \) alone, equation(59) gives

\[
I_{42}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{23}, \lambda_{24}) = \frac{128\pi^4}{\lambda_1(\lambda_1^2 - \lambda_{12}^2)(\lambda_3^2 - \lambda_{23}^2)} \ln \left[ \frac{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4}{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4} \right]. \quad (65)
\]

If \( \lambda_{23} \rightarrow \lambda_3 \) alone in equation(59), the result is

\[
I_{42}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{23}, \lambda_{24}) = \frac{128\pi^4}{(\lambda_1^2 - \lambda_{12}^2)\lambda_3(\lambda_4^2 - \lambda_{24}^2)} \ln \left[ \frac{\lambda_2 + \lambda_3 + \lambda_{12} + \lambda_4}{\lambda_2 + \lambda_3 + \lambda_{12} + \lambda_4} \right]. \quad (66)
\]

On the other hand, if \( \lambda_{24} \rightarrow \lambda_4 \) alone, equation(59) reduces to

\[
I_{42}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{23}, \lambda_4) = \frac{128\pi^4}{(\lambda_1^2 - \lambda_{12}^2)(\lambda_3^2 - \lambda_{23}^2)} \ln \left[ \frac{\lambda_2 + \lambda_{12} + \lambda_3 + \lambda_4}{\lambda_2 + \lambda_{12} + \lambda_3 + \lambda_4} \right]. \quad (67)
\]
In case \( \lambda_{12} \to \lambda_1 \) and \( \lambda_{23} \to \lambda_3 \) together, applying L'Hospital’s rule for 0/0 to the right hand side expressions in equation(65) or equation(66) as required, the following result is obtained:

\[
I_{42}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_1, \lambda_3, \lambda_{24}) = 64\pi^4\lambda_1(\lambda_3 + \lambda_{24})(\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4)(\lambda_1 + \lambda_2 + \lambda_3 + \lambda_{24})^{-1}. \tag{68}
\]

If, further, \( \lambda_{24} = \lambda_4 \), then

\[
I_{42}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_1, \lambda_3, \lambda_4) = 32\pi^4\lambda_3\lambda_4(\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4)^2^{-1}. \tag{69}
\]

In the most special case, if each of the exponential parameters (\( \lambda \)'s) in equation(59) is equal to \( \delta \), then equation(69) simplifies to

\[
I_{42}^g(\delta, \delta, \delta, \delta; \delta, \delta, \delta) = 2\pi^4\delta^{-5}. \tag{70}
\]

Adopting the same procedure as above, expressions for the following integrals are obtained from equation(67) taking limits \( \lambda_{12} \to \lambda_1 \) and \( \lambda_{23} \to \lambda_3 \), respectively:

\[
I_{42}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_1, \lambda_{23}, \lambda_4) = 64\pi^4\lambda_1(\lambda_3 + \lambda_{23})\lambda_4(\lambda_2 + \lambda_1 + \lambda_3 + \lambda_4)(\lambda_2 + \lambda_1 + \lambda_{23} + \lambda_4)^{-1}, \tag{71}
\]

\[
I_{42}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_1, \lambda_2, \lambda_4) = 64\pi^4(\lambda_1 + \lambda_{12})\lambda_3\lambda_4(\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4)(\lambda_2 + \lambda_{12} + \lambda_3 + \lambda_4)^{-1}. \tag{72}
\]

As expected, equation(69) is again established if either \( \lambda_{23} \) is replaced by \( \lambda_3 \) in equation(71) or \( \lambda_{12} \) is replaced by \( \lambda_1 \) in equation(72).

It is worth pointing out here that all the limiting expressions for \( I_{42}^g \) given in equations(61) and (65-72) can also be obtained directly from equation(53) by making use of equation(3) and/or equation(4) in the integral in equation(56) as per the desired limits and carrying out the integration. This statement has been actually verified by evaluating the integrals.

5.1(b) Evaluation of the generating integral \( I_{41}^g \)

The generating integral \( I_{41}^g \) as given by equation(52) can be recast as

\[
I_{41}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{13}, \lambda_{14}) = \int d\tau_1^2 \left[ r_1^{-1} \exp(-\lambda_1 r_1) \right] J(\lambda_2, \lambda_{12}, r_1)J(\lambda_3, \lambda_{13}, r_1)J(\lambda_4, \lambda_{14}, r_1), \tag{73}
\]

where the RJ’s are the integrals given by equations(1) and (3). Performing the evaluation as outlined in the case of the generating integral \( I_{42}^g \), the following closed-form expression is obtained for \( I_{41}^g \):

\[
I_{41}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{13}, \lambda_{14}) = BM, \tag{74}
\]

where \( B \) and \( M \) are functions given by

\[
B = 256\pi^4(\lambda_2^2 - \lambda_{12}^2)(\lambda_3^2 - \lambda_{13}^2)(\lambda_4^2 - \lambda_{14}^2)^{-1}. \tag{75}
\]
and

\[ M(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{13}, \lambda_{14}) = \sum_{i=1}^{8} M_i, \]  

(76)

with

\[
M_1 = (\lambda_1 + \lambda_{12} + \lambda_{13})\ln\left[ \frac{(\lambda_1 + \lambda_{12} + \lambda_{13} + \lambda_{14})}{(\lambda_1 + \lambda_{12} + \lambda_{13} + \lambda_4)} \right],
\]

\[
M_2 = (\lambda_1 + \lambda_{12} + \lambda_3)\ln\left[ \frac{(\lambda_1 + \lambda_{12} + \lambda_3 + \lambda_{14})}{(\lambda_1 + \lambda_{12} + \lambda_{13} + \lambda_{14})} \right],
\]

\[
M_3 = (\lambda_{12} + \lambda_1 + \lambda_{13})\ln\left[ \frac{(\lambda_{12} + \lambda_1 + \lambda_{13} + \lambda_4)}{(\lambda_{12} + \lambda_1 + \lambda_{13} + \lambda_{14})} \right],
\]

\[
M_4 = (\lambda_{12} + \lambda_1 + \lambda_3)\ln\left[ \frac{(\lambda_{12} + \lambda_1 + \lambda_3 + \lambda_{14})}{(\lambda_{12} + \lambda_1 + \lambda_{13} + \lambda_4)} \right],
\]

\[
M_5 = \lambda_{14}\ln\left[ \frac{(\lambda_1 + \lambda_{12} + \lambda_{13} + \lambda_{14})}{(\lambda_1 + \lambda_{12} + \lambda_4 + \lambda_{13})} \right],
\]

\[
M_6 = \lambda_{14}\ln\left[ \frac{(\lambda_{12} + \lambda_1 + \lambda_3 + \lambda_{14})}{(\lambda_{12} + \lambda_1 + \lambda_{13} + \lambda_{14})} \right],
\]

\[
M_7 = \lambda_4\ln\left[ \frac{(\lambda_1 + \lambda_3 + \lambda_4 + \lambda_{12})}{(\lambda_1 + \lambda_4 + \lambda_{12} + \lambda_{13})} \right],
\]

\[
M_8 = \lambda_4\ln\left[ \frac{(\lambda_2 + \lambda_1 + \lambda_4 + \lambda_{13})}{(\lambda_2 + \lambda_1 + \lambda_{13} + \lambda_4)} \right].
\]

Noting that \( r_{ij} = r_{ji} \) and \( \lambda_{ij} = \lambda_{ji} \), equation(52) for \( I_{41}^g \) is obtained from equation(53) for \( I_{42}^g \) by making the interchange (2 \( \Leftrightarrow \) 1) in equation(53). Comparing the expression for \( I_{42}^g \) given in the right hand side of equation(59) with that for \( I_{41}^g \) given in equation(74), it is clearly observed that the right hand side expression for \( I_{42}^g \) in equation(74) is exactly obtained from the right hand side expression for \( I_{42}^g \) in equation(59) by performing the interchange (2 \( \Leftrightarrow \) 1) in equation(59), as pointed out earlier. Thus we conclude that even without going through the process of evaluation, the closed-form expression for \( I_{41}^g \) can be obtained by inspection from that of \( I_{42}^g \).

**Limiting expressions for \( I_{41}^g \)**

If, as a special case, \( \lambda_{12} = \lambda_{13} = \lambda_{14} = 0 \) substituted on both sides of equation(74), an expression for the integral \( I_{41}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; 0, 0, 0) \) is obtained which is observed to be exactly identical with the one arrived at from the right hand side of equation(61) by making the interchange (2 \( \Leftrightarrow \) 1), as expected. Thus the following equality is obtained:

\[
I_{41}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; 0, 0, 0) = I_{42}^g(\lambda_1 \Rightarrow \lambda_2, \lambda_3, \lambda_4; 0, 0, 0); \quad (77)
\]

Various other limiting expressions for \( I_{41}^g \), similar to equations(65-72) in case of \( I_{42}^g \), can be easily obtained following the procedure adopted for \( I_{42}^g \).

**Expression for \( < r_{12}r_{13}/r_{14} > \)**

Sometimes it is required to obtain the expectation value \( < r_{12}r_{13}/r_{14} > \) in linear theories of atoms with four or more number of electrons. This can be achieved by differentiating both sides of equation(74) twice with respect to \( \lambda_{12} \) and twice with respect to \( \lambda_{13} \). Thus
the required integral is

\[ I_{41}(-1, -1, -1, -1; 1, 1, -1; \lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{13}, \lambda_{14}) = \frac{\partial^2}{\partial \lambda_{12} \partial \lambda_{13}} [BM]. \] (78)

Carrying out the differentiations on the right hand side, an analytical expression is obtained for the integral on the left hand side of equation (78), which is related to \( < r_{12} r_{13} / r_{14} > \).

If \( \lambda_{12} = \lambda_{13} = \lambda_{14} = 0 \), as a special case, then the following expression is obtained:

\[
I_{41}(-1, -1, -1, -1; 1, 1, -1; \lambda_1, \lambda_2, \lambda_3, \lambda_4; 0, 0, 0) \\
= \frac{4}{\lambda_2^4 \lambda_3^4} I_{41}^g (\lambda_1, \lambda_2, \lambda_3, \lambda_4; 0, 0, 0) \\
+ \frac{512 \pi^4}{\lambda_2^4 \lambda_3^4} \left[ \frac{1}{\lambda_1} - \frac{1}{\lambda_1 + \lambda_2} - \frac{1}{\lambda_1 + \lambda_3} + \frac{1}{\lambda_1 + \lambda_2 + \lambda_3} \right] \\
- \frac{1}{\lambda_2^3 (\lambda_1 + \lambda_4)^3} + \frac{1}{\lambda_3^3} \left( \frac{1}{\lambda_1} - \frac{1}{\lambda_1 + \lambda_3} - \frac{1}{\lambda_1 + \lambda_4} + \frac{1}{\lambda_1 + \lambda_3 + \lambda_4} \right). \] (79)

If, further, \( \lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = \delta \), then, the above equation simplifies to

\[
I_{41}(-1, -1, -1, -1; 1, 1, -1; \delta, \delta, \delta, \delta; 0, 0, 0) \\
= 512 \pi^4 \delta^{-9} (37/24 + 18 \ln 3 - 28 \ln 2). \] (80)

Following the same procedure as adopted in equation (78), the expectation values \( < r_{12} r_{14} / r_{13} > \) and \( < r_{13} r_{14} / r_{12} > \) can be obtained.

5.1 (c) Evaluation of the generating integrals \( I_{43}^g \) and \( I_{44}^g \)

Closed-form expression for \( I_{43}^g \) as defined in equation (54) can be obtained from that of \( I_{42}^g \) as given in the right hand side of equation (59) by performing the interchange \( (2 \rightleftharpoons 3) \) in equation (59). Alternatively, the integral \( I_{43}^g \) can be evaluated directly as was done in the case of \( I_{42}^g \) employing equations (1) and (3). It has been observed that the two expressions obtained for \( I_{43}^g \) by the above two alternative approaches do not appear to be identical. However, by minor manipulative algebra, both the expressions are shown to be exactly identical. In yet another alternative approach, expression for \( I_{43}^g \) can be obtained from the right hand side expression in equation (74) for \( I_{41}^g \), by making the interchange \( (1 \rightleftharpoons 3) \) in equation (74).

Expression for \( I_{44}^g \) as defined in equation (55) can be derived directly employing equations (1) and (3) as was done for \( I_{42}^g \). Alternatively, by inspection, its expression can be written as the one obtained either from equation (59) by the interchange \( (2 \rightleftharpoons 4) \), or from equation (74) by the interchange \( (1 \rightleftharpoons 4) \).

It is concluded, in general, that closed-form expression for \( I_{4i}^g \) can be obtained from the expression for \( I_{4j}^g \), by making interchange \( (j \rightleftharpoons i) \) in the expression for \( I_{4j}^g \), and vice versa, as pointed out earlier.

Various limiting expressions for \( I_{43}^g \) and \( I_{44}^g \) can be derived by following the same procedure adopted for \( I_{42}^g \) while obtaining expressions in equations (61) and (65-72).
5.2 Integrals represented by open square diagrams

**I.** There is one set of four general integrals involving exponential correlation corresponding to four equivalent open square diagrams, with one side of each square missing. Thus the respective integrals involve correlations of the form $(r_{ij}r_{jk}r_{kl})^{-1} \exp(-\lambda_{ij}r_{ij} - \lambda_{jk}r_{jk} - \lambda_{kl}r_{kl})$ with $i,j,k$ and $l$ cyclic, beginning with $i=1$. For example, for the first generating integral $i=1, j=2, k=3$ and $l=4$; for the second $i=2, j=3, k=4$ and $l=1$, etc.

**II.** There is another set of four such general four-electron integrals, each represented by an open square diagram with opposite sides of the square missing and the other two opposite sides connected by a diagonal. As an example, the correlation of the form $(r_{12}r_{13}r_{34})^{-1} \exp(-\lambda_{12}r_{12} - \lambda_{13}r_{13} - \lambda_{34}r_{34})$ is considered corresponding to an open square with opposite sides represented by $r_{12}$ and $r_{34}$, respectively, and connected by the diagonal represented by $r_{13}$. The other correlations considered are of the form $(r_{12}r_{24}r_{43})^{-1} \exp(-\lambda_{12}r_{12} - \lambda_{24}r_{24} - \lambda_{43}r_{43})$, $(r_{23}r_{31}r_{14})^{-1} \exp(-\lambda_{23}r_{23} - \lambda_{31}r_{31} - \lambda_{14}r_{14})$, and $(r_{23}r_{24}r_{41})^{-1} \exp(-\lambda_{23}r_{23} - \lambda_{24}r_{24} - \lambda_{41}r_{41})$.

5.2 (I) Integrals belonging to category (I)

The four general integrals belonging to the first category are denoted as (a) $K_{41}$, (b) $K_{42}$, (c) $K_{43}$ and (d) $K_{44}$, and defined as

$$K_{41}(i, j, k, l; m, n, p; \lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{23}, \lambda_{34}) = \int d\tau_1 d\tau_2 d\tau_3 d\tau_4 \int_{1}^{j} r_{12}^{m} r_{13}^{n} r_{24}^{p} \exp(-\lambda_{12}r_{12} - \lambda_{23}r_{23} - \lambda_{34}r_{34}).$$

(81)

with similar definitions for $K_{42}, K_{43}$ and $K_{44}$.

The integral $K_{41}$ can be related to the corresponding generating integral $K_{41}^q$, as usual, through parametric differentiation. Thus

$$K_{41}(i, j, k, l; m, n, p; \lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{23}, \lambda_{34}) = \left( -\frac{\partial}{\partial \lambda_1} \right)^{i+1} \left( -\frac{\partial}{\partial \lambda_2} \right)^{j+1} \left( -\frac{\partial}{\partial \lambda_3} \right)^{k+1} \left( -\frac{\partial}{\partial \lambda_4} \right)^{l+1} K_{41}^q,$$

(82)

where $K_{41}^q$ is the generating integral given by

$$K_{41}^q(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{23}, \lambda_{34}) = \int d\tau_1 d\tau_2 d\tau_3 d\tau_4 \int_{1}^{j} r_{12}^{m} r_{13}^{n} r_{24}^{p} \exp(-\lambda_{12}r_{12} - \lambda_{23}r_{23} - \lambda_{34}r_{34}).$$

(83)

with similar definitions for the other three integrals and the respective generating integrals.

(a) Analytic evaluation of $K_{41}^q$
The integral $K_{41}^g$ as defined in equation (83) can be written as

$$K_{41}^g = \int d\tau_2 d\tau_3 (r_2 r_3 r_{23})^{-1} \exp(-\lambda_2 r_2 - \lambda_3 r_3 - \lambda_{23} r_{23}) \times J(\lambda_1, \lambda_{12}, r_2) J(\lambda_4, \lambda_{34}, r_3),$$

where the J integrals are defined by equation (1) with their closed-form expressions given by equation (3). Substituting the expressions for the J’s in equation (84), it simplifies to

$$K_{41}^g = D[I_2(-2, -2, -1; \alpha_1, \beta_1, \gamma_1) - I_2(-2, -2, -1; \alpha_2, \beta_2, \gamma_2) - I_2(-2, -2, -1; \alpha_3, \beta_3, \gamma_3) + I_2(-2, -2, -1; \alpha_4, \beta_4, \gamma_4)],$$

where D is a function given by

$$D(\lambda_1, \lambda_{12}, \lambda_4, \lambda_{34}) = 16\pi^2[(\lambda_1^2 - \lambda_{12}^2)(\lambda_4^2 - \lambda_{34}^2)]^{-1},$$

and, in general,

$$I_2(-2, -2, -1; \alpha, \beta, \gamma) = \int d\tau_2 d\tau_3 (r_2 r_3 r_{23})^{-1} \times \exp(-\alpha r_2 - \beta r_3 - \gamma r_{23}),$$

with $\alpha_1 = \alpha_2 = \lambda_2 + \lambda_{12}$, $\alpha_3 = \alpha_4 = \lambda_1 + \lambda_2$, $\beta_1 = \beta_2 = \lambda_3 + \lambda_{34}$, $\beta_2 = \beta_4 = \lambda_3 + \lambda_4$ and $\gamma_1 = \gamma_2 = \gamma_3 = \gamma_4 = \lambda_{23}$.

The analytical expression for the integral defined in equation (87), in general, has been given in equation (25). Replacing the $I_2$ integrals in equation (85) by their closed-form expressions, and doing some simplifications, the following expression for $K_{41}^g$ is successfully obtained:

$$K_{41}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_{12}, \lambda_{23}, \lambda_{34}) = D N,$$

where the function D is given by equation (86) and the function N, which is the sum of the four $I_2$ integrals within the square brackets on the right hand side of equation (85), is given by

$$N(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{23}, \lambda_{34}) = \frac{8\pi^2}{\lambda_{23}} \left[ \ln \left( \frac{\lambda_{12} + \lambda_2 + \lambda_{23}}{\lambda_1 + \lambda_2 + \lambda_{23}} \right) \ln \left( \frac{\lambda_3 + \lambda_4 + \lambda_{23}}{\lambda_3 + \lambda_{34} + \lambda_{23}} \right) \right] + \text{dilog} \left( \frac{\lambda_2 + \lambda_1 + \lambda_3 + \lambda_{34}}{\lambda_2 + \lambda_{12} + \lambda_{23}} \right) + \text{dilog} \left( \frac{\lambda_2 + \lambda_1 + \lambda_3 + \lambda_{34}}{\lambda_3 + \lambda_{34} + \lambda_{23}} \right) - \text{dilog} \left( \frac{\lambda_2 + \lambda_1 + \lambda_3 + \lambda_{34}}{\lambda_2 + \lambda_{12} + \lambda_{23}} \right) - \text{dilog} \left( \frac{\lambda_2 + \lambda_1 + \lambda_3 + \lambda_{34}}{\lambda_3 + \lambda_{34} + \lambda_{23}} \right) - \text{dilog} \left( \frac{\lambda_2 + \lambda_1 + \lambda_3 + \lambda_{34}}{\lambda_2 + \lambda_{12} + \lambda_{23}} \right) - \text{dilog} \left( \frac{\lambda_2 + \lambda_1 + \lambda_3 + \lambda_{34}}{\lambda_3 + \lambda_{34} + \lambda_{23}} \right) + \text{dilog} \left( \frac{\lambda_2 + \lambda_1 + \lambda_3 + \lambda_{34}}{\lambda_2 + \lambda_{12} + \lambda_{23}} \right) + \text{dilog} \left( \frac{\lambda_2 + \lambda_1 + \lambda_3 + \lambda_{34}}{\lambda_3 + \lambda_{34} + \lambda_{23}} \right) \right].$$

It is worth pointing out here that an alternative analytical expression for the above integral has also been reported in [59] very recently. However, here, the following discussions are made relating to the right hand side expressions in equations (88) and (85) only.

**Limiting expressions for $K_{41}^g$**
If $\lambda_{23} \to 0$, the proper expressions for the $I_2$ integrals as per equation(29) are substituted in equation(85) to obtain, as a special case,

$$K_{\text{eq}}^{I_2}(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, 0, \lambda_{34}) = 256\pi^4[(\lambda_{23}^2 - \lambda_{12}^2)(\lambda_{23}^2 - \lambda_{34}^2)]^{-1}[T_1 + T_2 + T_3 + T_4],$$

(90)

where

$$T_1 = \frac{1}{\lambda_1 + \lambda_2} \ln \left( \frac{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4}{\lambda_3 + \lambda_4} \times \frac{\lambda_3 + \lambda_4}{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4} \right),$$

$$T_2 = \frac{1}{\lambda_3 + \lambda_4} \ln \left( \frac{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4}{\lambda_1 + \lambda_2} \times \frac{\lambda_2 + \lambda_12 + \lambda_3 + \lambda_4}{\lambda_3 + \lambda_4} \right),$$

$$T_3 = \frac{1}{\lambda_2 + \lambda_{12}} \ln \left( \frac{\lambda_2 + \lambda_{12} + \lambda_3 + \lambda_{34}}{\lambda_3 + \lambda_{34}} \times \frac{\lambda_3 + \lambda_4}{\lambda_2 + \lambda_{12} + \lambda_3 + \lambda_4} \right),$$

$$T_4 = \frac{1}{\lambda_3 + \lambda_{34}} \ln \left( \frac{\lambda_2 + \lambda_{12} + \lambda_3 + \lambda_{34}}{\lambda_2 + \lambda_{12}} \times \frac{\lambda_1 + \lambda_2}{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_{34}} \right),$$

which is exactly identical with equation(41) of the very recent paper [], wherein the integral on the left hand side of equation(90) has been evaluated directly. Expressions for the integrals $K_{\text{eq}}^{I_2}(\lambda_1, \lambda_2, \lambda_3, \lambda_4; 0, 0, \lambda_{34})$ and $K_{\text{eq}}^{I_2}(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, 0, 0)$ can be easily obtained from equation(90) by taking $\lambda_{12} = 0$ and $\lambda_{34} = 0$, respectively, on both sides. If both $\lambda_{12} = \lambda_{34} = 0$, then equation(90) simplifies to give

$$K_{\text{eq}}^{I_2}(\lambda_1, \lambda_2, \lambda_3, \lambda_4; 0, 0, 0) = \frac{256\pi^4}{\lambda_1^4\lambda_4^4} \left[ \frac{1}{\lambda_1 + \lambda_2} \ln \left( \frac{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4}{\lambda_3 + \lambda_4} \times \frac{\lambda_3}{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4} \right) \right.$$

$$+ \frac{1}{\lambda_3 + \lambda_4} \ln \left( \frac{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4}{\lambda_1 + \lambda_2} \times \frac{\lambda_2}{\lambda_2 + \lambda_3 + \lambda_4} \right)$$

$$+ \frac{1}{\lambda_2} \ln \left( \frac{\lambda_2 + \lambda_3}{\lambda_3} \times \frac{\lambda_3 + \lambda_4}{\lambda_2 + \lambda_3 + \lambda_4} \right) + \frac{1}{\lambda_3} \ln \left( \frac{\lambda_2 + \lambda_3}{\lambda_2} \times \frac{\lambda_1 + \lambda_2}{\lambda_1 + \lambda_2 + \lambda_3} \right) \left. \right],$$

(91)

which is exactly identical with equation(40) of [52] and equation(42) of [59]. If, further, $\lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = \delta$, then

$$K_{\text{eq}}^{I_2}(\delta, \delta, \delta, \delta; 0, 0, 0) = 256\pi^4(5 \ln 2 - 3 \ln 3) \times \delta^{-5},$$

(92)

which is identical with equation(41) of [52]. It is also observed in equation(90) that if $\lambda_{12} \to \lambda_1$, the right hand side expression assumes 0/0 form. Employing L’Hospital’s rule for 0/0, it can be shown that

$$K_{\text{eq}}^{I_2}(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_1, 0, \lambda_{34}) = \frac{128\pi^4}{\lambda_1(\lambda_1 + \lambda_2)^2(\lambda_3^2 - \lambda_{34}^2)} \ln \left( \frac{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_{34}}{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4} \times \frac{\lambda_3 + \lambda_4}{\lambda_3 + \lambda_{34}} \right).$$

(93)

If, further, $\lambda_{34} \to \lambda_4$, employing L’Hospital’s rule for 0/0, equation(93) simplifies to give

$$K_{\text{eq}}^{I_2}(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_1, 0, \lambda_4) = 64\pi^4 \left[ \lambda_1 \lambda_4(\lambda_1 + \lambda_2)(\lambda_3 + \lambda_4)(\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4) \right]^{-1}.$$  

(94)

In the most special case, if $\lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = \delta$, then
If $\lambda_{34} \to \lambda_4$ in equation (90), employing L’Hospital’s rule for $0/0$, the following integral is evaluated:

$$K_{41}^g(\delta, \delta, \delta; \delta, 0, \delta) = 4\pi^4 \delta^{-5}. \quad (95)$$

$$K_{41}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, 0, \lambda_4) = \frac{128\pi^4}{\lambda_4(\lambda_3 + \lambda_4)^2(\lambda_1^2 - \lambda_{12}^2)} \ln \left( \frac{\lambda_2 + \lambda_{12} + \lambda_3 + \lambda_4}{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4} \times \frac{\lambda_1 + \lambda_2}{\lambda_2 + \lambda_{12}} \right), \quad (96)$$

which, in the limit $\lambda_{12} \to \lambda_1$, reduces to equation (94) exactly, as expected. Taking $\lambda_{34} = 0$ on both sides of equation (93), a closed-form expression is obtained for the following integral:

$$K_{41}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_1, 0, 0) = \frac{128\pi^4}{\lambda_4(\lambda_1 + \lambda_2)^2\lambda_1^2} \ln \left( \frac{\lambda_1 + \lambda_2 + \lambda_3}{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4} \times \frac{\lambda_3 + \lambda_4}{\lambda_3} \right). \quad (97)$$

Substituting $\lambda_{12} = 0$ on both sides of equation (96), the following integral is evaluated:

$$K_{41}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; 0, 0, \lambda_4) = \frac{128\pi^4}{\lambda_4\lambda_1^2(\lambda_3 + \lambda_4)^2} \ln \left( \frac{\lambda_2 + \lambda_3 + \lambda_4}{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4} \times \frac{\lambda_1 + \lambda_2}{\lambda_2} \right). \quad (98)$$

If $\lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = \delta$, then equations (97) and (98) simplify to

$$K_{41}^g(\delta, \delta, \delta, \delta; 0, 0, 0) = K_{41}^g(\delta, \delta, \delta; 0, 0, \delta) = 32\pi^4 \ln(3/2)\delta^{-5}. \quad (99)$$

The integral defined by

$$K_{41}(-1, -1, 0, -1; -1, -1, -1; \lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{23}, \lambda_{34})$$

$$= \int d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 (r_1 r_2 r_4 r_{12} r_{23} r_{34})^{-1} \times \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_4 r_4 - \lambda_{12} r_{12} - \lambda_{23} r_{23} - \lambda_{34} r_{34}), \quad (100)$$

has been analytically evaluated, as a special case, by differentiating both sides of equation (88) with respect to $(-\lambda_3)$. The property mentioned in equation (28) is employed for the differentiation of the dilog functions. Proceeding this way and doing some lengthy, but straightforward algebra, an expression is obtained which is shown to be exactly identical with the expression reported earlier in equation (32) of paper I, wherein the integral was evaluated directly. Further, as pointed out in [59], equation (32) of paper I is also reproduced, as a special case, by taking $(-\partial/\partial \lambda_3)$ of equation (52) of [59], which gives an alternative expression for the integral $K_{41}^g$, reported very recently.

By taking $(-\partial/\partial \lambda_2)(\partial^2/\partial \lambda_{23}^2)$ of the integral in equation (100) and its closed-form expression in equation (32) of paper I, and then substituting $\lambda_{12} = \lambda_{23} = \lambda_{34} = 0$, the
following integral is evaluated as a special case:

\[
K_{41}(-1,0,0,-1;-1,1,-1;\lambda_1,\lambda_2,\lambda_3,\lambda_4;0,0,0)
= 512\pi^4 \left[ \frac{\lambda_3(\lambda_1 + 2\lambda_2 + \lambda_3)}{\lambda_3^3\lambda_2(\lambda_1 + \lambda_2)(\lambda_2 + \lambda_3)(\lambda_1 + \lambda_2 + \lambda_3)} \right.
+ \left. \frac{\lambda_4(2\lambda_3 + \lambda_4)(\lambda_1^2 + 3\lambda_1\lambda_2 + 3\lambda_1^2)}{\lambda_3^2(\lambda_3 + \lambda_4)^2\lambda_2^2(\lambda_1 + \lambda_2)^3} \right.
- \frac{\lambda_3(\lambda_1 + \lambda_3 + 2\lambda_2 + 2\lambda_4) + \lambda_4(\lambda_1 + \lambda_4 + 2\lambda_2)}{(\lambda_3 + \lambda_4)^4\lambda_2(\lambda_1 + \lambda_2)(\lambda_2 + \lambda_3 + \lambda_4)(\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4)} \right] \tag{101}
\]

A different expression for the above integral, obtained by an alternative method, has been reported in equation(51) of [52]. However, it has been verified that both the expressions yield the same number for the same set of values of \(\lambda_1, \lambda_2, \lambda_3\) and \(\lambda_4\) taken in both cases for calculation. Further, in the most special case, if \(\lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = \delta\), equation(101) also simplifies to equation(53) of [52], indicating that the derivation leading to equation(101) is correct.

An expression for another integral of interest, defined by

\[
K_{41}(-1,0,0,-1;-1,1,-1;\lambda_1,\lambda_2,\lambda_3,\lambda_4;\lambda_{12},\lambda_{23},\lambda_{34})
= \int d\bar{r}_1 d\bar{r}_2 d\bar{r}_3 d\bar{r}_4 (r_1 r_4 r_{12} r_{23} r_{34})^{-1}
\times \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_4 r_4 - \lambda_{12} r_{12} - \lambda_{23} r_{23} - \lambda_{34} r_{34}) \tag{102}
\]

has been obtained, as a special case, by differentiating the integral in equation(100) and its closed-form expression in equation(32) of paper I, with respect to \((-\lambda_2)\), and observed to be in conformity with equation(11) of the paper of Bonham [63], which was pointed out earlier in paper I. Substituting \(\lambda_{12} = \lambda_{23} = \lambda_{34} = 0\) in the closed-form expression for the integral defined in equation(102), the expressions in equation(37), and, as a special case in equation(38) of [52] are exactly reproduced.

All these observations point out that the derivation of the general expression leading to equation(88) is correct.

**Expression for \( < r_{12} r_{34} / r_{23} > \)**

As pointed out relating to equation(78), it may also be required to obtain the expectation value \( < r_{12} r_{34} / r_{23} > \) employing the expression for the generating integral \(K_{41}^d\) as per equation(88). This can be achieved by differentiating both sides of equation(88) twice with respect to \(\lambda_{12}\) and twice with respect to \(\lambda_{34}\) and making use of equation(28) for the differentiation of the dilog functions. Thus the following \(K_{41}\) integral is evaluated analytically:

\[
K_{41}(-1,-1,-1,1;\lambda_1,\lambda_2,\lambda_3,\lambda_4;\lambda_{12},\lambda_{23},\lambda_{34})
= \frac{\partial^2}{\partial \lambda_{12}^2} \frac{\partial^2}{\partial \lambda_{34}^2} \left[ D(\lambda_1,\lambda_{12},\lambda_4,\lambda_{34}) \times N(\lambda_1,\lambda_2,\lambda_3,\lambda_4;\lambda_{12},\lambda_{23},\lambda_{34}) \right] \tag{103}
\]

where D and N are functions given by equation(88) along with their expressions in equations(86) and (89), respectively.
In the limit \( \lambda_{12} = \lambda_{23} = \lambda_{34} \to 0 \), equation (103) is rewritten as
\[
K_{14}(-1, -1, -1, -1; 1, -1, 1; \lambda_1, \lambda_2, \lambda_3, \lambda_4; 0, 0, 0) = \lim_{\lambda_{12} \to 0, \lambda_{34} \to 0} \frac{\partial^2}{\partial \lambda_{12}^2} \frac{\partial^2}{\partial \lambda_{34}^2} K_{14}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, 0, \lambda_{34}),
\]
where the analytic expression for \( K_{14}^g \) above is given by equation (90). The differentiations, though lengthy but straightforward, are carried out and then the limits taken to obtain the following closed-form expression:
\[
K_{14}(-1, -1, -1, -1; 1, -1, 1; \lambda_1, \lambda_2, \lambda_3, \lambda_4; 0, 0, 0) = 256\pi^4 \left[ 4(\lambda_1 \lambda_4)^{-4} F_1 + 2\lambda_1^{-2} \lambda_4^{-2} F_2 + 2\lambda_1^{-4} \lambda_4^{-2} F_3 + (\lambda_1 \lambda_4)^{-2} F_4 \right],
\]
where \( F_1, F_2, F_3 \) and \( F_4 \) are functions given by
\[
F_1 = \frac{1}{\lambda_1 + \lambda_2} \ln \left( \frac{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4}{\lambda_1 + \lambda_2 + \lambda_3} \right) + \frac{1}{\lambda_3 + \lambda_4} \ln \left( \frac{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4}{\lambda_1 + \lambda_2 + \lambda_3} \right) + \frac{1}{\lambda_2} \ln \left( \frac{\lambda_2 + \lambda_3 + \lambda_4}{\lambda_2 + \lambda_3 + \lambda_4} \right) + \frac{1}{\lambda_3} \ln \left( \frac{\lambda_2 + \lambda_3 + \lambda_4}{\lambda_2 + \lambda_3 + \lambda_4} \right),
\]
\[
F_2 = \frac{1}{\lambda_3 + \lambda_4} \left\{ \frac{1}{(\lambda_2 + \lambda_3 + \lambda_4)^2} - \frac{1}{\lambda_2^2} \right\} + \frac{1}{\lambda_2^2} \left( \frac{\lambda_2 + \lambda_3}{\lambda_2 + \lambda_3 + \lambda_4} \right) + \frac{2}{\lambda_2^2} \ln \left( \frac{\lambda_2 + \lambda_3}{\lambda_2 + \lambda_3 + \lambda_4} \right),
\]
\[
F_3 = \frac{1}{\lambda_1 + \lambda_2} \left\{ \frac{1}{(\lambda_1 + \lambda_2 + \lambda_3)^2} - \frac{1}{\lambda_3^2} \right\} + \frac{1}{\lambda_3^2} \left( \frac{\lambda_2 + \lambda_3}{\lambda_2 + \lambda_3 + \lambda_4} \right) + \frac{2}{\lambda_3^2} \ln \left( \frac{\lambda_2 + \lambda_3}{\lambda_2 + \lambda_3 + \lambda_4} \right),
\]
\[
F_4 = \frac{2}{\lambda_2^2} \left\{ \frac{1}{\lambda_2^2} - \frac{1}{(\lambda_2 + \lambda_3)^2} \right\} + \frac{2}{\lambda_3^2} \left\{ \frac{1}{\lambda_3^2} - \frac{1}{(\lambda_2 + \lambda_3)^2} \right\} - \frac{4}{\lambda_2^2 (\lambda_2 + \lambda_3)^3} - \frac{6}{\lambda_3^2 (\lambda_2 + \lambda_3)^3} - \frac{6}{\lambda_3 (\lambda_2 + \lambda_3)^4}.
\]
In the most special case, if \( \lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = \delta \), then equation (105) simplifies to
\[
K_{14}(-1, -1, -1, -1; 1, -1, 1; \delta, \delta, \delta, \delta, 0, 0, 0) = 256\pi^4 \delta^{-9} \left[ 7/12 + 36 \ln 2 - 20 \ln 3 \right].
\]

**Expression for \( <r_{12} r_{23}/r_{34}> \)**

By employing the generating integral \( K_{14}^g \), as usual, an expression for \( <r_{12} r_{23}/r_{34}> \) can be obtained in general. Thus, both sides of equation (88) are differentiated twice with respect to \( \lambda_{12} \) and twice with respect to \( \lambda_{23} \) for evaluating the following integral analytically:
\[
K_{14}(-1, -1, -1, -1; 1, -1, 1; \lambda_1, \lambda_2, \lambda_3, \lambda_4) = \left( \frac{\partial^2}{\partial \lambda_{12}^2} \right) \left( \frac{\partial^2}{\partial \lambda_{23}^2} \right) \left[ D(\lambda_1, \lambda_{12}, \lambda_4, \lambda_{34}) \times N(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{23}, \lambda_{34}) \right].
\]
Expressions for the functions D and N are given by equations (86) and (89), respectively. Differentiation of the dilog functions in N can be performed by employing equation (28).

To simplify equation (107) further, the following observations are made, namely, (i) the function D does not depend on $\lambda_2$; (ii) as per equation (85), the function N is a sum of four different $I_2(−2, −2, −1; α, β, γ)$ integrals and the relations of various $α, β, γ$ parameters with $\lambda$ parameters are given along with equation (87), (iii) the parameter $γ$ for all the four $I_2$ integrals is equal to $λ_23$, and (iv) employing equation (87), it is easy to establish the relation

$$\left(\frac{\partial^2}{\partial γ^2}\right) I_2(−2, −2, −1; α, β, γ) = I_2(−2, −2, 1; α, β, γ).$$

(108)

Accordingly, equation (107) simplifies to give

$$K_{41}(−1, −1, −1, −1; 1, 1, 1, 1; λ_1, λ_2, λ_3, λ_4; λ_{12}, λ_{23}, λ_{34}) = \left(\frac{\partial^2}{\partial λ_{12}^2}\right)$$

$$\times \left[ D(λ_1, λ_{12}, λ_4, λ_{34}) \left\{ I_2(−2, −2, 1; α_1, β_1, λ_{23}) − I_2(−2, −2, 1; α_2, β_2, λ_{23}) − I_2(−2, −2, 1; α_3, β_3, λ_{23}) + I_2(−2, −2, 1; α_4, β_4, λ_{23}) \right\} \right].$$

(109)

Closed-form expression for $I_2(−2, −2, −1; α, β, γ)$ has been given in equation (25), and hence, through equation (108), all the four $I_2(−2, −2, 1; α, β, γ)$ integrals in equation (109) can be evaluated analytically. Then the differentiation with respect to $λ_{12}$ is performed twice keeping in mind that the function D and only the parameters $α_1$ and $α_2$ involve $λ_{12}$.

**Limiting expression if $λ_{12} = λ_{23} = λ_{34} = 0$**

First an expression for the integral $I_2(−2, −2, 1; α, β, γ)$ in the limit $γ → 0$ is obtained as given below.

Substituting equation (25) in equation (108), it becomes

$$I_2(−2, −2, 1; α, β, γ) = \left(\frac{\partial^2}{\partial γ^2}\right) \left[ 8π^2 γ^{−1} Q(α, β, γ) \right],$$

(110)

with the expression for the function $Q(α, β, γ)$ given by equation (26). Performing the differentiation on the right hand side, equation (110) reduces to

$$I_2(−2, −2, 1; α, β, γ) = \frac{8π^2}{γ^3} \times \left[ 2Q − 2γ \left(\frac{∂Q}{∂ γ}\right) + γ^2 \left(\frac{∂^2Q}{∂ γ^2}\right) \right].$$

(111)

It had been shown [] that $Q → 0$ as $γ → 0$. However, $\left(\frac{∂Q}{∂ γ}\right)$ and $\left(\frac{∂^2Q}{∂ γ^2}\right)$ both can be observed to be finite as $γ → 0$. Thus in the limit $γ → 0$, the right hand side expression in equation (111) assumes 0/0 form. Hence L’ Hospital’s rule for 0/0 is employed to obtain

$$I_2(−2, −2, 1; α, β, 0) = \left(\frac{8π^2}{3}\right) \left(\frac{∂^3Q}{∂ γ^3}\right) |_{γ=0}$$

$$= \frac{16π^2}{3} \left[ \frac{α + β}{α^2β^2} + \frac{2}{β^3} ln \left(\frac{α + β}{α}\right) + \frac{2}{α^3} ln \left(\frac{α + β}{β}\right) \right].$$

(112)
 Accordingly, if \( \lambda_{23} = 0 \), equation(109) is restated as

\[
K_{41}(-1, -1, -1; 1, 1, -1; \lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, 0, \lambda_{34}) = \left( \frac{\partial^2}{\partial \lambda_{12}^2} \right) \times \left[ D(\lambda_1, \lambda_{12}, \lambda_4, \lambda_{34}) \left\{ I_2(-2, -2, 1; \alpha_1, \beta_1, 0) - I_2(-2, -2, 1; \alpha_2, \beta_2, 0) \right. \right.
\]

\[
- I_2(-2, -2, 1; \alpha_3, \beta_3, 0) + I_2(-2, -2, 1; \alpha_4, \beta_4, 0) \right\} \right].
\]

Expressing the function \( D \), and \( \alpha \)'s and \( \beta \)'s, in terms of \( \lambda \)'s as per equations(86) and (87), respectively, and inserting equation(112) in equation(113), the differentiation with respect to \( \lambda_{12} \) is carried out twice. Then, substituting \( \lambda_{12} = \lambda_{34} = 0 \) in the resulting expression, the integral in equation(113) becomes

\[
K_{41}(-1, -1, -1, 1, 1, -1; \lambda_1, \lambda_2, \lambda_3, \lambda_4; 0, 0, 0) = \frac{512}{3} \cdot \frac{\pi^4}{\lambda_1^2 \lambda_4^2} \sum_{i=1}^{8} X_i, \tag{114}
\]

where

\[
X_1 = \frac{1}{\lambda_1^2} \left\{ \frac{\lambda_2 + \lambda_3}{\lambda_1^2 \lambda_3^2} + \frac{2}{\lambda_3^3} \ln \left( \frac{\lambda_2 + \lambda_3}{\lambda_2} \right) + \frac{2}{\lambda_2^3} \ln \left( \frac{\lambda_2 + \lambda_3}{\lambda_3} \right) \right\},
\]

\[
X_2 = -\frac{1}{\lambda_1^2} \left[ \frac{(\lambda_2 + \lambda_3 + \lambda_4)}{\lambda_2^2 (\lambda_3 + \lambda_4)} \right] + \frac{2}{(\lambda_3 + \lambda_4)^3} \ln \left( \frac{\lambda_2 + \lambda_3 + \lambda_4}{\lambda_2} \right) + \frac{2}{\lambda_2^3} \ln \left( \frac{\lambda_2 + \lambda_3 + \lambda_4}{\lambda_3 + \lambda_4} \right)
\]

\[
X_3 = \frac{1}{\lambda_1^2} \left\{ \frac{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4}{\lambda_1^2 (\lambda_1 + \lambda_2)^2} \right\} + \frac{2}{(\lambda_3 + \lambda_4)^3} \ln \left( \frac{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4}{\lambda_1 + \lambda_2} \right),
\]

\[
X_4 = \frac{1}{\lambda_1^2} \left\{ \frac{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4}{\lambda_1^2 (\lambda_1 + \lambda_2)^2} \right\},
\]

\[
X_5 = \frac{2}{(\lambda_1 + \lambda_2)^3} \ln \left( \frac{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4}{\lambda_1 + \lambda_2} \right),
\]

\[
X_6 = \frac{12}{\lambda_2^3} \ln \left( \frac{\lambda_2 + \lambda_3}{\lambda_3} \right) - \frac{6}{\lambda_3^3} \left( \frac{\lambda_2 + \lambda_3}{\lambda_2} \right),
\]

\[
X_7 = \frac{12}{\lambda_2^3} \left\{ \frac{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4}{\lambda_3 + \lambda_4} \right\} + \frac{6}{\lambda_3^3} \left( \frac{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4}{\lambda_3 + \lambda_4} \right),
\]

If \( \lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = \delta \), then equation(114) simplifies to

\[
K_{41}(-1, -1, -1, 1, 1, -1; \delta, \delta, \delta, \delta; 0, 0, 0) = (256/3) \pi^4 \delta^{-9} (5 + 65 \ln 2 - 33 \ln 3).
\]

Differentiating both sides of equation(114) with respect to \( -\lambda_3 \), a closed-form expression for the integral

\[
K_{41}(-1, -1, 0, -1; 1, 1, -1; \lambda_1, \lambda_2, \lambda_3, \lambda_4; 0, 0, 0) = \int d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 
\]

\[
\times (r_1 r_2 r_3) \times exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_4 r_4),
\]

\[
\tag{116}
\]

25
Comparing the integrand in the above integral with that given for the special case, the following equation is established:

\[ K_{41}(-1, -1, 0; -1, 1, 1, -1; \delta, \delta, \delta, 0, 0, 0) = \left( \frac{32\pi^4}{9} \right) \delta^{-10} [594 \ln 2 - 306 \ln 3 + 505]. \]  

(117)

Further, by taking \( \left( \frac{\partial}{\partial \lambda} \right) \left( \frac{\partial}{\partial \lambda} \right) \) of equation(114), a closed-form expression for the following integral

\[ K_{41}(-1, -1, 0; 1, 1, -1; \lambda_1, \lambda_2, \lambda_3, \lambda_4; 0, 0, 0) = \int d\tau_1^2 d\tau_2^2 d\tau_3^2 d\tau_4^2 \times (r_1 r_2)^{-1} (r_{12} r_{23} r_{34}) \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_4 r_4) \]  

(118)

is derived. If, in the most special case, \( \lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = \delta \) substituted in the expression for the above integral, it yields the following equation:

\[ K_{41}(-1, -1, 0; 1, 1, -1; \delta, \delta, \delta, 0, 0, 0) = \left( \frac{16\pi^4}{27} \right) \delta^{-11} [7344 \ln 2 - 3888 \ln 3 + 5167], \]  

(119)

which is exactly identical with equation(24) of the very recent report of King [59]. This observation clearly leads to the conclusion that the derivations leading to equations(114), (115), (117) and (119) are correct.

(b) Analytic evaluation of \( K_{42}^g \)

The generating integral \( K_{42}^g \) is defined, as usual, by the relation

\[ K_{42}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_23, \lambda_34, \lambda_{41}) = \int d\tau_1^2 d\tau_2^2 d\tau_3^2 d\tau_4^2 (r_1 r_2 r_3 r_4 r_{23} r_{34} r_{41})^{-1} \times \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_4 r_4 - \lambda_{23} r_{23} - \lambda_{34} r_{34} - \lambda_{41} r_{41}). \]  

(120)

Comparing the integrand in the above integral with that given for \( K_{41}^g \) in equation(83), it is observed that if a change \( (2 \leftrightarrow 4) \) is performed in the integrand in equation(83), the integrand on the right hand side of equation(120) is obtained, since \( \lambda_{ij} = \lambda_{ji} \) and \( r_{ij} = r_{ji} \). Hence, by observation, the following equation is established, starting from equations(88) and (89):

\[ K_{42}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_23, \lambda_34, \lambda_{41}) = \frac{16\pi^2}{(\lambda_2^2 - \lambda_{23}^2) (\lambda_3^2 - \lambda_{34}^2)} \times \frac{8\pi^2}{\lambda_{34}} \times \left[ \ln \left( \frac{\lambda_{41} + \lambda_4 + \lambda_{34}}{\lambda_1 + \lambda_4 + \lambda_{34}} \right) \times \ln \left( \frac{\lambda_3 + \lambda_2 + \lambda_{34}}{\lambda_3 + \lambda_{23} + \lambda_{34}} \right) \right. \]

\[ + \ \text{dilog} \left( \frac{\lambda_1 + \lambda_{41} + \lambda_3 + \lambda_{23}}{\lambda_4 + \lambda_{41} + \lambda_{34}} \right) + \ \text{dilog} \left( \frac{\lambda_4 + \lambda_{41} + \lambda_3 + \lambda_{23}}{\lambda_3 + \lambda_{23} + \lambda_{34}} \right) \]

\[ - \ \text{dilog} \left( \frac{\lambda_4 + \lambda_{41} + \lambda_3 + \lambda_2}{\lambda_4 + \lambda_{41} + \lambda_{34}} \right) - \ \text{dilog} \left( \frac{\lambda_4 + \lambda_{41} + \lambda_3 + \lambda_2}{\lambda_3 + \lambda_{23} + \lambda_{34}} \right) \]

\[ - \ \text{dilog} \left( \frac{\lambda_1 + \lambda_4 + \lambda_3 + \lambda_{23}}{\lambda_1 + \lambda_4 + \lambda_{34}} \right) - \ \text{dilog} \left( \frac{\lambda_1 + \lambda_4 + \lambda_3 + \lambda_{23}}{\lambda_3 + \lambda_{23} + \lambda_{34}} \right) \]

\[ + \ \text{dilog} \left( \frac{\lambda_1 + \lambda_4 + \lambda_3 + \lambda_2}{\lambda_1 + \lambda_4 + \lambda_{34}} \right) + \ \text{dilog} \left( \frac{\lambda_1 + \lambda_4 + \lambda_3 + \lambda_2}{\lambda_3 + \lambda_2 + \lambda_{34}} \right) \right]. \]  

(121)
It is worth pointing out here that the integral in equation (120) has also been evaluated directly adopting the same procedure as followed for the evaluation of the integral $K_{41}^g$ defined in equation (83), and subsequently, equation (121) is established as outlined below.

The integral in equation (120) can be rewritten as

$$K_{42}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{23}, \lambda_{34}, \lambda_{41}) = \int d\vec{r}_3 \ d\vec{r}_4 \ (r_3 r_4 r_{34})^{-1}$$ \times \exp(-\lambda_3 r_3 - \lambda_4 r_4 - \lambda_{34} r_{34}) \ J(\lambda_2, \lambda_{23}, r_3) \ J(\lambda_1, \lambda_{41}, r_4), \tag{122}$$

where the $J$'s are given by equations (1) and (3). Substituting the closed-form expressions for the $J$'s in equation (122), it simplifies to

$$K_{42}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{23}, \lambda_{34}, \lambda_{41}) = \frac{16\pi^2}{(\lambda_2^2 - \lambda_{23}^2)(\lambda_4^2 - \lambda_{41}^2)}$$ \times \left[ I_2(-2, -2, -1; \lambda_3 + \lambda_{23}, \lambda_4 + \lambda_{41}, \lambda_{34}) - I_2(-2, -2, -1; \lambda_3 + \lambda_{23}, \lambda_1 + \lambda_4, \lambda_{34}) \right.$$ \left. - I_2(-2, -2, -1; \lambda_2 + \lambda_3, \lambda_4 + \lambda_{41}, \lambda_{34}) + I_2(-2, -2, -1; \lambda_2 + \lambda_3, \lambda_1 + \lambda_4, \lambda_{34}) \right], \tag{123}$$

where, in general, the closed-form expression for the $I_2$ integral is given by equation (25). Substituting these expressions for various $I_2$ integrals in equation (123), and doing some simplifications, the expression in equation (121) is exactly reproduced.

Further, replacing the various $\alpha$, $\beta$ and $\gamma$ parameters in the right hand side expression in equation (85) by the corresponding $\lambda$ parameters given just after equation (87), and then making a change ($2 \leftrightarrow 4$) in the resulting expression, the right hand side expression in equation (123) is exactly reproduced, as expected.

**Limiting expressions for $K_{42}^g$**

In the limit $\lambda_{34} \to 0$, employing equation (29), the following integral is evaluated, as a special case, from equation (123):

$$K_{42}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{23}, 0, \lambda_{41}) = \frac{256\pi^4}{(\lambda_2^2 - \lambda_{23}^2)(\lambda_4^2 - \lambda_{41}^2)}$$ \times \left[ \frac{1}{\lambda_1 + \lambda_4} \ln \left( \frac{\lambda_2 + \lambda_3 + \lambda_1 + \lambda_4}{\lambda_2 + \lambda_3} \times \frac{\lambda_3 + \lambda_{23}}{\lambda_3 + \lambda_{23} + \lambda_1 + \lambda_4} \right) \right.$$ \left. + \frac{1}{\lambda_2 + \lambda_3} \ln \left( \frac{\lambda_2 + \lambda_3 + \lambda_1 + \lambda_4}{\lambda_1 + \lambda_4} \times \frac{\lambda_4 + \lambda_{41}}{\lambda_2 + \lambda_3 + \lambda_4 + \lambda_{41}} \right) \right.$$ \left. + \frac{1}{\lambda_4 + \lambda_{41}} \ln \left( \frac{\lambda_3 + \lambda_{23} + \lambda_4 + \lambda_{41}}{\lambda_3 + \lambda_{23}} \times \frac{\lambda_2 + \lambda_3}{\lambda_2 + \lambda_3 + \lambda_4 + \lambda_{41}} \right) \right.$$ \left. + \frac{1}{\lambda_3 + \lambda_{23}} \ln \left( \frac{\lambda_3 + \lambda_{23} + \lambda_1 + \lambda_{41}}{\lambda_4 + \lambda_{41}} \times \frac{\lambda_1 + \lambda_4}{\lambda_3 + \lambda_{23} + \lambda_1 + \lambda_4} \right) \right]. \tag{124}$$

Looking at the right hand side expressions in equations (90) and (124), it is observed that the latter expression can be obtained from the former by performing the change ($2 \leftrightarrow 4$) in the former, as expected. Also expressions for the integrals $K_{42}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{23}, 0, 0)$ and $K_{42}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; 0, 0, 0, \lambda_{41})$ can be easily obtained from equation (124) by substituting $\lambda_{41} = 0$ and $\lambda_{23} = 0$, respectively, on both sides. If both $\lambda_{41} = \lambda_{23} = 0$, then
equation (124) simplifies to give

\[
K^g_{42}(\lambda_1, \lambda_2, \lambda_3, \lambda_4; 0, 0, 0)
= \frac{256\pi^4}{(\lambda_2, \lambda_4^2, \lambda_3^2)^2} \left[ \frac{1}{\lambda_1 + \lambda_4} \ln \left( \frac{\lambda_2 + \lambda_3 + \lambda_4 + \lambda_1}{\lambda_2 + \lambda_3} \times \frac{\lambda_3}{\lambda_3 + \lambda_4 + \lambda_1} \right) + \frac{1}{\lambda_2 + \lambda_3} \ln \left( \frac{\lambda_2 + \lambda_3 + \lambda_4 + \lambda_1}{\lambda_2 + \lambda_3} \times \frac{\lambda_4}{\lambda_2 + \lambda_3 + \lambda_4} \right) + \frac{1}{\lambda_4} \ln \left( \frac{\lambda_3 + \lambda_4}{\lambda_3 + \lambda_4 + \lambda_1} \times \frac{\lambda_4}{\lambda_3 + \lambda_4 + \lambda_1} \right) \right].
\]  

(125)

Comparing the right hand side expressions in equations (91) and (125), it is clearly observed that the expression in equation (125) can also be obtained by making the change ($2 \rightarrow 4$) in the expression in equation (91), as expected. In the most special case, if $\lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = \delta$, then equation (125) reduces to

\[
K^g_{42}(\delta, \delta, \delta; 0, 0, 0) = 256\pi^4(5 \ln 2 - 3 \ln 3)\delta^{-5}.
\]  

(126)

Starting with equation (124), several limiting expressions can be obtained, by employing L’Hospital’s rule for 0/0, as was done in case of $K^g_{41}$. Thus, in the limit $\lambda_{41} \to \lambda_1$, equation (124) simplifies to

\[
K^g_{42}(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{23}, 0, \lambda_1)
= \frac{128\pi^4}{\lambda_1(\lambda_2^2 - \lambda_{23}^2)(\lambda_4 + \lambda_1)^2} \ln \left( \frac{\lambda_3 + \lambda_{23} + \lambda_4 + \lambda_1}{\lambda_2 + \lambda_3 + \lambda_4 + \lambda_1} \times \frac{\lambda_2 + \lambda_3}{\lambda_3 + \lambda_{23}} \right). \quad (127)
\]

If, further, $\lambda_{23} \to \lambda_2$, equation (127) becomes

\[
K^g_{42}(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_2, 0, \lambda_1)
= \frac{64\pi^4}{\lambda_1\lambda_2(\lambda_1 + \lambda_4)(\lambda_2 + \lambda_3)} \times \frac{1}{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4}.
\]  

(128)

If $\lambda_{23} \to \lambda_2$ first, then equation (124) gives

\[
K^g_{42}(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_2, 0, \lambda_{41})
= \frac{128\pi^4}{\lambda_2(\lambda_2 + \lambda_3)^2(\lambda_1^2 - \lambda_{41}^2)} \ln \left( \frac{\lambda_2 + \lambda_3 + \lambda_4 + \lambda_{41}}{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4} \times \frac{\lambda_1 + \lambda_4}{\lambda_4 + \lambda_{41}} \right).
\]  

(129)

If, further, $\lambda_{41} \to \lambda_1$, then equation (129) reduces to equation (128) exactly, as expected. Substituting $\lambda_{23} = 0$ in equation (127), the following integral is evaluated:

\[
K^g_{42}(\lambda_1, \lambda_2, \lambda_3, \lambda_4; 0, 0, \lambda_1)
= \frac{128\pi^4}{\lambda_1\lambda_2^2(\lambda_4 + \lambda_1)^2} \ln \left( \frac{\lambda_3 + \lambda_4 + \lambda_1}{\lambda_2 + \lambda_3 + \lambda_4 + \lambda_1} \times \frac{\lambda_2 + \lambda_3}{\lambda_3} \right).
\]  

(130)

If $\lambda_{41} = 0$, equation (129) simplifies to

\[
K^g_{42}(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_2, 0, 0)
= \frac{128\pi^4}{\lambda_2(\lambda_2 + \lambda_3)^2\lambda_1^2} \ln \left( \frac{\lambda_2 + \lambda_3 + \lambda_4}{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4} \times \frac{\lambda_1 + \lambda_4}{\lambda_4} \right).
\]  

(131)

If $\lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = \delta$, then equation (128) becomes

\[
K^g_{42}(\delta, \delta, \delta; 0, 0, \delta) = 4\pi^4/\delta^5,
\]  

(132)
and equations (130) and (131) simplify to give

\[ K_{42}^g(\delta, \delta, \delta, 0, 0, \delta) = K_{42}^g(\delta, \delta, \delta, 0, 0) = 32\pi^4 \ln(3/2)\delta^{-5} \]  

(133)

analogous with equation (99).

(c) Analytic evaluation of \( K_{43}^g \)

The generating integral \( K_{43}^g \) is defined by the equation

\[
K_{43}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{34}, \lambda_{41}, \lambda_{12}) = \int d\mathbf{r}_1^2 d\mathbf{r}_2^3 d\mathbf{r}_3^4 (r_1 r_2 r_3 r_4 r_{41} r_{12})^{-1} \\
\times \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_4 r_4 - \lambda_{34} r_{41} - \lambda_{12} r_{12}),
\]  

(134)

which can be recast as

\[
K_{43}^g = \int d\mathbf{r}_1^2 d\mathbf{r}_2^3 (r_1 r_4 r_{41})^{-1} \exp(-\lambda_1 r_1 - \lambda_4 r_4 - \lambda_{41} r_{41}) \\
\times J(\lambda_2, \lambda_{12}, r_1) J(\lambda_3, \lambda_{34}, r_4),
\]  

(135)

where the \( J \)'s are given by equations (1) and (3). Substituting the expressions for the \( J \)'s from equation (3) in the above equation, the following expression is obtained for \( K_{43}^g \):

\[
K_{43}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{34}, \lambda_{41}, \lambda_{12}) = \frac{16\pi^2}{(\lambda_3^2 - \lambda_{12}^2)(\lambda_4^2 - \lambda_{41}^2)} \\
\times \left[I_2(-2, -2, -1; \lambda_1 + \lambda_{12}, \lambda_2 + \lambda_{12}, \lambda_4 + \lambda_{12}) - I_2(-2, -2, -1; \lambda_1 + \lambda_{12}, \lambda_2 + \lambda_{12}, \lambda_4 + \lambda_{12}) - I_2(-2, -2, -1; \lambda_1 + \lambda_{12}, \lambda_2 + \lambda_{12}, \lambda_4 + \lambda_{12}) \right].
\]  

(136)

The general expression given for \( I_2(-2, -2, -1; \alpha, \beta, \gamma) \) in equation (25) can be employed in equation (136) to obtain the required closed-form expression for \( K_{43}^g \). Various limiting expressions for \( K_{43}^g \) can be obtained as was done for \( K_{41}^g \).

(d) Analytic evaluation of \( K_{44}^g \)

The generating integral \( K_{44}^g \) is defined by the equation

\[
K_{44}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{41}, \lambda_{12}, \lambda_{23}) = \int d\mathbf{r}_1^2 d\mathbf{r}_2^3 d\mathbf{r}_3^4 (r_1 r_2 r_3 r_4 r_{41} r_{12} r_{23})^{-1} \\
\times \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_4 r_4 - \lambda_{41} r_{41} - \lambda_{12} r_{12} - \lambda_{23} r_{23}),
\]  

(137)

and is rewritten as

\[
K_{44}^g = \int d\mathbf{r}_1^2 d\mathbf{r}_2^3 (r_1 r_2 r_{12})^{-1} \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_{12} r_{12}) \\
\times J(\lambda_3, \lambda_{23}, r_2) J(\lambda_4, \lambda_{41}, r_1).
\]  

(138)

Inserting equation (3) into equation (138), the following expression for \( K_{44}^g \) is obtained:

\[
K_{44}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{41}, \lambda_{12}, \lambda_{23}) = \frac{16\pi^2}{(\lambda_3^2 - \lambda_{23}^2)(\lambda_4^2 - \lambda_{41}^2)} \\
\times \left[I_2(-2, -2, -1; \lambda_1 + \lambda_{41}, \lambda_2 + \lambda_{23}, \lambda_{12}) - I_2(-2, -2, -1; \lambda_1 + \lambda_{41}, \lambda_2 + \lambda_{23}, \lambda_{12}) - I_2(-2, -2, -1; \lambda_1 + \lambda_{41}, \lambda_2 + \lambda_{23}, \lambda_{12}) + I_2(-2, -2, -1; \lambda_1 + \lambda_{41}, \lambda_2 + \lambda_{23}, \lambda_{12}) \right].
\]  

(139)
Replacing the $J_2$ integrals in equation(139) by their corresponding expressions as per equation(25), closed-form expression for the generating integral $K_{44}^g$ is easily obtained. Various limiting expressions for $K_{44}^g$ can be derived by following the same procedure as adopted for $K_{41}^g$.

5.2(II) Integrals belonging to category (II)

There are four general integrals belonging to category (II) of open square diagrams, corresponding to four different exponential correlation factors as mentioned earlier. These are denoted as (a) $K_{45}$, (b) $K_{46}$, (c) $K_{47}$ and (d) $K_{48}$, and the corresponding generating integrals as (a) $K_{45}^g$, (b) $K_{46}^g$, (c) $K_{47}^g$ and (d) $K_{48}^g$. The definition along with the method of analytic evaluation of each of these generating integrals is given below.

(a) Analytic evaluation of $K_{45}^g$

The generating integral $K_{45}^g$ is defined by the relation

$$K_{45}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{13}, \lambda_{34}) = \int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 d\mathbf{r}_4 (r_1 r_2 r_3 r_4 r_{12} r_{13} r_{34})^{-1} \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_4 r_4 - \lambda_{12} r_{12} - \lambda_{13} r_{13} - \lambda_{34} r_{34}),$$

which can be recast as

$$K_{45}^g = \int d\mathbf{r}_1 d\mathbf{r}_2 (r_1 r_2 r_{13})^{-1} \exp(-\lambda_1 r_1 - \lambda_3 r_3 - \lambda_{13} r_{13}) J(\lambda_2, \lambda_{12}, r_1) J(\lambda_4, \lambda_{34}, r_3),$$

where expressions for the $J$’s are given by equation(3). Inserting equation(3) in equation(141), the following equation is established:

$$K_{45}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{13}, \lambda_{34}) = \frac{16\pi^2}{(\lambda_2^2 - \lambda_{12}^2)(\lambda_4^2 - \lambda_{34}^2)} \times \left[I_2(-2, -2, -1; \lambda_1 + \lambda_{12}, \lambda_3 + \lambda_{34}, \lambda_{13}) - I_2(-2, -2, -1; \lambda_1 + \lambda_{12}, \lambda_3 + \lambda_{34}, \lambda_{13}) \right],$$

with expressions for the $I_2$ integrals given by equation(25).

It is easy to observe that if a change $(1 \leftrightarrow 2)$ is made in the integrand in equation(83) corresponding to $K_{41}^g$, the integrand for $K_{45}^g$ defined in equation(140) is obtained. Accordingly, it is easy to verify that the right hand side expression of equation(142) can be derived starting with the right hand side expression of equation(85), with $\alpha, \beta, \gamma$ parameters replaced by $\lambda$ parameters, and then making the interchange $(1 \leftrightarrow 2)$.

Inserting equation(25) in equation(142), the closed-form expression for the generating integral $K_{45}^g$ is derived, from which all the limiting expressions for $K_{45}^g$ can be obtained, following the procedure adopted for deriving equations(90-99) corresponding to $K_{41}^g$.

Expression for $< r_{12} r_{13} / r_{34} >$

An expression for $< r_{12} r_{13} / r_{34} >$ can be obtained making use of the generating
integral $K^{q}_{45}$. A closed-form expression for the following integral

$$K_{45}(-1, -1, -1, -1, 1, 1, -1; \lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{13}, \lambda_{34}) = \int \frac{d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 (r_1 r_2 r_3 r_4)^{-1} (r_{12} r_{13} / r_{34})}{(r_{12} r_{13} / r_{34})} \times \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_4 r_4 - \lambda_{12} r_{12} - \lambda_{13} r_{13} - \lambda_{34} r_{34})$$

(143)

can be obtained following similar procedure adopted for evaluating $< r_{12} r_{34} / r_{13} >$, employing equation(107). Substituting $\lambda_{12} = \lambda_{13} = \lambda_{34} = 0$ in the closed-form expression for the above integral, the following integral is evaluated:

$$K_{45}(-1, -1, -1, -1; 1, 1, -1; \lambda_1, \lambda_2, \lambda_3, \lambda_4; 0, 0, 0) = \frac{512 \pi^4}{3 \lambda^2 \lambda_4} \sum_{i=1}^{8} X_i(1 \Leftrightarrow 2).$$

(144)

Here, $X_i(1 \Leftrightarrow 2), i = 1, 2, \cdots, 8$, are the functions given by equation(114) followed by the interchange $(1 \Leftrightarrow 2)$. This integral has actually been evaluated and found to be consistent with the relation between $K^{q}_{41}$ and $K^{q}_{35}$.

**Expression for $< r_{12} r_{34} / r_{13} >$

Expressions for the integral

$$K_{45}(-1, -1, -1, -1; 1, 1, -1; \lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{13}, \lambda_{34}) = \int \frac{d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 (r_1 r_2 r_3 r_4)^{-1} (r_{12} r_{34} / r_{13})}{(r_{12} r_{34} / r_{13})} \times \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_4 r_4 - \lambda_{12} r_{12} - \lambda_{13} r_{13} - \lambda_{34} r_{34}),$$

(145)

and, the integral obtained as a special case from equation(145) with $\lambda_{12} = \lambda_{13} = \lambda_{34} = 0$, can be derived as was done relating to equations(90) and (103-106). In particular, a closed-form expression for $K^{q}_{35} (\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, 0, \lambda_{34})$ has been derived and shown to be exactly identical with the one obtained from the right hand side expression in equation(90) by making interchange $(1 \Leftrightarrow 2)$, as expected. Similarly, the expression derived for $K_{45}(-1, -1, -1, -1; 1, 1, -1; \lambda_1, \lambda_2, \lambda_3, \lambda_4; 0, 0, 0)$ has been shown to be exactly identical with the one obtained from the right hand side expression in equation(105) by performing the interchange $(1 \Leftrightarrow 2)$, as expected.

**(b) Analytic evaluation of $K^{q}_{46}$**

The generating integral $K^{q}_{46}$ is given by the equation

$$K^{q}_{46} (\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{24}, \lambda_{43}) = \int \frac{d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 (r_1 r_2 r_3 r_4 r_{12} r_{24} r_{43})^{-1}}{r_{12} r_{24} r_{43}} \times \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_4 r_4 - \lambda_{12} r_{12} - \lambda_{24} r_{24} - \lambda_{43} r_{43}),$$

(146)

which can be rewritten as

$$K^{q}_{46} = \int \frac{d\vec{r}_2 d\vec{r}_3 (r_2 r_3 r_{24})^{-1}}{r_{24}} \exp(-\lambda_2 r_2 - \lambda_4 r_4 - \lambda_{24} r_{24}) \times J(\lambda_1, \lambda_{12}, r_2) J(\lambda_3, \lambda_{43}, r_4),$$

(147)

where the $J$’s are given by equations(1) and (3). Replacing the $J$’s by their closed-form

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expressions, equation(147) simplifies to give

\[ K_{46}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{12}, \lambda_{24}, \lambda_{43}) = \frac{16\pi^2}{(\lambda_1^2 - \lambda_{12}^2)(\lambda_3^2 - \lambda_{24}^2)} \]

\[ \times \left[ I_2(-2, -2, -1; \lambda_2 + \lambda_{12}, \lambda_4 + \lambda_{24}, \lambda_{43}) - I_2(-2, -2, -1; \lambda_2 + \lambda_{12}, \lambda_3 + \lambda_{43}, \lambda_{24}) \right. \]

\[ - I_2(-2, -2, -1; \lambda_1 + \lambda_2, \lambda_4 + \lambda_{24}, \lambda_{43}) + I_2(-2, -2, -1; \lambda_1 + \lambda_2, \lambda_3 + \lambda_{24}, \lambda_{43}) \right], \quad (148) \]

where expressions for the \( I_2 \) integrals are given by equation(25).

Comparing equation(85) for the integral \( K_{41}^g \) with equation(148) for the integral \( K_{46}^g \), it is observed that if a change \((3 \Rightarrow 4)\) is made in the \( \lambda \) subscripts in equation(85), it leads to equation(148). This is as expected.

Similarly, comparing equation(148) for \( K_{46}^g \) and equation(136) for \( K_{44}^g \), it is observed that the closed-form expression for the former can be obtained from that for the latter by the interchange \((1 \Rightarrow 2)\) performed in the latter expression.

(c) Analytic evaluation of \( K_{47}^g \)

The generating integral \( K_{47}^g \) is defined as

\[ K_{47}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{23}, \lambda_{31}, \lambda_{14}) = \int d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 (r_1 r_2 r_3 r_4 r_{31} r_{14})^{-1} \]

\[ \times \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_4 r_4 - \lambda_{23} r_{23} - \lambda_{31} r_{31} - \lambda_{14} r_{14}), \quad (149) \]

which can be expressed as

\[ K_{47}^g = \int d\vec{r}_1 d\vec{r}_3 (r_1 r_3 r_{31})^{-1} \exp(-\lambda_1 r_1 - \lambda_3 r_3 - \lambda_{31} r_{31}) \]

\[ \times J(\lambda_2, \lambda_{23}, r_3) J(\lambda_4, \lambda_{14}, r_1), \quad (150) \]

with expressions for the \( J \)'s given in equation(3). Substituting these expressions in equation(150), it simplifies to

\[ K_{47}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{23}, \lambda_{31}, \lambda_{14}) = \frac{16\pi^2}{(\lambda_2^2 - \lambda_{23}^2)(\lambda_3^2 - \lambda_{31}^2)} \]

\[ \times \left[ I_2(-2, -2, -1; \lambda_1 + \lambda_{14}, \lambda_3 + \lambda_{23}, \lambda_{31}) - I_2(-2, -2, -1; \lambda_1 + \lambda_{14}, \lambda_2 + \lambda_3, \lambda_{31}) \right. \]

\[ - I_2(-2, -2, -1; \lambda_1 + \lambda_4, \lambda_3 + \lambda_{23}, \lambda_{31}) + I_2(-2, -2, -1; \lambda_1 + \lambda_4, \lambda_2 + \lambda_3, \lambda_{31}) \right], \quad (151) \]

with the \( I_2 \) integrals given by equation(25).

If the right hand side expression in equation(123) for \( K_{42}^g \) is compared with the right hand side expression in equation(151) for \( K_{47}^g \), it is clearly observed that the latter can be obtained from the former if an interchange \((4 \Rightarrow 1)\) is performed. This is consistent with the observation relating to the integrands for \( K_{42}^g \) and \( K_{47}^g \) defined in equations(120) and (149), respectively.

Similarly it is verified that the right hand side expression in equation(151) for \( K_{47}^g \) can be obtained from the right hand side expression in equation(139) for \( K_{44}^g \) by making interchange \((2 \Rightarrow 3)\) in equation(139), as expected.
(d) Analytic evaluation of $K_{48}^g$

The generating integral $K_{48}^g$ is defined by the relation

$$K_{48}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{23}, \lambda_{24}, \lambda_{41}) = \int d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 (r_1 r_2 r_3 r_4 r_{23} r_{24} r_{41})^{-1} \times \exp(-\lambda_1 r_1 - \lambda_2 r_2 - \lambda_3 r_3 - \lambda_4 r_4 - \lambda_{23} r_{23} - \lambda_{24} r_{24} - \lambda_{41} r_{41}),$$

which can be rewritten as

$$K_{48}^g = \int d\vec{r}_2 d\vec{r}_4 (r_2 r_4 r_{24})^{-1} \exp(-\lambda_2 r_2 - \lambda_4 r_4 - \lambda_{24} r_{24}) \times J(\lambda_3, \lambda_{23}, r_2) J(\lambda_1, \lambda_{41}, r_4).$$

Inserting equation(3) in equation(153), the following expression for $K_{48}^g$ is obtained:

$$K_{48}^g(\lambda_1, \lambda_2, \lambda_3, \lambda_4; \lambda_{23}, \lambda_{24}, \lambda_{41}) = \frac{16\pi^2}{(\lambda_3^2 - \lambda_{23}^2)(\lambda_4^2 - \lambda_{41}^2)} \times \left[ I_2(-2, -2, -1; \lambda_2 + \lambda_{23}, \lambda_4 + \lambda_{41}, \lambda_{24}) - I_2(-2, -2, -1; \lambda_2 + \lambda_{23}, \lambda_4 + \lambda_1, \lambda_{24}) - I_2(-2, -2, -1; \lambda_2 + \lambda_3, \lambda_4 + \lambda_{41}, \lambda_{24}) + I_2(-2, -2, -1; \lambda_2 + \lambda_3, \lambda_4 + \lambda_1, \lambda_{24}) \right],$$

with expressions for the $I_2$ integrals given by equation(25).

Comparing the right hand side expression in equation(123) for $K_{12}^g$ with that in equation(154) for $K_{48}^g$, it is observed that if a change $(3 \leftrightarrow 2)$ is performed in equation(123), expression in equation(154) is exactly reproduced, which is evident from integrands in equations(120) and (152).

All the limiting expressions for the generating integrals $K_{46}^g$, $K_{47}^g$ and $K_{48}^g$ can be derived in the same manner as was done for establishing equations(90-99) in the case of the generating integral $K_{41}^g$.

6. Conclusion

The integrals evaluated in this paper are likely to be utilized by those workers who do calculations employing Hy-CI and/or E-Hy-CI methods of variation. The programs sometimes developed by them for calculation of correlated integrals numerically can be tested with the exact values obtained from closed-form expressions of such integrals reported here.

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