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ORIGINAL PAPER

Analysis of atomic integrals involving explicit correlation factors for the three-electron case. I. Connection to the hypergeometric function ${}_3F_2$

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Abstract This work considers the solution of atomic three-electron integrals that involve explicit inter-electronic separation factors. The traditional Sack expansion is replaced by an alternative expansion, which avoids the breakup of the radial integrals into a number of factors depending on the lesser and greater of the inter-electronic separation distances. The present approach avoids the $N!$ increase in the number of required auxiliary functions, where N is the number of electrons. The new approach leads to additional infinite summations, but these summations either converge very quickly in a serial calculation, or can be effectively dealt with using the massively parallel architecture of a graphics processing unit. The new auxiliary functions that arise are discussed in detail.

Keywords Atomic three-electron integrals · Sack expansion · Hypergeometric functions

1 Introduction

There has been considerable progress over the past several years on the evaluation of the properties of atomic lithium and other related three-electron atomic species. A principal approach involved in these computational efforts has been the Hylleraas method [1–8]. Earlier progress can be found in the reviews [9,10]. The hybrid Hylleraas-CI technique and the exponentially correlated Gaussian approach have also

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proved to be very successful techniques [4,11–13]. There have also been extensions of the Hylleraas approach using both Slater-type functions and Gaussian functions to treat small molecular systems in a non-Born–Oppenheimer approach [12].

In the Hylleraas approach, the trial wave function involves an expansion in terms of explicit factors of the electron–electron separation distance, r_{ij}. In the conventional Hylleraas expansion, the wave function for the S states of a three-electron atomic system is expanded as

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \mathscr{A} \sum_{\mu=1}^{\mathscr{N}} C_\mu r_1^{i_\mu} r_2^{j_\mu} r_3^{k_\mu} r_{12}^{l_\mu} r_{13}^{m_\mu} r_{23}^{n_\mu} e^{-a_\mu r_1 - b_\mu r_2 - c_\mu r_3} \chi_\mu, \tag{1}$$

where r_i denotes an electron–nuclear separation, $\mathscr{A}$ is the antisymmetrizer, $\mathscr{N}$ is the number of basis functions, and χ_μ is a spin eigenfunction. The constants a_μ, b_μ and c_μ are >0, and the set of indices $\{i_\mu, j_\mu, k_\mu, l_\mu, m_\mu, n_\mu\}$ are integers that are ≥ 0. It can be shown that the expectation values for most properties of the atomic S-states are reducible to three-electron integrals of the form

$$I_3(i, j, k, l, m, n, a, b, c) = \int r_1^i r_2^j r_3^k r_{12}^l r_{13}^m r_{23}^n e^{-ar_1 - br_2 - cr_3} d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3, \tag{2}$$

where a, b and c are >0, and the set of indices $\{i, j, k, l, m, n\}$ are integers. For the evaluation of energy values and many other expectation values, the indices $\{i, j, k, l, m, n\}$ are each ≥ -1. In this paper will investigate an alternative strategy to the evaluation of the integrals appearing in Eq. (2). The motivation for seeking an alternative strategy is discussed in Sect. 2. We also note that the I_3 integrals arise in Hylleraas and Hylleraas-CI calculations on systems with more than three electrons, along with related integrals involving various angular factors.

The important work of Pachucki et al. [14] derives a closed form recursion formula for the three-electron correlated integrals. However, accurate integral evaluation using this closed form recursion scheme requires extended precision arithmetic. A significant number of publications have appeared where a series expansion approach has been employed to evaluate the required correlated integrals, and these can be evaluated in double precision arithmetic, or for very large basis sets, quadruple precision arithmetic might be required. It is not clear if the closed form recursion strategy can be extended to systems beyond the three-electron case. To the best of our knowledge, that has not been accomplished. Even if it can be, it is not clear what arithmetic precision level would be required for accurate evaluation of the recursion formula.

The approach we discuss is a series scheme, which in our opinion, could be extended to larger electron systems with appropriate treatment of the new auxiliary functions that arise. The present approach discussed in our work avoids the $N!$ growth in the number of auxiliary function evaluations, and this is both novel, in comparison with the standard series approach, and potentially important for calculations on larger N systems. The difference in the precision level of the arithmetic required in the series expansion method and the closed form recursion formula technique is a major distinction between the approaches.

More complicated integrals with r_{ij} factors in the exponentials have been studied for the three-electron case and some limited analytic work has been done for the four-electron case [15,16]. In a seminal publication, Puchalski et al. [5] have obtained extremely high accuracy for the ground state of the lithium atom using a relatively modest size basis set of exponentially correlated basis functions. Unfortunately, these calculations required extended precision arithmetic for parts of the calculations, with a factor of about 10^2 more cpu time being required in comparison with a standard Hylleraas basis set of the same size. In a very recent study [16], a stability analysis was carried out for some of the exponentially correlated integrals that arise for the four electron case. It was proved mathematically in [16] that extended precision arithmetic is required for the accurate evaluation of some of the analytic formulas involving higher powers on the pre-exponential terms, when exponentially correlated factors form part of the integrand. Some work has appeared over the past few years for the three electron case examining the role of compact expansions of exponential terms with r_{ij} factors. The convergence rate has been observed to be faster relative to similar compact expansions [17,18].

The plan of the paper is as follows. In Sect. 2 we briefly sketch the derivation of $I_3(i, j, k, l, m, n, a, b, c)$ in terms of the W-integral auxiliary function, and outline the principal issue associated with this approach, emphasizing what happens as we extend beyond the three-electron problem. In Sect. 3 we derive an expression for the I_3-integral using an alternative form of the Sack expansion for the Sack radial functions, and reduce the I_3-integral to a J_3 auxiliary function. We then examine some special cases of the J_3 auxiliary function, namely the K_2, J_2 functions (in Sects. 4 and 5), K_3, and a key special case of the K_3 integral with one zero argument (in Sect. 6). We show an important connection of the special case of the K_3 integral with one zero argument with the hypergeometric function ${}_3F_2$, and because this can be written as a finite sum, we discuss this special function and a number of special cases in detail in Sects. 7–13. In Sect. 14 we briefly discuss some simple closed form cases for the K_3 integral with one denominator index equal to zero. In the following section we discuss the general case of the K_3 integral and obtain a series form for the representation of this function. In Sect. 16 we evaluate the special case $K_3(i, j, k, l, 1, 1)$ in terms of the hypergeometric function ${}_3F_2$. Section 17 develops a general connection between the general K_3 integral and the hypergeometric function ${}_3F_2$. Section 18 discusses a reduction formula of J_3 to K_3. Sections 19 and 20 discuss some aspects of the numerical evaluation of the K_3 and I_3 integrals. A number of key recursion relations for the functions K_3 and J_3 are developed in part II of this study. Part II also includes the development of formulas that are more stable for the application of convergence accelerator techniques. The focus of this paper is on the mathematical developments. A future paper will discuss the numerical implementation strategy.

2 Reduction of the three-electron integral to auxiliary functions

In this section we concisely recap the standard reduction of the I-integrals to auxiliary functions. The I_3-integrals and some generalizations have received extensive discussion in the literature [14,19–44]. We will restrict consideration to the case where the indices $\{i, j, k, l, m, n\}$ are ≥ -1. The cases where the indices $\{l, m, n\}$ are allowed to be -2, which are required for the evaluation of relativistic effects [45,46] and some other properties [47,48], lead to significant additional complications, and some of these problems have been addressed in the literature [49–57].

The Sack expansion [58] is given by

$$r_{12}^{l} = \sum_{l_1=0}^{\infty} R_{ll_1}(r_1, r_2) P_{l_1}(\cos\theta_{12}), \tag{3}$$

where $P_{l_1}(\cos\theta_{12})$ denotes a Legendre polynomial and $R_{ll_1}(r_1, r_2)$ is a Sack radial function. Inserting the Sack expansion for each of the r_{ij} factors in Eq. (2), leads to

$$I_3(i, j, k, l, m, n, a, b, c) = \sum_{l_1=0}^{\infty}\sum_{m_1=0}^{\infty}\sum_{n_1=0}^{\infty} I_R(i, j, k, l, m, n, l_1, m_1, n_1, a, b, c) I_\Omega(l_1, m_1, n_1), \tag{4}$$

where the radial integrals are given by

$$I_R(i, j, k, l, m, n, l_1, m_1, n_1, a, b, c) = \int r_1^{i+2} r_2^{j+2} r_3^{k+2} R_{ll_1}(r_1, r_2) R_{mm_1}(r_1, r_3) R_{nn_1}(r_2, r_3) e^{-ar_1-br_2-cr_3} dr_1 dr_2 dr_3, \tag{5}$$

and the angular integrals by

$$I_\Omega(l_1, m_1, n_1) = \int P_{l_1}(\cos\theta_{12}) P_{m_1}(\cos\theta_{13}) P_{n_1}(\cos\theta_{23}) d\Omega_1 d\Omega_2 d\Omega_3. \tag{6}$$

The angular integral can be readily evaluated by employing the standard expansion of the Legendre polynomials in terms of spherical harmonics, leading to the result

$$I_\Omega(l_1, m_1, n_1) = \frac{64\pi^3 \delta_{l_1 m_1} \delta_{l_1 n_1} \delta_{m_1 n_1}}{(2l_1 + 1)^2}, \tag{7}$$

where $\delta_{l_1 n_1}$ denotes a Kronecker delta. Inserting this result for $I_\Omega(l_1, m_1, n_1)$ into Eq. (4) leads to

$$I_3(i, j, k, l, m, n, a, b, c) = 64\pi^3 \sum_{w=0}^{\infty} \frac{1}{(2w + 1)^2} I_R(i, j, k, l, m, n, w, w, w, a, b, c), \tag{8}$$

where

$$I_R(i,j,k,l,m,n,w,w,w,a,b,c) = \int r_1^{i+2} r_2^{j+2} r_3^{k+2} R_{lw}(r_1,r_2) R_{mw}(r_1,r_3) R_{nw}(r_2,r_3) e^{-ar_1-br_2-cr_3} dr_1 dr_2 dr_3. \tag{9}$$

The Sack radial function [58] can be written as

$$R_{lw}(r_1,r_2) = \frac{(-l/2)_w}{(1/2)_w} r_{12<}^{w} r_{12>}^{l-w} \sum_{u=0}^{\infty} a_{wlu} \left(\frac{r_{12<}}{r_{12>}}\right)^{2u}, \tag{10}$$

where $r_{12<} = \min(r_1, r_2)$ and $r_{12>} = \max(r_1, r_2)$, and the coefficients a_{wlu} are given by

$$a_{wlu} = \frac{\left(w - \frac{l}{2}\right)_u \left(-\frac{1}{2} - \frac{l}{2}\right)_u}{u! \left(w + \frac{3}{2}\right)_u}, \tag{11}$$

where $(\alpha)_n$ denotes a Pochhammer symbol, defined in terms of the gamma function $\Gamma(p)$ as

$$(p)_q = p(p+1)(p+2)\cdots(p+q-1) = \frac{\Gamma(p+q)}{\Gamma(p)}. \tag{12}$$

Inserting the expansions for the Sack radial functions into Eq. (8) leads to

$$\begin{aligned}
I_3(i,j,k,l,m,n,a,b,c) = 64\pi^3 \sum_{w=0}^{\infty} & \frac{(-l/2)_w(-m/2)_w(-n/2)_w}{(2w+1)^2\{(1/2)_w\}^3} \\
& \times \sum_{u=0}^{\infty} a_{wlu} \sum_{v=0}^{\infty} a_{wmv} \sum_{s=0}^{\infty} a_{wns} \\
& \times \{W(\mathrm{I}_1+\omega_1, \mathrm{J}_1+l-\omega_5, \mathrm{K}_1+m+n-\omega_3, a, b, c) \\
& + W(\mathrm{J}_1+\omega_2, \mathrm{I}_1+l-\omega_4, \mathrm{K}_1+m+n-\omega_3, b, a, c) \\
& + W(\mathrm{K}_1+\omega_3, \mathrm{J}_1+\omega_5+n, \mathrm{I}_1+l+m-\omega_1, c, b, a) \\
& + W(\mathrm{I}_1+\omega_1, \mathrm{K}_1+m-\omega_6, \mathrm{J}_1+l+n-\omega_2, a, c, b) \\
& + W(\mathrm{J}_1+\omega_2, \mathrm{K}_1+n+\omega_6, \mathrm{I}_1+l+m-\omega_1, b, c, a) \\
& + W(\mathrm{K}_1+\omega_3, \mathrm{I}_1+m+\omega_4, \mathrm{J}_1+l+n-\omega_2, c, a, b)\},
\end{aligned} \tag{13}$$

where the W-integral is defined by

$$W(p,q,s,\alpha,\beta,\gamma) = \int_0^{\infty} x^p e^{-\alpha x} dx \int_x^{\infty} y^q e^{-\beta y} dy \int_y^{\infty} z^s e^{-\gamma z} dz, \tag{14}$$

and the notational simplifications,

$$\mathrm{I}_1 = i + 2, \quad \mathrm{J}_1 = j + 2, \quad \mathrm{K}_1 = k + 2, \tag{15}$$

$$\omega_1 = 2u + 2v + 2w, \quad \omega_2 = 2u + 2s + 2w, \quad \omega_3 = 2v + 2s + 2w \tag{16}$$

$$\omega_4 = 2u - 2v, \quad \omega_5 = 2u - 2s, \quad \omega_6 = 2v - 2s, \tag{17}$$

have been employed. The W-integrals have received extensive study, and there are well-developed algorithms for the high precision evaluation of these auxiliary functions [59–70].

This study was motivated by desire to circumvent the W-integral approach. To apply the Hylleraas technique to a four-electron atomic system, the analogue of the W-integrals is given by [64,65,71]

$$\begin{aligned} &W_4(p, q, s, t, \alpha, \beta, \gamma, \delta) \\ &= \int_0^\infty x^p e^{-\alpha x} dx \int_x^\infty y^q e^{-\beta y} dy \int_y^\infty z^s e^{-\gamma z} dz \int_z^\infty w^t e^{-\delta w} dw, \end{aligned} \tag{18}$$

and there are 4! combinations of these integrals to contend with. Our objective in this work is to demonstrate an alternative strategy that circumvents this $N!$ increase in integral combinations as the number of electrons, N, increases. Other issues arise, and these are addressed in later sections.

3 An alternative expansion for the radial integrals

We now consider an alternative approach to evaluate the radial integrals $I_R(i, j, k, l, m, n, w, w, w, a, b, c)$. To do this we employ the following expansion for the Sack radial function [58]:

$$R_{lw}(r_1, r_2) = \frac{(-l/2)_w}{(1/2)_w} \frac{r_1^w r_2^w}{(r_1 + r_2)^{2w-l}} \sum_{u=0}^{\infty} b_{wlu} \left(\frac{r_1 r_2}{(r_1 + r_2)^2} \right)^u, \tag{19}$$

where the coefficients b_{wlu} are given by

$$b_{wlu} = \frac{4^u \left(w - \frac{l}{2}\right)_u (1 + w)_u}{u!(2 + 2w)_u}. \tag{20}$$

The radial integral can be written as

$$\begin{aligned} I_R(i, j, k, l, m, n, w, w, w, a, b, c) &= \frac{(-l/2)_w(-m/2)_w(-n/2)_w}{\{(1/2)_w\}^3} \sum_{u=0}^{\infty} b_{wlu} \sum_{v=0}^{\infty} b_{wmv} \sum_{s=0}^{\infty} b_{wns} \\ \times \int \frac{r_1^{i+2+2w+u+v} r_2^{j+2+2w+u+s} r_3^{k+2+2w+v+s}}{(r_1 + r_2)^{2w-l+2u}(r_1 + r_3)^{2w-m+2v}(r_2 + r_3)^{2w-n+2s}} &e^{-ar_1 - br_2 - cr_3} dr_1 dr_2 dr_3. \end{aligned} \tag{21}$$

Employing the substitutions $x = r_1,\ y = r_2$, and $z = r_3$, we introduce the auxiliary function

$$J_3(i, j, k, l, m, n, a, b, c) = \int_0^\infty \int_0^\infty \int_0^\infty \frac{x^i y^j z^k e^{-ax-by-cz}}{(x+y)^l (x+z)^m (y+z)^n} dx\, dy\, dz, \tag{22}$$

where a, b, and c are real numbers >0, and the indices $\{i, j, k, l, m, n\}$ are integers ≥ 0. There are additional constraints on the indices $\{i, j, k, l, m, n\}$, and these will be discussed in detail later. Equation (21) can be now written as

$$\begin{aligned} &I_R(i, j, k, l, m, n, w, w, w, a, b, c) \\ &= \frac{(-l/2)_w(-m/2)_w(-n/2)_w}{\{(1/2)_w\}^3} \sum_{u=0}^{\infty} b_{wlu} \sum_{v=0}^{\infty} b_{wmv} \sum_{s=0}^{\infty} b_{wns} \\ &\quad \times J_3(\mathrm{I}_1 + 2w + u + v, \mathrm{J}_1 + 2w + u + s, \mathrm{K}_1 + 2w + v + s, \\ &\quad \times 2w - l + 2u, 2w - m + 2v, 2w - n + 2s, a, b, c). \end{aligned} \tag{23}$$

The summation limits in Eq. (23) terminate at finite values when the indices $\{l, m, n\}$ are even integers because of a condition on one of the Pochhammer symbols that appear in the definition of the b_{wlu}, b_{wmv}, and b_{wns} coefficients, but are each non-terminating for odd integer values of the indices $\{l, m, n\}$. This latter case is the one of principal interest in this work. Two strategies are employed to deal with the multiple summations that appear. Convergence acceleration techniques can be judiciously applied to some rearranged forms of the final equations obtained. This approach will be detailed in part II of this work. The second method is to apply a graphical processing unit (GPU) evaluation strategy. In this approach, we can in effect, compute all the required terms in an individual non-terminating sum in essentially about the same time as it takes to evaluate the terms in a terminating sum. This is due to the massively parallel structure of the GPU device. The principal limitation of the current GPU devices is the restriction to double precision arithmetic. With more wide-spread usage of GPU devices for computational work, we expect this limitation to be removed. Further discussion on the numerical evaluation strategy will be given in a future paper.

4 The auxiliary functions K_2 and J_2

In this and the following sections the auxiliary functions required to evaluate Eq. (23) are considered. We start with two elementary auxiliary functions which are special cases of the J_3 function defined in Eq. (22), and in the following sections discuss the more complicated auxiliary functions. The first function considered is:

$$K_2(i, j, k) = \int_0^\infty \int_0^\infty \frac{x^i y^j e^{-x-y}}{(x+y)^k} dxdy, \tag{24}$$

with the constraints

$$i \geq 0, \quad j \geq 0, \quad i + j + 1 - k \geq 0. \tag{25}$$

With the change of variables $y = u - x$ followed by a change of integration order leads to

$$\begin{aligned} K_2(i, j, k) &= \int_0^\infty x^i dx \int_x^\infty (u - x)^j u^{-k} e^{-u} du \\ &= \int_0^\infty u^{-k} e^{-u} du \int_0^u (u - x)^j x^i dx \\ &= \int_0^\infty u^{i+j+1-k} e^{-u} du \int_0^1 (1 - v)^j v^i dv \\ &= (i + j + 1 - k)! B(i + 1, j + 1) \\ &= \frac{i!j!}{(i + j + 1)!} (i + j + 1 - k)!, \end{aligned} \tag{26}$$

where $B(x, y)$ is the beta function, defined in terms of the gamma function by [72]

$$B(a, b) = \int_0^1 t^{a-1} (1 - t)^{b-1} dt = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a + b)}, \text{ for } \operatorname{Re}(a) > 0 \text{ and } \operatorname{Re}(b) > 0. \tag{27}$$

The generalization of the $K_2(i, j, k)$ integral is as follows:

$$J_2(i, j, k, a, b) = \int_0^\infty \int_0^\infty \frac{x^i y^j e^{-ax-by}}{(x + y)^k} dx dy. \tag{28}$$

We now sketch the evaluation of $J_2(i, j, k, a, b)$. This auxiliary function can be directly recast in terms of a two-dimensional version of the W integral in Eq. (14) (sometimes referred to as the V auxiliary function), which has been discussed in the literature [20,59]. With the change of variables $x = uv$ and $y = u - uv$, Eq. (28) leads to

$$J_2(i, j, k, a, b) = \int_0^1 v^i (1 - v)^j dv \int_0^\infty u^{i+j+1-k} e^{-auv-bu(1-v)} du. \tag{29}$$

Let $L = (i + j - k + 1)$, then

$$J_2(i, j, k, a, b) = L! \int_0^1 \frac{v^i (1 - v)^j}{(av + b(1 - v))^{L+1}} dv. \tag{30}$$

For case (i), $a = b$, we have immediately from Eq. (30)

$$J_2(i, j, k, a, a) = a^{-L-1} K_2(i, j, k) = \frac{L!}{a^{L+1}} B(i + 1, j + 1). \tag{31}$$

For case (ii), $a \neq b$, assume without loss of generality that $a > b$. Let $a = b\alpha$ with $\alpha > 1$. Then

$$J_2(i, j, k, a, b) = \frac{L!}{b^{L+1}} \int_0^1 \frac{v^i (1-v)^j}{(1+(\alpha-1)v)^{L+1}} dv, \tag{32}$$

which can be rewritten using a binomial expansion, to give

$$\begin{aligned} J_2(i, j, k, a, b) &= \frac{L!}{b^{L+1}} \sum_{s=0}^{j} \binom{j}{s} (-1)^s \int_0^1 \frac{v^{i+s}}{(1+(\alpha-1)v)^{L+1}} dv \\ &= \frac{L!}{b^{\mathrm{L}+1}} \sum_{s=0}^{j} \binom{j}{s} \frac{(-1)^s}{(\alpha-1)^{i+s}} \int_0^1 \frac{[1+(\alpha-1)v-1]^{i+s}}{(1+(\alpha-1)v)^{L+1}} dv, \end{aligned} \tag{33}$$

where $\binom{j}{s}$ denotes a binomial coefficient. Expanding the numerator using the binomial expansion, leads to

$$\begin{aligned} J_2(i, j, k, a, b) &= \frac{L!}{b^{\mathrm{L}+1}} \sum_{s=0}^{j} \binom{j}{s} \frac{(-1)^s}{(\alpha-1)^{i+s}} \sum_{t=0}^{i+s} \binom{i+s}{t} (-1)^t \int_0^1 \frac{[1+(\alpha-1)v]^{i+s-t}}{(1+(\alpha-1)v)^{L+1}} dv \\ &= \frac{L!}{b^{\mathrm{L}+1}} \sum_{s=0}^{j} \binom{j}{s} \frac{(-1)^s}{(\alpha-1)^{i+s}} \sum_{t=0}^{i+s} \binom{i+s}{t} (-1)^t \int_0^1 (1+(\alpha-1)v)^{i+s-t-L-1} dv. \end{aligned} \tag{34}$$

The integral appearing in Eq. (34) can be evaluated as

$$\int_0^1 (1+(\alpha-1)v)^{m-1} dv = \begin{cases} \frac{\log\alpha}{\alpha-1} & \text{if } m = 0 \\ \frac{1-\alpha^m}{m(1-\alpha)} & \text{if } m \neq 0 \end{cases}, \tag{35}$$

so that

$$\begin{aligned} J_2(i, j, k, a, b) = \frac{L!}{b^{\mathrm{L}+1}} \sum_{s=0}^{j} \binom{j}{s} \frac{(-1)^s}{(\alpha-1)^{i+s+1}} \sum_{t=0}^{i+s} \binom{i+s}{t} (-1)^t \\ \times \begin{cases} \log(\alpha), & \text{if } L-i-s+t = 0 \\ \frac{(\alpha^{i+s-t-L}-1)}{i+s-t-L}, & \text{if } L-i-s+t \neq 0 \end{cases}. \end{aligned} \tag{36}$$

When the integer arguments of J_2 increase in size Eq. (36) becomes progressively more unstable for numerical evaluation. For example, for the case $i = 11$, $j = 9$, $k = 5$, $a = 2.3$, $b = 2.5$, separate calculation of the positive and negative parts of Eq. (36) establishes that 32 digits are loss when the positive and negative parts are combined to obtain the final value. In cases where the arguments for J_2 are large, the series expansion formulas Eqs. (39) and (40) given in the following section should be employed, and these are both stable for numerical evaluation.

5 Alternative approach to evaluate $J_2(i, j, k, a, b)$

In this section we consider an alternative scheme to evaluate the J_2 integrals. Without loss of generality assume $b > a$. Since

$$\mathrm{e}^{(-ax-by)} = \mathrm{e}^{(b-a)x}\mathrm{e}^{-b(x+y)}, \tag{37}$$

then with the change of variables $bx = s$ and $by = t$, it follows that

$$J_2(i, j, k, a, b) = \frac{1}{b^{i+j-k+2}} \int_0^\infty \int_0^\infty \frac{s^i t^j e^{\left(\frac{b-a}{b}\right)s} e^{-s-t}}{(s+t)^k} dsdt. \tag{38}$$

Employing a power series expansion for $e^{\left(\frac{b-a}{b}\right)s}$, we can write

$$\begin{aligned} J_2(i, j, k, a, b) &= \frac{1}{b^{i+j-k+2}} \sum_{\mu=0}^{\infty} \frac{\left(\frac{b-a}{b}\right)^\mu}{\mu!} \int_0^\infty \int_0^\infty \frac{x^{i+\mu} y^j e^{-x-y}}{(x+y)^k} dxdy \\ &= \frac{1}{b^{i+j-k+2}} \sum_{\mu=0}^{\infty} \left(\frac{b-a}{b}\right)^\mu \frac{K_2(i+\mu, j, k)}{\mu!}. \end{aligned} \tag{39}$$

The series expansion approach of Eq. (39) avoids the numerical instability issue that can arise using Eq. (36) when using larger integer arguments.

Alternatively, if $a < b \leq 2a$, then

$$\begin{aligned} J_2(i, j, k, a, b) &= \frac{1}{a^{i+j-k+2}} \sum_{\mu=0}^{\infty} (-1)^\mu \frac{\left(\frac{b-a}{a}\right)^\mu}{\mu!} \int_0^\infty \int_0^\infty \frac{x^i y^{j+\mu} e^{-x-y}}{(x+y)^k} dxdy \\ &= \frac{1}{a^{i+j-k+2}} \sum_{\mu=0}^{\infty} (-1)^\mu \left(\frac{b-a}{a}\right)^\mu \frac{K_2(i, j+\mu, k)}{\mu!}. \end{aligned} \tag{40}$$

Convergence acceleration techniques, for example, the Levin approach [73], are significantly more numerically stable when applied to series with alternating signs, which is the situation in Eq. (40). Sample values for the auxiliary functions K_2 and J_2 are presented in Tables 1 and 2.

Table 1 Sample values for the K_2 auxiliary function

Parameters			Integral
i	j	k	$K_2(i, j, k)$
1	1	1	$3.333333333333333333333333333333333 \times 10^{-1}$
2	1	1	$5.000000000000000000000000000000000 \times 10^{-1}$
2	2	1	$8.000000000000000000000000000000000 \times 10^{-1}$
2	2	2	$2.0000000000000000000000000000000000 \times 10^{-1}$
7	2	1	$1.0080000000000000000000000000000000 \times 10^{3}$
7	1	6	$8.333333333333333333333333333333333 \times 10^{-2}$
5	5	5	$2.5974025974025974025974025974025974 \times 10^{-1}$
12	2	10	$8.791208791208791208791208791208791 \times 10^{-2}$
1	3	5	$5.000000000000000000000000000000000 \times 10^{-2}$

Table 2 Sample values for the J_2 auxiliary function

Parameters					Integral
i	j	k	a	b	$J_2(i, j, k, a, b)$
1	1	1	2.1	2.2	$3.356180380735963591815495839220637 \times 10^{-2}$
2	2	1	2.5	2.4	$9.070834533153207178594989910647530 \times 10^{-3}$
2	2	2	4.6	8.3	$1.3056771755775946745334359397372531 \times 10^{-4}$
7	2	1	2	2	$9.843750000000000000000000000000000 \times 10^{-1}$
7	1	6	4.1	3	$3.723111304304961806557743692113333 \times 10^{-4}$
5	5	5	7.1	3.4	$3.1345963054263156697195206503365255 \times 10^{-6}$
12	2	10	1.9	2.7	$1.2168099834546693558405517235994899 \times 10^{-3}$
1	3	5	8.6	4.2	$8.989063450970709757771637791857777 \times 10^{-3}$

6 The auxiliary function K_3: the special case $m = 0$, l and $n > 0$

In this section we consider the evaluation of the auxiliary function

$$K_3(i, j, k, l, m, n) = \int_0^\infty \int_0^\infty \int_0^\infty \frac{x^i y^j z^k e^{-x-y-z}}{(x+y)^l (x+z)^m (y+z)^n} dx\, dy\, dz, \quad (41)$$

for the special case $m = 0$. This case will prove to be useful in a following section. Because of the inherent permutation symmetry for the auxiliary function $K_3(i, j, k, l, m, n)$, we can select any one of the indices l, m, or n to be zero. With the choice $m = 0$ and the change of variables $y = uv$ and $x = u - uv$, and rearranging the order of integration, we have

$$K_3(i, j, k, l, 0, n) = \int_0^1 v^j (1-v)^i dv \int_0^\infty \int_0^\infty \frac{u^{i+j-l+1} z^k e^{-u-z}}{(uv+z)^n} du dz. \quad (42)$$

With the further change of variables $u = xy$ and $z = x - xy$ then

$$K_3(i, j, k, l, 0, n) = \int_0^\infty x^{i+j+k+2-l-n} e^{-x} dx \int_0^1 v^j (1-v)^i dv \int_0^1 \frac{y^{i+j-l+1}(1-y)^k}{(1-y(1-v))^n} dy. \tag{43}$$

Set

$$\tau = i + j + k + 2 - l - n, \tag{44}$$

and consider the situation $\tau \geq 0$, hence

$$K_3(i, j, k, l, 0, n) = \tau! \int_0^1 v^j (1-v)^i dv \int_0^1 \frac{y^{i+j-l+1}(1-y)^k}{(1-y+yv)^n} dy. \tag{45}$$

Inserting the expansion

$$\frac{1}{(1-y(1-v))^n} = \sum_{\mu=0}^\infty \frac{(n)_\mu}{\mu!} y^\mu (1-v)^\mu, \tag{46}$$

into Eq. (45) leads to

$$K_3(i, j, k, l, 0, n) = \tau! \sum_{\mu=0}^\infty \frac{(n)_\mu}{\mu!} \int_0^1 v^j (1-v)^{i+\mu} dv \int_0^1 y^{i+j-l+1+\mu} (1-y)^k dy. \tag{47}$$

For $i + j + 1 - l \geq 0$ we have that

$$K_3(i, j, k, l, 0, n) = \tau! \sum_{\mu=0}^\infty \frac{(n)_\mu}{\mu!} B(j+1, i+1+\mu) B(i+j+2-l+\mu, k+1). \tag{48}$$

From Eq. (48) it follows by the symmetry of the kernel of the K_3 function that

$$K_3(k, j, i, n, 0, l) = K_3(i, j, k, l, 0, n), \tag{49}$$

and hence

$$K_3(k, j, i, n, 0, l) = \tau! \sum_{\mu=0}^\infty \frac{(l)_\mu}{\mu!} B(j+1, k+1+\mu) B(j+k+2-n+\mu, i+1). \tag{50}$$

The series in Eq. (48) can be written in term of the hypergeometric function ${}_3F_2$. Using the definition of the beta function given in Eq. (27), it follows that Eq. (48) can be expressed as

$$K_3(i,j,k,l,0,n) = j!k!\tau! \sum_{\mu=0}^{\infty} \frac{(n)_\mu}{\mu!} \frac{\Gamma(i+1+\mu)\Gamma(i+j+2-l+\mu)}{\Gamma(i+j+2+\mu)\Gamma(i+j+k+3-l+\mu)}. \tag{51}$$

Expressing the gamma functions in term of Pochhammer symbols yields

$$\begin{aligned} K_3(i,j,k,l,0,n) = j!k!\tau! &\frac{\Gamma(i+1)\Gamma(i+j+2-l)}{\Gamma(i+j+2)\Gamma(i+j+k+3-l)} \\ &\times \sum_{\mu=0}^{\infty} \frac{(n)_\mu}{\mu!} \frac{(i+1)_\mu (i+j+2-l)_\mu}{(i+j+2)_\mu (i+j+k+3-l)_\mu}. \end{aligned} \tag{52}$$

The ${}_3F_2$ hypergeometric function is defined by [74–84]

$${}_3F_2(a,b,c;d,e;z) = \sum_{\mu=0}^{\infty} \frac{(a)_\mu (b)_\mu (c)_\mu}{(d)_\mu (e)_\mu} \frac{z^\mu}{\mu!}, \tag{53}$$

so Eq. (52) can be written as

$$\begin{aligned} K_3(i,j,k,l,0,n) = j!k!\tau! &\frac{\Gamma(i+1)\Gamma(i+j+2-l)}{\Gamma(i+j+2)\Gamma(i+j+k+3-l)} \\ &\times {}_3F_2(n, i+1, i+j+2-l; i+j+2, i+j+k+3-l; 1). \end{aligned} \tag{54}$$

Several different results for $K_3(i,j,k,l,0,n)$ can be readily constructed in which the arguments of the hypergeometric function are different, and in some cases, leading to results which are slightly quicker to evaluate. For example,

$$\begin{aligned} K_3(i,j,k,l,0,n) = &\frac{i!j!k!(j+k+1-n)!(i+j+1-l)!}{(i+j+1)!(j+k+1)!} \\ &\times {}_3F_2(j+1, l, n; i+j+2, j+k+2; 1), \end{aligned} \tag{55}$$

and

$$\begin{aligned} K_3(i,j,k,l,0,n) = &\frac{i!k!(j+k+1-n)!(i+j+1-l)!(i+j+k+2-l-n)!}{(i+j+k+2-n)!(i+j+k+2-l)!} \\ &\times {}_3F_2(i+j+k+3-l-n, i+1, k+1; i+j \\ &\quad +k+3-n, i+j+k+3-l; 1). \end{aligned} \tag{56}$$

7 The generalized hypergeometric function ${}_3F_2$ with non-negative integer parameters and unit argument

Because of the key connection given in Eq. (54), we explore in this and the following few sections a number of results for the hypergeometric function ${}_3F_2$ which will allow the $m = 0$ case of K_3 to be efficiently evaluated at high speed. We will show that for the case of interest in this work, $\{a, b, c, d, e\} \in \mathbb{N}$, that

$$
{}_3F_2(a, b, c; d, e; 1) = c_1(a, b, c, d, e) + c_2(a, b, c, d, e)\pi^2, \tag{57}
$$

where $c_1, c_2 \in \mathbb{Q}$, and show how to determine explicit expressions for c_1 and c_2. It will become clear that these two functions involve relatively simple finite summations of gamma functions with integer arguments. Utilizing Eq. (57) allows Eq. (54) to be evaluated as a finite sum. We will abbreviate ${}_3F_2(a, b, c; d, e; 1)$ by ${}_3F_2(1)$ when we have no special need to discuss the other arguments. To establish Eq. (57) the Euler integral representation of ${}_3F_2$ (1) is employed. Resolution of the inner integral in this representation must be carefully performed; otherwise a sum of divergent integrals arises for the general case.

The generalized hypergeometric function ${}_3F_2(a, b, c; d, e; 1)$ converges for

$$
d + e - a - b - c > 0. \tag{58}
$$

The particular ${}_3F_2(1)$ studied in this work, is for the general case, neither Saalschützian, well-poised, nearly-poised, or balanced (see [75] p. 188 and [84] p. 70 for definitions). When those conditions do apply, simple expressions are obtained for the resulting values of ${}_3F_2(1)$.

From the work of Wimp [85] and Zeilberger [86] it is known that the general ${}_3F_2(a, b, c; d, e; z)$ cannot be expanded in a simple form in terms of gamma functions. In the case $\{a, b, c, d, e\} \in \mathbb{N}$, such an expansion is possible. The determination of the classes for which the generalized hypergeometric function can be written as a finite sum is an open problem [87].

Computer algebra schemes have become increasing useful for finding and manipulating various generalized hypergeometric functions [88–91]. Various special cases of the general results derived in this work for $\{a, b, c, d, e\} \in \mathbb{N}$ can be found in the latter two references as well as the book sources cited previously.

To establish equation Eq. (57) we will consider two main cases. The first one, which is more involved, arises when any of the values of a, b, and c are strictly smaller than both d and e. For this case, the Euler integral representation of ${}_3F_2(a, b, c; d, e; 1)$ will be employed. The second case occurs when one or two of a, b, and c are greater than or equal to one of d or e, which, without loss of generality, can be assumed to be $b \geq d$, is solved directly utilizing a result from Rösler [92].

The Euler integral representation of ${}_3F_2(a, b, c; d, e; 1)$ takes the following form [84]

$$
{}_3F_2(a,b,c;d,e;1) = \frac{\Gamma(d)\Gamma(e)}{\Gamma(b)\Gamma(c)\Gamma(d-b)\Gamma(e-c)} \times \int_0^1 t^{c-1}(1-t)^{e-c-1} I(a,b,d,t)dt, \tag{59}
$$

where

$$
I(a,b,d,t) = \int_0^1 \frac{s^{b-1}(1-s)^{d-b-1}}{(1-ts)^a} ds = \frac{\Gamma(b)\Gamma(d-b)}{\Gamma(d)} {}_2F_1(a,b;d;t). \tag{60}
$$

The strategy employed in this work is to reduce the $I(a,b,d,t)$ integral in Eq. (60) to a form such that the remaining integral is a beta function. The most straightforward and obvious way to deal with the $I(a,b,d,t)$ integral is to employ a binomial expansion for the numerator term followed by the change of variable $x = 1 - ts$, leaving a trivial integral to evaluate. Unfortunately, this approach fails for the general case, since it leads to a sum of several divergent integrals of the form of a beta function. It is therefore necessary to evaluate the $I(a,b,d,t)$ integral in a less than straightforward manner to resolve this divergence issue.

For the case that $e - c \geq 1$ and $d - b \geq 1$ with Eq. (58) also satisfied, the integral over s in the preceding result can be simplified as follows:

$$
I(a,b,d,t) = \sum_{k=0}^{d-b-1} \binom{d-b-1}{k} (-1)^k J(b-1+k, a-1, t), \tag{61}
$$

where we define

$$
J(m,j,t) = \int_0^1 \frac{s^m}{(1-ts)^{j+1}} ds = \frac{1}{t^{m+1}} B_t(m+1,-j), \tag{62}
$$

with $m, j \in \mathbb{Z}^+$ and where $B_z(a,b)$ denotes the incomplete beta function given by

$$
B_z(a,b) = \int_0^z t^{a-1}(1-t)^{b-1}dt, \text{ for } \operatorname{Re}(a) > 0 \text{ and } 0 < z < 1. \tag{63}
$$

For the case $m \geq j \geq 0$, a straightforward calculation leads to the recursion formula:

$$
J(m,j,t) = \frac{1}{jt(1-t)^j} - \frac{m}{jt} J(m-1, j-1, t), \tag{64}
$$

from which it follows by repeated application of the recursion formula, that

$$
J(m,j,t) = \frac{m!}{j!} \sum_{w=0}^{j-1} \frac{(-1)^w (j-1-w)!}{(m-w)! t^{w+1} (1-t)^{j-w}} + \frac{(-1)^j}{t^j} \binom{m}{j} J(m-j,0,t). \tag{65}
$$

Employing the result

$$J(m-j,0,t)=\sum_{w=0}^{\infty}\frac{t^w}{w+m-j+1}, \tag{66}$$

allows Eq. (65) to be rewritten as

$$\begin{aligned}J(m,j,t)&=(-1)^j\binom{m}{j}\sum_{w=0}^{\infty}\frac{t^w}{w+m+1}+(-1)^j\binom{m}{j}\sum_{w=0}^{j-1}\frac{t^{w-j}}{w+m-j+1}\\&\quad+\frac{m!}{j!}\sum_{w=0}^{j-1}\frac{(-1)^w(j-1-w)!}{(m-w)!t^{w+1}(1-t)^{j-w}}\\&=(-1)^j\binom{m}{j}\sum_{w=0}^{\infty}\frac{t^w}{w+m+1}\\&\quad+\frac{(-1)^j}{t^{j+1}(1-t)^j}\binom{m}{j}\sum_{w=1}^{j}\frac{t^w(1-t)^j}{w+m-j}\left[1+\frac{(m-j)!(w-1)!}{(t-1)^w(w+m-j-1)!}\right].\end{aligned} \tag{67}$$

Expanding the powers of $(1-t)$ in the numerator of the summand of the preceding equation and carrying out a summation rearrangement, leads to

$$\begin{aligned}&\sum_{w=1}^{j}\frac{t^w(1-t)^j}{(w+m-j)}\left[1+\frac{(m-j)!(w-1)!}{(t-1)^w(w+m-j-1)!}\right]=\sum_{p=1}^{j}(-t)^p\sum_{q=1}^{p}\frac{(-1)^q}{q+m-j}\binom{j}{p-q}\\&+\sum_{p=1}^{j}(-t)^p\sum_{q=1}^{p}\frac{(m-j)!(q-1)!}{(q+m-j)!}\binom{j-q}{p-q}\\&+(-t)^j\sum_{p=1}^{j}(-t)^p\sum_{q=p}^{j}\frac{(-1)^q}{q+m-j}\binom{j}{j+p-q}.\end{aligned} \tag{68}$$

To simplify Eq. (68) we make use of the result

$$\sum_{q=1}^{p}\left\{\frac{(-1)^q}{q+m-j}\binom{j}{p-q}+\frac{(m-j)!(q-1)!}{(q+m-j)!}\binom{j-q}{p-q}\right\}=0, \tag{69}$$

which can be proved in the following manner. For any $n\geq 0$ and $j\geq p\geq 1$ we show that

$$\sum_{q=1}^{p}\frac{n!(q-1)!}{(q+n)!}\binom{j-q}{p-q}=-\sum_{q=1}^{p}\frac{(-1)^q}{q+n}\binom{j}{p-q}. \tag{70}$$

Employing the partial fraction decomposition of $n!/(q+n)!$,

$$\frac{n!}{(q+n)!} = \sum_{k=1}^{q} \frac{(-1)^{k+1}}{(k-1)!(q-k)!} \frac{1}{k+n}, \tag{71}$$

then the left-hand side of Eq. (70), can be written as

$$\begin{aligned}
\sum_{q=1}^{p} \frac{n!(q-1)!}{(q+n)!} \binom{j-q}{p-q} &= -\sum_{q=1}^{p} \sum_{k=1}^{q} \frac{(-1)^k}{k+n} \frac{(q-1)!}{(k-1)!(q-k)!} \binom{j-q}{p-q} \\
&= -\sum_{k=1}^{p} \frac{(-1)^k}{k+n} \sum_{q=k}^{p} \binom{q-1}{k-1} \binom{j-q}{p-q} \\
&= -\sum_{q=1}^{p} \frac{(-1)^q}{q+n} \sum_{l=0}^{p-q} \binom{q+l-1}{l} \binom{j-q-l}{p-q-l},
\end{aligned} \tag{72}$$

where a summation rearrangement has been made. Employing the representation of the binomial coefficient:

$$\binom{n}{l} = (-1)^l \binom{l-n-1}{l}, \tag{73}$$

allows Eq. (72) to be recast as

$$\sum_{q=1}^{p} \frac{n!(q-1)!}{(q+n)!} \binom{j-q}{p-q} = (-1)^{p+1} \sum_{q=1}^{p} \frac{1}{q+n} \sum_{l=0}^{p-q} \binom{-q}{l} \binom{p-j-1}{p-q-l}. \tag{74}$$

Employing the Chu–Vandermonde identity [84]:

$$\sum_{l=0}^{m} \binom{a}{l} \binom{b}{m-l} = \binom{a+b}{m}, \tag{75}$$

then Eq. (74) simplifies to

$$\begin{aligned}
\sum_{q=1}^{p} \frac{n!(q-1)!}{(q+n)!} \binom{j-q}{p-q} &= -(-1)^p \sum_{q=1}^{p} \frac{1}{q+n} \binom{p-j-q-1}{p-q} \\
&= -\sum_{q=1}^{p} \frac{(-1)^q}{q+n} \binom{j}{p-q},
\end{aligned} \tag{76}$$

where Eq. (73) has been employed in the final step. This completes the proof of Eq. (69).

Using Eq. (69) allows Eq. (68) to be simplified, so that Eq. (67) reduces to

$$J(m,j,t) = (-1)^j \binom{m}{j} \sum_{w=0}^{\infty} \frac{t^w}{w+m+1} + \frac{1}{(1-t)^j} \binom{m}{j} \sum_{p=0}^{j-1} t^p \sum_{q=0}^{j-p-1} \frac{(-1)^q}{p+q+m+1-j} \binom{j}{q}. \quad (77)$$

In Eq. (77) the infinite sum can be expressed in the form:

$$\sum_{w=0}^{\infty} \frac{t^w}{w+m+1} = -t^{-m-1} \left\{ \ln(1-t) + \sum_{w=1}^{m} \frac{t^w}{w} \right\}, \text{ for } -1 \le t < 1, \quad (78)$$

but it will prove to more convenient for the evaluation of ${}_3F_2(1)$ to retain the form given in Eq. (77). Equation (78) will be useful for the derivation of some special cases.

For completeness we give the result for the case $j \ge m+1$ and $m \ge 0$. Employing the change of variable $w = (1-s)(1-ts)^{-1}$ followed by a binomial expansion, leads to

$$\begin{aligned} J(m,j,t) &= \frac{1}{(1-t)^j} \int_0^1 (1-w)^m (1-tw)^{j-m-1} dw \\ &= \frac{1}{(1-t)^j} \sum_{n=0}^{j-m-1} (-t)^n \binom{j-m-1}{n} \int_0^1 w^n (1-w)^m dw \\ &= \frac{1}{(1-t)^j} \sum_{n=0}^{j-m-1} (-t)^n \binom{j-m-1}{n} B(n+1, m+1), \end{aligned} \quad (79)$$

and hence

$$J(m,j,t) = \frac{(j-m-1)!m!}{j!(1-t)^j} \sum_{p=0}^{j-m-1} (-t)^p \binom{j}{p+m+1}. \quad (80)$$

8 The hypergeometric function for non-negative integer parameters

The results just developed can be used to obtain a simple finite summation formula for ${}_2F_1(a,b;c;t)$. From Eq. (60) for $\{a,b,c\} \in \mathbb{N}$, $c \ge b+1$, $-1 \le t < 1$, and without loss of generality we can take $1 \le a \le b$, so that

$$\begin{aligned} {}_2F_1(a,b;c;t) &= \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^1 s^{b-1}(1-s)^{c-b-1}(1-ts)^{-a} ds \\ &= \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \sum_{k=0}^{c-b-1} \binom{c-b-1}{k} (-1)^k J(b-1+k, a-1, t) \end{aligned}$$

$$
\begin{aligned}
&= \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \sum_{k=0}^{c-b-1} \binom{c-b-1}{k} (-1)^k t^{-b-k} B_t(b+k, 1-a) \\
&= \frac{\Gamma(c)}{\Gamma(b)} \sum_{k=0}^{c-b-1} \frac{(-1)^k}{\Gamma(c-b-k)\Gamma(k+1)} \\
&\quad \times \left[(-1)^a \binom{b+k-1}{a-1} t^{-b-k} \left\{ \ln(1-t) + \sum_{w=1}^{b+k-1} \frac{t^w}{w} \right\} \right. \\
&\quad \left. - \frac{1}{(1-t)^{a-1}} \binom{b+k-1}{a-1} \sum_{p=0}^{a-2} (-t)^p \sum_{q=p+1}^{a-1} \frac{(-1)^q}{q+b+k-a} \binom{a-1}{a+p-q} \right].
\end{aligned} \tag{81}
$$

For the particular case $\{a, b, c\} \in \mathbb{N}$, $c \geq a+1$, $c \geq b+1$, and $-1 \leq t < 1$, a slightly more compact result can be written in the following manner. With an appropriate change of integration variable we can write the $I(a, b, d, t)$ integral in Eq. (60) in the form

$$
\begin{aligned}
I(a, b, d, t) &= \frac{1}{(a-1)!} \int_0^\infty \int_0^\infty \frac{x^{b-1} y^{d-b-1} e^{-(1-t)x-y}}{(x+y)^{d-a}} dx dy \\
&= \frac{(1-t)^{d-a-b}}{(a-1)!} \int_0^\infty \int_0^\infty \frac{w^{b-1} y^{d-b-1} e^{-w-y}}{[w+(1-t)y]^{d-a}} dw dy.
\end{aligned} \tag{82}
$$

Repeated integration by parts with respect to the variable w leads to the result

$$
\begin{aligned}
I(a, b, d, t) &= \frac{(1-t)^{d-a-b}(-1)^{d-a-1}}{(a-1)!} \sum_{p=0}^{d-a-1} \frac{(-1)^p}{(d-a-1-p)!} \binom{b-1}{p} \\
&\quad \times \int_0^\infty \int_0^\infty \frac{w^{b-1-p} y^{d-b-1} e^{-w-y}}{[w+(1-t)y]} dw dy.
\end{aligned} \tag{83}
$$

With the change of integration variables $y = uv$ and $w = u(1-v)$ leads to

$$
\begin{aligned}
I(a, b, d, t) &= \frac{(1-t)^{d-a-b}(-1)^{d-a-1}}{(a-1)!} \sum_{p=0}^{d-a-1} \frac{(-1)^p (d-p-2)!}{(d-a-1-p)!} \binom{b-1}{p} \\
&\quad \times \int_0^1 \frac{v^{d-b-1}(1-v)^{b-p-1}}{1-tv} dv.
\end{aligned} \tag{84}
$$

Employing the preceding result with the variable switch $d \to c$ and using Eqs. (66) and (78), we have for $\{a, b, c\} \in \mathbb{N}$, $c \geq a+1$, $c \geq b+1$, and $a+b \geq c$, that

$$
{}_2F_1(a,b;c;t) = \frac{(-1)^{c-a}(1-t)^{c-a-b}\Gamma(c)}{\Gamma(a)\Gamma(b)\Gamma(c-b)t^{c-b}} \sum_{p=0}^{c-a-1} \frac{(-1)^p\Gamma(c-p-1)}{\Gamma(c-a-p)} \binom{b-1}{p}
\times \left\{ (1-\frac{1}{t})^{b-p-1}\ln(1-t) + \sum_{k=0}^{b-p-1} \binom{b-p-1}{k} (-t)^{-k} \sum_{w=1}^{k+c-b-1} \frac{t^w}{w} \right\}. \tag{85}
$$

For the particular case $a \geq d$ in Eq. (82), it follows directly (using the switch $d \to c$) for $c \geq b+1$ and $\{a, b, c\} \in \mathbb{N}$, that

$$
{}_2F_1(a,b;c;t) = \frac{(1-t)^{-b}\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \sum_{p=0}^{a-c} B(b+p, a-b-p) \binom{a-c}{p} (1-t)^{-p}. \tag{86}
$$

9 The function ${}_3F_2(a, b, c; d, e; 1)$ for $e - a - c \geq 0$ and $d - b \geq 1$

Because of the invariance of ${}_3F_2(a, b, c; d, e; 1)$ with respect to the interchange $a \leftrightarrow b \leftrightarrow c$, we can without loss of generality assume that $a \leq b$. Making use of the result for $J(m, j, t)$ given in Eq. (77), then Eq. (59) simplifies to

$$
{}_3F_2(a,b,c;d,e;1) = \frac{\Gamma(d)\Gamma(e)}{\Gamma(b)\Gamma(c)\Gamma(d-b)\Gamma(e-c)} \sum_{k=0}^{d-b-1} \binom{d-b-1}{k} \binom{b+k-1}{a-1} (-1)^{k+1}
\times \left\{ \sum_{p=0}^{a-2} (-1)^p \chi_{pk}(a,b) \int_0^1 t^{c+p-1}(1-t)^{e-a-c} dt
+ (-1)^a \sum_{p=0}^{\infty} \frac{(-1)^p}{p+k+b} \int_0^1 t^{c+p-1}(1-t)^{e-c-1} dt \right\}, \tag{87}
$$

where

$$
\chi_{pk}(a,b) = \sum_{q=p+1}^{a-1} \frac{(-1)^q}{q+k+b-a} \binom{a-1}{a+p-q}. \tag{88}
$$

Insertion of the beta functions into Eq. (87) leads to

$$
{}_3F_2(a,b,c;d,e;1) = \frac{\Gamma(d)\Gamma(e)}{\Gamma(b)\Gamma(c)\Gamma(d-b)\Gamma(e-c)} \sum_{k=0}^{d-b-1} \binom{d-b-1}{k} \binom{b+k-1}{a-1} (-1)^{k+1}
\times \left\{ \sum_{p=0}^{a-2} (-1)^p \chi_{pk}(a,b) B(c+p, e+1-a-c)
+ (-1)^a \sum_{j=0}^{e-c-1} \binom{e-c-1}{j} (-1)^j \sum_{p=0}^{\infty} \frac{1}{(p+k+b)(p+j+c)} \right\}, \tag{89}
$$

and hence, for $a \geq 1$, $b \geq 1$, $c \geq 1$, $d \geq 1$, $e \geq 1$, $d-b \geq 1$, $e-c \geq 1$, $a \leq b$, $e-a-c \geq 0$, and if $a \geq 2$, we have

$$
\begin{aligned}
{}_3F_2(a,b,c;d,e;1) = {} & \frac{\Gamma(d)\Gamma(e)}{\Gamma(b)\Gamma(c)\Gamma(d-b)\Gamma(e-c)} \sum_{k=0}^{d-b-1} \binom{d-b-1}{k} \binom{b+k-1}{a-1} (-1)^{k+1} \\
& \times \Bigg[\Gamma(e+1-a-c) \sum_{p=0}^{a-2} (-1)^p \chi_{pk}(a,b) \frac{\Gamma(c+p)}{\Gamma(e+1+p-a)} \\
& + (-1)^a \sum_{j=0}^{e-c-1} \binom{e-c-1}{j} (-1)^j \Lambda(k+b, j+c) \Bigg],
\end{aligned}
\tag{90}
$$

where

$$
\Lambda(u,v) = \begin{cases} \varsigma(2,u), & \text{for } u = v \\ \frac{\psi(u)-\psi(v)}{u-v} = \frac{1}{|u-v|} \sum_{l=\min\{u,v\}}^{\max\{u,v\}-1} \frac{1}{l}, & \text{for } u \neq v \end{cases},
\tag{91}
$$

and $\psi(k)$ denotes the digamma function and $\varsigma(2,k)$ designates the Hurwitz zeta function. An empty sum, that is $\sum_{q=n}^{m}$ for $n > m$, is assigned the value zero. The Hurwitz zeta function can be written as

$$
\varsigma(2,k) = \frac{\pi^2}{6} - \sum_{p=1}^{k-1} \frac{1}{p^2}.
\tag{92}
$$

Inserting Eqs. (91) and (92) into Eq. (90) leads to the key result, Eq. (57), where

$$
\begin{aligned}
c_1(a,b,c,d,e) = {} & \frac{\Gamma(d)\Gamma(e)}{\Gamma(b)\Gamma(c)\Gamma(d-b)\Gamma(e-c)} \sum_{k=0}^{d-b-1} \binom{d-b-1}{k} \binom{b+k-1}{a-1} (-1)^{k+1} \\
& \times \Bigg[\Gamma(e+1-a-c) \sum_{p=0}^{a-2} (-1)^p \chi_{pk}(a,b) \frac{\Gamma(c+p)}{\Gamma(e+1+p-a)} \\
& + (-1)^a \sum_{j=0}^{e-c-1} \binom{e-c-1}{j} (-1)^j \\
& \times \begin{cases} -\sum_{p=1}^{j+c-1} \frac{1}{p^2} & \text{for } j = k+b-c \\ \frac{1}{|k+b-j-c|} \sum_{l=\min\{k+b,j+c\}}^{\max\{k+b,j+c\}-1} \frac{1}{l} & \text{for } j \neq k+b-c \end{cases} \Bigg]
\end{aligned}
\tag{93}
$$

and

$$c_2(a,b,c,d,e) = \frac{(-1)^{a+b+c+1}}{6} \frac{\Gamma(d)\Gamma(e)}{\Gamma(b)\Gamma(c)\Gamma(d-b)\Gamma(e-c)} \times \sum_{k=0}^{d-b-1} \binom{d-b-1}{k} \binom{b+k-1}{a-1} \sum_{j=0}^{e-c-1} \binom{e-c-1}{j} \delta_{j(k+b-c)}. \tag{94}$$

10 ${}_3F_2(a, b, c; d, e; 1)$ for the case $d \leq a + b$

To handle the situation where $d \leq a+b$ we proceed in the following manner. Substituting Eq. (84) into Eq. (59) leads to

$$\begin{aligned} {}_3F_2(a,b,c;d,e;1) = {} & \frac{(-1)^{d-a-1}\Gamma(d)\Gamma(e)}{\Gamma(a)\Gamma(b)\Gamma(c)\Gamma(d-b)\Gamma(e-c)} \sum_{p=0}^{d-a-1} \frac{(-1)^p (d-p-2)!}{(d-a-1-p)!} \binom{b-1}{p} \\ & \times \sum_{k=0}^{b-p-1} \binom{b-p-1}{k} (-1)^k \int_0^1 t^{c-1}(1-t)^{e+d-a-b-c-1} \\ & \times J(d+k-p-1, 0, t)dt. \end{aligned} \tag{95}$$

Employing Eq. (66) leads to

$$\begin{aligned} {}_3F_2(a,b,c;d,e;1) = {} & \frac{(-1)^{d-a-1}\Gamma(d)\Gamma(e)}{\Gamma(a)\Gamma(b)\Gamma(c)\Gamma(d-b)\Gamma(e-c)} \sum_{p=0}^{d-a-1} \frac{(-1)^p (d-p-2)!}{(d-a-1-p)!} \binom{b-1}{p} \\ & \times \sum_{k=0}^{b-p-1} \binom{b-p-1}{k} (-1)^k \sum_{w=0}^{\infty} \frac{1}{w+d+k-p} \\ & \times \int_0^1 t^{c+w-1}(1-t)^{e+d-a-b-c-1} dt \\ = {} & \frac{(-1)^{d-a-1}\Gamma(d)\Gamma(e)}{\Gamma(a)\Gamma(b)\Gamma(c)\Gamma(d-b)\Gamma(e-c)} \sum_{p=0}^{d-a-1} \frac{(-1)^p (d-p-2)!}{(d-a-1-p)!} \binom{b-1}{p} \\ & \times \sum_{k=0}^{b-p-1} \binom{b-p-1}{k} (-1)^k \sum_{j=0}^{e+d-a-b-c-1} \binom{e+d-a-b-c-1}{j} (-1)^j \\ & \times \sum_{w=0}^{\infty} \frac{1}{(w+d+k-p)(w+j+c)}, \end{aligned} \tag{96}$$

and hence, for $a \geq 1, b \geq 1, c \geq 1, d \geq 2, e \geq 1, d-b \geq 1, e-c \geq 1, d-a-1 \geq 0$, $b+a \geq d$, and $d+e-a-b-c \geq 1$, we have

$$
\begin{aligned}
{}_3F_2(a,b,c;d,e;1) = {} & \frac{(-1)^{d-a-1}\Gamma(d)\Gamma(e)}{\Gamma(a)\Gamma(b)\Gamma(c)\Gamma(d-b)\Gamma(e-c)} \sum_{p=0}^{d-a-1} \frac{(-1)^p (d-p-2)!}{(d-a-1-p)!} \binom{b-1}{p} \\
& \times \sum_{k=0}^{b-p-1} \binom{b-p-1}{k} (-1)^k \sum_{j=0}^{e+d-a-b-c-1} \\
& \times \binom{e+d-a-b-c-1}{j} (-1)^j \Lambda(k+d-p, j+c). \qquad (97)
\end{aligned}
$$

Equation (97) can be expressed in the form of Eq. (57) in the same manner indicated to obtain Eqs. (93) and (94).

11 ${}_3F_2(a, b, c; d, e; 1)$ for the case $d - b \leq 0$

To complete the proof of Eq. (57), it is necessary to consider the case where $d-b \leq 0$. For this case we avoid the Euler integral relationship and employ a result given by Rösler [92]:

$$
{}_3F_2(a, b+m, c; b, e; 1) = \frac{\Gamma(e)}{\Gamma(e-a)\Gamma(e-c)} \sum_{j=0}^{m} \binom{m}{j} \frac{(a)_j (c)_j}{(b)_j} \Gamma(e-a-c-j), \qquad (98)
$$

where $m \in \mathbb{Z}^+$. Equation (98) requires $e \geq 1$, $e-a \geq 1$, $e-c \geq 1$, $e-a-c \geq 1$, and $d-b \leq 0$. There are a number of extensions of this result to general ${}_pF_q$ and to general arguments [93–98]. In this form the right-hand side of the equation can be identified with $c_1(a, b+m, c, b, e)$ and the c_2 term is zero.

To ascertain which of Eqs. (90), (97), or (98) should be employed, taking explicit account of the symmetry of ${}_3F_2(a, b, c; d, e; 1)$ with respect to interchanges of a, b, and c or between d and e, proceed as follows. Determine first if either d or e is $\leq$ any of a, b, and c, then assign b to any of $\{a, b, c\}$ and d to whichever of $\{d, e\}$ satisfies the preceding condition. Thus if the condition is met we have $d - b \leq 0$ and Eq. (98) can be employed. If both d and e are $> \max\{a, b, c\}$ then $d - b \geq 1$, and if $e - a - c \geq 0$ apply Eq. (90), and if $e - a - c < 0$ then with the switch $d \leftrightarrow e$ and $c \leftrightarrow b$ leads to $d < a + b$ and so apply Eq. (97).

12 Some special cases for ${}_3F_2$ (1)

In this section we consider some special cases of ${}_3F_2(1)$ that can be written in a reasonably compact form. Several of these cases are particularly useful for the rapid evaluation of ${}_3F_2(1)$ for the evaluation of the $m = 0$ case of the K_3 auxiliary function. A particularly simple case of Eq. (90) occurs for $a = 1$, $b = 1$, $d = 2$, $e = c + 1$, so that for $c \in \mathbb{N}$:

$$
{}_3F_2(1,1,c;2,c+1;1)=\begin{cases}\frac{\pi^2}{6}, & \text{for } c=1\\ \frac{c}{c-1}\sum_{w=1}^{c-1}\frac{1}{w}, & \text{for } c\geq 2\end{cases}. \tag{99}
$$

The case $a=1$, $d=b+1$, $e=c+1$, where the latter two conditions fix the first condition (for the nonnegative integer case), also reduces to a compact sum, so for $b, c \in \mathbb{N}$:

$$
{}_3F_2(1,b,c;b+1,c+1;1)=\frac{bc}{c-b}\sum_{w=b}^{c-1}\frac{1}{w}, \text{ for } c>b. \tag{100}
$$

The special case of the preceding result for $b=c$ follows directly from Eq. (90) to yield for $b\in\mathbb{N}$:

$$
{}_3F_2(1,b,b;b+1,b+1;1)=b^2\left(\frac{\pi^2}{6}-\sum_{w=1}^{b-1}\frac{1}{w^2}\right)=b^2\varsigma(2,b). \tag{101}
$$

In a similar fashion, we obtain for $e-b\geq 1$, and $b, e\in\mathbb{N}$,

$$
{}_3F_2(1,b,b;b+1,e;1)=\frac{b\Gamma(e)}{\Gamma(b)\Gamma(e-b)}\left\{\varsigma(2,e-b)-\sum_{p=1}^{b-1}\frac{B(p,e-b)}{p}\right\}. \tag{102}
$$

For the case $c-b\geq 1$, $e-b\geq -1$, and $e-c\geq 1$,

$$
\begin{aligned}
&{}_3F_2(1,b,c;b+1,e;1)\\
&=\frac{b\Gamma(e)}{\Gamma(c)\Gamma(e-c)}\left\{B(c-b,e-c)\{\psi(e-b)-\psi(e-c)\}-\sum_{p=1}^{b-1}\frac{B(c-b+p,e-c)}{p}\right\}.
\end{aligned} \tag{103}
$$

For the case $b\geq 1$, $c\geq 1$, $d-b\geq -1$, and $e-c\geq 1$, we obtain

$$
\begin{aligned}
{}_3F_2(1,b,c;d,e;1)=&\frac{\Gamma(d)\Gamma(e)}{\Gamma(b)\Gamma(c)\Gamma(d-b)\Gamma(e-c)}\sum_{k=0}^{d-b-1}(-1)^k\binom{d-b-1}{k}\\
&\times\sum_{j=0}^{e-c-1}\binom{e-c-1}{j}(-1)^j\Lambda(k+b,j+c).
\end{aligned} \tag{104}
$$

The case $e-c\geq a$ and $a\geq b+1$ reduces to

$$
{}_3F_2(a,b,c;b+1,e;1)=\frac{b\Gamma(a-b)\Gamma(b)\Gamma(e)}{\Gamma(c)\Gamma(e-c)}\sum_{k=0}^{a-b-1}\frac{(-1)^k B(k+c,e-a-c+1)}{\Gamma(k+b+1)\Gamma(a-b-k)}. \tag{105}
$$

To obtain the special case ${}_3F_2(1, 1, 1; m+2, m+2; 1)$ for $m \in \mathbb{Z}^+$, it is advantageous to first carry out a pair of Thomae transformations. Let $s = d + e - a - b - c$, then the Thomae transformation takes the form [99]

$$ {}_3F_2(a, b, c; d, e; 1) = \frac{\Gamma(d)\Gamma(e)\Gamma(s)}{\Gamma(a)\Gamma(s+b)\Gamma(s+c)} {}_3F_2(d-a, e-a, s; s+b, s+c; 1). \tag{106} $$

Applying this transformation to ${}_3F_2(1, 1, 1; m+2, m+2; 1)$ yields

$$ \begin{aligned} {}_3F_2(1, 1, 1; m+2, m+2; 1) &= \left[\frac{\Gamma(m+2)}{\Gamma(2m+2)}\right]^2 \\ &\times \Gamma(2m+1) {}_3F_2(m+1, m+1, 2m+1; 2m+2, 2m+2; 1). \end{aligned} \tag{107} $$

Applying a second Thomae transformation to the preceding result yields

$$ {}_3F_2(1, 1, 1; m+2, m+2; 1) = \frac{(m+1)}{(2m+1)} {}_3F_2(1, m+1, m+1; m+2, 2m+2; 1), \tag{108} $$

which simplifies on using Eqs. (59), (60), and (62) to yield

$$ {}_3F_2(1, 1, 1; m+2, m+2; 1) = (m+1)^2 \binom{2m}{m} \int_0^1 t^m (1-t)^m J(m, 0, t) dt. \tag{109} $$

Utilizing Eqs. (77) and (78) leads to

$$ {}_3F_2(1, 1, 1; m+2, m+2; 1) = (m+1)^2 \binom{2m}{m} \left\{ \frac{\pi^2}{6} - \sum_{w=1}^{m} \frac{1 + wB(w, m+1)}{w^2} \right\}. \tag{110} $$

A similar approach can be taken to evaluate ${}_3F_2(1, 1, 1; m+2, n+2; 1)$ for $m, n \in \mathbb{Z}^+$, with the result that

$$ \begin{aligned} {}_3F_2(1, 1, 1; m+2, n+2; 1) &= (m+1)(n+1) \binom{m+n}{m} \\ &\times \left\{ \frac{\pi^2}{6} - \sum_{w=1}^{m} \frac{1}{w^2} - \sum_{w=1}^{n} \frac{B(w, m+1)}{w} \right\}. \end{aligned} \tag{111} $$

A slightly more tedious calculation by the same approach yields for $m \in \mathbb{Z}^+$,

$$ \begin{aligned} {}_3F_2(1, 1, 2; m+3, m+3; 1) &= \frac{(m+2)^2}{m+1} + (2m+1)(m+2)^2 \binom{2m}{m} \left\{ \frac{1}{(m+1)^2} \right. \\ &\left. + \sum_{w=1}^{m} \left\{ \frac{1}{w^2} + \frac{B(w, m+1)}{w} - \frac{B(w, m+2)}{m+1} \right\} - \frac{\pi^2}{6} \right\}. \end{aligned} \tag{112} $$

The case ${}_3F_2(n, n, n; n+1, 2n; 1)$ for $n \in \mathbb{N}$, can be evaluated in a straightforward fashion making use of the result

$$J(n, n, t) = (-t)^{-n-1} \left\{ \log(1-t) - \sum_{w=1}^{n} \frac{1}{w} \left(\frac{t}{t-1} \right)^{w} \right\}, \tag{113}$$

to yield

$${}_3F_2(n, n, n; n+1, 2n; 1) = (-1)^n \frac{n^2}{2} \binom{2n}{n} \left\{ -\frac{\pi^2}{6} + \sum_{w=1}^{n-1} \frac{1 - (-1)^w w B(w, n-w)}{w^2} \right\}. \tag{114}$$

For $m, n \in \mathbb{N}$ and $m \geq 2n$ we obtain

$$\begin{aligned} {}_3F_2(n, n, n; n+1, m; 1) = \frac{(-1)^n n\Gamma(m)}{\Gamma(m-n)\Gamma(n)} & \left\{ \sum_{w=1}^{m-n-1} \frac{1}{w^2} \right. \\ & \left. - \sum_{w=1}^{n-1} \frac{(-1)^w B(w, m-n-w)}{w} - \frac{\pi^2}{6} \right\}, \end{aligned} \tag{115}$$

and for $m, n, p \in \mathbb{N}$ with $p - n \geq 1$ and $m - n - p \geq 0$ yields

$$\begin{aligned} {}_3F_2(n, n, p; n+1, m; 1) = \frac{(-1)^{n+1} n\Gamma(m)}{\Gamma(m-p)\Gamma(p)} & \left\{ \sum_{w=1}^{n-1} \frac{(-1)^w B(w+p-n, m-p-w)}{w} \right. \\ & \left. + \frac{\Gamma(m-p)\Gamma(p-n)}{\Gamma(m-n)} \sum_{w=0}^{p-n-1} \frac{1}{w+m-p} \right\}. \end{aligned} \tag{116}$$

13 Recursive reduction of ${}_3F_2$ (1)

In some cases it may be possible to improve the speed of computation for Eq. (90) by selectively decreasing some of the parameter values. This can be done in a recursive fashion. From the standard recursion formula for contiguous generalized hypergeometric functions [84]

$$\begin{aligned} {}_3F_2(a, b+1, c; d, e+1; 1) = {}& {}_3F_2(a, b, c; d, e; 1) \\ & + \frac{ac(e-b)}{de(e+1)} {}_3F_2(a+1, b+1, c+1; d+1, e+2; 1), \end{aligned} \tag{117}$$

we can write for $n \in \mathbb{Z}^+$

$$\begin{aligned} & {}_3F_2(a+n, b+n, c+n; d+n, e+2n; 1) \\ & = \frac{(d)_n}{(a)_n (b)_n (e-c)_n} \sum_{p=1}^{n+1} \alpha(n+1, p) {}_3F_2(a, b, c+p-1; d, e+p-1; 1), \end{aligned} \tag{118}$$

where the α coefficient satisfies

$$\alpha(q,1) = (-1)^{q+1}(e+2n-2q+2)_{2(q-1)}, \tag{119}$$
$$\alpha(q,q) = (e+2n-q)_{q-1}(e+2n-q+1)_{q-1}, \tag{120}$$

and

$$\alpha(q,p) = \beta(q-1,p-1)\alpha(q-1,p-1) - \beta(q-1,p)\alpha(q-1,p), \tag{121}$$

with

$$\beta(q-1,p-1) = (e+2n-2q+p-1)(e+2n-2q+p). \tag{122}$$

The maximum reduction results when n is selected as

$$n = \min\{a-1, b-1, c-1, d-1, \lfloor (e-1)/2 \rfloor\}, \tag{123}$$

where $\lfloor x \rfloor$ denotes the floor function; the largest integer $\leq x$.

14 Some special cases for the $m = 0$ K_3 auxiliary function

If $l = j+k+2$, then from Eq. (52)

$$\begin{aligned} K_3(i,j,k,j+k+2,0,n) &= j!k!\tau!\frac{\Gamma(i-k)}{\Gamma(i+j+2)}\sum_{\mu=0}^{\infty}\frac{(n)_\mu}{\mu!}\frac{(i-k)_\mu}{(i+j+2)_\mu} \\ &= \frac{(i-n)!j!k!(i-k-1)!}{(i+j+1)!}{}_2F_1(n,i-k;i+j+2;1). \end{aligned} \tag{124}$$

By the Gauss summation formula [84]

$${}_2F_1(a,b;c;1) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}. \tag{125}$$

Applying this result to Eq. (124) leads to

$$\begin{aligned} K_3(i,j,k,j+k+2,0,n) &= \frac{(i-n)!j!k!(i-k-1)!}{(i+j+1)!}\frac{\Gamma(i+j+2)\Gamma(j+k+2-n)}{\Gamma(i+j+2-n)\Gamma(j+k+2)} \\ &= \frac{(i-n)!j!k!(i-k-1)!(l-n-1)!}{(i+j+1-n)!(l-1)!}, \end{aligned} \tag{126}$$

which is valid for $i \geq n$, $i \geq k+1$, $l \geq n+1$, and $i+j+1-n \geq 0$. Similarly, it can be shown that when $n = i+j+2$,

$$K_3(i,j,k,l,0,i+j+2) = \frac{i!j!(k-l)!(k-i-1)!(n-l-1)!}{(k+j+1-l)!(n-1)!}, \tag{127}$$

which is valid for $k \geq l$, $k \geq i+1$, $n \geq l+1$, and $k+j+1-l \geq 0$. Some further discussion of $K_3\,(i, j, k, l, 0, n)$ is relegated to part II of this work.

15 The general case $l, m,$ and $n > 0$ for K_3

We now turn our attention to the more general form of the K_3 auxiliary function. With the change of variables $y = uv$ and $x = u - uv$ we have

$$\begin{aligned} K_3(i, j, k, l, m, n) &= \int_0^\infty \int_0^\infty \int_0^\infty \frac{x^i y^j z^k e^{-x-y-z}}{(x+y)^l (x+z)^m (y+z)^n} dx dy dz \\ &= \int_0^1 v^j (1-v)^i dv \int_0^\infty \int_0^\infty \frac{u^{i+j-l+1} z^k e^{-u-z}}{(u-uv+z)^m (uv+z)^n} du dz. \end{aligned} \tag{128}$$

Let $\sigma = i+j+k+2-l-m-n$ and with the additional change of variables $z = uw$, then

$$\begin{aligned} K_3(i, j, k, l, m, n) &= \int_0^1 v^j (1-v)^i dv \int_0^\infty \frac{w^k}{(1-v+w)^m (v+w)^n} dw \\ &\quad \times \int_0^\infty u^{i+j+k+2-l-m-n} e^{-u(1+w)} du \\ &= \sigma! \int_0^1 v^j (1-v)^i dv \int_0^\infty \frac{w^k}{(1-v+w)^m (v+w)^n (1+w)^{\sigma+1}} dw. \end{aligned} \tag{129}$$

Let $w = u - 1$ and set $u = \frac{1}{x}$, then

$$\begin{aligned} K_3(i, j, k, l, m, n) &= \sigma! \int_0^1 v^j (1-v)^i dv \int_1^\infty \frac{(u-1)^k}{(u-v)^m (v+u-1)^n u^{\sigma+1}} du \\ &= \sigma! \int_0^1 v^j (1-v)^i dv \int_0^1 \frac{x^{\sigma+m+n-k-1}(1-x)^k}{(1-xv)^m (1-x(1-v))^n} dx. \end{aligned} \tag{130}$$

Employing the expansions

$$\frac{1}{(1-xv)^m} = \sum_{\mu_1=0}^\infty \frac{(m)_{\mu_1}}{\mu_1!} x^{\mu_1} v^{\mu_1}, \tag{131}$$

and

$$\frac{1}{(1-x(1-v))^n} = \sum_{\mu_2=0}^\infty \frac{(n)_{\mu_2}}{\mu_2!} x^{\mu_2} (1-v)^{\mu_2}, \tag{132}$$

leads to

$$K_3(i, j, k, l, m, n) = \sigma! \sum_{\mu_1=0}^{\infty} \sum_{\mu_2=0}^{\infty} \frac{(m)_{\mu_1}}{\mu_1!} \frac{(n)_{\mu_2}}{\mu_2!} \times \int_0^1 v^{j+\mu_1}(1-v)^{i+\mu_2} dv \int_0^1 x^{\sigma+m+n-k-1+\mu_1+\mu_2}(1-x)^k dx. \tag{133}$$

For the case that $\sigma + m + n - k - 1 \geq 0$

$$K_3(i, j, k, l, m, n) = \sigma! \sum_{\mu_1=0}^{\infty} \sum_{\mu_2=0}^{\infty} \frac{(m)_{\mu_1}}{\mu_1!} \frac{(n)_{\mu_2}}{\mu_2!} B(j + 1 + \mu_1, i + 1 + \mu_2) \times B(\sigma + m + n - k + \mu_1 + \mu_2, k + 1). \tag{134}$$

A discussion of how to turn this expression into a form suitable for a numerically stable application of convergence accelerators is discussed in part II of this work. From this result we can deduce the following constraints:

$$i + j + 1 - l \geq 0, \tag{135}$$

$$i + k + 1 - m \geq 0, \tag{136}$$

$$j + k + 1 - n \geq 0, \tag{137}$$

and

$$i + j + k + 2 - l - m - n \geq 0. \tag{138}$$

Further discussion on the constraints that are required for convergent K_3 and J_3 integrals is given in part II, as well as a discussion on connecting the general K_3 integrals to the $m = 0$ case of this integral by recursion.

16 Formula for $K_3(i, j, k, l, 1, 1)$ in terms of ${}_3F_2$ (1)

In this section we develop a general formula for the special case $K_3\,(i, j, k, l, 1, 1)$ which is useful both as a means for the rapid evaluation of this case when it arises, and also in checking formulas evaluated numerically. Start from Eq. (130), setting $m = n = 1$ and carrying out a partial fraction separation of the denominator terms, leads to

$$K_3(i, j, k, l, m, n) = \sigma!\{f(i, j, k, l) + f(j, i, k, l)\}, \tag{139}$$

where

$$f(i, j, k, l) = \int_0^1 \frac{(1-x)^k x^{i+j+1-l}}{(2-x)} dx \int_0^1 \frac{(1-v)^i v^j}{(1-xv)} dv. \tag{140}$$

By making the appropriate binomial expansion and taking advantage of Eqs. (59) and (60), it follows that

$$
\begin{aligned}
f(i,j,k,l) = 2^{i+j-l} \Bigg\{ & 2(-1)^k g(i,j) \\
& + \frac{i!j!}{(i+j+1)!} \Bigg[-k! \sum_{p=0}^{i+j-l} \frac{p!}{2^p(k+1+p)!} {}_3F_2(1, j+1, p+1; i+j \\
& +2, k+2+p; 1) \\
& + (-1)^k \sum_{p=1}^{k} \binom{k}{p} (-2)^p \sum_{q=0}^{p-1} \binom{p-1}{q} \frac{1}{(-2)^q(1+q)} {}_3F_2(1, j \\
& +1, q+1; i+j+2, q+2; 1) \Bigg] \Bigg\},
\end{aligned} \tag{141}
$$

with

$$
g(i,j) = \int_0^1 (1-v)^i v^j dv \int_0^{1/2} \frac{1}{(1-w)(1-2vw)} dw. \tag{142}
$$

The function $g(i,j)$ can be evaluated as

$$
g(i,i) = \frac{1}{2^{2i+1}} \left\{ \frac{\pi^2}{4} - \sum_{t=0}^{i-1} \frac{(2t)!!}{(t+1)(2t+1)!!} \right\}, \tag{143}
$$

and without loss of generality, because of the permutation symmetry between i and j, take $j \ge i$ and set $\eta = j - i$, then

$$
\begin{aligned}
g(i,j) + g(j,i) = \frac{1}{2^{i+j+1}} \Bigg\{ & \frac{\pi^2}{2} - 2 \sum_{p=0}^{i-1} \frac{2^p p!}{(p+1)(2p+1)!!} \\
& + 2^i i! \sum_{q=1}^{\lfloor \eta/2 \rfloor} \binom{\eta}{2q} \frac{(q-1)!}{(2i+2q-1)!!} \left[\frac{2^q}{(i+q)} + \sum_{p=1}^{q-1} \frac{2^p(2q-2p-1)!!}{(i+p)(q-p)!} \right] \Bigg\},
\end{aligned} \tag{144}
$$

where the $\lfloor\rfloor$ brackets on the summation limit denote the floor function. From Eqs. (139 to 144) we obtain the sample values:

$$
K_3(1,1,1,1,1,1) = 5 - \frac{\pi^2}{2}, \tag{145}
$$

$$
K_3(2,2,2,2,1,1) = \frac{385}{3} - 13\pi^2, \tag{146}
$$

$$
K_3(5,4,3,2,1,1) = -\frac{10445964}{7} + 151200\pi^2. \tag{147}
$$

17 Connection of the general case K_3 with ${}_3F_2$ (1)

In this section a connection between the K_3 auxiliary function with general arguments and the hypergeometric function ${}_3F_2(1)$ is derived. We start with the following equality

$$\begin{aligned}
&\int_0^\infty \int_0^\infty \int_0^\infty \frac{(x+y+z)^p x^i y^j z^k e^{-x-y-z}}{(x+y)^l (x+z)^m (y+z)^n} dx\, dy\, dz \\
&= \lim_{a\to 1} (-1)^p \frac{d^p}{da^p} \int_0^\infty \int_0^\infty \int_0^\infty \frac{x^i y^j z^k e^{-a(x+y+z)}}{(x+y)^l (x+z)^m (y+z)^n} dx\, dy\, dz \\
&= \lim_{a\to 1} (-1)^p \frac{d^p}{da^p} a^{-(i+j+k+3-l-m-n)} \int_0^\infty \int_0^\infty \int_0^\infty \frac{x^i y^j z^k e^{-x-y-z}}{(x+y)^l (x+z)^m (y+z)^n} dx\, dy\, dz \\
&= (\sigma)_p K_3(i,j,k,l,m,n), \qquad (148)
\end{aligned}$$

with $\sigma = i+j+k+3-l-m-n$. Then we can write

$$K_3(i,j,k,l,m,n) = \frac{1}{(\sigma)_p} \int_0^\infty \int_0^\infty \int_0^\infty \frac{(x+y+z)^p x^i y^j z^k e^{-x-y-z}}{(x+y)^l (x+z)^m (y+z)^n} dx\, dy\, dz. \qquad (149)$$

Let $p = l+m+n$, and hence

$$2^p (x+y+z)^p = ((x+y)+(x+z)+(y+z))^{l+m+n}, \qquad (150)$$

and with appropriate binomial expansions it follows that

$$\begin{aligned}
&\frac{2^p (x+y+z)^p}{(x+y)^l (x+z)^m (y+z)^n} = \sum_{\mu=0}^{l+m-1} \binom{l+m+n}{\mu} \sum_{v=0}^{\mu} \binom{\mu}{v} \frac{(y+z)^{l+m-\mu}}{(x+y)^{l-\mu+v} (x+z)^{m-v}} \\
&+ \sum_{\mu=l+m}^{l+m+n} \binom{l+m+n}{\mu} \sum_{v=0}^{m-1} \binom{\mu}{v} \frac{(x+y)^{\mu-v-l}}{(x+z)^{m-v} (y+z)^{-l-m+\mu}} \\
&+ \sum_{\mu=l+m}^{l+m+n} \binom{l+m+n}{\mu} \sum_{v=m}^{\mu} \binom{\mu}{v} \frac{(x+z)^{v-m}}{(x+y)^{l-\mu+v} (y+z)^{-l-m+\mu}} \\
&= \sum_{\mu=0}^{l+m-1} \binom{l+m+n}{\mu} \sum_{v=0}^{\mu} \binom{\mu}{v} \sum_{w=0}^{l+m-\mu} \binom{l+m-\mu}{w} \frac{y^{l+m-\mu-w} z^w}{(x+y)^{l-\mu+v} (x+z)^{m-v}} \\
&+ \sum_{\mu=l+m}^{l+m+n} \binom{l+m+n}{\mu} \sum_{v=0}^{m-1} \binom{\mu}{v} \sum_{w=0}^{\mu-v-l} \binom{\mu-v-l}{w} \frac{x^{\mu-v-l-w} y^w}{(x+z)^{m-v} (y+z)^{-l-m+\mu}} \\
&+ \sum_{\mu=l+m}^{l+m+n} \binom{l+m+n}{\mu} \sum_{v=m}^{\mu} \binom{\mu}{v} \sum_{w=0}^{v-m} \binom{v-m}{w} \frac{x^{v-m-w} z^w}{(x+y)^{l-\mu+v} (y+z)^{-l-m+\mu}}.
\end{aligned} \qquad (151)$$

Inserting Eqs. (150) and (151) into Eq. (149) an setting $\sigma_1 = (\sigma)_p 2^p$ yields

$$
\begin{aligned}
K_3(i, j, k, l, m, n) &= \frac{1}{\sigma_1} \int_0^\infty \int_0^\infty \int_0^\infty \frac{2^p (x+y+z)^p x^i y^j z^k e^{-x-y-z}}{(x+y)^l (x+z)^m (y+z)^n} dx\, dy\, dz \\
&= \frac{1}{\sigma_1} \left\{ \sum_{\mu=0}^{l+m-1} \binom{l+m+n}{\mu} \sum_{v=0}^{\mu} \binom{\mu}{v} \sum_{w=0}^{l+m-\mu} \binom{l+m-\mu}{w} \right. \\
&\times \int_0^\infty \int_0^\infty \int_0^\infty \frac{x^i y^j z^k y^{l+m-\mu-w} z^w e^{-x-y-z}}{(x+y)^{l-\mu+v} (x+z)^{m-v}} dx\, dy\, dz \\
&+ \sum_{\mu=l+m}^{l+m+n} \binom{l+m+n}{\mu} \sum_{v=0}^{m-1} \binom{\mu}{v} \sum_{w=0}^{\mu-v-l} \binom{\mu-v-l}{w} \\
&\times \int_0^\infty \int_0^\infty \int_0^\infty \frac{x^i y^j z^k x^{\mu-v-l-w} y^w e^{-x-y-z}}{(x+z)^{m-v} (y+z)^{-l-m+\mu}} dx\, dy\, dz \\
&+ \sum_{\mu=l+m}^{l+m+n} \binom{l+m+n}{\mu} \sum_{v=m}^{\mu} \binom{\mu}{v} \sum_{w=0}^{v-m} \binom{v-m}{w} \\
&\times \left. \int_0^\infty \int_0^\infty \int_0^\infty \frac{x^i y^j z^k x^{v-m-w} z^w e^{-x-y-z}}{(x+y)^{l-\mu+v} (y+z)^{-l-m+\mu}} dx\, dy\, dz \right\} \\
&= \frac{1}{\sigma_1} \left\{ \sum_{\mu=0}^{l+m-1} \binom{l+m+n}{\mu} \sum_{v=0}^{\mu} \binom{\mu}{v} \sum_{w=0}^{l+m-\mu} \binom{l+m-\mu}{w} \right. \\
&\times K_3(j+l+m-\mu-w, i, k+w, l-\mu+v, 0, m-v) \\
&+ \sum_{\mu=l+m}^{l+m+n} \binom{l+m+n}{\mu} \sum_{v=0}^{m-1} \binom{\mu}{v} \sum_{w=0}^{\mu-v-l} \binom{\mu-v-l}{w} \\
&\times K_3(i+\mu-v-l-w, k, j+w, m-v, 0, \mu-l-m) \\
&+ \sum_{\mu=l+m}^{l+m+n} \binom{l+m+n}{\mu} \sum_{v=m}^{\mu} \binom{\mu}{v} \sum_{w=0}^{v-m} \binom{v-m}{w} \\
&\times \left. K_3(i+v-m-w, j, k+w, l-\mu+v, 0, \mu-l-m) \right\}. \qquad (152)
\end{aligned}
$$

Employing Eq. (54) leads to the result

$$
\begin{aligned}
&K_3(i, j, k, l, m, n) \\
&= \frac{1}{\sigma_1} \left\{ \sum_{\mu=0}^{l+m-1} \binom{l+m+n}{\mu} \sum_{v=0}^{\mu} \binom{\mu}{v} \sum_{w=0}^{l+m-\mu} \binom{l+m-\mu}{w} \right. \\
&\quad \times K_3(j+l+m-\mu-w, i, k+w, l-\mu+v, 0, m-v)
\end{aligned}
$$

$$
\begin{aligned}
&+\sum_{\mu=l+m}^{l+m+n}\binom{l+m+n}{\mu}\sum_{v=0}^{m-1}\binom{\mu}{v}\sum_{w=0}^{\mu-v-l}\binom{\mu-v-l}{w}\\
&\times K_3(i+\mu-v-l-w,k,j+w,m-v,0,\mu-l-m)\\
&+\sum_{\mu=l+m}^{l+m+n}\binom{l+m+n}{\mu}\sum_{v=m}^{\mu}\binom{\mu}{v}\sum_{w=0}^{v-m}\binom{v-m}{w}\\
&\times K_3(i+v-m-w,j,k+w,l-\mu+v,m,0,\mu-l-m)\ \Bigg\}\\
=\ &\frac{(i+j+k+2)!}{\sigma_1}\Bigg\{i!\sum_{\mu=0}^{l+m-1}\binom{l+m+n}{\mu}\sum_{v=0}^{\mu}\binom{\mu}{v}\sum_{w=0}^{l+m-\mu}\binom{l+m-\mu}{w}\\
&\times\frac{(j+l+m-\mu-w)!(k+w)!(i+j+1+m-v-w)!}{(i+j+1+l+m-\mu-w)!(i+j+k+2+m-v)!}\\
&\times{}_3F_2(m-v,j+l+m+1-\mu-w,i+j+2+m-v-w;\\
&\times i+j+2+l+m-\mu-w,i+j+k+3+m-v;1)\\
&+k!\sum_{u=0}^{n}\binom{l+m+n}{u+l+m}\sum_{v=0}^{m-1}\binom{u+l+m}{v}\sum_{w=0}^{u+m-v}\binom{u+m-v}{w}\\
&\times\frac{(i+u+m-v-w)!(j+w)!(i+k+1+u-w)!}{(i+k+1+u+m-v-w)!(i+j+k+2+u)!}\\
&\times{}_3F_2(u,i+1+u+m-v-w,i+k+2+u-w;\\
&\times i+k+2+u+m-v-w,i+j+k+3+u;1)\\
&+j!\sum_{u=0}^{n}\binom{l+m+n}{u+l+m}\sum_{p=0}^{u+l}\binom{u+l+m}{p+m}\sum_{w=0}^{p}\binom{p}{w}\\
&\times\frac{(i+p-w)!(k+w)!(i+j+1+u-w)!}{(i+j+1+p-w)!(i+j+k+2+u)!}\\
&\times{}_3F_2(u,i+1+p-w,i+j+2+u-w;i\\
&+j+2+p-w,i+j+k+3+u;1)\Bigg\}. \qquad (153)
\end{aligned}
$$

The preceding result is most useful as an evaluation strategy when the indices $\{l, m, n\}$ are not very large, otherwise numerical evaluation of $K_3(i, j, k, l, m, n)$ is best carried out using the result in Eq. (134). Sample values for the auxiliary function K_3 are presented in Table 3.

18 Reduction of the auxiliary function J_3 to K_3

The J_3 integral defined in Eq. (22) reduces in the case that $m = 0$ and $n = 0$ to the J_2 auxiliary function, and for $a = b = c$ it reduces to the K_3 auxiliary function. The J_3 integrals have obvious permutation symmetry, so without loss of generality we will assume that $c \geq b \geq a$. Since

Table 3 Sample values for the K_3 auxiliary function

Parameters						Integral
i	j	k	l	m	n	$K_3(i, j, k, l, m, n)$
1	1	1	1	0	0	1/3
1	1	1	1	1	0	$1.3039559891064138116550900012384886 \times 10^{-1}$
1	1	1	1	1	1	$6.5197799455320690582754500061924432 3432 \times 10^{-2}$
1	1	1	1	2	2	$8.8766483287943390881896208338493 7 \times 10^{-2}$
2	3	4	1	2	3	$9.4011075481535348537046658476394 3 \times 10^{-3}$
1	9	1	4	3	2	$5.6055851663319028318325681440841 44 \times 10^{-1}$
1	9	1	1	2	1	$6.6325757400221429219621639928541971 \times 10^{2}$
9	1	1	1	2	1	$1.3764657675029150947043942353265134 \times 10^{2}$
5	5	5	7	3	2	$1.4891638853148397457310518024446 \times 10^{-4}$
12	2	10	9	7	2	$9.2098333848884251695140452279230013 \times 10^{-4}$
1	3	6	3	4	3	$1.8705536541001030893626545330943 \times 10^{-3}$

$$\mathrm{e}^{(-ax-by-cz)} = \mathrm{e}^{(c-a)x}\mathrm{e}^{(c-b)y}\mathrm{e}^{-c(x+y+z)}, \tag{154}$$

then with the change of variables $cx = s$, $cy = t$, and $cz = u$, we have

$$J_3(i, j, k, l, m, n, a, b, c) = \frac{1}{c^{i+j+k-l-m-n+3}} \times \int_0^\infty \int_0^\infty \int_0^\infty \frac{s^i t^j u^k e^{\left(\frac{c-a}{c}\right)s} e^{\left(\frac{c-b}{c}\right)t} e^{-s-t-u}}{(s+t)^l (s+u)^m (t+u)^n} dsdtdu. \tag{155}$$

Employing a power series expansion for $e^{\left(\frac{c-a}{c}\right)s}$ and $e^{\left(\frac{c-b}{c}\right)t}$, we can write

$$J_3(i, j, k, l, m, n, a, b, c) = \frac{1}{c^{i+j+k-l-m-n+3}} \sum_{\mu=0}^{\infty} \sum_{v=0}^{\infty} \frac{\left(\frac{c-a}{c}\right)^{\mu}}{\mu!} \frac{\left(\frac{c-b}{c}\right)^{v}}{v!} \times \int_0^\infty \int_0^\infty \int_0^\infty \frac{x^{i+\mu} y^{j+v} z^k e^{-x-y-z}}{(x+y)^l (x+z)^m (y+z)^n} dxdydz, \tag{156}$$

which can be expressed using a summation rearrangement, as

$$J_3(i, j, k, l, m, n, a, b, c) = \frac{1}{c^{i+j+k-l-m-n+3}} \sum_{\mu=0}^{\infty} \sum_{v=0}^{\mu} \frac{\left(\frac{c-a}{c}\right)^{\mu-v}}{(\mu-v)!} \frac{\left(\frac{c-b}{c}\right)^{v}}{v!} \times \int_0^\infty \int_0^\infty \int_0^\infty \frac{x^{i+\mu-v} y^{j+v} z^k e^{-x-y-z}}{(x+y)^l (x+z)^m (y+z)^n} dxdydz. \tag{157}$$

Table 4 Sample values for the J_3 auxiliary function

Parameters									Integral
i	j	k	l	m	n	a	b	c	$J_3(i, j, k, l, m, n, a, b, c)$
1	1	1	1	0	1	4.5	4.6	4.8	$2.8264894520045896962463335099932 \times 10^{-4}$
1	1	1	1	1	1	2	2	3.4	$4.6430833705857903627338362188 \times 10^{-3}$
1	1	1	2	1	2	4.2	3.1	2.2	$2.8441545418151529520503899995 \times 10^{-2}$
1	2	3	2	3	2	1.7	2.1	4.4	$8.5275454075465462436568001938 2 \times 10^{-4}$
1	9	1	4	3	2	0.1	0.2	0.2	$2.0611142974180393470174568766 0 \times 10^{3}$
1	9	1	1	2	1	6.4	1.8	6.4	$1.7259537230263809948507901150 5 \times 10^{-1}$
9	1	1	1	2	1	2.1	3.1	4.1	$2.0567447192257066872622309104 8 \times 10^{-2}$
5	5	5	7	3	2	2.2	2.7	3.2	$3.1498517526739136062727331353 2 \times 10^{-7}$

This approach will be particularly stable when two of the exponents are equal, or fairly close to each other. Sample values for the auxiliary function J_3 are presented in Table 4. In part II we will give an alternative recursive approach to the evaluation of J_3.

19 Numerical evaluation of K_3

Employing the asymptotic estimate for the gamma function [72], we have that

$$\frac{\Gamma(z+b)}{\Gamma(z+c)} \approx z^{b-c} \text{ as } z \to \infty. \tag{158}$$

The series in Eq. (48) can be written as

$$\begin{aligned} &K_3(i, j, k, l, 0, n) \\ &\quad = \frac{j!k!\tau!}{(n-1)!} \sum_{\mu=0}^{\infty} \frac{\Gamma(n+\mu)}{\Gamma(\mu+1)} \frac{\Gamma(i+1+\mu)\Gamma(i+j+2-l+\mu)}{\Gamma(i+j+2+\mu)\Gamma(i+j+k+3-l+\mu)}. \end{aligned} \tag{159}$$

Making use of Eq. (158) leads to the asymptotic behavior for $K_3(i, j, k, l, 0, n)$ as

$$K_3(i, j, k, l, 0, n) \sim \sum_{\mu} \frac{1}{\mu^{i+j+3-l}}. \tag{160}$$

Similarly it can be shown that the asymptotic behavior of the series in Eq. (50) is

$$K_3(i, j, k, l, 0, n) \sim \sum_{\mu} \frac{1}{\mu^{j+k+3-n}}. \tag{161}$$

The convergence of the series in Eqs. (48) and (50) is governed by the factors $i+j+3-l$ and $j+k+3-n$, respectively. If either one of these factors is large, a direct summation technique may be effective in the evaluation of the $K_3(i, j, k, l, 0, n)$ integrals. But, when these factors are small, the series in Eqs. (48) and (50) converge too slowly. In these cases, application of convergence acceleration techniques is a requirement.

For the calculation of the I_3 integrals required for an energy evaluation, which have a maximum of one of the indices $\{l, m, n\}$ in Eq. (2) being -1, the other indices being > -1, then the series expansion in Eq. (134) converges quickly.

20 Summary of principal results

To summarize, we can write

$$I_3(i, j, k, l, m, n, a, b, c) = 64\pi^3 \sum_{w=0}^{\infty} \frac{I_R(i, j, k, l, m, n, w, w, w, a, b, c)}{(2w+1)^2}, \tag{162}$$

with

$$\begin{aligned} I_R(i, j, k, l, m, n, w, w, w, a, b, c) &= \frac{(-l/2)_w(-m/2)_w(-n/2)_w}{(2w+1)^2\{(1/2)_w\}^3} \sum_{l_1=0}^{\infty} \sum_{m_1=0}^{\infty} \sum_{n_1=0}^{\infty} \\ &\times \frac{4^{l_1+m_1+n_1}(w-\frac{l}{2})_{l_1}(w-\frac{m}{2})_{m_1}(w-\frac{n}{2})_{n_1}(1+w)_{l_1}(1+w)_{m_1}(1+w)_{n_1}}{l_1!m_1!n_1!(2+2w)_{l_1}(2+2w)_{m_1}(2+2w)_{n_1}} J_3(i+2 \\ &+2w+l_1+m_1, j+2+2w+l_1+n_1, k+2+2w+m_1+n_1, 2w-l \\ &+2l_1, 2w-m+2m_1, 2w-n+2n_1, a, b, c), \end{aligned} \tag{163}$$

and

$$\begin{aligned} J_3(\mathrm{I,J,K,L,M,N}, a, b, c) &= \frac{1}{c^{\mathrm{I+J+K-L-M-N+3}}} \sum_{s=0}^{\infty} \sum_{t=0}^{s} \frac{1}{(s-t)!t!} \left(\frac{c-a}{c}\right)^{s-t} \left(\frac{c-b}{c}\right)^{t} \\ &\times K_3(\mathrm{I}+s-t, \mathrm{J}+t, \mathrm{K,L,M,N}), \end{aligned} \tag{164}$$

where

$$\mathrm{I} = i+2+2w+l_1+m_1, \quad \mathrm{J} = j+2+2w+l_1+n_1, \quad \mathrm{K} = k+2+2w+m_1+n_1, \tag{165}$$

$$\mathrm{L} = 2w-l+2l_1, \quad \mathrm{M} = 2w-m+2m_1, \quad \mathrm{N} = 2w-n+2n_1. \tag{166}$$

The I integrals can be evaluated from Eq. (162), using Eqs. (163) and (164) to express $I_R(i, j, k, l, m, n, w, w, w, a, b, c)$ in terms of the J_3 integrals and hence the K_3 auxiliary functions, and employ Eq. (134) to evaluate the latter integrals. Where possible we take advantage of all the special cases we have outlined, in particular, the case where one of $\{l, m, n\}$ is zero for the K_3 auxiliary function. Also, the symmetry properties of J_3 or K_3 have been utilized when a permutation of parameters leads to quicker converging sums.

21 Conclusion

In this paper, we have presented a different evaluation strategy for the calculation of correlated three-electron integrals, which avoids the $N!$ growth issue in the number of required auxiliary function evaluations. It is shown that the new auxiliary functions that arise can be related directly to the hypergeometric function ${}_3F_2(1)$. General formulas and a number of special cases of ${}_3F_2(1)$ are presented which allow for the rapid evaluation of the new auxiliary functions encountered. A future study will detail the numerical evaluation strategy.

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