Analysis of some integrals arising in the atomic three-electron problem

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A detailed analysis is presented for the evaluation of atomic integrals of the form $\int r_1^i r_2^j r_3^k r_{23}^{-2} r_{31}^m r_{12}^n e^{-\alpha r_1 - \beta r_2 - \gamma r_3} d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3$, which arise in several contexts of the three-electron atomic problem. All convergent integrals with $i \geq -2$, $j \geq -2$, $k \geq -2$, $m \geq -1$, and $n \geq -1$ are examined. These integrals are solved by two distinct procedures. A majority of the integrals can be evaluated by a reduction of the three-electron integrals to integrals arising in the atomic two-electron integral problem. A second approach allows all integrals with the aforementioned indices to be evaluated by the use of Sack's expansion [J. Math. Phys. **5**, 245 (1964)] of the interelectronic separation, which leads to a reduction of the above nine-dimensional integrals to a set of three-dimensional integrals. A discussion is given for the numerical evaluation of the three-dimensional integrals that arise.

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I. INTRODUCTION

The purpose of this paper is to present the evaluation of certain one-center atomic integrals of the form

$$I(i,j,k,l,m,n,\alpha,\beta,\gamma)=\int r_1^i r_2^j r_3^k r_{23}^l r_{31}^m r_{12}^n \times e^{-\alpha r_1-\beta r_2-\gamma r_3} \times d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 \quad (1)$$

which will be referred to as the I integrals. In Eq. (1), r_s denotes the electron-nuclear separations and r_{pq} denotes the interelectronic separations. Henceforth, r_{23}, r_{31}, and r_{12} will be abbreviated by u_1, u_2, and u_3, respectively. Because these I integrals form the core of calculations on three-electron systems [1–9], or more generally, four-particle systems [10], using Hylleraas-type basis functions, there has been considerable attention devoted to their evaluation in the literature [1,2,11–18]. A generalization of Eq. (1) has recently been investigated [19]. For the aforementioned calculations, the I integrals required have l,m,n each ≥ -1.

The present work considers I integrals when one of l, m, or n is equal to -2, and the other two values are ≥ -1. I integrals of this form arise in the evaluation of certain relativistic contributions for three-electron systems using Hylleraas-type basis functions. These integrals also represent the major impediment to the evaluation of lower bounds to the energy, using formulas dependent on matrix elements of the square of the Hamiltonian. Very little work has been previously published for the I integrals containing a factor r_{ij}^{-2}. Some special cases of Eq. (1) which arise in the context of the two-electron atomic problem can be found scattered throughout the literature [20–27].

The approach taken in this work is to divide the I integrals into two major categories. The first group is determined by the set of conditions

$$l=-2;\ m,n \geq -1 \text{ and } m,n \text{ not both odd}\ . \quad (2)$$

The second group is defined by

$$l=-2,\quad m,n \geq -1 \text{ and } m,n \text{ odd or even}\ . \quad (3)$$

This division separates the I integrals into a group that can be evaluated in closed form (group 1), and a second set for which no analytic solutions appear possible. This separation of I integrals resembles the situation known in the literature for the case l,m,n each ≥ -1. One result for the I integral in the latter situation when l, m, and n are all odd is an infinite series [12].

II. SOME PRELIMINARY INTEGRALS

A major component of the evaluation strategy for the group-1 I integrals is their reduction to simpler integrals that appear in the two-electron atomic problem. In these simpler integrals only one interelectronic separation appears. In Sec. III it will be demonstrated that the I integrals defined by the conditions given in Eq. (2) can be reduced to integrals of the form

$$\mathcal{J}(i,j,l,\alpha,\beta)=\int r_1^i r_2^j u_3^l e^{-\alpha r_1-\beta r_2} d\mathbf{r}_1 d\mathbf{r}_2\ . \quad (4)$$

Two principal cases for Eq. (4) are required, and they are both treated below.

A. Integral $\mathcal{J}(i,j,l,\alpha,\beta)$ for $i,j,l \ge -1$

This integral has been discussed at length in the literature [28,29]. This is the basic atomic integral arising in the two-electron problem (more generally, the three-particle problem) using Hylleraas-type basis functions. Since this integral is central to the results of Sec. III, we present explicit formulas for its evaluation. Additional results for this integral can be found in the literature.

The standard simplification for all the $\mathcal{J}$ integrals in this work is to convert to perimetric coordinates [30],

$$x = r_1 + r_2 - u_3 \,, \tag{5a}$$

$$y = r_2 + u_3 - r_1 \,, \tag{5b}$$

$$z = u_3 + r_1 - r_2 \,, \tag{5c}$$

and

$$d\mathbf{r}_1\, d\mathbf{r}_2 = \frac{\pi^2}{4}(x+y)(y+z)(z+x)\,dx\,dy\,dz \,. \tag{5d}$$

If Eq. (5) is employed in Eq. (4), then for i,j,l each ≥ -1,

$$\mathcal{J}(i,j,l,\alpha,\beta) = 16\pi^2 \sum_{r=0}^{i+1} \sum_{s=0}^{j+1} \sum_{t=0}^{l+1} \binom{i+1}{r} \binom{j+1}{s} \binom{l+1}{t} \frac{(i+j+2-r-s)!(l+1+s-t)!(r+t)!}{(\alpha+\beta)^{i+j+3-r-s}\alpha^{r+t+1}\beta^{s+l+2-t}} \tag{6}$$

where $\binom{m}{n}$ denotes a binomial coefficient throughout this work. Using integration by parts, it can be shown that the $\mathcal{J}$ integrals satisfy the general recursion formula

$$\begin{aligned}\alpha\beta\mathcal{J}(i,j,l,\alpha,\beta) &= \beta(i+1)\mathcal{J}(i-1,j,l,\alpha,\beta) + \alpha(j+1)\mathcal{J}(i,j-1,l,\alpha,\beta) \\ &\quad + (\alpha+\beta)(l+1)\mathcal{J}(i,j,l-1,\alpha,\beta) - (i+1)(j+1)\mathcal{J}(i-1,j-1,l,\alpha,\beta) \\ &\quad - (i+1)(l+1)\mathcal{J}(i-1,j,l-1,\alpha,\beta) - (j+1)(l+1)\mathcal{J}(i,j-1,l-1,\alpha,\beta) \\ &\quad - l(l+1)\mathcal{J}(i,j,l-2,\alpha,\beta) + \frac{16\pi^2(i+j+2)!}{(\alpha+\beta)^{i+j+3}}\delta_{l,-1}\end{aligned} \tag{7}$$

where $\delta_{s,t}$ denotes the Kronecker δ. The $\mathcal{J}$ integrals can be numerically evaluated in the sequence $\mathcal{J}(-1,-1,l,\alpha,\beta)$, $\mathcal{J}(i,-1,-1,\alpha,\beta)$, $\mathcal{J}(i,-1,l,\alpha,\beta)$, $\mathcal{J}(i,j,-1,\alpha,\beta)$, and finally $\mathcal{J}(i,j,l,\alpha,\beta)$. Various recursion formulas for particular cases can be obtained from Eq. (7) or by direct consideration of Eq. (4).

B. Integral $\mathcal{J}(i,j,-2,\alpha,\beta)$ for $i,j \ge -1$

$\mathcal{J}$ integrals in this group have been discussed in the literature, though less extensively than those described in Sec. II A. These integrals arise in the calculation of certain relativistic expectation values, and applications involving the square of the Hamiltonian for two-electron systems using a Hylleraas basis set. A number of special cases have been discussed in the literature [20–27].

The restrictions for convergence of the above integrals are

$$i+j+3 \ge 0 \tag{8}$$

with

$$i \ge -2 \quad \text{and} \quad j \ge -2 \,. \tag{9}$$

The simplest case to consider is $i \ge -1$, $j \ge -1$.

Converting Eq. (4) to perimetric coordinates, the following result can be established:

$$\begin{aligned}\mathcal{J}(i,j,-2,\alpha,\beta) &= \frac{16\pi^2}{(\alpha+\beta)^{i+j+3}} \sum_{r=0}^{i+1} \sum_{s=0}^{j+1} \binom{i+1}{r} \binom{j+1}{s} (i+j+2-r-s)!(\alpha+\beta)^{r+s} \\ &\quad \times \left[\sum_{t=0}^{r-1} \sum_{k=0}^{r-t-1} \binom{r}{t} \frac{(-1)^t(r-t-1)!(s+t+k)!}{k!\beta^{s+t+k+1}\alpha^{r-k-t}} \right. \\ &\quad \left. + (-1)^r(s+r)!S_{rs}(\alpha,\beta) \right] \quad (i \ge -1, j \ge -1)\end{aligned} \tag{10}$$

where

$$S_{rs}(\alpha,\beta) = \frac{1}{(\beta-\alpha)^{r+s+1}} \left[\ln(\beta/\alpha) - \sum_{k=1}^{r+s} \frac{1}{k} \left[\frac{\beta-\alpha}{\beta} \right]^k \right] . \tag{11}$$

In Eqs. (10) and (11), and throughout the rest of paper, the standard summation convention $\sum_{k=n}^{m}=0$, when $m<n$, is employed. For the situation when α and β are approximately the same, Eq. (11) can be reexpressed in a format more suitable for numerical evaluation, namely,

$$S_{rs}(\alpha,\beta)=\frac{1}{\beta^{r+s+1}}\sum_{k=0}^{\infty}\frac{\epsilon^k}{(k+r+s+1)} \tag{12}$$

where

$$\epsilon=\frac{\beta-\alpha}{\beta}\ . \tag{13}$$

The following recursion formulas can be established by integration by parts:

$$(\alpha^2-\beta^2)\mathcal{I}(-1,j+1,-2,\alpha,\beta)=(j+2)(j+1)\mathcal{I}(-1,j-1,-2,\alpha,\beta)-2\beta(j+2)\mathcal{I}(-1,j,-2,\alpha,\beta)+\frac{16\pi^2(j+1)!}{\beta^{j+2}}\quad(j\geq-1) \tag{14}$$

with

$$\mathcal{I}(-1,-1,-2,\alpha,\beta)=\frac{16\pi^2}{\alpha^2-\beta^2}\ln(\alpha/\beta)\ ; \tag{15}$$

and the general result

$$\begin{aligned}(\alpha^2-\beta^2)\mathcal{I}(i,j,-2,\alpha,\beta)&=j(j+1)\mathcal{I}(i,j-2,-2,\alpha,\beta)-i(i+1)\mathcal{I}(i-2,j,-2,\alpha,\beta)\\&\quad+2\alpha(i+1)\mathcal{I}(i-1,j,-2,\alpha,\beta)-2\beta(j+1)\mathcal{I}(i,j-1,-2,\alpha,\beta)\\&\quad\times16\pi^2\left[\ln(\alpha/\beta)\delta_{i,-1}\delta_{j,-1}+\left[\frac{j!\delta_{i,-1}}{\beta^{j+1}}\right]_{j\geq0}-\left[\frac{i!\delta_{j,-1}}{\alpha^{i+1}}\right]_{i\geq0}\right]\quad\text{for } i\geq-1, j\geq-1\ .\end{aligned} \tag{16}$$

The necessary input for the recursion formula Eq. (16), $\mathcal{I}(i,-1,-2,\alpha,\beta)$ and $\mathcal{I}(-1,j,-2,\alpha,\beta)$, can be obtained using Eqs. (14) and (15). For the situation where $\alpha\approx\beta$, an alternative to Eq. (14) is

$$(\alpha+\beta)\mathcal{I}(-1,j,-2,\alpha,\beta)=(j+1)\mathcal{I}(-1,j-1,-2,\alpha,\beta)+16\pi^2(j+1)!S_{j1}(\alpha,\beta) \tag{17}$$

where $S_{rs}(\alpha,\beta)$ has been defined in Eq. (11) and can be numerically evaluated for the case $a\approx\beta$ using Eq. (12). An alternative recursive scheme to Eq. (16) with all positive factors is

$$\begin{aligned}(\alpha+\beta)\mathcal{I}(i,j,-2,\alpha,\beta)&=(i+1)\mathcal{I}(i-1,j,-2,\alpha,\beta)\\&\quad+(j+1)\mathcal{I}(i,j-1,-2,\alpha,\beta)\\&\quad+f(j+1,i+1,\beta,\alpha)\end{aligned} \tag{18}$$

where

$$f(i,j,\alpha,\beta)=16\pi^2\int_0^{\infty}e^{-\alpha x}x^i dx\int_0^{\infty}\frac{e^{-\beta y}y^j}{(x+y)}dy\ . \tag{19}$$

Evaluation of $f(i,j,\alpha,\beta)$ gives

$$f(i,j,\alpha,\beta)=\frac{16\pi^2(-1)^i}{(\beta-\alpha)^{i+j+1}}[(i+j)!\ln(\beta/\alpha)+\mathcal{R}_{ij}(\alpha,\beta)-\mathcal{R}_{ji}(\beta,\alpha)] \tag{20}$$

with

$$\mathcal{R}_{ij}(\alpha,\beta)=\sum_{m=1}^{i}\binom{i}{m}(i+j-m)!(m-1)!\left[\frac{\alpha-\beta}{\alpha}\right]^m, \tag{21}$$

or for the case $\alpha\approx\beta$, $f(i,j,\alpha,\beta)$ can be expressed in terms of the hypergeometric function ${}_2F_1$,

$$\begin{aligned}f(i,j,\alpha,\beta)&=\frac{16\pi^2 i!j!}{\alpha^i\beta^{j+1}(i+j+1)}\times{}_2F_1(j+1,1;i+j+2,\epsilon)\\&=\frac{i!(i+j)!}{\alpha^i\beta^{j+1}}\sum_{k=0}^{\infty}\frac{(j+k)!\epsilon^k}{(i+j+k+1)!}\end{aligned} \tag{22}$$

with ϵ given in Eq. (13).

C. Integral $\mathcal{I}(-2,j,-2,\alpha,\beta)$ for $j\geq-1$

The $\mathcal{I}$ integral of this subsection can be evaluated by converting to perimetric coordinates to yield

$$\mathcal{J}(-2,j,-2,\alpha,\beta)=16\pi^2\sum_{m=0}^{j+1}\begin{bmatrix} j+1 \\ m \end{bmatrix}\int_0^\infty e^{-\alpha z}F(j+1-m,\alpha+\beta,z)F(m,\beta,z)dz \tag{23}$$

with [31]

$$F(m,\beta,z)=\int_0^\infty \frac{y^m e^{-\beta y}dy}{y+z} =(-z)^m\left[e^{\beta z}E_1(\beta z)+\sum_{k=1}^{m}(-1)^k(k-1)!(\beta z)^{-k}\right] \tag{24}$$

where $E_1(x)$ is the exponential integral. Substitution of Eq. (24) into Eq. (23) leads to

$$\begin{aligned}\mathcal{J}(-2,j,-2,\alpha,\beta)=16\pi^2(-1)^{j+1}\Bigg\{&\frac{2^{j+1}}{\beta^{j+2}}K_1\left[j+1,-2,\frac{\alpha+\beta}{\beta}\right] \\ &+\sum_{m=0}^{j+1}\begin{bmatrix} j+1 \\ m \end{bmatrix}\Bigg[\frac{1}{(\alpha+\beta)^{j+2}}U\left[j,m,\frac{\alpha+\beta}{\beta},\frac{-\beta}{\alpha+\beta}\right] \\ &+\frac{1}{\beta^{j+2}}U\left[j,j+1-m,\frac{\beta}{\alpha+\beta},\frac{\alpha-\beta}{\beta}\right] \\ &+\frac{1}{\alpha^{j+2}}\sum_{l=1}^{j+1-m}\sum_{k=1}^{m}(-1)^{l+k}(l-1)!(k-1)! \\ &\times(j+1-l-k)!\left[\frac{\alpha}{\alpha+\beta}\right]^l\left[\frac{\alpha}{\beta}\right]^k\Bigg]\Bigg\}\end{aligned} \tag{25}$$

where

$$U(j,m,a,b)=\sum_{n=1}^{m}(-1)^n(n-1)!a^n\mathcal{L}(j+1-n,b)\ , \tag{26}$$

$$\mathcal{L}(m,a)=\int_0^\infty x^m e^{-ax}E_1(x)dx\ , \tag{27}$$

and

$$K_1(m,a,b)=\int_0^\infty x^m e^{-ax}E_1(x)E_1(bx)dx\ . \tag{28}$$

The function $\mathcal{L}(m,a)$ satisfies

$$\mathcal{L}(m,a)=\frac{m}{a}\mathcal{L}(m-1,a)-\frac{1}{a}\frac{(m-1)!}{(a+1)^m}\quad(m\geq 1) \tag{29}$$

with

$$\mathcal{L}(0,a)=\frac{1}{a}\ln(1+a)\ ; \tag{30}$$

and

$$\mathcal{L}(m,a)=\frac{m!}{a^{m+1}}\left[\ln(1+a)-\sum_{k=1}^{m}\frac{1}{k}\left[\frac{a}{1+a}\right]^k\right]\ . \tag{31}$$

By noting the expansion

$$\ln(1+a)=\sum_{k=1}^{\infty}\left[\frac{a}{1+a}\right]^k\frac{1}{k}\quad\text{for } a\geq -\tfrac{1}{2}\ , \tag{32}$$

it is clear that Eq. (31) is *not* numerically stable for large m, nor is the formula suitable for small a. In place of Eq. (31), the following two expressions are numerically stable for both large m and small $|a|$:

$$\mathcal{L}(m,a)=\frac{m!}{(1+a)^{m+1}}\times\left[\frac{1}{m+1}+\sum_{n=1}^{\infty}\left[\frac{a}{1+a}\right]^n\frac{1}{n+m+1}\right]\quad\text{for } a\geq 0 \tag{33}$$

and

$$\begin{aligned}\mathcal{L}(m,a)=\frac{m!}{(1+a)^{m+1}}\Bigg\{&\frac{1}{m+1}+\left[\frac{a}{1+a}\right]\frac{1}{m+2} \\ &+\sum_{n=1}^{\infty}\left[\frac{a}{1+a}\right]^{2n}\left[\frac{1}{2n+m+1}+\left[\frac{a}{1+a}\right]\frac{1}{2n+m+2}\right]\Bigg\}\quad\text{for } a\geq -\tfrac{1}{2}\ .\end{aligned} \tag{34}$$

The function $K_1(m,a,b)$ and its generalization are examined in detail in Appendix A. Special cases of the Sec. II C integral occur in several places in this investigation. With the restriction that $\alpha\neq\beta$, a more compact expression than Eq. (25) can be obtained by noting

$$\mathcal{I}(-2,j,-2,\alpha,\beta)=(-1)^{j+1}\frac{\partial^{j+1}}{\partial\beta^{j+1}}\mathcal{I}(-2,-1,-2,\alpha,\beta) \tag{35}$$

where

$$\mathcal{I}(-2,-1,-2,\alpha,\beta)=16\pi^2\int_0^\infty\int_0^\infty\int_0^\infty\frac{e^{-\alpha(x+z)-\beta(x+y)}}{(z+x)(z+y)}dx\,dy\,dz\ . \tag{36}$$

$\mathcal{I}(-2,-1,-2,\alpha,\beta)$ may be expressed directly in terms of the $K_1(m,a,b)$ integrals [Eq. (28)] or alternatively, evaluated by expressing the factors $(z+x)$ and $(z+y)$ as Laplace transforms, with the result

$$\begin{aligned}\mathcal{I}(-2,-1,-2,\alpha,\beta)&=\frac{16\pi^2}{\beta}\int_\tau^\infty\frac{\ln x\,dx}{x^2-1}\\&=\frac{16\pi^2}{\beta}K_1(0,-2,1+\tau)\end{aligned} \tag{37}$$

with $\tau=\alpha/\beta$ and $K_1(0,-2,1+\tau)$ is given in Eqs. (A6) and (A7). Inserting Eq. (37) into Eq. (35) yields

$$\begin{aligned}\mathcal{I}(-2,j,-2,\alpha,\beta)=\frac{8\pi^2(j+1)!}{\beta^{j+2}}\Bigg[&2K_1(0,-2,1+\tau)-\frac{2\alpha\beta}{\alpha^2-\beta^2}\ln(\alpha/\beta)+\ln(\beta/\alpha)\sum_{m=2}^{j+1}\frac{\beta^m}{m}\left[\frac{1}{(\beta+\alpha)^m}-\frac{1}{(\beta-\alpha)^m}\right]\\&+\sum_{m=2}^{j+1}\frac{\beta^m}{m}\sum_{n=1}^{m-1}\frac{1}{n\beta^n}\left[\frac{1}{(\beta-\alpha)^{m-n}}-\frac{1}{(\beta+\alpha)^{m-n}}\right]\Bigg]\quad\text{for } j\geq 0\ .\end{aligned} \tag{38}$$

The preceding equation is obviously not numerically stable when $\alpha\approx\beta$. Even for moderate differences between α and β, the formula quickly loses numerical significance as j increases, a fact readily observed by computing separately the positive and negative contributions to the term in square brackets. In such cases, Eq. (25) is superior for numerical computation.

D. Integral $\mathcal{I}(-2,j,l,\alpha,\beta)$ for $j\geq-2$ and $l\geq-1$

For $j\geq-1$ and $l\geq-1$ the following result is readily derived:

$$\begin{aligned}\mathcal{I}(-2,j,l,\alpha,\beta)=\frac{16\pi^2}{\beta^{l+2}\alpha^{j+2}}\sum_{m=0}^{l+1}\sum_{n=0}^{j+1}&\binom{l+1}{m}\binom{j+1}{n}(l+1+n-m)!(-1)^m\left[\frac{\alpha}{\beta}\right]^{n-m}\\&\times\Bigg[\mathcal{L}(j+1-n+m,\beta/\alpha)-\left[\frac{\alpha}{\alpha+\beta}\right]^{j+1+m-n}\\&\qquad\times\sum_{p=0}^{m-1}(-1)^p p!(j+m-n-p)!\left[\frac{\alpha+\beta}{\alpha}\right]^p\Bigg]\ .\end{aligned} \tag{39}$$

For the case $j=-2$ and $l\geq-1$, the integral simplifies to

$$\mathcal{I}(-2,-2,l,\alpha,\beta)=16\pi^2\sum_{m=0}^{l+1}\binom{l+1}{m}\int_0^\infty e^{-(\alpha+\beta)x}F(l+1-m,\beta,x)F(m,\alpha,x)dx \tag{40}$$

where $F(m,\alpha,x)$ is defined in Eq. (24). The above expression can be simplified to yield

$$\begin{aligned}\mathcal{I}(-2,-2,l,\alpha,\beta)=16\pi^2(-1)^{l+1}\Bigg[&\frac{2^{l+1}}{\alpha^{l+2}}K_1(l+1,0,\beta/\alpha)\\&+\sum_{m=0}^{l+1}\binom{l+1}{m}\Bigg[V(l,m,\alpha,\beta)+V(l,l+1-m,\beta,\alpha)\\&\qquad+\sum_{k=1}^{m}\sum_{n=1}^{l+1-m}\frac{(k-1)!(n-1)!(-1)^{k+n}(l+1-k-n)!}{\alpha^k\beta^n(\alpha+\beta)^{l+2-k-n}}\Bigg]\Bigg]\end{aligned} \tag{41}$$

where

$$V(l,m,\alpha,\beta)=\sum_{k=1}^{m}\frac{(-1)^k(k-1)!\mathcal{L}(l+1-k,\alpha/\beta)}{\alpha^k\beta^{l+2-k}} \tag{42}$$

and $K_1(l+1,0,\beta/\alpha)$ can be computed from Eq. (A11).

E. A generalized $\mathcal{J}$ integral

The first integral that we consider in this section is

$$\mathcal{K}(i,j,l,\alpha,\beta,\gamma)=\int r_1^i r_2^j r_{12}^l E_1(\alpha r_2)e^{-\beta r_1-\gamma r_2}d\mathbf{r}_1\,d\mathbf{r}_2 \; . \tag{43}$$

This integral does not arise in any context for the two-electron problem. This special integral arises in the next section, and is treated here, because of its relationship to other integrals examined above.

Three cases for the $\mathcal{K}$ integral will be examined. (a) $i\geq -1$, $j\geq -1$, $l\geq -1$, (b) $i\geq -1$, $j\geq -1$, $l=-2$, and (c) $i=-2$, $j\geq -1$, $l=-2$. For case (a), conversion of the integral to perimetric coordinates yields the result

$$\mathcal{K}(i,j,l,\alpha,\beta,\gamma)=\frac{16\pi^2}{\beta\alpha^{i+j+l+5}}\sum_{r=0}^{i+1}\sum_{s=0}^{j+1}\sum_{t=0}^{l+1}\begin{bmatrix}i+1\\ r\end{bmatrix}\begin{bmatrix}j+1\\ s\end{bmatrix}\begin{bmatrix}l+1\\ t\end{bmatrix}(r+t)!\left[\frac{\alpha}{\beta}\right]^{r+t} \times G\left[i+j+2-r-s,s+l+1-t,\frac{\beta+\gamma}{\alpha},\frac{\gamma}{\alpha}\right] \tag{44}$$

where

$$G(i,j,a,b)=\int_0^\infty x^i e^{-ax}dx\int_0^\infty y^j e^{-by}E_1(x+y)dy \; . \tag{45}$$

The above integral can be simplified to yield

$$G(i,j,a,b)=\mathcal{G}(i,j,a,b)+\mathcal{G}(j,i,b,a) \tag{46}$$

with

$$\mathcal{G}(i,j,a,b)=\frac{i!}{a^{i+1}(b-a)^{j+1}}\left[\ln(1+a)\sum_{m=0}^{i}\left[\frac{a}{a-b}\right]^m\frac{(j+m)!}{m!} - \sum_{m=1}^{i}\left[\frac{a}{a-b}\right]^m\sum_{n=1}^{m}\frac{1}{n}\left[\frac{a-b}{a+1}\right]^n\left[\frac{(j+m-n)!}{(m-n)!}\right]\right] \quad \text{for } a\neq b \; . \tag{47}$$

The case $a=b$ is not required in Eq. (44) since $\beta>0$ in this expression. For the second case $(i\geq -1, j\geq -1, l=-2)$ $\mathcal{K}$ can be reduced to the form

$$\mathcal{K}(i,j,-2,\alpha,\beta,\gamma)=16\pi^2\sum_{r=0}^{i+1}\sum_{s=0}^{j+1}\begin{bmatrix}i+1\\ r\end{bmatrix}\begin{bmatrix}j+1\\ s\end{bmatrix}\int_0^\infty e^{-(\beta+\gamma)x}x^{i+j+2-r-s}dx\int_0^\infty e^{-\gamma y}y^s E_1(\alpha(x+y))F(r,\beta,y)dy \tag{48}$$

where the function $F(r,\beta,y)$ is given by Eq. (24). The preceding integral can be simplified to yield

$$\mathcal{K}(i,j,-2,\alpha,\beta,\gamma)=16\pi^2\sum_{r=0}^{i+1}\sum_{s=0}^{j+1}\begin{bmatrix}i+1\\ r\end{bmatrix}\begin{bmatrix}j+1\\ s\end{bmatrix}(-1)^r \times\left[\frac{1}{\alpha^{i+j+4}}\sum_{k=1}^{r}(-1)^k(k-1)!\left[\frac{\alpha}{\beta}\right]^k G\left[i+j+2-r-s,r+s-k,\frac{\beta+\gamma}{\alpha},\frac{\gamma}{\alpha}\right] + H(i+j+2-r-s,r+s,\beta+\gamma,\gamma-\beta,\alpha,\beta)\right] \tag{49}$$

where

$$H(m,n,a,b,c,d)=\int_0^\infty x^m e^{-ax}dx\int_0^\infty y^n e^{-by}E_1(c(x+y))E_1(dy)dy \; . \tag{50}$$

The function H can be simplified using the result

$$\int_0^\infty x^n e^{-ax}E_1(x+y)dx=\frac{n!}{a^{n+1}}\left[E_1(y)-e^{ay}\sum_{i=0}^{n}\left[\frac{a}{1+a}\right]^i E_{i+1}((1+a)y)\right] \tag{51}$$

to obtain

$$H(m,n,a,b,c,d)=\frac{m!}{a^{m+1}c^{n+1}}\left[K_1\left[n,\frac{b}{c},\frac{d}{c}\right]-\left[\frac{c}{d}\right]^{n+1}\sum_{j=1}^{m+1}\left[\frac{a}{a+c}\right]^{j-1}K_j\left[n,\frac{b-a}{d},\frac{a+c}{d}\right]\right]. \tag{52}$$

The $K_j(m,\mathscr{a},\mathscr{b})$ integrals required in Eq. (52) have $\mathscr{a}=-1$. Use of the recursive formula Eq. (A14) together with the result for $K_1(0,-1,\mathscr{b})$ [Eq. (A10)] provides a route to these functions. $K_1(0,\mathscr{a},\mathscr{b})$ for $\mathscr{a}>0$ and $\mathscr{b}>0$ is also required in Eq. (52), and this may be obtained using Eq. (A8), or Eq. (A9) if $\mathscr{a}$ is small.

The integral $\mathscr{H}(-2,j\geq-1,l\geq-1,\alpha,\beta,\gamma)$ is also needed for the evaluation of certain I integrals. This particular $\mathscr{H}$ integral can be evaluated in a manner analogous to Eq. (48), leading to a result similar to Eq. (49).

The third case ($i=-2$, $j\geq-1$, $l=-2$) is by far the most obdurate. We consider first the case $j=-1$. Conversion to perimetric coordinates gives

$$\mathscr{H}(-2,-1,-2,\alpha,\beta,\gamma)=\frac{16\pi^2}{\alpha}\int_0^\infty e^{-ax}dx\int_0^\infty e^{-by}E_1(x+y)dy\int_0^\infty\frac{e^{-cz}dz}{(z+x)(z+y)} \tag{53}$$

with $a=(\beta+\gamma)/\alpha$, $b=\gamma/\alpha$, and $c=\beta/\alpha$. Inserting the definition of the exponential integral and writing $(z+x)^{-1}$ and $(z+y)^{-1}$ as Laplace transforms yields after some manipulation

$$\mathscr{H}(-2,-1,-2,\alpha,\beta,\gamma)=\frac{16\pi^2}{\alpha}\mathfrak{R}(a,b) \tag{54}$$

with

$$\mathfrak{R}(a,b)=\int_1^\infty\frac{dt\,K_1(0,-2,1+\tau)}{t(t+b)} \tag{55}$$

and $\tau=c/(t+b)\equiv(a-b)/(t+b)$, and $K_1(0,-2,1+\tau)$ is given in Eqs. (A6) or (A7). The integral appearing in Eq. (55) is rather tedious to evaluate, particularly in a form suitable for numerical evaluation. If $c-b\leq1$ then $0<\tau\leq1$ and Eq. (55) must be evaluated using Eq. (A7a). If $c-b\geq1$ then Eq. (55) can be written as

$$\mathfrak{R}(a,b)=\int_1^{c-b}\frac{dt}{t(t+b)}K_1(0,-2,1+\tau)+\int_{c-b}^\infty\frac{dt}{t(t+b)}K_1(0,-2,1+\tau)\ , \tag{56}$$

where for the first integral in Eq. (56) $\tau\geq1$, and for the second integral $0<\tau\leq1$, and both Eqs. (A7a) and (A7c) are needed in the evaluation of the integral. In each of the preceding three integrals [Eqs. (55) and (56)], integrands containing a product of a pair of log functions are encountered. Generally, such integrals can be reduced (through some tedious algebra) to Euler's dilogarithm function and its generalization, the trilogarithm function [32]. We have opted instead to carry out appropriate series expansion of parts of the integrands, in the hope of obtaining results suitable for numerical evaluation. For $c-b\leq1$ denote $\mathfrak{R}(a,b)$ by $\mathfrak{R}_1$ and employ Eq. (A7a), then with the variable change $t=c\tau^{-1}-b$

$$\mathfrak{R}_1=\frac{\pi^2}{4b}\ln(1+b)-\frac{1}{c}\sum_{n=0}^\infty\frac{1}{(2n+1)^2}\left[\frac{c}{b}\right]^{2n+2}\left[\ln(1+b)-\sum_{k=1}^{2n+1}\left[\frac{b}{b+1}\right]^k\frac{1}{k}\right]$$
$$+\tfrac{1}{2}\int_0^{c/(1+b)}\frac{\ln\tau\ln[(1+\tau)/(1-\tau)]d\tau}{c-\tau b}\ . \tag{57}$$

The second factor on the right-hand side (in square brackets) will not be stable for numerical evaluation. Expanding $\ln(1+b)$ in a power series yields for the summation in Eq. (57)

$$\sum_{n=0}^\infty\frac{1}{(2n+1)^2}\left[\frac{c}{1+b}\right]^{2n+1}\sum_{j=0}^\infty\left[\frac{b}{1+b}\right]^j\frac{1}{j+2n+2} \tag{58}$$

which is clearly more suitable for numerical computation. The integral in Eq. (57) can be expressed as

$$\tfrac{1}{2}\int_0^{c/(1+b)}\frac{\ln\tau\ln[(1+\tau)/(1-\tau)]d\tau}{c-\tau b}=\frac{1}{b+1}\sum_{k=1}^\infty\frac{1}{2k-1}\left[\frac{c}{b+1}\right]^{2k-1}$$
$$\times\sum_{m=0}^\infty\left[\frac{b}{b+1}\right]^m\frac{\{(m+2k)\ln[c/(1+b)]-1\}}{(m+2k)^2}\ . \tag{59}$$

Alternative forms for the above integral involving only one infinite summation can be derived, but will be less suitable for numerical evaluation. Collecting Eqs. (58) and (59), Eq. (57) becomes

$$\mathfrak{K}_1=\frac{\pi^2}{4b}\ln(1+b)-\frac{1}{c}\sum_{k=0}^{\infty}\left[\frac{c}{1+b}\right]^{2k+2}\frac{1}{(2k+1)}\sum_{n=0}^{\infty}\left[\frac{b}{b+1}\right]^{n}\frac{1}{(n+2k+2)}\times\left[\ln\left[\frac{b+1}{c}\right]+\frac{(n+4k+3)}{(n+2k+2)(2k+1)}\right]. \tag{60}$$

Denote by $\mathfrak{K}_2$ the second integral on the right-hand side of Eq. (56). Introducing the change of variable $t=c\tau^{-1}-b$ and employing Eq. (A7a) leads after straightforward algebra to the result

$$\mathfrak{K}_2=-\frac{\pi^2}{4b}\ln\left[\frac{c-b}{c}\right]-\frac{1}{c}\sum_{m=0}^{\infty}\left[\frac{b}{c}\right]^{m}\sum_{n=0}^{\infty}\frac{(4n+m+3)}{[(2n+1)(2n+2+m)]^2}. \tag{61}$$

The remaining integral in Eq. (56) is

$$\mathfrak{K}_3=\sum_{n=0}^{\infty}\frac{1}{(2n+1)^2}\int_1^{c/(b+1)}\frac{\tau^{-2n-1}}{(c-\tau b)}d\tau+\tfrac{1}{2}\int_1^{c/(b+1)}\frac{\ln\tau\ln[(\tau+1)/(\tau-1)]}{c-\tau b}d\tau. \tag{62}$$

The first integral in Eq. (62) is straightforward and is evaluated to yield

$$\frac{1}{c}\left[\frac{b}{c}\right]^{2n}\left[\ln(c-b)+\sum_{m=1}^{2n}\frac{1}{b^i i}[c^i-(b+1)^i]\right], \tag{63}$$

and the remaining integral can be evaluated as

$$\frac{1}{2b}\ln\left[\frac{c+b}{c-b}\right]\left[\ln\left[\frac{c}{b}\right]\ln(c-b)+\tfrac{1}{2}\ln^2\left[\frac{b+1}{b}\right]-\tfrac{1}{2}\ln^2\left[\frac{b}{c}\right]-\mathrm{Li}_2\left[\frac{c-b}{c}\right]+\mathrm{Li}_2\left[\frac{1}{b+1}\right]\right]+\frac{1}{c}\sum_{k=1}^{\infty}\frac{1}{2k+1}\left[\frac{b}{c}\right]^{2k}\sum_{n=1}^{2k}\left\{\left[\frac{c}{b}\right]^{n}\frac{1}{n^2}-\frac{1}{n}\left[\frac{b+1}{b}\right]^{n}\left[\ln\left[\frac{c}{b+1}\right]+\frac{1}{n}\right]\right\}, \tag{64}$$

where $\mathrm{Li}_2(x)$ is Euler's dilogarithm function. Combining Eqs. (62)–(64) gives the final result for $\mathfrak{K}_3$.

For the case of general j, $\mathcal{K}(-2,j,-2,\alpha,\beta,\gamma)$ can be evaluated in closed form after some rather tedious and lengthy algebra. The details are presented in Appendix B.

III. $I(i,j,k,-2,m,n,\alpha,\beta,\gamma)$ m AND n *NOT* BOTH ODD

In this section the I integral with i,j,k each ≥ -2 and $m,n \geq -1$, and with the restriction that m and n are *not both odd* is considered. For this case, the I integrals can be reduced to a set of $\mathcal{I}$ integrals, the latter integrals having been discussed in detail in the preceding section. Without loss of generality n is assumed even in the following development. The symmetry exhibited by the I integrals, namely,

$$\begin{aligned}I(i,j,k,l,m,n,\alpha,\beta,\gamma)&=I(i,k,j,l,n,m,\alpha,\gamma,\beta)\\&=I(j,i,k,m,l,n,\beta,\alpha,\gamma)\\&=I(j,k,i,m,n,l,\beta,\gamma,\alpha)\\&=I(k,j,i,n,m,l,\gamma,\beta,\alpha)\\&=I(k,i,j,n,l,m,\gamma,\alpha,\beta)\end{aligned} \tag{65}$$

can be employed to interchange m and n.

The Sack expansion of the function u_2^m takes the form [33]

$$u_2^m=\sum_{p=0}^{\infty}R_{mp}(r_3,r_1)P_p(\cos\theta_{31}) \tag{66}$$

where $P_p(\cos\theta)$ are the Legendre polynomials and $R_{mp}(r_3,r_1)$ denotes the radial functions. Several formulas for R_{mp} are given by Sack. If the above expansion for u_2^m and the analogous expansion for u_3^n are inserted into the expression for the I integral of the Sec. III title, then

$$I(i,j,k,-2,m,n,\alpha,\beta,\gamma)=\int r_1^i r_2^j r_3^k u_1^{-2} u_2^m u_3^n e^{-\alpha r_1-\beta r_2-\gamma r_3} d\mathbf{r}_1\, d\mathbf{r}_2\, d\mathbf{r}_3$$
$$=\sum_{p=0}^{\infty}\sum_{l_1=0}^{\infty}\int r_1^i r_2^j r_3^k u_1^{-2} e^{-\alpha r_1-\beta r_2-\gamma r_3} R_{mp}(r_3,r_1) R_{nl_1}(r_1,r_2)$$
$$\times P_p(\cos\theta_{31}) P_{l_1}(\cos\theta_{12}) d\mathbf{r}_1\, d\mathbf{r}_2\, d\mathbf{r}_3 \ . \quad (67)$$

Employing the standard expansion of the Legendre polynomials in terms of spherical harmonics

$$P_l(\cos\theta_{31})=\frac{4\pi}{2l+1}\sum_{m=-l}^{l} Y_{lm}^*(\theta_3,\phi_3) Y_{lm}(\theta_1,\phi_1) \ , \quad (68)$$

and inserting this into Eq. (67) yields

$$I(i,j,k,-2,m,n,\alpha,\beta,\gamma)=\sum_{p=0}^{\infty}\sum_{l_1=0}^{\infty}\left[\frac{4\pi}{2p+1}\right]\left[\frac{4\pi}{2l_1+1}\right]$$
$$\times\sum_{M=-p}^{p}\sum_{M_1=-l_1}^{l_1}\int r_1^{i+2} r_2^j r_3^k u_1^{-2} e^{-\alpha r_1-\beta r_2-\gamma r_3}$$
$$\times R_{mp}(r_3,r_1) R_{nl_1}(r_1,r_2) dr_1\, d\mathbf{r}_2\, d\mathbf{r}_3$$
$$\times\int Y_{pM}^*(\theta_3,\phi_3) Y_{pM}(\theta_1,\phi_1) Y_{l_1M_1}^*(\theta_1,\phi_1)$$
$$\times Y_{l_1M_1}(\theta_2,\phi_2) d\Omega_1 \ . \quad (69)$$

Employing

$$\int Y_{l_1M_1}^*(\theta_1,\phi_1) Y_{pM}(\theta_1,\phi_1) d\Omega_1=\delta_{p,l_1}\delta_{M,M_1} \quad (70)$$

in Eq. (69) leads to

$$I(i,j,k,-2,m,n,\alpha,\beta,\gamma)=4\pi\sum_{p=0}^{\infty}\frac{1}{(2p+1)}\int r_1^{i+2} r_2^j r_3^k u_1^{-2} R_{mp}(r_3,r_1) R_{np}(r_1,r_2) e^{-\alpha r_1-\beta r_2-\gamma r_3} P_p(\cos\theta_{23}) dr_1\, d\mathbf{r}_2\, d\mathbf{r}_3 \ . \quad (71)$$

Two distinct expansions of the Sack radial function are employed:

$$R_{mp}(r_3,r_1)=\frac{(-m/2)_p}{(\frac{1}{2})_p} r_{13>}^{m-p} r_{13<}^p \sum_{t=0}^{\infty} a_{pmt}\left[\frac{r_{13<}}{r_{13>}}\right]^{2t} \quad (72)$$

where

$$a_{pmt}=\frac{(p-m/2)_t(-\frac{1}{2}-m/2)_t}{t!(p+\frac{3}{2})_t}, \quad (73)$$

$(a)_b$ denotes a Pochhammer symbol, $r_{13>}$ denotes the greater of (r_1,r_3), and $r_{13<}$ denotes the lesser of (r_1,r_3). The second expansion employed is

$$R_{np}(r_1,r_2)=\frac{(-n/2)_p}{(\frac{1}{2})_p}\frac{r_1^p r_2^p}{(r_1+r_2)^{2p-n}}\sum_{u=0}^{\infty} b_{pnu}\left[\frac{4r_1r_2}{(r_1+r_2)^2}\right]^u \quad (74)$$

where

$$b_{pnu}=\frac{(p-n/2)_u(1+p)_u}{u!(2+2p)_u} \ . \quad (75)$$

If these expansions are inserted into Eq. (71) then

$$I(i,j,k-2,m,n,\alpha,\beta,\gamma)=4\pi\sum_{p=0}^{\infty}\sum_{t=0}^{\infty}\sum_{u=0}^{\infty}\frac{2^{2u}(-m/2)_p(-n/2)_p}{(2p+1)[(1/2)_p]^2}a_{pmt}b_{pnu}$$
$$\times\int r_2^{j+p+u}r_3^k u_1^{-2}e^{-\beta r_2-\gamma r_3}P_p(\cos\theta_{23})$$
$$\times\mathcal{g}(i+2+p+u,m-p-2t,p+2t,n-2p-2u,\alpha,r_2,r_3)d\mathbf{r}_2\,d\mathbf{r}_3 \qquad (76)$$

with

$$\mathcal{g}(L,M,N,P,\alpha,r_2,r_3)=\int_0^\infty e^{-\alpha r_1}r_1^L r_{13>}^M r_{13<}^N(r_1+r_2)^P dr_1 \,. \qquad (77)$$

On noting the property of the Pochhammer symbol (for integer k)

$$(-k)_l=0,\quad l>k\;, \qquad (78)$$

then the p summation in Eq. (76) terminates at $p=n/2$ (recall the even restriction placed on n at the start of this section) and the u summation terminates at $(n/2-p)$. It is clear that the power P in Eq. (77) is always ≥ 0, which allows a finite binomial expansion of the $(r_1+r_2)^P$ factor. On splitting the range $[0,\infty)$ into $[0,r_3]$ and $[r_3,\infty)$ in Eq. (77), $\mathcal{g}$ is evaluated to be

$$\mathcal{g}(L,M,N,P,\alpha,r_2,r_3)=\sum_{v=0}^{P}\begin{bmatrix}P\\v\end{bmatrix}r_2^v r_3^M\alpha^{-(L+N+P-v+1)}$$
$$\times\left[(L+P+N-v)!-e^{-\alpha r_3}Z(L+P+N-v,\alpha,r_3)+\begin{Bmatrix}(\alpha r_3)^{N-M}e^{-\alpha r_3}Z(L+M+P-v,\alpha,r_3)\\ r_3^{N-M}\alpha^{L+P+N-v+1}E_1(\alpha r_3)\end{Bmatrix}\right] \qquad (79)$$

with

$$Z(q,\alpha,r_3)=q!\sum_{z=0}^{q}\frac{(\alpha r_3)^z}{z!}\,. \qquad (80)$$

An analysis of the factor $(L+M+P-v)$ [see Eq. (76)] shows that the minimum value is zero for even m and -1 for odd m, assuming the lowest i value possible. The top factor in the braces in Eq. (79) is employed when $(L+M+P-v)\geq 0$, otherwise the term involving the exponential integral is employed.

The Legendre polynomial appearing in Eq. (76) can be expanded as

$$P_p(\cos\theta_{23})=\sum_{q=0}^{[p/2]}\sum_{r=0}^{p-2q}\sum_{s=0}^{p-2q-r}(-1)^{q+r}\begin{bmatrix}p-2q\\r\end{bmatrix}\begin{bmatrix}p-2q-r\\s\end{bmatrix}(2p-2q)!\frac{r_2^{p-2q-2r-2s}r_3^{-p+2q+2s}r_{23}^{2r}}{2^{2p-2q}q!(p-q)!(p-2q)!} \qquad (81)$$

where $[p/2]=p/2$ for p even or $(p-1)/2$ for p odd.

If the above expressions for $\mathcal{g}$ and $P_p(\cos\theta_{23})$ are inserted into Eq. (76) and the following notational simplifications introduced:

$$\mathfrak{z}_1=i+2+n+2t-u-v\;, \qquad (82)$$

$$\mathfrak{z}_2=j+2p+u-2q-2r-2s+v\;, \qquad (83)$$

$$\mathfrak{z}_3=k+m-2p+2q+2s-2t\;, \qquad (84)$$

$$\mathfrak{z}_4=k+2q+2s+2t\;, \qquad (85)$$

$$\mathfrak{z}_5=i+2+m+n-2p-u-v-2t\;, \qquad (86)$$

then Eq. (76) yields

$$I(i,j,k,-2,m,n,\alpha,\beta,\gamma)=\frac{4\pi}{\alpha^{i+n+3}}\sum_{p=0}^{p_{\max}}\sum_{q=0}^{[p/2]}\sum_{r=0}^{p-2q}\sum_{s=0}^{p-2q-r}\sum_{t=0}^{t_{\max}}\sum_{u=0}^{u_{\max}}\sum_{v=0}^{n-2p-2u}\frac{(-1)^{q+r}}{(2p+1)}a_{pmt}b_{pnu}$$
$$\times\frac{\begin{bmatrix} n-2p-2u \\ v \end{bmatrix}(2p-2q)!(-m/2)_p(-n/2)_p}{r!s!(p-2q-r-s)!q!(p-q)![(\frac{1}{2})_p]^2 4^{p-q-u}\alpha^{2t-u-v}}$$
$$\times\Bigg[\mathfrak{z}_1!\mathcal{J}(\mathfrak{z}_2,\mathfrak{z}_3,2r-2,\beta,\gamma)-\mathfrak{z}_1!\sum_{w=0}^{\mathfrak{z}_1}\frac{\alpha^w}{w!}\mathcal{J}(\mathfrak{z}_2,\mathfrak{z}_3+w,2r-2,\beta,\alpha+\gamma)$$
$$+\left[\frac{\mathfrak{z}_5!}{\alpha^{m-2p-4t}}\sum_{w=0}^{\mathfrak{z}_5}\frac{\alpha^w}{w!}\mathcal{J}(\mathfrak{z}_2,\mathfrak{z}_4+w,2r-2,\beta,\alpha+\gamma)\right]_{\mathfrak{z}_5\geq 0}$$
$$+\alpha^{\mathfrak{z}_1+1}\mathcal{K}(\mathfrak{z}_2,\mathfrak{z}_4,2r-2,\alpha,\beta,\gamma)\delta_{\mathfrak{z}_5,-1}\Bigg] \tag{87}$$

and all the $\mathcal{J}$ and $\mathcal{K}$ integrals needed are defined and evaluated in Sec. II. Equation (87) is one of the two principal results of this investigation. It represents the reduction of the three-electron integral problem for the case under consideration to the two-electron case.

The maximum limits on the p, t, and u summations, denoted by $p_{\max}$, $t_{\max}$, and $u_{\max}$, respectively, are determined by the appropriate Pochhammer symbols appearing in Eq. (87). $p_{\max}=n/2$ or, if m is also even, then $p_{\max}=\min(m/2,n/2)$. $u_{\max}=n/2-p$ and $t_{\max}=(m+1)/2$ if m is odd or $t_{\max}=m/2-p$ if m is even.

The following restrictions can be put on the use of Eq. (87). The odd-m–odd-n exclusion has already been referred to at the start of this section. By reference to Eq. (82) the following condition must hold:

$$\mathfrak{z}_1\geq 0 \Longrightarrow i\geq -2\ . \tag{88}$$

For $r=0$ in Eq. (87) the integrals $\mathcal{J}(\mathfrak{z}_2,\mathfrak{z}_3,-2,\alpha,\beta)$, $\mathcal{J}(\mathfrak{z}_2,\mathfrak{z}_4,-2,\alpha,\beta)$, and $\mathcal{K}(\mathfrak{z}_2,\mathfrak{z}_4,-2,\alpha,\beta,\gamma)$ must be convergent. By reference to Eqs. (83)–(85) the following constraints can be deduced. For m even,

$$\begin{aligned} &i\geq -2\ ,\\ &j\geq -2\ ,\\ &k\geq -2\ ,\\ &j+k\geq -3\ ,\\ &j+k+m\geq -3\ , \end{aligned} \tag{89}$$

and (with n even and ≥ 0 assumed) for m odd,

$$\begin{aligned} &i\geq -2\ ,\\ &j\geq -2\ ,\\ &k\geq n-1\ ,\\ &j+k-n\geq -2\ . \end{aligned} \tag{90}$$

The $\mathcal{K}$ integral in Eq. (87) arises only when $i=-2$ and m is odd. Since n is restricted to even values and $k\geq n-1$, only $\mathcal{K}$ integrals for $\mathfrak{z}_4\geq -1$ arise.

Table I presents results for various I integrals evaluated using Eq. (87). A wide selection of I integrals are presented which utilize the different $\mathcal{J}$ and $\mathcal{K}$ integrals that arise in this expression. The first 42 entries in the table were checked independently using the approach discussed in the next section. The number of decimal digits of precision that matched was in the range 19–27, with the smaller number of matching digits occurring for larger values of m and n, and large values of the sum $i+j+k+m+n$. For the remaining entries in Table I, the methods of the next section are somewhat slower and were used to generate approximately 12–15 significant figures for the I integrals, in order to compare with the results from Eq. (87). This match does provide an important check, but leaves some uncertainty in the number of significant figures being generated using Eq. (87) for these cases. However, there appears to be no reason to expect any major change in the number of significant figures being generated for these entries using Eq. (87). All the numerical evaluations in this work were carried out on a Cray 1M in double precision (which yields approximately 28 decimal digits).

IV. $I(i,j,k,-2,m,n,\alpha,\beta,\gamma)$— THE GENERAL CASE

In this section the general integral $I(i,j,k,-2,m,n,\alpha,\beta,\gamma)$ $(m\geq 1, n\geq 1)$ is reduced to simpler integrals. Unfortunately, the relative simplicity of the result obtained in Sec. III is lost for the general case.

A. Expansion formula for r_{ij}^{-2}

To evaluate the general case a suitable expansion for r_{ij}^{-2} is required The following approach is based on the

TABLE I. Values of $I(i,j,k,l,m,n,\alpha,\beta,\gamma)$ computed using Eq. (87).

i	j	k	l	m	n	α	β	γ	I
0	0	0	−2	0	0	2.0	2.0	2.0	$2.067\,085\,112\,019\,988\,011\,698\,421\,00 \times 10^{1}$
0	0	0	−2	0	0	5.0	5.0	5.0	$3.386\,712\,247\,533\,548\,358\,366\,692\,97 \times 10^{-2}$
0	0	0	−2	0	0	2.7	2.9	0.65	$2.069\,431\,027\,531\,892\,717\,303\,914\,29 \times 10^{1}$
0	0	0	−2	0	2	2.7	2.9	0.65	$5.834\,638\,925\,250\,533\,005\,404\,820\,65 \times 10^{1}$
0	0	0	−2	0	4	2.7	2.9	0.65	$3.434\,050\,939\,387\,686\,769\,519\,490\,8 \times 10^{2}$
0	0	−1	−2	2	4	2.7	2.9	0.65	$2.399\,706\,201\,578\,161\,234\,002\,003\,8 \times 10^{3}$
2	2	2	−2	0	0	2.7	2.9	0.65	$3.051\,914\,096\,585\,057\,305\,590\,024\,6 \times 10^{2}$
2	2	2	−2	0	2	2.7	2.9	0.65	$2.350\,220\,972\,043\,034\,399\,333\,867\,8 \times 10^{3}$
2	2	2	−2	0	4	2.7	2.9	0.65	$3.179\,460\,482\,863\,080\,485\,056\,679\,6 \times 10^{4}$
1	1	1	−2	0	2	2.7	2.9	0.65	$2.303\,824\,600\,389\,656\,487\,454\,977\,7 \times 10^{2}$
1	1	1	−2	0	4	2.7	2.9	0.65	$2.155\,598\,471\,373\,367\,692\,201\,820\,4 \times 10^{3}$
1	1	1	−2	1	0	2.7	2.9	0.65	$1.654\,915\,009\,958\,514\,078\,982\,271\,0 \times 10^{2}$
3	3	2	−2	0	4	2.7	2.9	0.65	$1.892\,395\,797\,843\,513\,878\,591\,765 \times 10^{5}$
3	3	2	−2	2	4	2.7	2.9	0.65	$8.382\,093\,933\,453\,153\,119\,689\,782 \times 10^{6}$
3	3	3	−2	2	2	2.7	2.9	0.65	$2.750\,777\,067\,630\,129\,348\,914\,527 \times 10^{6}$
3	3	3	−2	2	4	2.7	2.9	0.65	$5.518\,061\,029\,454\,149\,476\,487\,148 \times 10^{7}$
3	3	2	−2	−1	0	2.7	2.9	0.65	$2.573\,361\,421\,526\,794\,238\,287\,725 \times 10^{2}$
3	3	2	−2	−1	2	2.7	2.9	0.65	$2.352\,124\,263\,232\,767\,920\,735\,299 \times 10^{3}$
3	2	3	−2	−1	0	2.7	2.9	0.65	$5.357\,654\,836\,588\,144\,700\,825\,901 \times 10^{2}$
3	2	3	−2	−1	2	2.7	2.9	0.65	$4.580\,429\,171\,980\,893\,713\,536\,495 \times 10^{3}$
3	2	3	−2	1	0	2.7	2.9	0.65	$1.661\,934\,415\,781\,205\,486\,972\,822 \times 10^{4}$
3	2	3	−2	1	2	2.7	2.9	0.65	$1.655\,254\,412\,226\,743\,522\,888\,135 \times 10^{5}$
3	2	3	−2	3	0	2.7	2.9	0.65	$1.262\,075\,100\,417\,932\,549\,496\,420 \times 10^{6}$
3	2	3	−2	3	2	2.7	2.9	0.65	$1.316\,185\,845\,361\,141\,014\,644\,198 \times 10^{7}$
0	0	0	−2	4	4	2.7	2.9	0.65	$1.423\,236\,982\,236\,386\,168\,558\,231 \times 10^{5}$
0	0	0	−2	6	4	0.5	0.5	1.0	$2.358\,198\,302\,782\,912\,116\,458\,407 \times 10^{16}$
−1	0	0	−2	−1	0	2.7	2.9	0.65	$2.067\,321\,071\,227\,145\,287\,680\,895 \times 10^{1}$
−1	0	0	−2	0	0	2.7	2.9	0.65	$2.793\,731\,887\,168\,055\,168\,360\,284 \times 10^{1}$
−1	0	0	−2	0	2	2.7	2.9	0.65	$5.577\,394\,740\,719\,449\,871\,403\,270 \times 10^{1}$
−1	0	0	−2	0	4	2.7	2.9	0.65	$2.474\,991\,388\,450\,957\,507\,219\,897 \times 10^{2}$
−1	0	0	−2	1	0	2.7	2.9	0.65	$6.030\,719\,203\,675\,633\,061\,583\,526 \times 10^{1}$
−1	2	3	−2	0	0	2.7	2.9	0.65	$1.144\,010\,541\,077\,014\,596\,095\,036 \times 10^{3}$
−1	2	3	−2	0	2	2.7	2.9	0.65	$5.153\,289\,329\,234\,846\,352\,545\,967 \times 10^{3}$
−1	−1	3	−2	0	0	2.7	2.9	0.65	$1.106\,225\,242\,658\,711\,311\,585\,232 \times 10^{3}$
−1	−1	3	−2	0	2	2.7	2.9	0.65	$1.725\,301\,862\,323\,040\,537\,224\,447 \times 10^{3}$
−1	−1	3	−2	0	4	2.7	2.9	0.65	$6.739\,279\,036\,920\,982\,069\,090\,995 \times 10^{3}$
−1	−1	3	−2	2	2	2.7	2.9	0.65	$8.383\,204\,201\,213\,800\,191\,615\,640 \times 10^{4}$
−2	−1	−1	−2	0	0	2.7	2.9	0.65	$1.376\,066\,844\,627\,906\,944\,819\,661 \times 10^{2}$
−2	−1	−1	−2	0	2	2.7	2.9	0.65	$9.138\,865\,880\,993\,483\,437\,450\,698 \times 10^{1}$
−2	−1	−1	−2	0	4	2.7	2.9	0.65	$1.914\,808\,553\,442\,016\,138\,095\,538 \times 10^{2}$
−2	−1	−1	−2	2	2	2.7	2.9	0.65	$2.975\,496\,827\,447\,503\,261\,280\,484 \times 10^{2}$
−2	−1	−1	−2	2	4	2.7	2.9	0.65	$1.001\,224\,088\,412\,704\,075\,110\,145 \times 10^{3}$
−2	−2	−1	−2	0	0	2.7	2.9	0.65	$6.404\,335\,322\,907\,260\,289\,063\,400 \times 10^{2}$
−2	−2	−1	−2	2	2	2.7	2.92	2.65	$1.715\,887\,878\,071\,845\,875\,610\,635 \times 10^{2}$
−2	−2	0	−2	2	4	2.7	2.9	0.65	$2.867\,034\,747\,696\,047\,768\,426\,855 \times 10^{3}$
−2	−2	1	−2	2	2	2.7	2.9	0.65	$4.793\,502\,392\,148\,070\,693\,668\,806 \times 10^{3}$
−2	−2	1	−2	2	4	2.7	2.9	0.65	$1.050\,013\,709\,895\,394\,890\,960\,258 \times 10^{4}$
−2	−2	2	−2	2	2	2.7	2.9	0.65	$2.820\,676\,020\,288\,631\,555\,890\,723 \times 10^{4}$
−1	−2	−1	−2	2	2	2.7	2.9	0.65	$8.133\,653\,681\,661\,903\,522\,531\,843 \times 10^{2}$
−1	−2	1	−2	3	0	2.7	2.9	0.65	$2.066\,569\,861\,842\,100\,263\,569\,142 \times 10^{4}$
−1	−2	2	−2	−1	2	2.7	2.9	0.65	$2.168\,791\,565\,210\,574\,301\,222\,774 \times 10^{2}$
−1	−2	2	−2	1	2	2.7	2.9	0.65	$3.576\,974\,714\,380\,302\,751\,730\,570 \times 10^{3}$
−2	−2	0	−2	−1	0	2.7	2.9	0.65	$4.623\,806\,824\,305\,902\,305\,315\,834 \times 10^{2}$
−2	−2	0	−2	1	0	2.7	2.9	0.65	$6.473\,942\,674\,258\,305\,779\,561\,337 \times 10^{2}$
−2	−2	1	−2	−1	0	2.7	2.9	0.65	$3.477\,322\,585\,501\,385\,971\,888\,241 \times 10^{2}$
−2	−2	1	−2	3	0	2.7	2.9	0.65	$5.363\,393\,270\,088\,623\,464\,144\,902 \times 10^{4}$
−2	−2	2	−2	−1	2	2.7	2.9	0.65	$2.986\,965\,412\,857\,829\,505\,998\,896 \times 10^{2}$

work of Sack [33]. The Sack expansion of r_{12}^{-2} takes the form

$$r_{12}^{-2}=\sum_{l=0}^{\infty} R_{-2l}(r_1,r_2)P_l(\cos\theta_{12}) . \tag{91}$$

The R functions of Sack can be expressed as hypergeometric functions. If Eq. (27a) of Sack's paper is employed then

$$R_{-2l}(r_1,r_2)=\frac{(1)_l r_1^l r_2^l}{(\frac{1}{2})_l(r_1^2+r_2^2)^{l+1}} \times F(\tfrac{1}{2}l+1,\tfrac{1}{2}l+\tfrac{1}{2};\tfrac{3}{2}+l;\rho^2) \tag{92}$$

where

$$\rho=\frac{2r_1r_2}{r_1^2+r_2^2} . \tag{93}$$

Equation (92) can be cast in terms of the Legendre functions of the second kind [34] to yield

$$R_{-2l}(r_1,r_2)=\frac{2l+1}{2r_1r_2}Q_l(1/\rho) . \tag{94}$$

Sack [33] was aware of the connection between the R functions and the Legendre functions of the second kind, but he did not pursue the connection. Now using the following result [35]:

$$Q_l(z)=Q_0(z)P_l(z)-W_{l-1}(z) \tag{95}$$

where $W_{l-1}(z)$ is a polynomial in z, then

$$r_{12}^{-2}=\sum_{l=0}^{\infty}\frac{2l+1}{2r_1r_2}\left[Q_0\left[\frac{1}{\rho}\right]P_l\left[\frac{1}{\rho}\right]-W_{l-1}\left[\frac{1}{\rho}\right]\right] \times P_l(\cos\theta_{12}) . \tag{96}$$

Using the value of $Q_0(1/\rho)$ and the expansion of $P_l(1/\rho)$, the first factor in the square brackets in Eq. (96) can be expressed as

$$Q_0\left[\frac{1}{\rho}\right]P_l\left[\frac{1}{\rho}\right]=\tfrac{1}{2}\ln\left|\frac{1+1/\rho}{1-1/\rho}\right|\sum_{r=0}^{[l/2]}\frac{(-1)^r(2l-2r)!}{2^l r!(l-r)!(l-2r)!}\left[\frac{1}{\rho}\right]^{l-2r}$$
$$=\frac{1}{(4r_1r_2)^l}\sum_{r=0}^{[l/2]}(-4)^r\begin{bmatrix}2l-2r\\ l\end{bmatrix}\begin{bmatrix}l\\ r\end{bmatrix}(r_1r_2)^{2r}(r_1^2+r_2^2)^{l-2r}\ln\left|\frac{r_1+r_2}{r_1-r_2}\right| . \tag{97}$$

If $(r_1^2+r_2^2)^{l-2r}$ is expanded as a binomial series and a summation rearrangement is made, Eq. (97) simplifies to

$$Q_0\left[\frac{1}{\rho}\right]P_l\left[\frac{1}{\rho}\right]=\frac{1}{(4r_1r_2)^l}\ln\left|\frac{r_1+r_2}{r_1-r_2}\right|\sum_{\kappa=0}^{l} r_1^{2\kappa}r_2^{2l-2\kappa}\sum_{v=0}^{\min[\kappa,l-\kappa]}(-4)^v\begin{bmatrix}l\\ v\end{bmatrix}\begin{bmatrix}2l-2v\\ l\end{bmatrix}\begin{bmatrix}l-2v\\ \kappa-v\end{bmatrix} . \tag{98}$$

From Ref. [36] it can be deduced that

$$W_{l-1}(x)=\frac{(2l-1)!!}{l!}\sum_{\mu=0}^{[(l-1)/2]}x^{l-1-2\mu}\sum_{v=0}^{\mu}\frac{(-1)^v l!(2l-1-2v)!!}{(2\mu-2v+1)(2v)!!(l-2v)!(2l-1)!!} \tag{99}$$

and hence

$$W_{l-1}\left[\frac{1}{\rho}\right]=\rho^{-l+1}\sum_{\mu=0}^{[(l-1)/2]}\rho^{2\mu}\sum_{v=0}^{\mu}\frac{(-1)^v(2l-1-2v)!!}{(2\mu-2v+1)2^v v!(l-2v)!}$$
$$=2^{-l}\rho^{-l+1}\sum_{\mu=0}^{[(l-1)/2]}\rho^{2\mu}\sum_{v=0}^{\mu}\frac{(-1)^v}{(2\mu-2v+1)}\begin{bmatrix}2l-2v\\ l\end{bmatrix}\begin{bmatrix}l\\ v\end{bmatrix} . \tag{100}$$

Inserting the expression for ρ and employing a binomial expansion for $(r_1^2+r_2^2)^{l-1-2\mu}$, followed by a summation rearrangement, leads to

$$W_{l-1}\left[\frac{1}{\rho}\right]=2^{-2l+1}\sum_{\kappa=0}^{l-1}r_1^{-l+1+2\kappa}r_2^{l-2\kappa-1}\sum_{j=0}^{\min[\kappa,l-\kappa-1]}4^j\begin{bmatrix}l-2j-1\\ \kappa-j\end{bmatrix}\sum_{v=0}^{j}\frac{(-1)^v\begin{bmatrix}l\\ v\end{bmatrix}\begin{bmatrix}2l-2v\\ l\end{bmatrix}}{2j-2v+1} . \tag{101}$$

Inserting Eqs. (98) and (101) into Eq. (96) yields

$$\frac{1}{r_{12}^2}=\sum_{l=0}^{\infty}\left[\frac{2l+1}{2}\right]4^{-l}\left[\ln\left|\frac{r_1+r_2}{r_1-r_2}\right|\sum_{\kappa=0}^{l}r_1^{2\kappa-l-1}r_2^{l-2\kappa-1}\sum_{v=0}^{\min[\kappa,l-\kappa]}(-4)^v\begin{bmatrix}l\\v\end{bmatrix}\begin{bmatrix}2l-2v\\l\end{bmatrix}\begin{bmatrix}l-2v\\\kappa-v\end{bmatrix}\right.$$
$$\left.-2\sum_{\kappa=0}^{l-1}r_1^{-l+2\kappa}r_2^{l-2\kappa-2}\sum_{j=0}^{\min[\kappa,l-\kappa-1]}4^j\begin{bmatrix}l-2j-1\\\kappa-j\end{bmatrix}\sum_{v=0}^{j}\frac{(-1)^v\begin{bmatrix}l\\v\end{bmatrix}\begin{bmatrix}2l-2v\\l\end{bmatrix}}{2j-2v+1}\right]P_l(\cos\theta_{12})\ . \tag{102}$$

An alternative to the above approach is to carry out a Neumann expansion in a series of Legendre polynomials.

The Neumann expansion approach was considered in a recent paper by Pauli and Kleindienst [24]. Ignoring a few minor misprints in their expression for r_{12}^{-2} (l should read l_{12} in two binomial coefficients), they have miscalculated the summation limits in three places, as well as incorrectly giving one binomial factor, which is readily observed to be inconsistent with the summation limits. An alternative approach to the expansion of r_{12}^{-2}, which was not exploited in the present investigation, is [37]

$$r_{12}^{-2}=\sum_{n=0}^{\infty}\frac{r_{12<}^{n}}{r_{12>}^{n+2}}\mathcal{C}_n^1(\cos\theta_{12}) \tag{103}$$

where $\mathcal{C}_n^1(\cos\theta)$ are the Gegenbauer polynomials. This form has obvious similarities with the well-known expansion of r_{12}^{-1} in terms of Legendre polynomials, however the "complexities" of the expansion are carried with the angular term. This expansion may merit detailed investigation. An alternative expansion for r_{12}^{-2} given in the literature [38] was explored in our initial investigations, but not employed for the final results of this section.

B. Evaluation of the I integrals using Eq. (102)

Utilizing the expression derived above for r_{ij}^{-2} a general formula for the I integral can be developed. Inserting Eq. (102) for r_{23}^{-2} into Eq. (1) yields

$$I(i,j,k,-2,m,n,\alpha,\beta,\gamma)$$
$$=\int\sum_{p=0}^{\infty}\sum_{l_1=0}^{\infty}\sum_{l=0}^{\infty}\left[\frac{2l+1}{2}\right]4^{-l}P_l(\cos\theta_{23})r_1^ir_2^jr_3^ke^{-\alpha r_1-\beta r_2-\gamma r_3}R_{mp}(r_3,r_1)R_{nl_1}(r_1,r_2)P_p(\cos\theta_{31})P_{l_1}(\cos\theta_{12})$$
$$\times\left[\sum_{\kappa=0}^{l}r_2^{-l-1+2\kappa}r_3^{l-1-2\kappa}\ln\left|\frac{r_2+r_3}{r_2-r_3}\right|\right.$$
$$\times\sum_{v=0}^{\min[\kappa,l-\kappa]}(-4)^v\begin{bmatrix}l\\r\end{bmatrix}\begin{bmatrix}2l-2v\\l\end{bmatrix}\begin{bmatrix}l-2v\\\kappa-v\end{bmatrix}$$
$$\left.-2\sum_{\kappa=0}^{l-1}r_2^{-l+2\kappa}r_3^{l-2\kappa-2}\sum_{j=0}^{\min[\kappa,l-\kappa-1]}4^j\begin{bmatrix}l-2j-1\\\kappa-j\end{bmatrix}\sum_{v=0}^{j}\frac{(-1)^v\begin{bmatrix}l\\v\end{bmatrix}\begin{bmatrix}2l-2v\\l\end{bmatrix}}{2j-2v+1}\right]d\mathbf{r}_1\,d\mathbf{r}_2\,d\mathbf{r}_3 \tag{104}$$

where the Sack expansion given in Eq. (66) has been employed. To simplify the notation set

$$\mathcal{F}(l,\kappa)=\sum_{v=0}^{\min[\kappa,l-\kappa]}(-4)^v\begin{bmatrix}l\\v\end{bmatrix}\begin{bmatrix}2l-2v\\l\end{bmatrix}\begin{bmatrix}l-2v\\\kappa-v\end{bmatrix} \tag{105}$$

and

$$\mathcal{G}(l,\kappa)=2\sum_{j=0}^{\min[\kappa,l-\kappa-1]}4^j\begin{bmatrix}l-2j-1\\\kappa-j\end{bmatrix}\sum_{v=0}^{j}\frac{(-1)^v\begin{bmatrix}l\\v\end{bmatrix}\begin{bmatrix}2l-2v\\l\end{bmatrix}}{2j-2v+1}\ . \tag{106}$$

The angle integral in Eq. (104) is

$$I_\Omega=\int P_l(\cos\theta_{23})P_p(\cos\theta_{31})P_{l_1}(\cos\theta_{12})d\Omega_1\,d\Omega_2\,d\Omega_3 \tag{107}$$

which can be evaluated on employing Eq. (68) to give

$$I_\Omega=\frac{64\pi^3}{(2l+1)^2}\delta_{l_1,p}\delta_{l,l_1}\delta_{p,l}\ . \tag{108}$$

So Eq. (104) simplifies to

$$I(i,j,k,-2,m,n,\alpha,\beta,\gamma)=32\pi^3\sum_{l=0}^{\infty}\frac{4^{-l}}{(2l+1)}\int R_{ml}(r_3,r_1)R_{nl}(r_1,r_2)r_1^{i+2}r_2^{j+2}r_3^{k+2}e^{-\alpha r_1-\beta r_2-\gamma r_3}$$
$$\times\left[\sum_{\kappa=0}^{l}r_2^{-l-1+2\kappa}r_3^{l-1-2\kappa}\ln\left|\frac{r_2+r_3}{r_2-r_3}\right|\mathcal{F}(l,\kappa)-\sum_{\kappa=0}^{l-1}r_2^{-l+2\kappa}r_3^{l-2\kappa-2}\mathcal{G}(l,\kappa)\right]dr_1\,dr_2\,dr_3\ . \tag{109}$$

Inserting the Sack expansions for $R_{ml}(r_3,r_1)$ and $R_{nl}(r_1,r_2)$ into Eq. (109) yields

$$I(i,j,k,-2,m,n,\alpha,\beta,\gamma)=32\pi^3\sum_{l=0}^{\infty}\frac{4^{-l}(-m/2)_l(-n/2)_l}{(2l+1)[(\frac{1}{2})_l]^2}\sum_{t=0}^{\infty}a_{lmt}\sum_{s=0}^{\infty}a_{lns}$$
$$\times\left[\sum_{\kappa=0}^{l}\mathcal{F}(l,\kappa)\int r_{13>}^{m-l-2t}r_{13<}^{l+2t}r_{12>}^{n-l-2s}r_{12<}^{l+2s}r_1^{i+2}r_2^{j+1-l+2\kappa}r_3^{k+1+l-2\kappa}\ln\left|\frac{r_2+r_3}{r_2-r_3}\right|\times e^{-\alpha r_1-\beta r_2-\gamma r_3}dr_1\,dr_2\,dr_3\right.$$
$$\left.-\sum_{\kappa=0}^{l-1}\mathcal{G}(l,\kappa)\int r_{13>}^{m-l-2t}r_{13<}^{l+2t}r_{12>}^{n-l-2s}r_{12<}^{l+2s}r_1^{i+2}r_2^{j+2-l+2\kappa}r_3^{k+l-2\kappa}e^{-\alpha r_1-\beta r_2-\gamma r_3}dr_1\,dr_2\,dr_3\right] \tag{110}$$

where a_{lns} is defined in Eq. (73). To simplify the notation define

$$\mathcal{R}_1\equiv\mathcal{R}_1(i,j,k,m,n,l,s,t,\alpha,\beta,\gamma)=\sum_{\kappa=0}^{l}\mathcal{F}(l,\kappa)\int r_{13>}^{m-l-2t}r_{13<}^{l+2t}r_{12>}^{n-l-2s}r_{12<}^{l+2s}r_1^{i+2}r_2^{j+1-l+2\kappa}r_3^{k+1+l-2\kappa}\ln\left|\frac{r_2+r_3}{r_2-r_3}\right|e^{-\alpha r_1-\beta r_2-\gamma r_3}dr_1\,dr_2\,dr_3 \tag{111}$$

and

$$\mathcal{R}_2\equiv\mathcal{R}_2(i,j,k,m,n,l,s,t,\alpha,\beta,\gamma)=-\sum_{\kappa=0}^{l-1}\mathcal{G}(l,\kappa)\int r_{13>}^{m-l-2t}r_{13<}^{l+2t}r_{12>}^{n-l-2s}r_{12<}^{l+2s}r_1^{i+2}r_2^{j+2-l+2\kappa}r_3^{k+l-2\kappa}e^{-\alpha r_1-\beta r_2-\gamma r_3}dr_1\,dr_2\,dr_3\ . \tag{112}$$

The $\mathcal{R}_2$ integral can be simplified by splitting the integration range for the six choices $0\le r_i\le r_j\le r_k<\infty$, with the result that

$$\begin{aligned}\mathcal{R}_2=-\sum_{\kappa=0}^{l-1}\mathcal{G}(l,\kappa)[&W(i+2+2l+2t+2s,j+2+n-2l-2s+2\kappa,k+m-2t-2\kappa,\alpha,\beta,\gamma)\\&+W(j+2+2s+2\kappa,i+2+n+2t-2s,k+m-2t-2\kappa,\beta,\alpha,\gamma)\\&+W(k+2t+2l-2\kappa,j+2+2s+2\kappa,i+2+m+n-2l-2t-2s,\gamma,\beta,\alpha)\\&+W(i+2+2l+2s+2t,k+m-2t-2\kappa,j+2+n-2l-2s+2\kappa,\alpha,\gamma,\beta)\\&+W(j+2+2s+2\kappa,k+2l+2t-2\kappa,i+2+m+n-2l-2s-2t,\beta,\gamma,\alpha)\\&+W(k+2l+2t-2\kappa,i+2+m+2s-2t,j+2+n-2l-2s+2\kappa,\gamma,\alpha,\beta)]\end{aligned} \tag{113}$$

where

$$W(L,M,N,a,b,c)=\int_0^\infty x^Le^{-ax}dx\int_x^\infty y^Me^{-by}dy\int_y^\infty z^Ne^{-cz}dz\ . \tag{114}$$

The W integrals appearing in Eq. (114) have been discussed in several places in the literature [1,2,12,14,18]. Efficient algorithms for their evaluation are available [12].

In a similar fashion the $\mathcal{R}_1$ integral can be split up as a sum of six integrals to yield

$$\mathcal{R}_1=\sum_{\kappa=0}^{l}\mathcal{F}(l,\kappa)[W_{L_1}(i+2+2l+2s+2t,j+1+n-2l-2s+2\kappa,k+1+m-2t-2\kappa,\alpha,\beta,\gamma)$$
$$+W_{L_1}(i+2+2l+2s+2t,k+1+m-2t-2\kappa,j+1+n-2l-2s+2\kappa,\alpha,\gamma,\beta)$$
$$+W_{L_2}(k+1+2l+2t-2\kappa,j+1+2s+2\kappa,i+2+m+n-2l-2s-2t,\gamma,\beta,\alpha)$$
$$+W_{L_2}(j+1+2s+2\kappa,k+1+2l+2t-2\kappa,i+2+m+n-2l-2t-2s,\beta,\gamma,\alpha)$$
$$+W_{L_3}(j+1+2s+2\kappa,i+2+n+2t-2s,k+1+m-2t-2\kappa,\beta,\alpha,\gamma)$$
$$+W_{L_3}(k+1+2l+2t-2\kappa,i+2+m+2s-2t,j+1+n-2l-2s+2\kappa,\gamma,\alpha,\beta)] \quad (115)$$

where

$$W_{L_1}(L,M,N,a,b,c)=\int_0^\infty x^L e^{-ax}dx\int_x^\infty y^M e^{-by}dy\int_y^\infty z^N e^{-cz}\ln\left|\frac{z+y}{z-y}\right|dz\ , \quad (116)$$

$$W_{L_2}(L,M,N,a,b,c)=\int_0^\infty x^L e^{-ax}dx\int_x^\infty y^M e^{-by}\ln\left|\frac{y+x}{y-x}\right|dy\int_y^\infty z^N e^{-cz}dz\ , \quad (117)$$

and

$$W_{L_3}(L,M,N,a,b,c)=\int_0^\infty x^L e^{-ax}dx\int_x^\infty y^M e^{-by}dy\int_y^\infty z^N e^{-cz}\ln\left|\frac{z+x}{z-x}\right|dz\ . \quad (118)$$

The above integrals can be simplified down to two-dimensional integrals, and a complete discussion of these is given in Appendix C. Since the whole analysis of the general case being considered in this section hinges on the solution of the W_{L_1}, W_{L_2}, and W_{L_3} integrals, a complete discussion of their evaluation is given in Appendix D. Some representative values for the above W_{L_1}, W_{L_2}, and W_{L_3} integrals are given in Table II.

So the final result obtained is

$$I(i,j,k,-2,m,n,\alpha,\beta,\gamma)=32\pi^3\sum_{w=0}^{\infty}\frac{4^{-w}(-m/2)_w(-n/2)_w}{(2w+1)[(\frac{1}{2})_w]^2}\sum_{s=0}^{\infty}a_{wns}\sum_{t=0}^{\infty}a_{wmt}[\mathcal{R}_1(i,j,k,m,n,w,s,t,\alpha,\beta,\gamma)$$
$$+\mathcal{R}_2(i,j,k,m,n,w,s,t,\alpha,\beta,\gamma)] \quad (119)$$

with Eqs. (115) and (113) providing a route for the evaluation of $\mathcal{R}_1$ and $\mathcal{R}_2$. Equation (119) is a principal result of this study.

As discussed in detail in Appendix D, the slow integrals to compute are W_{L_1}, W_{L_2}, and particularly W_{L_3} with negative values for L, M, and N. By inspection of Eq. (115) the following observations can be made. If m and n are both even in Eq. (119), then with

$$i\geq -2,\quad j\geq -1,\quad k\geq -1 \quad (120)$$

no W_L integrals with negative arguments arise, and the computational time required for the evaluation of the I integral is relatively short. If m is even, and n is odd and

$$i\geq -1,\quad j\geq m,\quad k\geq -1\ , \quad (121)$$

or m is odd and n is even and

$$i\geq -1,\quad j\geq -1,\quad k\geq n\ , \quad (122)$$

W_L integrals with negative arguments do not arise, and as above, the computational time for the I integral is short. When m and n are both odd, W_L integrals with negative arguments arise, and the computational speed for the evaluation of the I integrals is somewhat slow, particularly if more than about 10 significant figures are required. A good fraction of the evaluation time is tied up in the calculation of W_{L_3} integrals with negative arguments. Equation (119) has been employed to calculate a large number of I integrals. This formula has provided an important check on the result of Sec. III.

In Table III some results are presented for I integrals not accessible by the methods of Sec. III. The number of significant figures presented was determined by successively decreasing the summation cutoff tolerance for the several infinite sums involved in the calculations (see Appendices C and D for details).

V. CONCLUSION

In this work a major integral bottleneck for accurate calculations on three-electron atomic systems has been resolved. Two formulas have been developed, one formula being able to handle most cases and being computationally quick, the other being general, but less rapid in computational speed.

There are still some open issues. There arise in certain atomic three-electron calculations integrals even more recalcitrant than those investigated in this work. These have factors of the form $r_{ij}^{-2}r_{ik}^{-2}$ $(j\neq k)$ in the integrand. The principal advice that can be provided is to choose the basis set judiciously, so that these integrals do not arise. It would, however, be nice to see procedures developed to solve these integrals.

A generalization of the title integral can be made by inserting the factor $e^{\alpha_{12}r_{12}+\alpha_{31}r_{31}+\alpha_{23}r_{23}}$. Evaluation of these integrals would allow additional flexibility in the choice of trial basis functions, and aid in the accurate calculation of properties for three-electron systems.

The analysis of Sec. IV would be greatly enhanced if faster and computationally stable algorithms could be found which improve on the results of Appendix D. Work is in progress to develop fast and efficient specialized numerical quadrature procedures to deal with the W_L integrals.

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APPENDIX A: EVALUATION OF $K_j(m,a,b)$

This appendix evaluates the function $K_j(m,a,b)$, defined by

$$K_j(m,a,b)=\int_0^\infty x^m e^{-ax}E_j(bx)E_1(x)dx,\quad j\geq 1\ , \tag{A1}$$

where $E_j(x)$ is the exponential integral. Special cases and generalizations of Eq. (A1) have been discussed in the literature [39–41]. Several special cases of this function which are needed in Sec. II are examined.

1. Case (i) $m=0$, $j=1$

Inserting the definition of $E_1(x)$ into Eq. (A1) leads to

$$K_1(0,a,b)=\int_{a+b}^\infty \frac{\ln(1+x)}{x(x-a)}dx\ . \tag{A2}$$

The integral in Eq. (A2) can be evaluated according to the values of a and b. For $(a+b)\geq 0$

TABLE II. Values for the functions $W_{L_1}(L,M,N,a,b,c)$, $W_{L_2}(L,M,N,a,b,c)$, and $W_{L_3}(L,M,N,a,b,c)$ for $a=2.7$, $b=2.9$, and $c=0.65$.

L	M	N	W_{L_1}	W_{L_2}	W_{L_3}
1	2	3	$1.332\,608\,340\,516\,097\,042\,381\,627\,50\times10^{-1}$	$2.988\,187\,511\,654\,956\,809\,890\,176\,09\times10^{-1}$	$5.352\,514\,091\,973\,446\,887\,573\,221\,06\times10^{-2}$
2	2	2	$2.119\,463\,339\,019\,491\,876\,285\,240\,78\times10^{-2}$	$4.182\,249\,452\,212\,097\,350\,142\,363\,21\times10^{-2}$	$1.058\,735\,819\,836\,258\,231\,687\,995\,28\times10^{-2}$
0	0	−1	$8.025\,525\,662\,784\,285\,311\,433\,011\,8\times10^{-2}$	$7.611\,490\,494\,767\,222\,964\,007\,693\,4\times10^{-2}$	$2.761\,390\,585\,597\,0\times10^{-2}$
0	−1	0	$1.587\,746\,108\,058\,152\,730\,940\,490\,4\times10^{-1}$	$3.936\,360\,219\,418\,632\,057\,939\,254\,0\times10^{-1}$	$6.044\,759\,670\,738\times10^{-2}$
−1	0	0		$7.699\,111\,080\,235\,621\,792\,157\,242\,3\times10^{-1}$	$1.383\,706\,663\,995\times10^{-1}$
0	−1	−1	$4.259\,663\,398\,034\,221\,678\,875\,194\,9\times10^{-1}$		$1.660\,849\,370\,09\times10^{-1}$
−1	0	−1		$1.163\,134\,344\,880\,376\,987\,210\,004\,6$	$3.493\,885\,957\,26\times10^{-1}$
−1	−1	0			$9.876\,051\,123\,09\times10^{-1}$
0	0	−2	$2.685\,305\,385\,865\,521\,944\,010\,578\,7\times10^{-1}$	$2.063\,887\,260\,462\,241\,345\,000\,015\,0\times10^{-1}$	$9.745\,924\,763\,3\times10^{-2}$
2	−2	−2	$7.813\,540\,282\,797\,574\,279\,094\,356\,8\times10^{-2}$	$1.120\,556\,509\,348\,349\,755\,934\,694\,9\times10^{-1}$	$4.797\,783\,484\,57\times10^{-2}$
4	−1	−4	$4.550\,694\,383\,451\,418\,283\,893\,332\,9\times10^{-3}$	$5.011\,420\,658\,446\,222\,072\,458\,035\,4\times10^{-3}$	$2.986\,668\,378\,08\times10^{-3}$

TABLE III. Values of $I(i,j,k,l,m,n,\alpha,\beta,\gamma)$ generated using Eq. (119).

i	j	k	l	m	n	α	β	γ	I
0	0	0	−2	1	1	2.5	2.5	0.6	$2.035\,406\,498\,2\times 10^{2}$
−1	−1	−1	−2	1	1	2.7	2.9	0.65	$7.290\,827\,5\times 10^{1}$
1	1	1	−2	1	1	2.7	2.7	2.7	7.187 646 24
0	0	0	−2	−1	−1	2.7	2.9	0.65	$1.527\,0\times 10^{1}$
0	0	0	−2	−1	1	2.7	2.9	0.65	$1.698\,678\,25\times 10^{1}$

$$K_1(0,a,b)=\begin{cases}\dfrac{1}{a}\left[\mathrm{Li}_2\left[\dfrac{a+b}{1+a+b}\right]-\mathrm{Li}_2\left[\dfrac{b}{1+a+b}\right]-\ln(1+a)\ln\left[\dfrac{b}{1+a+b}\right]\right] & \text{for } 1+a>0 \quad \text{(A3a)}\\[2ex] \dfrac{1}{a}\left[\mathrm{Li}_2\left[\dfrac{a+b}{1+a+b}\right]+\mathrm{Li}_2\left[\dfrac{1+a+b}{b}\right]-\dfrac{\pi^2}{3}+\tfrac{1}{2}\ln^2\left[\dfrac{1+a+b}{b}\right]\right. \\ \qquad\left.-\ln(-a-1)\ln\left[\dfrac{b}{1+a+b}\right]\right] & \text{for } 1+a<0 \quad \text{(A3b)}\end{cases}$$

and for $0<1+a+b\leq 1$

$$K_1(0,a,b)=\begin{cases}-\dfrac{1}{2}\left[\mathrm{Li}_2(-a-b)+\mathrm{Li}_2\left[\dfrac{b}{1+a+b}\right]+\tfrac{1}{2}\ln^2(a+b+1)\right. \\ \qquad\left.+\ln(1+a)\ln\left[\dfrac{b}{1+a+b}\right]\right] & \text{for } 1+a>0 \quad \text{(A4a)}\\[2ex] -\dfrac{1}{2}\left[\dfrac{\pi^2}{3}+\mathrm{Li}_2(-a-b)-\mathrm{Li}_2\left[\dfrac{1+a+b}{b}\right]+\tfrac{1}{2}\ln^2(1+a+b)-\tfrac{1}{2}\ln^2\left[\dfrac{1+a+b}{b}\right]\right. \\ \qquad\left.+\ln(-1-a)\ln\left[\dfrac{b}{1+a+b}\right]\right] & \text{for } 1+a<0\,. \quad \text{(A4b)}\end{cases}$$

$\mathrm{Li}_2(x)$ denotes Euler's dilogarithm function, which can be evaluated from the series representation (see Chap. 1 of Ref. [32])

$$\mathrm{Li}_2(x)=\sum_{n=1}^{\infty}\frac{x^n}{n^2}\,. \tag{A5}$$

Some special cases of Eqs. (A3) and (A4) which are used explicitly in Sec. II, or have been employed in the numerical phase of the project, are

$$K_1(0,-2,1+\tau)=\begin{cases}\dfrac{1}{2}\left[\dfrac{\pi^2}{3}+\mathrm{Li}_2(1-\tau)-\mathrm{Li}_2\left[\dfrac{1}{1+\tau}\right]-\ln^2(1+\tau)\right], & 0\leq\tau\leq 1 \quad \text{(A6a)}\\[2ex] \dfrac{1}{2}\left[\dfrac{\pi^2}{3}-\mathrm{Li}_2\left[\dfrac{\tau}{\tau+1}\right]-\mathrm{Li}_2\left[\dfrac{\tau-1}{\tau}\right]-\dfrac{1}{2}\ln^2\left[\dfrac{\tau}{\tau+1}\right]\right], & \tau\geq 1 \quad \text{(A6b)}\end{cases}$$

$$=\begin{cases}\tfrac{1}{2}\ln\tau\ln\left[\dfrac{1+\tau}{1+\tau}\right]+\dfrac{\pi^2}{4}-\displaystyle\sum_{n=0}^{\infty}\frac{\tau^{2n+1}}{(2n+1)^2}, & 0\leq\tau\leq 1 \quad \text{(A7a)}\\[2ex] \dfrac{\pi^2}{8}, & \tau=1 \quad \text{(A7b)}\\[2ex] \dfrac{1}{2}\ln\tau\ln\left[\dfrac{\tau+1}{\tau-1}\right]+\displaystyle\sum_{n=0}^{\infty}\frac{1}{(2n+1)^2\tau^{2n+1}}, & \tau\geq 1\,. \quad \text{(A7c)}\end{cases}$$

For $a \geq 0$ and $b > 0$

$$K_1(0,a,b) = \frac{1}{a}\left[\mathrm{Li}_2\left[\frac{a+b}{1+a+b}\right] - \mathrm{Li}_2\left[\frac{b}{1+a+b}\right] - \ln(1+a)\ln\left[\frac{b}{1+a+b}\right]\right]. \quad (A8)$$

For small a a form for Eq. (A8) suitable for numerical evaluation is

$$K_1(0,a,b) = \ln\left[\frac{1+a+b}{b}\right]\sum_{j=0}^{\infty}\frac{(-a)^j}{j+1} + \frac{1}{b}\sum_{n=1}^{\infty}\frac{1}{n^2}\left[\frac{b}{1+a+b}\right]^n \sum_{j=0}^{n-1}\left[1+\frac{a}{b}\right]^j. \quad (A9)$$

The special case $a = -1$ is also utilized in Sec. II; the result is

$$K_1(0,-1,b) = \begin{cases} \dfrac{\pi^2}{6} + \frac{1}{2}\ln^2(b) + \mathrm{Li}_2(1-b), & 0 < b \leq 1 \quad (A10a) \\ \dfrac{\pi^2}{6} - \mathrm{Li}_2\left[\dfrac{b-1}{b}\right], & b \geq 1. \quad (A10b) \end{cases}$$

2. Case (ii) $m > 0$, $j = 1$

The following recursion formula can be readily established by integration by parts

$$K_1(m,a,b) = \frac{m}{a}K_1(m-1,a,b) - \frac{1}{ab^m}\mathcal{L}\left[m-1,\frac{1+a}{b}\right] - \frac{1}{a}\mathcal{L}(m-1,a+b) \quad \text{for } m \geq 1 \quad (A11)$$

where the function $\mathcal{L}(m,\alpha)$ is defined in Eq. (27). The special case $a=0$ can be directly evaluated from Eq. (A1) to yield

$$K_1(m,0,b) = \frac{1}{m+1}\left[\mathcal{L}(m,b) + \frac{1}{b^{m+1}}\mathcal{L}\left[m,\frac{1}{b}\right]\right], \quad m \geq 0. \quad (A12)$$

3. Case (iii) $j > 1$

If the recursion formula

$$E_j(\beta x) = \frac{1}{j-1}[e^{-\beta x} - \beta x E_{j-1}(\beta x)], \quad j \geq 2 \quad (A13)$$

is inserted into Eq. (A1) the following result is obtained:

$$K_j(m,a,b) = \frac{1}{j-1}[\mathcal{L}(m,a+b) - bK_{j-1}(m+1,a,b)] \quad \text{for } j \geq 2. \quad (A14)$$

Several of the formulas of this appendix could involve the evaluation of the dilogarithm function for arguments numerically close to 1. In such cases, Eq. (A5) is not numerically suitable. A superior approach is to employ the Euler result [32]

$$\mathrm{Li}_2(x) = \frac{\pi^2}{6} - \ln x\,\ln(1-x) - \mathrm{Li}_2(1-x). \quad (A15)$$

APPENDIX B: EVALUATION OF $\mathcal{K}(-2,j,-2,\alpha,\beta,\gamma)$

The $\mathcal{K}$ integral of this appendix is rather tedious to evaluate. For the case of general j ($j \geq -1$), Eq. (43), after conversion to perimetric coordinates, can be simplified to

$$\mathcal{K}(-2,j,-2,\alpha,\beta,\gamma) = \frac{16\pi^2}{\gamma^{j+2}}(j+1)!\sum_{s=0}^{j+1}(-1)^s\int_0^{\omega}\frac{z^{j+1}}{1-z}I_\kappa(j+1-s,s,\tau)dz \quad (B1)$$

with

$$I_\kappa(m,n,\tau) = \int_{\tau-1}^{\infty}\frac{\left[\ln(1+x) + \sum_{i=1}^{n}(-x)^i/i\right]dx}{(x+2)^{m+1}x^{n+1}} \quad (B2)$$

and

$$\omega = \frac{b}{b+1}, \quad b = \frac{\gamma}{\alpha}, \quad \tau = \frac{c}{b}z, \quad c = \frac{\beta}{\alpha}. \quad (B3)$$

The function $I_\kappa(m,n,\tau)$ satisfies

$$I_\kappa(m,0,\tau)=\frac{1}{2^m}K_1(0,-2,1+\tau)+g_\kappa(m,\tau) \quad \text{for } m\geq 0 \tag{B4}$$

and

$$I_\kappa(m,n,\tau)=-\left[\frac{m+1}{n}\right]I_\kappa(m+1,n-1,\tau)+f_\kappa(m,n,\tau) \quad \text{for } n\geq 1 \tag{B5}$$

with

$$g_\kappa(m,\tau)=\frac{1}{2^{m+1}}\left\{\sum_{i=1}^{m}\frac{2^i}{i}\left[\ln\left[\frac{\tau}{\tau+1}\right]-\frac{\ln\tau}{(\tau+1)^i}\right]+\sum_{i=1}^{m-1}\frac{1}{i(1+\tau)^i}\sum_{n=i+1}^{m}\frac{2^n}{n}\right\} \tag{B6}$$

and

$$f_\kappa(m,n,\tau)=\frac{1}{n}\left\{\frac{1}{(\tau+1)^{m+1}(\tau-1)^n}\left[\ln\tau+\sum_{i=1}^{n}\frac{(1-\tau)^i}{i}\right]\right.$$
$$\left.-(-1)^n\left[\ln\left[\frac{\tau}{\tau+1}\right]+\frac{1}{n(\tau+1)^{m+1}}+\sum_{i=1}^{m}\frac{1}{i(1+\tau)^i}\right]\right\} \quad (n\geq 1)\ . \tag{B7}$$

The K_1 function in Eq. (B4) is discussed in Appendix A. The next step is the evaluation of the integrals

$$\int_0^\omega \frac{z^{j+1}}{1-z}I_\kappa(m,0,\tau)dz \quad \text{and} \quad \int_0^\omega \frac{z^{j+1}}{1-z}f_\kappa(m,n,\tau)dz$$

which together with Eqs. (B4)–(B7) provide a route for the evaluation of the integrals required in Eq. (B1).

Solution of the integral involving the K_1 function leads to

$$\int_0^\omega \frac{z^{j+1}}{1-z}K_1(0,-2,1+\tau)dz=\sum_{p=j+1}^{\infty}\omega^{p+1}\left[\frac{\pi^2}{4(p+1)}+\sum_{k=0}^{\infty}\frac{\mu^{2k+1}}{(2k+1)(2k+p+2)}\right.$$
$$\left.\times\left[\ln\mu-\frac{(4k+p+3)}{(2k+1)(2k+p+2)}\right]\right] \quad \text{for } \mu\leq 1 \tag{B8}$$

and

$$\int_0^\omega \frac{z^{j+1}}{1-z}K_1(0,-2,1+\tau)dz=\ln\mu\sum_{p=[j/2]+1}^{\infty}\frac{\{\frac{1}{2}\ln\mu+[1/(2p+1)]\}}{(2p+1)\lambda^{2p+1}}$$
$$+\sum_{p=j+1}^{\infty}\frac{1}{\lambda^{p+1}}\left[\left[\frac{\pi^2}{8}+\sum_{k=1}^{\infty}\frac{1}{(2k+p)^2}\right]\frac{1}{(p+1)}\right.$$
$$\left.+\sum_{k=0}^{\infty}{}'\left[\frac{1}{(p-2k)^2}-\frac{1}{(p-2k)(2k+1)^2}\right]\right]$$
$$+\frac{1}{\lambda}\sum_{p=j+1}^{\infty}\omega^p\sum_{k=0}^{\infty}{}'\frac{1}{(p-2k)\mu^{2k}}\left[\ln\mu+\frac{1}{(2k+1)^2}-\frac{1}{(p-2k)}\right] \quad \text{for } \mu>1 \tag{B9}$$

where

$$\mu=c(1+b)^{-1}\ , \tag{B10a}$$

$$\lambda=cb^{-1}\ . \tag{B10b}$$

The prime on the summation denotes the omission of the singular term $p=2k$ in the sum.

The details for the evaluation of the remaining integrals necessary to evaluate Eq. (B1) can be obtained from the Physics Auxiliary Publication Service [42]. The last five entries reported in Table I have been evaluated by employing the analysis of Appendix B.

APPENDIX C: INTEGRALS REQUIRED FOR THE EVALUATION OF W_L

In this appendix, the focus is the evaluation of the integral

$$V_L(L,M,a,b)=\int_0^\infty x^L e^{-ax}dx\int_x^\infty y^M e^{-by}\ln\left|\frac{y+x}{y-x}\right|dy\ . \tag{C1}$$

This integral is utilized in the evaluation of the W_L integrals, which are discussed below.

By appropriate expansion of the log term appearing in Eq. (C1) the following limits on L and M can be determined in order that the integral converge:

$$L \geq -1 \; , \tag{C2}$$

$$M+L \geq -1 \; . \tag{C3}$$

The analysis can most conveniently be broken up into two cases: (i) $L \geq 0$, $M \geq 0$ and (ii) integrals where L or M or both are negative.

1. Case (i) $L \geq 0$, $M \geq 0$

With the change of variable $y-x=xz$, Eq. (C1) can be written as

$$V_L(L,M,a,b)=\sum_{m=0}^{M}\binom{M}{m}\int_0^\infty x^{L+M+1}e^{-(a+b)x}dx\int_0^\infty z^m e^{-bxz}\ln\left|\frac{z+2}{z}\right|dz \; . \tag{C4}$$

Now

$$\int_0^\infty z^m e^{-bxz}\ln\left|\frac{z+2}{z}\right|dz=\frac{m!}{(bx)^{m+1}}[\ln(2bx)-S_m+\gamma]+2^{m+1}\int_0^\infty z^m e^{-2bxz}\ln(1+z)dz \tag{C5}$$

where γ is Euler's constant, S_m is defined by

$$S_m=\sum_{k=1}^{m}\frac{1}{k}, \quad S_0=0 \; ,$$

and the integral appearing on the right-hand side of Eq. (C5) can be evaluated to be

$$\int_0^\infty z^m e^{-2bxz}\ln(1+z)dz=\frac{(-1)^m m!}{2bx}\left[e^{2bx}E_1(2bx)\sum_{k=0}^{m}\frac{(-1)^k}{(m-k)!(2bx)^k}+\sum_{l=1}^{m}\frac{1}{(2bx)^l}\sum_{t=l}^{m}\frac{(-1)^t(S_t-S_{t-l})}{(m-t)!(t-l)!}\right] \; . \tag{C6}$$

Inserting Eqs. (C5) and (C6) into Eq. (C4) leads to

$$\begin{aligned} V_L(L,M,a,b)=\frac{M!}{b}\sum_{m=0}^{M}\frac{1}{(M-m)!}\Bigg\{ & \frac{(L+M-m)!}{b^m(a+b)^{L+M-m+1}}\left[\ln\left[\frac{2b}{a+b}\right]+S_{L+M-m}-S_m\right] \\ & +(-2)^m\Bigg[\frac{1}{(2b)^{L+M+1}}\sum_{k=0}^{m}\frac{(-1)^k\mathcal{L}(L+M-k,(a-b)/2b)}{(m-k)!} \\ & +\frac{1}{(a+b)^{L+M+1}}\sum_{l=1}^{m}(L+M-l)!\left[\frac{a+b}{2b}\right]^l \\ & \times\sum_{j=l}^{m}\frac{(-1)^j(S_j-S_{j-l})}{(m-j)!(j-l)!}\Bigg]\Bigg\} \end{aligned} \tag{C7}$$

where $\mathcal{L}(L+M-k,(a-b)/2b)$ is defined in Eq. (27).

Equation (C7) has been tested for a range of values of L, M, a, and b. Computing the positive and negative contributions to $V_L(L,M,a,b)$ in Eq. (C7) shows that the formula downgrades for large values of M. The particular values of M for which this becomes a serious difficulty are governed by the selected values of a and b. Under such circumstances Eq. (C15) given below should be utilized, though this result is slower to evaluate. Equation (C1) can also be conveniently reduced to a single quadrature, namely,

$$V_L(L,M,a,b)=(L+M+1)!\int_0^\infty\frac{(1+y)^M\ln\left|\frac{2+y}{y}\right|}{(a+b+by)^{L+M+2}}dy \; . \tag{C8}$$

Equation (C8) has been employed as a check on Eq. (C7).

The following recursion formula can be established by integration by parts:

$$V_L(L-1,M+1,a,b)=\frac{1}{b}[(L+M+1)V_L(L-1,M,a,b)-aV_L(L,M,a,b)] \; . \tag{C9}$$

The recursion formula above requires $V_L(L,0,a,b)$, which for $a\neq b$ can be conveniently computed using

$$V_L(L,0,a,b)=\frac{L!}{b(a^2-b^2)^{L+1}}\left[(a-b)^{L+1}S_L-(a+b)^{L+1}\sum_{k=1}^{L}\frac{1}{k}\left[\frac{a-b}{a+b}\right]^k\right.$$
$$\left.+[(a+b)^{L+1}-(a-b)^{L+1}]\ln\left[\frac{a+b}{2b}\right]\right], \tag{C10}$$

which has been obtained by employing

$$V_L(L,0,a,b)=(-1)^L\frac{\partial^L}{\partial a^L}V_L(0,0,a,b) . \tag{C11}$$

Equation (C9) appears to be reasonably stable for numerical computation.

2. Case (ii) L and/or M negative

Reversing the order of integration in Eq. (C1) and introducing the change of variable $x=yz$ leads to

$$V_L(L,M,a,b)=\int_0^\infty y^{L+M+1}e^{-by}dy\int_0^1 z^L e^{-azy}\ln\left|\frac{1+z}{1-z}\right|dz . \tag{C12}$$

Now using the change of variable $z=1-x$,

$$\int_0^1 z^L e^{-ayz}\ln(1+z)dz=e^{-ay}\int_0^1 e^{ayx}(1-x)^L\ln(2-x)dx$$
$$=e^{-ay}\sum_{k=0}^{\infty}\frac{(ay)^k}{k!}\int_0^1(1-x)^L x^k\ln(2-x)dx \tag{C13}$$

and similarly,

$$\int_0^1 z^L e^{-ayx}\ln(1-z)dz=e^{-ay}\sum_{k=0}^{\infty}\frac{(ay)^k}{k!}\int_0^1(1-x)^L x^k\ln x\,dx . \tag{C14}$$

Substituting Eqs. (C13) and (C14) into Eq. (C12) leads to

$$V_L(L,M,a,b)=\frac{1}{(a+b)^{L+M+2}}\sum_{k=0}^{\infty}\left[\frac{a}{a+b}\right]^k\frac{(L+M+1+k)!}{k!}\mathfrak{F}(L,k) \tag{C15}$$

with

$$\mathfrak{F}(L,k)=\int_0^1(1-x)^L x^k\ln(2-x)dx-\int_0^1(1-x)^L x^k\ln x\,dx . \tag{C16}$$

Since the second integral in Eq. (C16) is negative, the summation in Eq. (C15) is numerically stable. The evaluation of the two integrals appearing in Eq. (C16) can be treated as two cases, (i) $L=-1$ or (ii) $L\geq 0$.

$$\int_0^1(1-x)^L x^k\ln x\,dx=\begin{cases}-\zeta(2,k+1) & \text{for } L=-1 \quad \text{(C17a)}\\ \dfrac{-k!L!}{(k+L+1)!}\displaystyle\sum_{j=0}^{L}\frac{1}{k+1+j} & \text{for } L\geq 0 \quad \text{(C17b)}\end{cases}$$

where $\zeta(m,n)$ is the generalized zeta function, which can be evaluated as

$$\zeta(2,k+1)=\frac{\pi^2}{6}-\sum_{j=1}^{k}\frac{1}{j^2} . \tag{C18}$$

Equation (C18) is suitable for numerical evaluation except for large values of k, where the formula

$$\zeta(2,k+1)=\sum_{j=0}^{\infty}\frac{1}{(j+k+1)^2} \tag{C19}$$

is employed in connection with Kummer's comparison method. In practical calculations, large values of k are not required in Eq. (C17). The summation in Eq. (C17b) can be expressed as $(S_{L+k+1}-S_k)$. The other integral appearing in

Eq. (C16) can be expressed as

$$\int_0^1 (1-x)^L x^k \ln(2-x)dx = \begin{cases} \dfrac{\pi^2}{12} - \ln 2 \sum_{j=1}^{k} \dfrac{2^j}{j} + \sum_{j=0}^{k-1} 2^j \sum_{m=1}^{k-j} \dfrac{1}{m(m+j)} & \text{for } L=-1 \quad \text{(C20a)} \\ 2^{k+1} \sum_{j=0}^{L} \dfrac{(-2)^j \begin{bmatrix} L \\ j \end{bmatrix}}{k+j+1} \left[\ln 2 - \sum_{m=1}^{k+j+1} \dfrac{1}{2^m m} \right] & \text{for } L \ge 0 \ . \quad \text{(C20b)} \end{cases}$$

Several alternative formulas for both cases of Eq. (C20) have been derived. Equation (C20) is numerically stable only for small values of k. For larger values of k the following results are employed:

$$\int_0^1 (1-x)^L x^k \ln(2-x)dx = \frac{\pi^2}{12} - \sum_{j=1}^{k} \frac{1}{j} \sum_{n=1}^{\infty} \frac{1}{2^n (n+j)} \quad \text{for } L=-1 \ , \tag{C21}$$

$$\int_0^1 x^k \ln(2-x)dx = \frac{2}{k+1} \sum_{n=2}^{\infty} \frac{1}{2^n(n+k)} \quad \text{for } L=0 \ , \tag{C22}$$

and

$$\int_0^1 (1-x)^L x^k \ln(2-x)dx = k! \sum_{j=1}^{\infty} \frac{(-1)^{j+1}(L+j)!}{j(L+j+k+1)!} \ , \tag{C23a}$$

$$= \frac{k!L!}{(k+L+1)!} \sum_{j=1}^{\infty} \frac{1}{2^j j} \left[1 - \prod_{m=1}^{j} \left[\frac{k+m}{L+1+k+m} \right] \right] \quad \text{for } L>0 \ . \tag{C23b}$$

Equation (C23b) has the advantage of being a sum of positive terms, so it is likely to be more suitable for numerical evaluation.

A principle advantage of the above approach is that the $\mathfrak{F}(L,k)$ integrals are *independent* of the parameters a and b, and so a matrix array of these integrals need only be computed once and stored. This in turn means that the evaluation of the V_L integrals using Eq. (C15) is computationally quick.

APPENDIX D: THE W_L INTEGRALS

The W_L integrals appearing in Sec. IV are defined in Eqs. (116)–(118). Appendix D indicates the strategy for the evaluation of these integrals. A straightforward analysis shows that the integrals converge when the following conditions hold: for W_{L_1},

$$L \ge 0 \ , \tag{D1a}$$

$$L+M \ge -2 \ , \tag{D1b}$$

$$L+M+N \ge -2 \ ; \tag{D1c}$$

for W_{L_2},

$$L \ge -1 \ , \tag{D2a}$$

$$L+M \ge -1 \ , \tag{D2b}$$

$$L+M+N \ge -2 \ ; \tag{D2c}$$

and for W_{L_3},

$$L \ge -1 \ , \tag{D3a}$$

$$L+M \ge -2 \ , \tag{D3b}$$

$$L+M+N \ge -2 \ . \tag{D3c}$$

As for the V_L integrals, analysis of the W_L integrals is most conveniently handled by considering two categories; (i) all L,M,N indices positive, or (ii) cases where one or more of the L,M,N indices are negative.

1. Case (i) W_L integrals, positive L,M,N

The approach taken below is to reduce the W_L integrals to the V_L integrals wherever possible. The latter integrals have been thoroughly discussed in Appendix C.

For W_{L_2} the following result holds:

$$W_{L_2}(L,M,N,a,b,c) = \int_0^\infty x^L e^{-ax} dx \times \int_x^\infty y^M e^{-by} \ln \left| \frac{y+x}{y-x} \right| dy \times \left[\frac{N! e^{-cy}}{c^{N+1}} \sum_{v=0}^{N} \frac{(cy)^v}{v!} \right] \tag{D4}$$

and hence

$$W_{L_2}(L,M,N,a,b,c)=\frac{N!}{c^{N+1}}\sum_{v=0}^{N}\frac{c^v}{v!}V_L(L,M+v,a,b+c). \quad \text{(D5)}$$

For W_{L_1}, Eq. (116) can be written, after changing the order of integration with respect to y and x, as

$$W_{L_1}(L,M,N,a,b,c)=\int_0^\infty y^M e^{-by}g(y)dy\int_0^y x^L e^{-ax}dx \quad \text{(D6)}$$

where

$$g(y)=\int_y^\infty z^N e^{-cz}\ln\left|\frac{z+y}{z-y}\right|dz . \quad \text{(D7)}$$

Equation (D7) can be recast as

$$\begin{aligned}W_{L_1}(L,M,N,a,b,c)&=\int_0^\infty y^M e^{-by}g(y)dy\left[\int_0^\infty x^L e^{-ax}dx-\int_y^\infty x^L e^{-ax}dx\right]\\&=\frac{L!}{a^{L+1}}\left[\int_0^\infty y^m e^{-by}g(y)dy-\sum_{v=0}^{L}\frac{a^v}{v!}\int_0^\infty y^{M+v}e^{-(a+b)y}g(y)dy\right]\end{aligned} \quad \text{(D8)}$$

and hence

$$W_{L_1}(L,M,N,a,b,c)=\frac{L!}{a^{L+1}}\left[V_L(M,N,b,c)-\sum_{v=0}^{L}\frac{a^v}{v!}V_L(M+v,N,a+b,c)\right] . \quad \text{(D9)}$$

For W_{L_3}, Eq. (138) can be expressed as

$$\begin{aligned}W_{L_3}(L,M,N,a,b,c)=&\int_0^\infty x^L e^{-ax}dx\int_x^\infty y^M e^{-by}dy\int_x^\infty z^N e^{-cz}\ln\left|\frac{z+x}{z-x}\right|dz\\&-\int_0^\infty x^L e^{-ax}dx\int_x^\infty y^M e^{-by}dy\int_x^y z^N e^{-cz}\ln\left|\frac{z+x}{z-x}\right|dz .\end{aligned} \quad \text{(D10)}$$

The first integral on the right-hand side of Eq. (D10) can be simplified as follows:

$$\begin{aligned}\int_0^\infty x^L e^{-ax}dx\int_x^\infty y^M c^{-by}dy\int_x^\infty z^N e^{-cz}\ln\left|\frac{z+x}{z-x}\right|dx&=\int_0^\infty x^{L+M+1}e^{-ax}dx\int_x^\infty z^N e^{-cz}\ln\left|\frac{z+x}{z-x}\right|dx\int_1^\infty w^M e^{-bxw}dw\\&=\frac{M!}{b^{M+1}}\sum_{v=0}^{M}\frac{b^v}{v!}V_L(L+v,N,a+b,c) .\end{aligned} \quad \text{(D11)}$$

On interchanging the order of integration in Eq. (D10), first with respect to x and y, then with respect to x and z, yields

$$\int_0^\infty x^L e^{-ax}dx\int_x^\infty y^M e^{-by}dy\int_x^y z^N e^{-cz}\ln\left|\frac{z+x}{z-x}\right|dz=\int_0^\infty y^M e^{-by}dy\int_0^y z^N e^{-cz}dz\int_0^z x^L e^{-ax}\ln\left|\frac{z+x}{z-x}\right|dx . \quad \text{(D12)}$$

Equation (D12) can be rearranged to the form

$$\begin{aligned}\int_0^\infty x^L e^{-ax}dx\int_x^\infty y^M e^{-by}dy\int_x^y z^N e^{-cz}\ln\left|\frac{z+x}{z-x}\right|dz&=\int_0^\infty x^L e^{-ax}dx\int_x^\infty z^N e^{-cz}\ln\left|\frac{z+x}{z-x}\right|dz\int_z^\infty y^M e^{-by}dy\\&=\frac{M!}{b^{M+1}}\sum_{v=0}^{M}\frac{b^v}{v!}\int_0^\infty x^L e^{-ax}dx\int_x^\infty z^{N+v}e^{-(b+c)z}\ln\left|\frac{z+x}{z-x}\right|dz .\end{aligned} \quad \text{(D13)}$$

Combining Eqs. (D11) and (D13) leads to

$$W_{L_3}(L,M,N,a,b,c)=\frac{M!}{b^{M+1}}\sum_{v=0}^{M}\frac{b^v}{v!}[V_L(L+v,N,a+b,c)-V_L(L,N+v,a,b+c)] . \quad \text{(D14)}$$

Equations (D5), (D9), and (D14) represent the results for the W_L integrals for the all positive L,M,N case. Attention is now focused on the W_L integrals for cases where one (or more) of the indices L,M,N is negative.

2. Case (ii) W_L integrals; negative values of L, M, or N

The strategy employed for this case is the same as above, that is, an attempt is made to simplify the W_L integrals to expressions involving the V_L integrals.

For W_{L_1}, since $L \geq 0$ [Eq. (D1a)], Eq. (116) can be simplified to yield Eq. (D9). When significant figure loss is likely to arise, then W_{L_1} can be written as

$$W_{L_1}(L,M,N,a,b,c)=\int_0^\infty y^M e^{-by}dy \int_y^\infty z^N e^{-cz}\ln\left|\frac{z+y}{z-y}\right| dz \int_0^y x^L e^{-ax}dx$$
$$=\frac{L!}{a}\sum_{v=1}^{\infty}\frac{a^v}{(v+L)!}V_L(L+M+v,N,a+b,c) \ . \tag{D15}$$

This form for W_{L_1} eliminates the possibility of significant figure loss by subtraction of terms of similar size, as may occur in the use of Eq. (D9).

For W_{L_2}, Eq. (117) can be simplified to

$$W_{L_2}(L,M,N,a,b,c)=\int_0^\infty y^M e^{-by}dy \int_y^\infty z^N e^{-cz}dz \int_0^y x^L e^{-ax}\ln\left|\frac{y+x}{y-x}\right| dx$$
$$=\sum_{v=0}^{\infty}\frac{a^v}{v!}\mathfrak{F}(L,v)\int_0^\infty y^{L+M+v+1}e^{-(a+b)y}dy\int_y^\infty z^N e^{-cz}dz$$
$$=\sum_{v=0}^{\infty}\frac{a^v}{v!}\mathfrak{F}(L,v)V(L+M+1+v,N,a+b,c) \tag{D16}$$

where $V(L,M,a,b)$ is defined by

$$V(L,M,a,b)=\int_0^\infty x^L e^{-ax}dx\int_x^\infty y^M e^{-by}dy \ . \tag{D17}$$

Methods for the evaluation of this integral have been discussed in the literature [12,14].

For W_{L_3} for negative L, M, or N, several subcases are considered according to (i) $M \geq 0$ with $L<0$, $N \geq 0$ or $L \geq 0$, $N<0$ or $L<0$, $N<0$. (ii) $M<0$ and either L or $N<0$ [but not both; note Eq. (D3c)].

For subcase (i), Eq. (D14) can be reexpressed as

$$\begin{aligned}W_{L_3}(L,M,N,a,b,c)=\frac{M!}{b^{M+1}}\Bigg\{&\sum_{m=M+1}^{\infty}\frac{(-b)^m}{m!}\sum_{j=0}^{M}\frac{b^j}{j!}[V_L(L+j+m,N,a,c)-V_L(L,N+j+m,a,c)]\\&+\sum_{m=0}^{M}\frac{(-b)^m}{m!}\sum_{j=M-m+1}^{M}\frac{b^j}{j!}[V_L(L+j+m,N,a,c)-V_L(L,N+j+m,a,c)]\\&+\sum_{m=0}^{M}\frac{(-b)^m}{m!}\sum_{j=0}^{M-m}\frac{b^j}{j!}[V_L(L+j+m,N,a,c)-V_L(L,N+j+m,a,c)]\Bigg\} \ .\end{aligned} \tag{D18}$$

The last double sum in Eq. (D18) equals zero, therefore Eq. (D18) simplifies to

$$\begin{aligned}W_{L_3}(L,M,N,a,b,c)=\frac{M!}{b!}\Bigg\{&\sum_{m=0}^{M}\frac{(-b)^m}{m!}\sum_{j=M-m+1}^{M}\frac{b^j}{j!}[V_L(L+j+m,N,a,c)-V_L(L,N+j+m,a,c)]\\&+\sum_{m=M+1}^{\infty}\frac{(-b)^m}{m!}\sum_{j=0}^{M}\frac{b^j}{j!}[V_L(L+j+m,N,a,c)-V_L(L,N+j+m,a,c)]\Bigg\} \ .\end{aligned} \tag{D19}$$

When round-off errors are likely because of the subtraction of terms of similar size in Eq. (D19), the approach indicated in Eq. (D20) should be employed.

For the second subcase, use the change of variable $z=vy$ in Eq. (118), reverse the order of integration over x and y, and then introduce the variable change $x=yt$ to obtain

$$W_{L_3}(L,M,N,a,b,c)=\int_0^\infty y^{L+M+N+2}e^{-by}dy\int_0^1 t^L e^{-ayt}dt\int_1^\infty v^N e^{-cyv}\ln\left|\frac{v+t}{v-t}\right|dv$$
$$=2\sum_{k=1}^\infty \frac{1}{(2k-1)}\int_0^\infty y^{L+M+N+2}e^{-by}dy\int_1^\infty v^{N+1-2k}e^{-cyv}dv\int_0^1 t^{L-1+2k}e^{-ayt}dt$$
$$=2\sum_{k=1}^\infty \frac{(L+2k-1)!}{(2k-1)}\sum_{m=0}^\infty \frac{a^m}{(L+2k+m)!}\int_0^\infty y^{L+M+N+2}e^{-(a+b)y}dy\int_1^\infty v^{N+1-2k}e^{-cyv}dv$$
$$=2\sum_{k=1}^\infty \frac{(L+2k-1)!}{(2k-1)}\sum_{m=0}^\infty \frac{a^m}{(L+2k+m)!}V(L+M+m+2k,N+1-2k,a+b,c)\ . \qquad \text{(D20)}$$

The above result will actually handle both subcases (i) and (ii), and has the advantage that it represents a sum of positive terms. An alternative form of Eq. (D20) is possible with the infinite sum over index m replaced by a finite sum, but this is at the expense of introducing a difference of terms in the infinite sum over the index k.

The major impediment in the approach discussed in Sec. IV is the fast computation of the W_{L_3} integrals with negative arguments. This becomes particularly problematic if a large number of significant figures are required for the I integrals. The best approach to the computation of I integrals requiring a number of the recalcitrant W_L integrals is to build up and store arrays of the V and V_L integrals as a function of the variables a, b, and c. This avoids redundant calculation of the reoccurring V, V_L, and W_L integrals.

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[42] See AIP Document No. PAPS PLRAA-44-7108-8 for eight pages of equations on the evaluation of the integrals of Appendix B. Order by PAPS number and journal reference from American Institute of Physics, Physics Auxiliary Publication Service, 335 East 45th Street, New York, NY 10017. The price is $1.50 for each microfiche or $5.00 for photocopies up to 30 pages. Airmail additional.