Recursion relations for the four-electron subsidiary integral $W_4(k,l,m,n;\theta,\alpha,\beta,\gamma)$

Chun Li,[1,*] Liming Wang,[2] and Zong-Chao Yan[3]

[1]*Department of Mathematics, Nanjing University, Nanjing, Jiangsu, People's Republic of China 210093*

[2]*Department of Physics, Henan Normal University, Xinxiang, Henan, People's Republic of China 453007*

[3]*Department of Physics, University of New Brunswick, Fredericton, New Brunswick, Canada E3B 5A3*

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The subsidiary integral $W_4(k,l,m,n;\,\theta,\alpha,\beta,\gamma)$ plays an essential role in the variational calculation of four-electron atomic systems using Hylleraas coordinates. With respect to the case where the ratio $\theta/(\theta+\alpha+\beta+\gamma)\sim 1$, an important special situation that may occur in the evaluation of the Bethe logarithm, existing approaches for evaluating the W_4 integral become impractical due to the problem of slow convergence. Based on our recent work for the three-electron subsidiary integral $W_3(l,m,n;\,\alpha,\beta,\gamma)$, we present a computationally efficient and numerically stable method, in which the W_4 integral can be expressed in terms of either a finite series or a finite recursion relation. Numerical experimentation is presented to validate our method.

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I. INTRODUCTION

Few-body atomic and molecular systems can serve as a testing ground for various computational methods and for physical theories, such as relativistic and quantum electrodynamic (QED) effects, provided both atomic-structure calculation and experimental measurement can be done to a sufficiently high precision. In addition to atomic hydrogen and helium, where high-order relativistic and QED effects have been tested in various ways, recent advances in variational calculations of lithium energy levels have opened another avenue for testing these effects in this three-electron system [1,2]. For a light atom containing more than one electron, from a computational point of view, the central problem is how to build electron-electron correlations in wave functions. It is well accepted that a variational calculation in Hylleraas coordinates, which explicitly includes the electron-electron distances $r_{ab}=|\mathbf{r}_a-\mathbf{r}_b|$ in variational basis functions, is regarded as the most powerful method among existing theoretical approaches in obtaining the energy eigenvalues of the Hamiltonian with high accuracy [3–5]. Although Hylleraas-type calculations have been done successfully for three-electron systems, its extension to four-electron systems is still quite limited [6]. One bottleneck is lack of viable computational methods to deal with the issue of slow convergence for the overlap integrals where five or all six powers j_{ab} in $r_{ab}^{j_{ab}}$ ($b>a$, $a,b=1,2,3,4$) are odd integers. Another potential bottleneck is the effective evaluation of the extremely slowly converged subsidiary integral $W_4(k,l,m,n;\,\theta,\alpha,\beta,\gamma)$ when the ratio $\theta/(\theta+\alpha+\beta+\gamma)\sim 1$, as it may happen in the evaluation of the Bethe logarithm in the leading QED corrections, using the Drake-Goldman method [7]. It should be mentioned that, although a variational calculation in full Hylleraas coordinates is not available for four-electron atomic systems at this moment, a variational calculation using explicitly correlated Gaussian functions [8,9] has been performed recently for some low-lying states of beryllium, including the leading relativistic and QED corrections. However, this type of function suffers from undesirable short-distance (Kato cusps) and long-range (asymptotic) behavior that may eventually limit its accuracy. Other approaches for four-electron systems include Hylleraas configuration-interaction basis functions [10], as well as selective Hylleraas basis functions [6] to explicitly avoid the situation where five or all six powers in $r_{ab}^{j_{ab}}$ are odd. The purpose of this paper is to present an effective approach based on a set of recursion relations for dealing with the four-electron subsidiary integral W_4, with particular attention being paid to the case of $\theta/(\theta+\alpha+\beta+\gamma)\sim 1$. The present approach is a significant extension of our recent work [11] on the evaluation of the three-electron subsidiary integral $W_3(l,m,n;\alpha,\beta,\gamma)$ (we adopt the notation W_3 hereafter to replace W defined in [11]). The four-electron subsidiary integral W_4 has been investigated by some authors [12–15], but none of them have addressed the issue of slow convergence when $\theta/(\theta+\alpha+\beta+\gamma)\sim 1$.

For a four-electron atomic system, the wave function is constructed from the following functions in Hylleraas coordinates (for the sake of simplicity we consider S states only):

$$r_1^{j_1} r_2^{j_2} r_3^{j_3} r_4^{j_4} r_{12}^{j_{12}} r_{13}^{j_{13}} r_{14}^{j_{14}} r_{23}^{j_{23}} r_{24}^{j_{24}} r_{34}^{j_{34}} e^{-\alpha r_1-\beta r_2-\gamma r_3-\theta r_4}. \tag{1}$$

The construction of the Hamiltonian and overlap matrix elements is thus reduced to evaluating the following basic integral:

$$\begin{aligned} I(j_1,j_2,j_3,j_4,j_{12},j_{13},j_{14},j_{23},j_{24},j_{34}) &= \int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 d\mathbf{r}_4\, r_1^{j_1} r_2^{j_2} r_3^{j_3} r_4^{j_4} r_{12}^{j_{12}} r_{13}^{j_{13}} r_{14}^{j_{14}} \\ &\quad\times r_{23}^{j_{23}} r_{24}^{j_{24}} r_{34}^{j_{34}} e^{-\alpha r_1-\beta r_2-\gamma r_3-\theta r_4}, \end{aligned} \tag{2}$$

where the nonlinear parameter dependence of I has been suppressed. The factors involving the interelectronic coordinates r_{ab} can be expanded using Perkins expansion [16],

$$r_{12}^{j} = \sum_{q=0}^{M_{12}} P_q(\cos\theta_{12}) \sum_{k=0}^{L_{12}} C_{jqk}\, r_{12<}^{q+2k} r_{12>}^{j-q-2k}. \tag{3}$$

In the above, for even j's, $M_{12}=\frac{1}{2}j$, $L_{12}=\frac{1}{2}j-q$; for odd ones, $M_{12}=\infty$, $L_{12}=\frac{1}{2}(j+1)$; $r_{12<}=\min(r_1,r_2)$,

*lichun@nju.edu.cn

$r_{12>}=\max(r_1,r_2)$, and the coefficients are

$$C_{jqk}=\frac{2q+1}{j+2}\binom{j+2}{2k+1}\prod_{t=0}^{S_{qj}}\frac{2k+2t-j}{2k+2q-2t+1}$$

with $S_{qj}=\min[q-1,\frac{1}{2}(j+1)]$. After expanding each $r_{ab}^{j_{ab}}$ in the basic integral (2), we obtain the following formal multiple series:

$$I(j_1,j_2,j_3,j_4,j_{12},j_{13},j_{14},j_{23},j_{24},j_{34})=\sum_{q_{12}=0}^{M_{12}}\sum_{q_{13}=0}^{M_{13}}\sum_{q_{14}=0}^{M_{14}}\sum_{q_{23}=0}^{M_{23}}\sum_{q_{24}=0}^{M_{24}}\sum_{q_{34}=0}^{M_{34}}\sum_{k_{12}=0}^{L_{12}}\sum_{k_{13}=0}^{L_{13}}\sum_{k_{14}=0}^{L_{14}}\sum_{k_{23}=0}^{L_{23}}\sum_{k_{24}=0}^{L_{24}}\sum_{k_{34}=0}^{L_{34}}$$
$$\times I_{\rm ang}(q_{12},q_{13},q_{14},q_{23},q_{24},q_{34})I_{\rm R}(q_{12},q_{13},q_{14},q_{23},q_{24},q_{34};k_{12},k_{13},k_{14},k_{23},k_{24},k_{34}), \tag{4}$$

where the angular part $I_{\rm ang}$ can be expressed as [15,17]

$$I_{\rm ang}(q_{12},q_{13},q_{14},q_{23},q_{24},q_{34})=(4\pi)^4(-1)^{q_{12}+q_{34}}\begin{pmatrix}q_{12}&q_{13}&q_{14}\\0&0&0\end{pmatrix}\begin{pmatrix}q_{12}&q_{23}&q_{24}\\0&0&0\end{pmatrix}\begin{pmatrix}q_{13}&q_{23}&q_{34}\\0&0&0\end{pmatrix}$$
$$\times\begin{pmatrix}q_{14}&q_{24}&q_{34}\\0&0&0\end{pmatrix}\begin{Bmatrix}q_{12}&q_{23}&q_{24}\\q_{34}&q_{14}&q_{13}\end{Bmatrix}, \tag{5}$$

and the radial part $I_{\rm R}$ can be written as

$$I_{\rm R}(q_{12},q_{13},q_{14},q_{23},q_{24},q_{34};k_{12},k_{13},k_{14},k_{23},k_{24},k_{34})=C_{j_{12}q_{12}k_{12}}C_{j_{13}q_{13}k_{13}}C_{j_{14}q_{14}k_{14}}C_{j_{23}q_{23}k_{23}}C_{j_{24}q_{24}k_{24}}C_{j_{34}q_{34}k_{34}}$$
$$\times W_{\rm R}(q_{12},q_{13},q_{14},q_{23},q_{24},q_{34};k_{12},k_{13},k_{14},k_{23},k_{24},k_{34}), \tag{6}$$

with $W_{\rm R}$ being a sum [12,13,15] of 24 subsidiary integrals W_4 defined below:

$$W_4(k,l,m,n;\theta,\alpha,\beta,\gamma)=\int_0^\infty dv\,v^ke^{-\theta v}\int_v^\infty dx\,x^le^{-\alpha x}\int_x^\infty dy\,y^me^{-\beta y}\int_y^\infty dz\,z^ne^{-\gamma z}$$
$$=\int_0^\infty dz\,z^ne^{-\gamma z}\int_0^z dy\,y^me^{-\beta y}\int_0^y dx\,x^le^{-\alpha x}\int_0^x dv\,v^ke^{-\theta v}. \tag{7}$$

In the above θ, α, β, and γ are positive real numbers, k, l, m, and n are integers satisfying the requirements $k\geqslant 0$, $k+l+1\geqslant 0$, $k+l+m+2\geqslant 0$, and $k+l+m+n+3\geqslant 0$. An analytical formula for the W_4 integral can be derived [15]:

$$W_4(k,l,m,n;\theta,\alpha,\beta,\gamma)=\frac{k!}{(\theta+\alpha+\beta+\gamma)^{k+l+m+n+4}}\sum_{p=0}^\infty\frac{(k+l+1+p)!}{(k+1+p)!}\left(\frac{\theta}{\theta+\alpha+\beta+\gamma}\right)^p$$
$$\times\sum_{q=0}^\infty\frac{(k+l+m+n+3+p+q)!}{(k+l+2+p+q)!}\left(\frac{\theta+\alpha}{\theta+\alpha+\beta+\gamma}\right)^q\frac{1}{k+l+m+3+p+q}$$
$$\times{}_2F_1\left(1,k+l+m+n+p+q+4;k+l+m+p+q+4;\frac{\theta+\alpha+\beta}{\theta+\alpha+\beta+\gamma}\right), \tag{8}$$

where ${}_2F_1$ is the Gauss hypergeometric function. The W_4 integral can further be reduced to the following infinite series [15]:

$$W_4(k,l,m,n;\theta,\alpha,\beta,\gamma)=k!\sum_{p=0}^\infty\frac{\theta^p}{(k+p+1)!}W_3(k+l+p+1,m,n;\theta+\alpha,\beta,\gamma), \tag{9}$$

where W_3 is the three-electron subsidiary integral defined by

$$W_3(l,m,n;\,\alpha,\beta,\gamma)=\int_0^\infty dx\,x^le^{-\alpha x}\int_x^\infty dy\,y^me^{-\beta y}\int_y^\infty dz\,z^ne^{-\gamma z}=\int_0^\infty dz\,z^ne^{-\gamma z}\int_0^z dy\,y^me^{-\beta y}\int_0^y dx\,x^le^{-\alpha x}. \tag{10}$$

In the above, α, β, and γ are all positive real numbers, and l, m, and n are integers with constraints $l\geqslant 0$, $l+m+1\geqslant 0$ and $l+m+n+2\geqslant 0$. An analytical expression for the W_3 integral is given by [18]

$$W_3(l,m,n;\,\alpha,\beta,\gamma)=\frac{l!}{(\alpha+\beta+\gamma)^{l+m+n+3}}\sum_{p=0}^\infty\frac{(l+m+n+p+2)!}{(l+1+p)!(l+m+2+p)}\left(\frac{\alpha}{\alpha+\beta+\gamma}\right)^p{}_2$$
$$\times F_1\left(1,l+m+n+p+3;l+m+p+3;\frac{\alpha+\beta}{\alpha+\beta+\gamma}\right). \tag{11}$$

One can see from (9) and (11) that the rate of convergence of W_4, as an infinite series in p, is largely determined by the ratio $\theta/(\theta+\alpha+\beta+\gamma)$. When this ratio is not close to 1, the infinite series formula (9) will converge rapidly. However, when this ratio is close to 1, as it may appear in the calculation of the Bethe logarithm using the Drake-Goldman method [7], the use of this infinite series expression is not practical at all, in spite of the fact that the similar problem of slow convergence for the three-electron subsidiary integral W_3 has been completely solved recently [11]. Here we propose a finite-term method for the evaluation of the W_4 integral with special attention to the case of $\theta/(\theta+\alpha+\beta+\gamma)\sim 1$. Our method is valid not only for the most general conditions on (k,l,m,n), i.e., $k\geqslant 0$, $k+l+1\geqslant 0$, $k+l+m+2\geqslant 0$, and $k+l+m+n+3\geqslant 0$, but is also computationally efficient and numerically stable in the range of $\theta/(\theta+\alpha+\beta+\gamma)\sim 1$.

It should be pointed out that, although a finite-step calculation for W_4 was mentioned in King's work [13], it is only for the following two cases: (1) For $n\geqslant 0$, a finite recurrence relation [Eq. (45) in [13]] is presented, which is the same as (14) (see below). However, the implementation of the W_3 integral is different from ours. (2) Another recurrence relation [Eq. (46) in [13]] for $n<0$, together with the constraints $l\geqslant 0$, $l+m+1\geqslant 0$, and $l+m+n+2\geqslant 0$, is presented, which is different from that given here. Kleindienst *et al.* [14] also discussed two ways of calculating the W_4 integral: the first is the infinite-series relation (9); the second seems to be a finite-term calculation outwardly, but it is a truncation of a multiple series by using some integration and differentiation techniques. Neither King [13] nor Kleindienst *et al.* [14] have addressed a finite-step procedure under the most general conditions on (k,l,m,n), as well as under the special condition of $\theta/(\theta+\alpha+\beta+\gamma)\sim 1$.

II. RECURSION RELATIONS FOR THE SUBSIDIARY INTEGRAL

For the sake of convenience, we first list two definite integral formulas that will be used subsequently:

$$\int_y^\infty dx x^n e^{-\lambda x} = \frac{n!}{\lambda^{n+1}} e^{-\lambda y}\sum_{k=0}^{n}\frac{\lambda^k y^k}{k!} \tag{12}$$

and

$$\int_0^\infty dx x^n e^{-\lambda x} = \frac{n!}{\lambda^{n+1}}, \tag{13}$$

where n is a non-negative integer and λ is a positive real number.

A. Case 1: $n\geqslant 0$

For the integral representation of W_4 in (7), using (12), the integration over z can be performed first, yielding the following finite expression for W_4 [13]:

$$\begin{aligned} W_4(k,l,m,n;\theta,\alpha,\beta,\gamma) &= \frac{n!}{\gamma^{n+1}}\sum_{p=0}^{n}\frac{\gamma^p}{p!}\int_0^\infty dv\, v^k e^{-\theta v}\int_v^\infty dx\, x^l e^{-\alpha x}\int_x^\infty dy\, y^{p+m} e^{-(\beta+\gamma)y} \\ &= \frac{n!}{\gamma^{n+1}}\sum_{p=0}^{n}\frac{\gamma^p}{p!} W_3(k,l,m+p;\theta,\alpha,\beta+\gamma). \end{aligned} \tag{14}$$

It is obvious from (14) that the requirements for W_3 to exist are automatically satisfied, i.e., $k\geqslant 0$, $k+l+1\geqslant 0$, and $k+l+(m+p)+2\geqslant 0$. For the evaluation of W_3 above, the recursion relations established in [11] will be used.

B. Case 2: $n<0$

In this section we use $-n$ to substitute for n so that n is now positive. It should be restated here that the requirements imposed on (k,l,m,n) become $k\geqslant 0$, $k+l+1\geqslant 0$, $k+l+m+2\geqslant 0$, and $k+l+m-n+3\geqslant 0$. For simplicity, we define

$$\Lambda_4(k,l,m,n) := W_4(k,l,m,-n;\theta,\alpha,\beta,\gamma) = \int_0^\infty dv\, v^k e^{-\theta v}\int_v^\infty dx\, x^l e^{-\alpha x}\int_x^\infty dy\, y^m e^{-\beta y}\int_y^\infty dz\, z^{-n} e^{-\gamma z}.$$

Performing integration by parts over z, we obtain the following recursion relation for $n>1$:

$$\Lambda_4(k,l,m,n) = \frac{1}{n-1}W_3(k,l,m+1-n;\theta,\alpha,\beta+\gamma) - \frac{\gamma}{n-1}\Lambda_4(k,l,m,n-1). \tag{15}$$

In order to complete the calculation for $\Lambda_4(k,l,m,n)$, it suffices to find a way to calculate the boundary term $\Lambda_4(k,l,m,1)$, which will be our main focus below.

III. BOUNDARY TERM $\Lambda_4(k,l,m,1)$

The boundary term $\Lambda_4(k,l,m,1)$ reads

$$\Lambda_4(k,l,m,1) = \int_0^\infty dv\, v^k e^{-\theta v}\int_v^\infty dx\, x^l e^{-\alpha x}\int_x^\infty dy\, y^m e^{-\beta y}\int_y^\infty \frac{1}{z}e^{-\gamma z}dz \tag{16}$$

with the requirements that $k\geqslant 0$, $k+l+1\geqslant 0$, and $k+l+m+2\geqslant 0$.

A. $k \geqslant 0, l \geqslant 0, m \geqslant 0$

Interchanging the integration order of (16) yields

$$\begin{aligned}\Lambda_4(k,l,m,1) &= \int_0^\infty dz\,\frac{1}{z}e^{-\gamma z}\int_0^z dy\,y^m e^{-\beta y}\int_0^y dx\,x^l e^{-\alpha x}\int_0^x dv\,v^k e^{-\theta v}\\ &= \int_0^\infty dz\,\frac{1}{z}e^{-\gamma z}\int_0^z dy\,y^m e^{-\beta y}\int_0^y dx\,x^l e^{-\alpha x}\frac{k!}{\theta^{k+1}}\left(1-e^{-\theta x}\sum_{p=0}^{k}\frac{\theta^p x^p}{p!}\right)\\ &= \frac{k!}{\theta^{k+1}}\left[W_3(l,m,-1;\alpha,\beta,\gamma)-\sum_{p=0}^{k}\frac{\theta^p}{p!}W_3(l+p,m,-1;\theta+\alpha,\beta,\gamma)\right].\end{aligned} \tag{17}$$

B. $k \geqslant 0, l < 0, m \geqslant 0$

Similarly, we replace l by $-l$ such that $l > 0$ in this section. Let

$$E_3(k,l,m) := \Lambda_4(k,-l,m,1) = \int_0^\infty dz\,\frac{1}{z}e^{-\gamma z}\int_0^z dy\,y^m e^{-\beta y}\int_0^y dx\,\frac{1}{x^l}e^{-\alpha x}\int_0^x dv\,v^k e^{-\theta v}. \tag{18}$$

Write $H(x) := \int_0^x dv\,v^k e^{-\theta v}$. Taking the x integral by parts for $l > 1$ yields the formula

$$\int_0^y dx\,x^{-l}e^{-\alpha x}H(x) = \frac{1}{1-l}\left[y^{1-l}e^{-\alpha y}\int_0^y dx\,x^k e^{-\theta x} - \int_0^y dx\,x^{k+1-l}e^{-(\theta+\alpha)x} + \alpha\int_0^y dx\,x^{1-l}e^{-\alpha x}H(x)\right]. \tag{19}$$

Using (19), one can obtain the recursive relation

$$E_3(k,l,m) = \frac{1}{1-l}[W_3(k,m-l+1,-1;\theta,\alpha+\beta,\gamma) - W_3(k-l+1,m,-1;\theta+\alpha,\beta,\gamma)] + \frac{\alpha}{1-l}E_3(k,l-1,m). \tag{20}$$

Thus the problem has now become the evaluation of the sub-boundary term

$$E_3(k,1,m) = \int_0^\infty dz\,\frac{e^{-\gamma z}}{z}\int_0^z dy\,y^m e^{-\beta y}\int_0^y dx\,\frac{e^{-\alpha x}}{x}\int_0^x dv\,v^k e^{-\theta v} \tag{21}$$

for $k \geqslant 0$ and $m \geqslant 0$. With the help of (12) and (13), we have

$$\begin{aligned}E_3(k,1,m) &= \int_0^\infty dz\,\frac{e^{-\gamma z}}{z}\int_0^z dy\,y^m e^{-\beta y}\int_0^y dx\,\frac{e^{-\alpha x}}{x}\frac{k!}{\theta^{k+1}}\left(1-e^{-\theta x}-e^{-\theta x}\sum_{p=1}^{k}\frac{\theta^p x^p}{p!}\right)\\ &= \frac{k!}{\theta^{k+1}}\left[\int_0^\infty dz\,\frac{e^{-\gamma z}}{z}\int_0^z dy\,y^m e^{-\beta y}\int_0^y dx\,e^{-\alpha x}\frac{1-e^{-\theta x}}{x} - \sum_{p=1}^{k}\frac{\theta^p}{p!}W_3(p-1,m,-1;\theta+\alpha,\beta,\gamma)\right].\end{aligned} \tag{22}$$

Now the evaluation of $E_3(k,1,m)$ reduces to a triple integral in the right-hand side of (22). For the sake of simplicity, we set $\tilde{H}(y) = \int_0^y dx\,e^{-\alpha x}\frac{1-e^{-\theta x}}{x}$. Integrating by parts for $m > 1$ reads

$$\begin{aligned}\int_0^z dy\,y^m e^{-\beta y}\tilde{H}(y) &= -\frac{1}{\beta}\int_0^z de^{-\beta y}\,y^m\tilde{H}(y)\\ &= \frac{1}{\beta}\left[m\int_0^z dy\,y^{m-1}e^{-\beta y}\tilde{H}(y) + \int_0^z dy\,y^{m-1}\frac{1-e^{-\theta y}}{e^{(\alpha+\beta)y}} - z^m e^{-\beta z}\int_0^z dy\,e^{-\alpha y}\frac{1-e^{-\theta y}}{y}\right]\end{aligned} \tag{23}$$

and then one arrives at

$$\begin{aligned}G_1(m) &:= \int_0^\infty dz\,\frac{e^{-\gamma z}}{z}\int_0^z dy\,y^m e^{-\beta y}\int_0^y dx\,e^{-\alpha x}\frac{1-e^{-\theta x}}{x}\\ &= \frac{m}{\beta}G_1(m-1) + \frac{1}{\beta}\int_0^\infty dz\,\frac{e^{-\gamma z}}{z}\int_0^z dy\,y^{m-1}\frac{1-e^{-\theta y}}{e^{(\alpha+\beta)y}} - \frac{1}{\beta}\int_0^\infty dz\,z^{m-1}e^{-(\beta+\gamma)z}\int_0^z dy\,e^{-\alpha y}\frac{1-e^{-\theta y}}{y}\\ &:= \frac{m}{\beta}G_1(m-1) + \frac{1}{\beta}G_{11}(m-1) - \frac{1}{\beta}G_{12}(m-1).\end{aligned} \tag{24}$$

Using (12) and (13) we have

$$\begin{aligned} G_{11}(m-1) &= \int_0^\infty dz\,\frac{e^{-\gamma z}}{z}\int_0^z dy\,y^{m-1}e^{-(\alpha+\beta)y} - \int_0^\infty dz\,\frac{e^{-\gamma z}}{z}\int_0^z dy\,y^{m-1}e^{-(\theta+\alpha+\beta)y} \\ &= \frac{(m-1)!}{(\alpha+\beta)^m}\left[\ln\frac{\alpha+\beta+\gamma}{\gamma} - \sum_{q=1}^{m-1}\frac{1}{q}\left(\frac{\alpha+\beta}{\alpha+\beta+\gamma}\right)^q\right] \\ &\quad - \frac{(m-1)!}{(\theta+\alpha+\beta)^m}\left[\ln\frac{\theta+\alpha+\beta+\gamma}{\gamma} - \sum_{q=1}^{m-1}\frac{1}{q}\left(\frac{\theta+\alpha+\beta}{\theta+\alpha+\beta+\gamma}\right)^q\right] \end{aligned} \tag{25}$$

and

$$\begin{aligned} G_{12}(m-1) &= \int_0^\infty dy\,e^{-\alpha y}\,\frac{1-e^{-\theta y}}{y}\int_y^\infty dz\,z^{m-1}e^{-(\beta+\gamma)z} \\ &= \int_0^\infty dy\,\frac{1-e^{-\theta y}}{y}e^{-(\alpha+\beta+\gamma)y}\,\frac{(m-1)!}{(\beta+\gamma)^m}\sum_{q=0}^{m-1}\frac{(\beta+\gamma)^q y^q}{q!} \\ &= \frac{(m-1)!}{(\beta+\gamma)^m}\left[\ln\frac{\theta+\alpha+\beta+\gamma}{\alpha+\beta+\gamma} + \sum_{q=1}^{m-1}\frac{(\beta+\gamma)^q}{q!}\int_0^\infty dy\,y^{q-1}e^{-(\alpha+\beta+\gamma)y}(1-e^{-\theta y})\right] \\ &= \frac{(m-1)!}{(\beta+\gamma)^m}\left\{\ln\frac{\theta+\alpha+\beta+\gamma}{\alpha+\beta+\gamma} + \sum_{q=1}^{m-1}\frac{1}{q}\left[\left(\frac{\beta+\gamma}{\alpha+\beta+\gamma}\right)^q - \left(\frac{\beta+\gamma}{\theta+\alpha+\beta+\gamma}\right)^q\right]\right\}. \end{aligned} \tag{26}$$

It should be pointed out that, when evaluating the two terms in the two square brackets in (25) respectively with the logarithmic arguments being close to 1, numerical cancellation could happen between the two terms. However, the cancellation can be avoided by using the following stable expression:

$$\ln\frac{a+b}{b} - \sum_{p=1}^{M}\frac{1}{p}\left(\frac{a}{a+b}\right)^p = \sum_{p=M+1}^{\infty}\frac{1}{p}\left(\frac{a}{a+b}\right)^p. \tag{27}$$

The remaining term for evaluating $G_1(m)$ recursively is

$$G_1(0) = \int_0^\infty dz\,\frac{e^{-\gamma z}}{z}\int_0^z dy\,e^{-\beta y}\int_0^y dx\,e^{-\alpha x}\,\frac{1-e^{-\theta x}}{x} := F(\theta,\alpha,\beta,\gamma). \tag{28}$$

Differentiating $F(\theta,\alpha,\beta,\gamma)$ with respect to α, one has

$$\begin{aligned} \frac{\partial F}{\partial\alpha} &= -\int_0^\infty dz\,\frac{e^{-\gamma z}}{z}\int_0^z dy\,e^{-\beta y}\int_0^y dx\,e^{-\alpha x}(1-e^{-\theta x}) \\ &= \frac{1}{\theta+\alpha}\int_0^\infty dz\,\frac{e^{-\gamma z}}{z}\int_0^z dy\,e^{-\beta y}(1-e^{-(\theta+\alpha)y}) - \frac{1}{\alpha}\int_0^\infty dz\,\frac{e^{-\gamma z}}{z}\int_0^z dy\,e^{-\beta y}(1-e^{-\alpha y}) \\ &= \frac{1}{\theta+\alpha}\left(\frac{1}{\beta}\ln\frac{\beta+\gamma}{\gamma} - \frac{1}{\theta+\alpha+\beta}\ln\frac{\theta+\alpha+\beta+\gamma}{\gamma}\right) - \frac{1}{\alpha}\left(\frac{1}{\beta}\ln\frac{\beta+\gamma}{\gamma} - \frac{1}{\alpha+\beta}\ln\frac{\alpha+\beta+\gamma}{\gamma}\right), \end{aligned} \tag{29}$$

where (12), (13), and the following formula

$$\int_0^\infty dx\,\frac{1-e^{-ax}}{x}e^{-bx} = \ln\frac{a+b}{b} \tag{30}$$

were used in the last step. Noticing the two facts that $F(\theta,\alpha,\beta,\gamma)\to 0$ as $\alpha\to\infty$ and $\frac{\partial F}{\partial\alpha}$ can be written in the form $F_1(\theta+\alpha) - F_1(\alpha)$ with

$$F_1(t) = \frac{1}{t}\left(\frac{1}{\beta}\ln\frac{\beta+\gamma}{\gamma} - \frac{1}{t+\beta}\ln\frac{t+\beta+\gamma}{\gamma}\right),$$

one immediately concludes that

$$F(\theta,\alpha,\beta,\gamma) = -\int_\alpha^\infty dt\,\frac{\partial F(\theta,t,\beta,\gamma)}{\partial t} = -\int_\alpha^\infty dt\,[F_1(\theta+t) - F_1(t)] = -\left[\int_{\theta+\alpha}^\infty dt\,F_1(t) - \int_\alpha^\infty dt\,F_1(t)\right] = \int_\alpha^{\theta+\alpha} dt\,F_1(t). \tag{31}$$

It should be mentioned here that there exists an important integration formula [19]

$$\int_{\xi_1}^{\xi_2} \frac{\ln(c+e\xi)}{a+b\xi} d\xi = \frac{1}{b} \ln \frac{bc-ae}{b} \ln \frac{a+b\xi_2}{a+b\xi_1} - \frac{1}{b}\mathrm{Li}_2\left[\frac{e(a+b\xi_2)}{ae-bc}\right] + \frac{1}{b}\mathrm{Li}_2\left[\frac{e(a+b\xi_1)}{ae-bc}\right], \tag{32}$$

with $\mathrm{Li}_2(z)$ being the dilogarithmic function defined by $\mathrm{Li}_2(z) := -\int_0^z \xi^{-1}\ln(1-\xi)d\xi$. With the help of the above formula, we have

$$F(\theta,\alpha,\beta,\gamma) = \int_\alpha^{\theta+\alpha} dt\, F_1(t) = \frac{1}{\beta}\left[\mathrm{Li}_2\left(-\frac{\theta+\alpha}{\beta+\gamma}\right) - \mathrm{Li}_2\left(-\frac{\alpha}{\beta+\gamma}\right) + \mathrm{Li}_2\left(-\frac{\alpha+\beta}{\gamma}\right) - \mathrm{Li}_2\left(-\frac{\theta+\alpha+\beta}{\gamma}\right)\right]. \tag{33}$$

C. $k \geqslant 0, l \geqslant 0, m < 0$

Similarly, we replace m by $-m$ such that $m > 0$ in this section. Let

$$M_3(k,l,m) := \Lambda_4(k,l,-m,1) = \int_0^\infty dz\, \frac{1}{z} e^{-\gamma z} \int_0^z dy\, y^{-m} e^{-\beta y} \int_0^y dx\, x^l e^{-\alpha x} \int_0^x dv\, v^k e^{-\theta v} \tag{34}$$

with the requirements that $k \geqslant 0$, $k+l+1 \geqslant 0$, and $k+l-m+2 \geqslant 0$. Following a similar procedure as in (19)–(22), we arrive at the following recursion relation for $m > 1$:

$$M_3(k,l,m) = \frac{\beta}{1-m} M_3(k,l,m-1) + \frac{1}{1-m}[W_3(k,l,-m;\theta,\alpha,\beta+\gamma) - W_3(k,l+1-m,-1;\theta,\alpha+\beta,\gamma)]. \tag{35}$$

Now this recursion relation for $M_3(k,l,m)$ traces back to $M_3(k,l,1)$. Performing the v integral by using (12) and (13) yields

$$\begin{aligned} M_3(k,l,1) &= \frac{k!}{\theta^{k+1}}\left[\int_0^\infty dz\, \frac{e^{-\gamma z}}{z} \int_0^z dy\, \frac{e^{-\beta y}}{y} \int_0^y dx\, x^l e^{-\alpha x} - \sum_{p=0}^k \frac{t^p}{p!} \int_0^\infty dz\, \frac{e^{-\gamma z}}{z} \int_0^z dy\, \frac{e^{-\beta y}}{y} \int_0^y dx\, x^{l+p} e^{-(\theta+\alpha)x}\right] \\ &:= \frac{k!}{\theta^{k+1}}\left[J(l;\alpha,\beta,\gamma) - \sum_{p=0}^k \frac{t^p}{p!} J(l+p;\theta+\alpha,\beta,\gamma)\right]. \end{aligned} \tag{36}$$

With the help of the two formulas in [11]

$$\begin{aligned} \tilde{F}(a,b,c) &:= \int_0^\infty dz\, \frac{e^{-cz}}{z} \int_0^z dy\, \frac{e^{-by}}{y}(1-e^{-ay}) \\ &= \frac{1}{2}\left[\ln^2\left(\frac{b+c}{b}\right) - \ln^2\left(\frac{a+b+c}{a+b}\right) + \ln^2\left(\frac{a+b}{c}\right)\right] + \mathrm{Li}_2\left(\frac{c}{b+c}\right) - \mathrm{Li}_2\left(\frac{c}{a+b+c}\right) - \frac{1}{2}\ln^2\left(\frac{b}{c}\right) \end{aligned} \tag{37}$$

and

$$\int_0^\infty dz\, \frac{e^{-bz}}{z} \int_0^z dy\, e^{-ay} y^{p-1} = \frac{(p-1)!}{a^p}\left[\ln \frac{a+b}{b} - \sum_{q=1}^{p-1} \frac{1}{q}\left(\frac{a}{a+b}\right)^q\right] \tag{38}$$

for a positive integer p, one obtains

$$J(l;\alpha,\beta,\gamma) = \frac{l!}{\alpha^{l+1}}\left\{\tilde{F}(\alpha,\beta,\gamma) - \sum_{q=1}^{l} \frac{1}{q}\left(\frac{\alpha}{\alpha+\beta}\right)^q\left[\ln\left(\frac{\alpha+\beta+\gamma}{\gamma}\right) - \sum_{r=1}^{q-1} \frac{1}{r}\left(\frac{\alpha+\beta}{\alpha+\beta+\gamma}\right)^r\right]\right\}, \tag{39}$$

which gives rise to $M_3(k,l,1)$ immediately from (36).

D. $k \geqslant 0, l < 0, m < 0$

Similarly, we replace l and m by $-l$ and $-m$, respectively, with l and m being now positive. Let

$$N_3(k,l,m) := \Lambda_4(k,-l,-m,1) = \int_0^\infty dz\, \frac{1}{z} e^{-\gamma z} \int_0^z dy\, y^{-m} e^{-\beta y} \int_0^y dx\, x^{-l} e^{-\alpha x} \int_0^x dv\, v^k e^{-\theta v} \tag{40}$$

with the requirements of $k \geqslant 0$, $k-l+1 \geqslant 0$, and $k-l-m+2 \geqslant 0$. With a similar procedure as in (19)–(22), we obtain the following recursion relation for $l > 1$:

$$N_3(k,l,m) = \frac{\alpha}{1-l} N_3(k,l-1,m) + \frac{1}{1-l}[W_3(k,-l-m+1,-1;\theta,\alpha+\beta,\gamma) - W_3(k-l+1,-m,-1;\theta+\alpha,\beta,\gamma)], \tag{41}$$

as well as the recursion relation for $m > 1$:

$$N_3(k,1,m) = \frac{\beta}{1-m} N_3(k,1,m-1) + \frac{1}{1-m}[W_3(k,-1,-m;\theta,\alpha,\beta+\gamma) - W_3(k,-m,-1;\theta,\alpha+\beta,\gamma)]. \tag{42}$$

By using (12) and (13), the initial term for this recursion relation is

$$N_3(k,1,1) = \frac{k!}{\theta^{k+1}}\bigg[\int_0^\infty dz\, \frac{e^{-\gamma z}}{z} \int_0^z dy\, \frac{e^{-\beta y}}{y} \int_0^y dx\, \frac{e^{-\alpha x}}{x}(1-e^{-\theta x}) - \sum_{p=1}^{k} \frac{\theta^p}{p!} \int_0^\infty dz\, \frac{e^{-\gamma z}}{z} \int_0^z dy\, \frac{e^{-\beta y}}{y} \int_0^y dx\, e^{-(\theta+\alpha)x} x^{p-1}\bigg] := \frac{k!}{\theta^{k+1}}[\Phi(\theta,\alpha,\beta,\gamma) - \Psi(k;\theta,\alpha,\beta,\gamma)]. \tag{43}$$

Recalling (37) and (38), $\Psi(k;\theta,\alpha,\beta,\gamma)$ takes the following form:

$$\Psi(k;\theta,\alpha,\beta,\gamma) = \sum_{p=1}^{k} \frac{1}{p}\left(\frac{\theta}{\theta+\alpha}\right)^p \left\{\tilde{F}(\theta+\alpha,\beta,\gamma) - \sum_{q=1}^{p-1} \frac{1}{q}\left(\frac{\theta+\alpha}{\theta+\alpha+\beta}\right)^q \times \left[\ln\left(\frac{\theta+\alpha+\beta+\gamma}{\gamma}\right) - \sum_{r=1}^{q-1} \frac{1}{r}\left(\frac{\theta+\alpha+\beta}{\theta+\alpha+\beta+\gamma}\right)^r\right]\right\}. \tag{44}$$

As for $\Phi(\theta,\alpha,\beta,\gamma)$, differentiating it with respect to α reads

$$\frac{\partial \Phi}{\partial \alpha} = \int_0^\infty dz\, \frac{e^{-\gamma z}}{z} \int_0^z dy\, \frac{e^{-\beta y}}{y} \int_0^y dx\, e^{-(\theta+\alpha)x} - \int_0^\infty dz\, \frac{e^{-\gamma z}}{z} \int_0^z dy\, \frac{e^{-\beta y}}{y} \int_0^y dx\, e^{-\alpha x} := \Phi_1(\theta+\alpha) - \Phi_1(\alpha) \tag{45}$$

with

$$\Phi_1(\alpha) = \frac{1}{\alpha}\left\{\mathrm{Li}_2\left(\frac{\gamma}{\beta+\gamma}\right) - \mathrm{Li}_2\left(\frac{\gamma}{\alpha+\beta+\gamma}\right) - \frac{1}{2}\ln^2\left(\frac{\beta}{\gamma}\right) + \frac{1}{2}\left[\ln^2\left(\frac{\beta+\gamma}{\beta}\right) - \ln^2\left(\frac{\alpha+\beta+\gamma}{\alpha+\beta}\right) + \ln^2\left(\frac{\alpha+\beta}{\gamma}\right)\right]\right\}. \tag{46}$$

Based on the same reasoning leading to (31), we have

$$\Phi(\theta,\alpha,\beta,\gamma) = \int_\alpha^{\theta+\alpha} dt\, \Phi_1(t) = \int_\alpha^{\theta+\alpha} dt\, \frac{1}{t}\left[\mathrm{Li}_2\left(\frac{\gamma}{\beta+\gamma}\right) + \frac{1}{2}\ln^2\left(\frac{\beta+\gamma}{\beta}\right) - \frac{1}{2}\ln^2\left(\frac{\beta}{\gamma}\right)\right] - \int_\alpha^{\theta+\alpha} dt\, \frac{1}{t}\mathrm{Li}_2\left(\frac{\gamma}{t+\beta+\gamma}\right) - \int_\alpha^{\theta+\alpha} dt\, \frac{1}{2t}\ln^2\left(\frac{t+\beta+\gamma}{t+\beta}\right) + \int_\alpha^{\theta+\alpha} dt\, \frac{1}{2t}\ln^2\left(\frac{t+\beta}{\gamma}\right) := I_0 + I_1 + I_2 + I_3. \tag{47}$$

The I_0 integral can be easily obtained:

$$I_0 = \left[\mathrm{Li}_2\left(\frac{\gamma}{\beta+\gamma}\right) + \frac{1}{2}\ln^2\left(\frac{\beta+\gamma}{\beta}\right) - \frac{1}{2}\ln^2\left(\frac{\beta}{\gamma}\right)\right]\ln\left(\frac{\theta+\alpha}{\alpha}\right). \tag{48}$$

Recalling the dilogarithm specified below (32) and taking the integration by parts, we find

$$I_1 = \mathrm{Li}_2\left(\frac{\gamma}{\alpha+\beta+\gamma}\right)\ln\alpha - \mathrm{Li}_2\left(\frac{\gamma}{\theta+\alpha+\beta+\gamma}\right)\ln(\theta+\alpha) + \int_\alpha^{\theta+\alpha} dt\, \ln(t)\ln\left(\frac{t+\beta}{t+\beta+\gamma}\right)\frac{1}{t+\beta+\gamma}. \tag{49}$$

Meanwhile, the latter two integrals in (47) satisfy

$$I_2 = \frac{1}{2}\ln\alpha\ln^2\left(\frac{\alpha+\beta+\gamma}{\alpha+\beta}\right) - \frac{1}{2}\ln(\theta+\alpha)\ln^2\left(\frac{\theta+\alpha+\beta+\gamma}{\theta+\alpha+\beta}\right) + \int_\alpha^{\theta+\alpha} dt\, \ln(t)\ln\left(\frac{t+\beta+\gamma}{t+\beta}\right)\frac{1}{t+\beta+\gamma} - \int_\alpha^{\theta+\alpha} dt\, \ln(t)\ln\left(\frac{t+\beta+\gamma}{t+\beta}\right)\frac{1}{t+\beta} \tag{50}$$

and

$$I_3 = \frac{1}{2}\ln(\theta+\alpha)\ln^2\left(\frac{\theta+\alpha+\beta}{\gamma}\right) - \frac{1}{2}\ln(\alpha)\ln^2\left(\frac{\alpha+\beta}{\gamma}\right) + \ln(\gamma)\left[\ln(\theta+\alpha)\ln\left(\frac{\theta+\alpha+\beta}{\beta}\right) - \ln(\alpha)\ln\left(\frac{\alpha+\beta}{\beta}\right)\right] + \ln(\gamma)\left[\mathrm{Li}_2\left(-\frac{\theta+\alpha}{\beta}\right) - \mathrm{Li}_2\left(-\frac{\alpha}{\beta}\right)\right] - \int_\alpha^{\theta+\alpha} dt\, \ln(t)\ln(t+\beta)\frac{1}{t+\beta}, \tag{51}$$

respectively. It follows from (48)–(51) that

$$\Phi(\theta,\alpha,\beta,\gamma) = \mathcal{I} - \int_\alpha^{\theta+\alpha} dt\, \ln(t)\ln(t+\beta+\gamma)\frac{1}{t+\beta} := \mathcal{I} - I_s, \tag{52}$$

where

$$\mathcal{I} = \ln\left(\frac{\theta+\alpha}{\alpha}\right)\left[\mathrm{Li}_2\left(\frac{\gamma}{\beta+\gamma}\right) + \frac{1}{2}\ln\left(\frac{\beta+\gamma}{\gamma}\right)\ln\left(\frac{(\beta+\gamma)\gamma}{\beta^2}\right)\right] + \mathrm{Li}_2\left(\frac{\gamma}{\alpha+\beta+\gamma}\right)\ln\alpha - \mathrm{Li}_2\left(\frac{\gamma}{\theta+\alpha+\beta+\gamma}\right)\ln(\theta+\alpha)$$
$$+ \frac{1}{2}\ln(\alpha)\ln\left(\frac{\alpha+\beta+\gamma}{\gamma}\right)\ln\left(\frac{(\alpha+\beta+\gamma)\gamma}{(\alpha+\beta)^2}\right) - \frac{1}{2}\ln(\theta+\alpha)\ln\left(\frac{\theta+\alpha+\beta+\gamma}{\gamma}\right)\ln\left(\frac{(\theta+\alpha+\beta+\gamma)\gamma}{(\theta+\alpha+\beta)^2}\right)$$
$$+ \ln(\gamma)\left[\ln(\theta+\alpha)\ln\left(\frac{\theta+\alpha+\beta}{\beta}\right) - \ln(\alpha)\ln\left(\frac{\alpha+\beta}{\beta}\right)\right] + \ln(\gamma)\left[\mathrm{Li}_2\left(-\frac{\theta+\alpha}{\beta}\right) - \mathrm{Li}_2\left(-\frac{\alpha}{\beta}\right)\right].$$

Now the evaluation of $\Phi(\theta,\alpha,\beta,\gamma)$ is reduced to the definite integral I_s. The change of variable $u = (t+\beta)/\beta$ gives rise to the following expression immediately:

$$I_s = \int_{u_1}^{u_2} du\left[\frac{\ln\beta\,\ln\gamma}{u} + \frac{\ln\beta\,\ln(1+cu)}{u} + \frac{\ln\gamma\,\ln|1-u|}{u} + \frac{\ln|1-u|\,\ln(1+cu)}{u}\right]$$
$$= \ln\beta\ln\gamma\ln\frac{u_2}{u_1} + \ln\beta\,[\mathrm{Li}_2(-cu_1) - \mathrm{Li}_2(-cu_2)] + \ln\gamma\,[\mathrm{Li}_2(u_1) - \mathrm{Li}_2(u_2)] + \int_{u_1}^{u_2} du\frac{\ln|1-u|\,\ln(1+cu)}{u}, \qquad (53)$$

where $c = \beta/\gamma$, $u_1 = (\alpha+\beta)/\beta$, and $u_2 = (\theta+\alpha+\beta)/\beta$. Denoting by I_s^* the integral appearing in the last term of (53), we find

$$I_s^* = \frac{1}{2}\left\{\ln^2(c)\ln\left(\frac{w_2}{w_1}\right) + 2\ln(c)[\mathrm{Li}_2(w_1) - \mathrm{Li}_2(w_2)] + [\mathcal{F}(w_2) - \mathcal{F}(w_1)] + [\mathcal{F}(-cu_2) - \mathcal{F}(-cu_1)]\right.$$
$$\left. + [\mathcal{F}(u_2) - \mathcal{F}(u_1)] - [\mathcal{F}(\tilde{w}_2) - \mathcal{F}(\tilde{w}_1)]\right\}, \qquad (54)$$

where $w_i = \frac{1+c}{c(1-u_i)}$ and $\tilde{w}_i = \frac{u_i(1+c)}{u_i-1}$ for $i = 1,2$, and the auxiliary function $\mathcal{F}$ is defined by

$$\mathcal{F}(\xi) = \ln|\xi|\,\ln^2|\xi-1| + 2\ln|\xi-1|\,\mathrm{Li}_2(1-\xi) - 2\mathrm{Li}_3(1-\xi) \qquad (55)$$

with $\mathrm{Li}_3(\xi)$ the trilogarithmic function [20,21] defined by $\mathrm{Li}_3(\xi) := \int_0^\xi \frac{\mathrm{Li}_2(\eta)}{\eta}d\eta$. In order to remove ambiguities for multiple-valued problems, $\ln(x)$ is understood as $\ln|x|$ for $x < 0$, and $\mathrm{Li}_2(x)$ and $\mathrm{Li}_3(x)$ are

$$\mathrm{Li}_2(x) = \frac{\pi^2}{3} - \mathrm{Li}_2(x^{-1}) - \frac{1}{2}\ln^2 x \qquad (56)$$

and

$$\mathrm{Li}_3(x) = \frac{\pi^2}{3}\ln x + \mathrm{Li}_3(x^{-1}) - \frac{1}{6}\ln^3 x \qquad (57)$$

TABLE I. Values of $W_4(k,l,m,n;\theta,\alpha,\beta,\gamma)$ with $(\theta,\alpha,\beta,\gamma) = (2.1,1.6,1.0,0.8)$ for the first $(k,l,m,n) = (4,3,1,-2)$ and $(\theta,\alpha,\beta,\gamma) = (3.6,2.5,1.5,1.1)$ for the remaining ones. For each (k,l,m,n), we list two quadruple FORTRAN values of W_4, where the first one is obtained using the recursive method and the second one is obtained using (8). [X] indicates the power of 10^X.

(k,l,m,n)	$W_4(k,l,m,n;\theta,\alpha,\beta,\gamma)$
$(4,3,1,-2)$	6.407706007018718040867766170534678 [−4]
	6.407706007018718040867766170534240 [−4]
$(4,3,2,-2)$	1.225819152498255647777409301906053 [−5]
	1.225819152498255647777409301906012 [−5]
$(0,3,2,-2)$	3.390075950061788847980390618485692 [−4]
	3.390075950061788847980390618485658 [−4]
$(4,6,5,-2)$	3.804439168009192177902570317632892 [−4]
	3.804439168009192177902570317632809 [−4]
$(4,3,0,-2)$	6.536176807512103122943273916266838 [−6]
	6.536176807512103122943273916266331 [−6]
$(4,3,6,-3)$	6.412291381304496379807410314518402 [−5]
	6.412291381304496379807410314518460 [−5]
$(4,3,6,2)$	3.477569221454161773218604728474131 [−2]
	3.477569221454161773218604728474138 [−2]

TABLE II. Values of $W_4(k,l,m,n;\theta,\alpha,\beta,\gamma)$ with $(\theta,\alpha,\beta,\gamma) = (3.6,2.5,1.5,1.1)$ and (k,l,m,n) being generated from $(4,2,2,2)$ with all possible negative sign choices. For each (k,l,m,n), we list two quadruple FORTRAN values of W_4, where the first one is obtained using the recursive method and the second one is obtained using (8). [X] indicates the power of 10^X.

(k,l,m,n)	$W_4(k,l,m,n;\theta,\alpha,\beta,\gamma)$
$(4,2,2,2)$	4.819662720799299029439114765171396 [−4]
	4.819662720799299029439114765171399 [−4]
$(4,-2,2,2)$	6.779880249449667776523412349957551 [−4]
	6.779880249449667776523412349957545 [−4]
$(4,2,-2,2)$	8.617361420158524690721813293468132 [−5]
	8.617361420158524690721813293468073 [−5]
$(4,2,2,-2)$	1.123135156079134344568286930590841 [−5]
	1.123135156079134344568286930590816 [−5]
$(4,-2,-2,2)$	8.904237776472281777971693390725130 [−4]
	8.904237776472281777971693390725994 [−4]
$(4,-2,2,-2)$	3.867768663362658337756916820585075 [−5]
	3.867768663362658337756916820586540 [−5]
$(4,2,-2,-2)$	9.397848209296999727653893885192435 [−6]
	9.397848209296999727653893885194976 [−6]
$(4,-2,-2,-2)$	7.105319773033728311846144013385863 [−4]
	7.105319773033728311846144013385257 [−4]

TABLE III. Values of W_4 for $n \geqslant 0$ with $(k,l,m,n) = (40,10,20,10)$ and $(\alpha,\beta,\gamma) = (3.5,1.1,0.4)$. For a given θ, two values of W_4 are presented using the recursive method, where the first entry is calculated by FORTRAN in quadruple precision and the second by MAPLE in multiple precision. [X] indicates the power of 10^X.

θ	$\frac{\theta}{\theta+\alpha+\beta+\gamma}$	$W_4(k,l,m,n;\theta,\alpha,\beta,\gamma)$
15.0	0.75	2.72453498647625756643993668191560 [28]
		2.7245349864762575664399366819156022663 [28]
20.0	0.8	2.83280866972294521071985732849751 [23]
		2.8328086697229452107198573284975111824 [23]
45.0	0.9	1.18053485618692796394570132172308 [9]
		1.1805348561869279639457013217230797267 [9]
495.0	0.99	2.373343287216544723748873509937717 [−34]
		2.3733432872165447237488735099377184964 [−34]
4995.0	0.999	1.637640316762922087489047781716579 [−75]
		1.6376403167629220874890477817165781222 [−75]
49995.0	0.9999	1.578280661834121777472027137948787 [−116]
		1.5782806618341217774720271379487877262 [−116]
499995.0	0.99999	1.572467218847705012359378032580944 [−157]
		1.5724672188477050123593780325809431084 [−157]
4999995.0	0.999999	1.571887082294971933107418240416460 [−198]
		1.5718870822949719331074182404164596573 [−198]
49999995.0	0.9999999	1.571829080699870378345418745351643 [−239]
		1.5718290806998703783454187453516432456 [−239]

for $x > 1$, respectively. Similarly to the way of numerically evaluating $\mathrm{Li}_2(x)$ in [19], we investigate the trilogarithmic function below.

(I) If x lies in the range $-1/2 \leqslant x < 2/3$, $\mathrm{Li}_3(x)$ can be calculated by using the following power series expansion:

$$\mathrm{Li}_3(x) = \sum_{n=1}^{N} \frac{x^n}{n^3} + R_N(x), \tag{58}$$

with N being large enough so that the truncation error bound

$$|R_N(x)| \leqslant \frac{|x|^{N+1}}{(N+1)^3(1-|x|)} \tag{59}$$

is small enough to guarantee the required accuracy.

(II) For $x \leqslant -2$,

$$\mathrm{Li}_3(x) = \mathrm{Li}_3\left(\frac{1}{x}\right) - \frac{\pi^2}{6}\ln(-x) - \frac{1}{6}\ln^3(-x) \tag{60}$$

with $\mathrm{Li}_3(1/x)$ evaluated by using (I).

TABLE IV. Values of W_4 for $n \geqslant 0$ with $(k,l,m,n) = (40,-10,20,10)$ and $(\alpha,\beta,\gamma) = (3.5,1.1,0.4)$. For a given θ, two values of W_4 are presented using the recursive method, where the first entry is calculated by FORTRAN in quadruple precision and the second by MAPLE in multiple precision. [X] indicates the power of 10^X.

θ	$\frac{\theta}{\theta+\alpha+\beta+\gamma}$	$W_4(k,l,m,n;\theta,\alpha,\beta,\gamma)$
15.0	0.75	3.51654946995816684965874944541588 [20]
		3.5165494699581668496587494454162959798 [20]
20.0	0.8	1.82100070983003518804949804061464 [17]
		1.8210007098300351880494980406146359971 [17]
45.0	0.9	1.89613791618796333144217430096769 [7]
		1.8961379161879633314421743009676910052 [7]
495.0	0.99	9.795720000776817442907094504837701 [−26]
		9.7957200007768174429070945048377050896 [−26]
4995.0	0.999	9.208929536477765863678890212637938 [−58]
		9.2089295364777658636788902126379393714 [−58]
49995.0	0.9999	9.152689486928382814098609465976611 [−90]
		9.1526894869283828140986094659766120187 [−90]
499995.0	0.99999	9.147089218698421633005885100442584 [−122]
		9.1470892186984216330058851004425865743 [−122]
4999995.0	0.999999	9.146529428607362656584002096409819 [−154]
		9.1465294286073626565840020964098205816 [−154]
49999995.0	0.9999999	9.146473451964942600268994789690104 [−186]
		9.1464734519649426002689947896901060674 [−186]

TABLE V. Values of W_4 for $n \geqslant 0$ with $(k,l,m,n) = (40,10,-20,10)$ and $(\alpha,\beta,\gamma) = (3.5,1.1,0.4)$. For a given θ, two values of W_4 are presented using the recursive method, where the first entry is calculated by FORTRAN in quadruple precision and the second by MAPLE in multiple precision. [X] indicates the power of 10^X.

θ	$\frac{\theta}{\theta+\alpha+\beta+\gamma}$	$W_4(k,l,m,n;\theta,\alpha,\beta,\gamma)$
15.0	0.75	1.52308914698078940739995793347317 [1]
		1.5230891469807894073999579334722203458 [1]
20.0	0.8	9.545534563199629277902797602372884 [−3]
		9.5455345631996292779027976023689423635 [−3]
45.0	0.9	1.135575381001893618179480020366452 [−12]
		1.1355753810018936181794800203665617549 [−12]
495.0	0.99	1.260673980650920374068408010393664 [−45]
		1.2606739806509203740684080103936647375 [−45]
4995.0	0.999	1.283777349651987038077202085918517 [−78]
		1.2837773496519870380772020859185177136 [−78]
49995.0	0.9999	1.286256190233811103585738108257018 [−111]
		1.2862561902338111035857381082570188914 [−111]
499995.0	0.99999	1.286505870845184435066665074690149 [−144]
		1.2865058708451844350666650746901501813 [−144]
4999995.0	0.999999	1.286530856993136577891420821832037 [−177]
		1.2865308569931365778914208218320379582 [−177]
49999995.0	0.9999999	1.286533355788922313987503800156406 [−210]
		1.2865333557889223139875038001564064514 [−210]

(III) For $-2 < x < -1/2$,

$$\mathrm{Li}_3(x) = -\mathrm{Li}_3\left(\frac{1}{1-x}\right) - \mathrm{Li}_3\left(\frac{x}{x-1}\right) + \mathrm{Li}_3(1) - \frac{\pi^2}{6}\ln(1-x) - \frac{1}{2}\ln\left(\frac{x}{x-1}\right)\ln^2(1-x) - \frac{1}{6}\ln^3(1-x). \tag{61}$$

It is easy to see that $\frac{1}{1-x}$ and $\frac{x}{x-1}$ both lie in the range $(1/3,2/3)$, which allows us to compute $\mathrm{Li}_3(\frac{1}{1-x})$ and $\mathrm{Li}_3(\frac{x}{x-1})$ using (I).

(IV) For $2/3 \leqslant x < 1$, we use the following identity:

$$\mathrm{Li}_3(x) = -\mathrm{Li}_3\left(\frac{x-1}{x}\right) - \mathrm{Li}_3(1-x) + \mathrm{Li}_3(1) + \frac{\pi^2}{6}\ln(1-x) - \frac{1}{2}\ln(x)\ln^2(1-x) + \frac{1}{6}\left[\ln^3\left(\frac{x}{1-x}\right) + \ln^3(1-x)\right] \tag{62}$$

TABLE VI. Values of W_4 for $n \geqslant 0$ with $(k,l,m,n) = (40,-10,-20,10)$ and $(\alpha,\beta,\gamma) = (3.5,1.1,0.4)$. For a given θ, two values of W_4 are presented using the recursive method, where the first entry is calculated by FORTRAN in quadruple precision and the second by MAPLE in multiple precision. [X] indicates the power of 10^X.

θ	$\frac{\theta}{\theta+\alpha+\beta+\gamma}$	$W_4(k,l,m,n;\theta,\alpha,\beta,\gamma)$
15.0	0.75	1.06816189243673833018014689178016 [0]
		1.0681618924367383301801468917801606972 [0]
20.0	0.8	5.730133195384882447788965394449981 [−2]
		5.7301331953848824477889653944499868717 [−2]
45.0	0.9	6.672431661640159070743519313762207 [−6]
		6.6724316616401590707435193137622120235 [−6]
495.0	0.99	6.409169809995467848831577254891414 [−19]
		6.4091698099954678488315772548914188826 [−19]
4995.0	0.999	6.384195742630979666044717605548649 [−32]
		6.3841957426309796660447176055486527952 [−32]
49995.0	0.9999	6.381711650490512740275485192787110 [−45]
		6.3817116504905127402754851927871159820 [−45]
499995.0	0.99999	6.381463374232566384701069504288033 [−58]
		6.3814633742325663847010695042880372913 [−58]
4999995.0	0.999999	6.381438547936144609315007687555769 [−71]
		6.3814385479361446093150076875557746864 [−71]
49999995.0	0.9999999	6.381436065319795972407039143736353 [−84]
		6.3814360653197959724070391437363573262 [−84]

TABLE VII. Values of W_4 for $n < 0$ with $(k,l,m,n) = (40,10,5,-25)$ and $(\alpha,\beta,\gamma) = (3.5,1.1,0.4)$. For a given θ, two values of W_4 are presented using the recursive method, where the first entry is calculated by FORTRAN in quadruple precision and the second by MAPLE in multiple precision. [X] indicates the power of 10^X.

θ	$\frac{\theta}{\theta+\alpha+\beta+\gamma}$	$W_4(k,l,m,n;\theta,\alpha,\beta,\gamma)$
15.0	0.75	6.169829531313502398960164186375392 [−12]
		6.1698295313135023989601641863910645176 [−12]
20.0	0.8	3.620361020700878145986390977151464 [−15]
		3.6203610207008781459863909771580037710 [−15]
45.0	0.9	2.990570800056888995818227896562259 [−25]
		2.9905708000568889958182278965604520022 [−25]
495.0	0.99	4.632849047409620808031140192728108 [−59]
		4.6328490474096208080311401927281081942 [−59]
4995.0	0.999	4.901241465050573329978190364235030 [−93]
		4.9012414650505733299781903642350299418 [−93]
49995.0	0.9999	4.929932990242740563591838093543859 [−127]
		4.9299329902427405635918380935438594145 [−127]
499995.0	0.99999	4.932822283467293345527190413166810 [−161]
		4.9328222834672933455271904131668099268 [−161]
4999995.0	0.999999	4.933111416003836909850262035207493 [−195]
		4.9331114160038369098502620352074916423 [−195]
49999995.0	0.9999999	4.933140331291461315099851327469129 [−229]
		4.9331403312914613150998513274691291220 [−229]

to evaluate $\mathrm{Li}_3(x)$, where the two trilogarithm arguments $\frac{x-1}{x}$ and $1-x$ both lie in the range $[-1/2,1/3)$ and thus the corresponding trilogarithms can be computed by (I), with the special value of $\mathrm{Li}_3(1)$ being considered below.

(V) For $x = 1$,

$$\mathrm{Li}_3(1) = \frac{8}{7}\mathrm{Li}_3\left(\frac{1}{2}\right) + \frac{2\pi^2}{21}\ln 2 - \frac{4}{21}\ln^3 2 = \zeta(3) \quad (63)$$

with $\mathrm{Li}_3(1/2)$ being evaluated using procedure (I) or, more commonly, using the Riemann zeta function value $\zeta(3)$ to evaluate $\mathrm{Li}_3(1)$.

(VI) For $1 < x \leqslant 3/2$,

$$\begin{aligned}\mathrm{Li}_3(x) = {} & -\mathrm{Li}_3(1-x) - \mathrm{Li}_3\left(1-\frac{1}{x}\right) + \mathrm{Li}_3(1) \\ & + \frac{\pi^2}{6}\ln(x) + \frac{1}{2}\ln(x)\ln^2\left(1-\frac{1}{x}\right) \\ & + \frac{1}{6}\left[\ln^3\left(\frac{1}{x-1}\right) + \ln^3\left(1-\frac{1}{x}\right) - \ln^3(x)\right] \quad (64)\end{aligned}$$

with the first two terms in the right-hand side being evaluated using procedure (I).

TABLE VIII. Values of W_4 for $n < 0$ with $(k,l,m,n) = (40,-10,5,-25)$ and $(\alpha,\beta,\gamma) = (3.5,1.1,0.4)$. For a given θ, two values of W_4 are presented using the recursive method, where the first entry is calculated by FORTRAN in quadruple precision and the second by MAPLE in multiple precision. [X] indicates the power of 10^X.

θ	$\frac{\theta}{\theta+\alpha+\beta+\gamma}$	$W_4(k,l,m,n;\theta,\alpha,\beta,\gamma)$
15.0	0.75	2.671462819061004216593186254998596 [−13]
		2.6714628190610042165931862549985965151 [−13]
20.0	0.8	1.220127599168729853159041634148152 [−14]
		1.2201275991687298531590416341481519767 [−14]
45.0	0.9	8.053867937886302281876066336377980 [−19]
		8.0538679378863022818760663363779800209 [−19]
495.0	0.99	8.673172242041309982988010984738373 [−33]
		8.6731722420413099829880109847383753767 [−33]
4995.0	0.999	8.739454441821909539915087573223001 [−47]
		8.7394544418219095399150875732230018720 [−47]
49995.0	0.9999	8.746129289807819439910154055087924 [−61]
		8.7461292898078194399101540550879249651 [−61]
499995.0	0.99999	8.746797244233662031986239540782027 [−75]
		8.7467972442336620319862395407820280940 [−75]
4999995.0	0.999999	8.746864044375891625295590274636182 [−89]
		8.7468640443758916252955902746361811817 [−89]
49999995.0	0.9999999	8.746870724437114413371486876946360 [−103]
		8.7468707244371144133714868769463594092 [−103]

TABLE IX. Values of W_4 for $n < 0$ with $(k,l,m,n) = (40,10,-5,-25)$ and $(\alpha,\beta,\gamma) = (3.5,1.1,0.4)$. For a given θ, two values of W_4 are presented using the recursive method, where the first entry is calculated by FORTRAN in quadruple precision and the second by MAPLE in multiple precision. [X] indicates the power of 10^X.

θ	$\frac{\theta}{\theta+\alpha+\beta+\gamma}$	$W_4(k,l,m,n;\theta,\alpha,\beta,\gamma)$
15.0	0.75	9.0507424083816701756741677357230 19 [−14]
		9.05074240838167017567416773572317770 02 [−14]
20.0	0.8	4.58787214982689237049326801990167 0 [−16]
		4.5878721498268923704932680199016763003 [−16]
45.0	0.9	3.1888561277634058198223195656136 52 [−23]
		3.1888561277634058198223195656136519043 [−23]
495.0	0.99	3.726624254141271979606145766499850 [−47]
		3.7266242541412719796061457664998504935 [−47]
4995.0	0.999	3.789503725765687534027199149521775 [−71]
		3.7895037257656875340271991495217748388 [−71]
49995.0	0.9999	3.795899386608692779472249941358632 [−95]
		3.7958993866086927794722499413586326535 [−95]
499995.0	0.99999	3.796540049909219060258914914185551 [−119]
		3.7965400499092190602589149141855513998 [−119]
4999995.0	0.999999	3.796604127231929727161889309319503 [−143]
		3.7966041272319297271618893093195025884 [−143]
49999995.0	0.9999999	3.796610535074147912626344941777762 [−167]
		3.7966105350741479126263449417777614341 [−167]

(VII) For $x > 3/2$,

$$\mathrm{Li}_3(x) = \mathrm{Li}_3\left(\frac{1}{x}\right) + \frac{\pi^2}{3}\ln(x) - \frac{1}{6}\ln^3(x) \tag{65}$$

with $\mathrm{Li}_3(1/x)$ being evaluated using procedure (I).

IV. NUMERICAL TESTS

In implementing W_4 numerically, we will encounter many evaluations of W_3. The recursion relations for W_3 developed in [11] will be used throughout. The recursion relations derived here for W_4 are implemented in FORTRAN in quadruple-precision arithmetic (about 32 digits), or in MAPLE using multiple precision. Table I presents some numerical results computed by FORTRAN with the choices of two quadruplets (k,l,m,n) and $(\theta,\alpha,\beta,\gamma)$, which are those used by Frolov [15]. For each group of eight parameters, we give two values for the corresponding W_4 integral, where the first one is calculated by the recursion relations and the second one by the analytical expression (8). It is seen that the two values match remarkably well and are in agreement with [15]. Notice that all the integer quadruplets given in [15] admit only one negative tuple, which

TABLE X. Values of W_4 for $n < 0$ with $(k,l,m,n) = (40,-10,-5,-25)$ and $(\alpha,\beta,\gamma) = (3.5,1.1,0.4)$. For a given θ, two values of W_4 are presented using the recursive method, where the first entry is calculated by sc fortran in quadruple precision and the second by MAPLE in multiple precision. [X] indicates the power of 10^X.

θ	$\frac{\theta}{\theta+\alpha+\beta+\gamma}$	$W_4(k,l,m,n;\theta,\alpha,\beta,\gamma)$
15.0	0.75	1.446053405943977577931788157246515 [−9]
		1.4460534059439775779317881572465151518 [−9]
20.0	0.8	5.972332267119546335455001257005701 [−10]
		5.9723322671195463354550012570057017855 [−10]
45.0	0.9	3.795817906804137739996499543483194 [−11]
		3.7958179068041377399964995434831935686 [−11]
495.0	0.99	3.854388578173303539516189758406969 [−15]
		3.8543885781733035395161897584069688995 [−15]
4995.0	0.999	3.860341348023986736367975574390631 [−19]
		3.8603413480239867363679755743906307629 [−19]
49995.0	0.9999	3.860937599840697501494260221095425 [−23]
		3.8609375998406975014942602210954245510 [−23]
499995.0	0.99999	3.860997234788874645491563631465142 [−27]
		3.8609972347888746454915636314651422450 [−27]
4999995.0	0.999999	3.861003198381375649691397004282718 [−31]
		3.8610031983813756496913970042827180983 [−31]
49999995.0	0.9999999	3.861003794741602601242464815860655 [−35]
		3.8610037947416026012424648158606544066 [−35]

is not sufficient for testing our recursion relations. Thus, we present some numerical values in Table II with all possible negative choices for tuples in the integer quadruplet (k,l,m,n), where the absolute values of the four integers are (4,2,2,2). It is clear that our recursive method is equivalent to the analytical expression (8). For bigger integers with the ratio $\theta/(\theta+\alpha+\beta+\gamma)$ close to 1, calculation by using (8) is very time consuming, which is slower than using the recursive method by a factor of 100 or even 1000 times. Thus, as a benchmark, instead of using (8), we use MAPLE in multiple precision (up to 300 digists) to calculate W_4 recursively for comparison with the results using the same recursive method in FORTRAN quadruple precision. Tables III–X list the values of W_4, where the first four tables are for the case of $n \geqslant 0$ and the remaining tables are for $n < 0$, with the ratio $\theta/(\theta+\alpha+\beta+\gamma)$ ranging from 0.75 to 0.999 999 9. It can be seen that the results from using the recursive method in FORTRAN are in perfect agreement with the benchmark results of MAPLE.

V. CONCLUSION

We have developed a recursive method to calculate the four-electron subsidiary integral $W_4(k,l,m,n;\,\theta,\alpha,\beta,\gamma)$, which covers the most general conditions: $k \geqslant 0$, $k+l+1 \geqslant 0$, $k+l+m+2 \geqslant 0$, and $k+l+m+n+3 \geqslant 0$. Extensive numerical experimentation has demonstrated that this method is computationally efficient and numerically stable, including the case of $\theta/(\theta+\alpha+\beta+\gamma) \sim 1$.

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