Analytic evaluation of three-electron integrals

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An analytic formula for the three-electron generating integral $I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}) := \int (r_1 r_2 r_3 r_{12} r_{23} r_{31})^{-1} \exp(-\alpha_1 r_1 - \alpha_2 r_2 - \alpha_3 r_3 - \alpha_{12} r_{12} - \alpha_{23} r_{23} - \alpha_{31} r_{31}) d^3r_1 d^3r_2 d^3r_3$ is given which is valid for all values of $\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}$ for which this integral converges. A large class of integrals can be evaluated analytically by taking derivatives of I with respect to the α's. More general integrals whose integrands contain products of spherical harmonics can also be evaluated analytically. In particular, all of the matrix element integrals which arise in a variational calculation on the lithium atom with Hylleraas-type basis functions can be evaluated in closed form. Certain difficult two-electron integrals can be obtained as a limiting case. Two-center two-electron molecular integrals can be obtained via an inverse Laplace transform; this observation is used to discuss the computation and convergence of series expansions for these molecular integrals.

I. INTRODUCTION

The well-known Rayleigh-Ritz variational method is widely used for calculating energies and wave functions for bound states of atoms and molecules. The success of such a calculation depends on its rate of convergence. The rate of convergence depends in turn on the ability of the basis functions used in the variational calculation to approximate the behavior of the exact wave function in the neighborhood of its singularities. The most important singularities are the cusps which occur at those points in configuration space where two or more interparticle distances are zero.[1-5] Getting the two-particle cusp behavior correct is the primary consideration in the design of better variational trial functions; three-particle cusps and pairs of two-particle cusps are believed to be less important. The wave function in the neighborhood of the point where particles i and j approach each other with no other particles close together has the form $\psi_0 + |\mathbf{r}_i - \mathbf{r}_j| \psi_{ij}$ where ψ_0 and ψ_{ij} are analytic functions of the Cartesian coordinates. Thus the proper two-particle cusp behavior can be built in by using a variational trial function of the form

$$\tilde{\psi} = \psi_0 + \sum_{\substack{i,j \\ (i<j)}} |\mathbf{r}_i - \mathbf{r}_j| \psi_{ij} , \tag{1.1}$$

where ψ_0 and the ψ_{ij} are finite sums of products of one-particle functions. For atoms, Slater orbitals, which make it easy to get the electron-nucleus cusp behavior correct, are the obvious choice for these one-particle functions.

The use of trial functions such as (1.1) is not a new idea. An extensive discussion of (1.1) and related ideas for getting the two-particle cusp behavior right has been given recently by Kutzelnigg.[6] Unfortunately, the widespread use of $|\mathbf{r}_i - \mathbf{r}_j|$ correlation factors has so far been precluded by the lack of analytic formulas for certain of the matrix element integrals which arise. The present paper opens the door to the practical use of trial functions such as (1.1) by evaluating the previously intractable three-electron integral

$$J(n_1,n_2,n_3,n_{12},n_{23},n_{31};\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}) := \int r_1^{n_1-1} r_2^{n_2-1} r_3^{n_3-1} r_{12}^{n_{12}-1} r_{23}^{n_{23}-1} r_{31}^{n_{31}-1} \exp(-\alpha_1 r_1 - \alpha_2 r_2 - \alpha_3 r_3 - \alpha_{12} r_{12} - \alpha_{23} r_{23} - \alpha_{31} r_{31}) d^3r_1 d^3r_2 d^3r_3 \tag{1.2}$$

for all non-negative integers $n_1,n_2,n_3,n_{12},n_{23},n_{31}$, where $r_{ij} := |\mathbf{r}_i - \mathbf{r}_j|$. Here $a := b$ means $a = b$ by definition. This is achieved by deriving an analytic formula for the generating integral

$$I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}) := \int (r_1 r_2 r_3 r_{12} r_{23} r_{31})^{-1} \exp(-\alpha_1 r_1 - \alpha_2 r_2 - \alpha_3 r_3 - \alpha_{12} r_{12} - \alpha_{23} r_{23} - \alpha_{31} r_{31}) d^3r_1 d^3r_2 d^3r_3 . \tag{1.3}$$

The integral (1.2) is obtained from (1.3) by differentiation:

$$J(n_1,n_2,n_3,n_{12},n_{23},n_{31};\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}) = \left[-\frac{\partial}{\partial\alpha_1}\right]^{n_1} \left[-\frac{\partial}{\partial\alpha_2}\right]^{n_2} \left[-\frac{\partial}{\partial\alpha_3}\right]^{n_3} \left[-\frac{\partial}{\partial\alpha_{12}}\right]^{n_{12}} \left[-\frac{\partial}{\partial\alpha_{23}}\right]^{n_{23}} \left[-\frac{\partial}{\partial\alpha_{31}}\right]^{n_{31}} I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}) . \tag{1.4}$$

Integrals more general than (1.2), in which the integrand of (1.2) has been multiplied by one or more factors of the form

$$r_1^{l_1} r_2^{l_2} r_3^{l_3} Y_{l_1 m_1}(\theta_1,\phi_1) Y_{l_2 m_2}(\theta_2,\phi_2) Y_{l_3 m_3}(\theta_3,\phi_3) ,$$

where the Y_{lm} are spherical harmonics, can also be evaluated analytically.

The appearance of the three-electron integral (1.2) is not limited to atomic calculations with variational trial functions of the form (1.1). All of the matrix element integrals which arise in a variational calculation on the lithium atom with Hylleraas-type basis functions of the form

$$\Phi(l_1,m_1,l_2,m_2,l_3,m_3;n_1,n_2,n_3,n_{12},n_{23},n_{31};\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})$$
$$:=r_1^{n_1+l_1}r_2^{n_2+l_2}r_3^{n_3+l_3}r_{12}^{n_{12}}r_{23}^{n_{23}}r_{31}^{n_{31}}\exp[-(\alpha_1r_1+\alpha_2r_2+\alpha_3r_3+\alpha_{12}r_{12}+\alpha_{23}r_{23}+\alpha_{31}r_{31})/2]$$
$$\times Y_{l_1m_1}(\theta_1,\phi_1)Y_{l_2m_2}(\theta_2,\phi_2)Y_{l_3m_3}(\theta_3,\phi_3) \tag{1.5}$$

can be reduced to finite sums of integrals of the form (1.2). The availability of an analytic formula for (1.2) should make is possible to use basis functions like (1.5) in variational approximations to the solutions of the inhomogeneous three-particle Schrödinger equations which arise in perturbation theory. Certain difficult two-electron integrals can be obtained as limiting cases of (1.2), as is discussed in Sec. II D. The integral (1.3) is the Laplace transform of certain two-electron two-center integrals which appear in molecular calculations, as is discussed in more detail in Sec. II E. Finally, of course, there is the hope that the methods which have yielded an analytic formula for (1.1) can be extended to other previously intractable matrix element integrals.

The initial evaluation of three-electron integrals such as (1.2) is due to James and Coolidge,[7] who were the first to use the Hylleraas-type basis functions (1.5) on lithium. Improvements were made by Burke,[8] by Larsson,[9] by Ho and Page,[10] and by Ho;[11] in each of these papers the main difficulty was the form (1.2). In order to make such integrals tractable, restrictions were usually placed on the α's and the n's. The calculations by James and Coolidge,[7] Burke,[8] Larsson,[9] Ho and Page,[10] and Ho[11] all had $\alpha_{12}=\alpha_{23}=\alpha_{31}=0$. Additionally, James and Coolidge, and Burke required that only one of $n_{12}-1$, $n_{23}-1$, and $n_{31}-1$ be nonzero at a time. The main technique used by these authors, and extended by others,[12–17] is expansion in terms of spherical harmonics and/or Legendre polynomials. These approaches then exploit in varying orders: (1) coordinate system manipulations, (2) relations among the spherical harmonics and Legendre polynomials, and (3) integrations over the angular coordinates, with the result being a linear combination of a set of standard integrals. For some combinations of the parameters, the sum is finite. For other combinations, it is an infinite sum that may or may not have a rapid convergence rate. The main difficulty, though, is that some of the standard integrals involve double and triple integrations over the radial variables. and have linked limits of integration. Because of the varying convergence rates and the computational difficulties associated with the standard integrals, the accuracy of the evaluations has been limited.

An example of a different approach is presented in a paper by Bonham.[18] There are three major differences between his work and that described above. First of all, he includes the factor $(-\alpha_{12}r_{12}-\alpha_{23}r_{23}-\alpha_{31}r_{31})$ in the exponential. Secondly, he gets the various powers of the r's by differentiation of the integral with respect to the appropriate α's, thus producing a standard integral to evaluate. Finally, he performs Fourier transformations on this integral, of the type used in this paper, to obtain an integral whose integrand contains only rational functions. His result, after performing the standard integrations, is a finite sum of integrals that have no linked limits of integrations, and are, at worst, triple integrals. Although his result has a very clean appearance, it is numerically inefficient because different integrals have to be evaluated for different values of the n's.

This paper is organized as follows: Section II collects and discusses results. Section III shows how these results can be used for the efficient recursive evaluation of a collection of integrals of the form (1.2). Derivations have been relegated to Sec. IV. Section II has been further subdivided as follows: Sec. II A gives the analytic formulas for the generating integral (1.3). Section II B discusses the symmetries of (1.3); Sec. II C discusses the singularities and specifies the branches of the multiple valued functions which occur in the formulas of Sec. II A. Section II D provides an example of the branch tracking which must be done to make sure that the correct branches of the multiple-valued functions are chosen in particular applications. Section II E outlines the $\alpha_3\to\infty$ limit of (1.3), which yields formulas for certain difficult two-electron integrals and provides another example of how to keep track of the branches of the multiple-valued functions. Section II F discusses the two-center two-electron molecular integral. The extension of the analysis to evaluate integrals whose integrands contains spherical harmonics is outlined in Sec. II G.

II. RESULTS

This section presents the formula for the generating integral (1.3), discusses its symmetries and singularities, shows how it is related to certain difficult two-electron integrals and to molecular two-center two-electron integrals, and outlines the extension to more general integrals which contain spherical harmonics.

A. A formula for the generating integral

The analytic formula for the generating integral (1.2) is

$$I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})$$
$$=\frac{16\pi^3}{\sigma}\left[\sum_{j=1}^{3}u(\beta_0^{(0)}\beta_0^{(j)})+\sum_{j=0}^{3}\sum_{k=0}^{3}v(\gamma_k^{(j)}/\sigma)\right], \tag{2.1}$$

where the functions u and v are defined by

$$u(z) := \mathrm{Li}_2(z) - \mathrm{Li}_2(1/z) \tag{2.2}$$

and

$$v(z) := \tfrac{1}{2}\mathrm{Li}_2[\tfrac{1}{2}(1-z)] - \tfrac{1}{4}\ln^2[\tfrac{1}{2}(1-z)] - \tfrac{1}{2}\mathrm{Li}_2[\tfrac{1}{2}(1+z)] + \tfrac{1}{4}\ln^2[\tfrac{1}{2}(1+z)] \tag{2.3}$$

with $\mathrm{Li}_2(z)$ the dilogarithm function,[19] defined by

$$\mathrm{Li}_2(z) := -\int_0^z \zeta^{-1}\ln(1-\zeta)\,d\zeta \ . \tag{2.4}$$

The reader should be warned that the functions u and v are multiple valued; thus the analytic formula (2.1) holds only if the branches of u and v are chosen correctly, as is discussed in more detail in Secs. II C, II D, and II E below. The quantity σ is the square root of a homogeneous sixth-degree polynomial in the α's:

$$\begin{aligned}\sigma := [&\alpha_1^2\alpha_{23}^2(\alpha_1^2-\alpha_2^2-\alpha_3^2-\alpha_{12}^2+\alpha_{23}^2-\alpha_{31}^2)\\ &+\alpha_2^2\alpha_{31}^2(-\alpha_1^2+\alpha_2^2-\alpha_3^2-\alpha_{12}^2-\alpha_{23}^2+\alpha_{31}^2)\\ &+\alpha_3^2\alpha_{12}^2(-\alpha_1^2-\alpha_2^2+\alpha_3^2+\alpha_{12}^2-\alpha_{23}^2-\alpha_{31}^2)\\ &+\alpha_1^2\alpha_2^2\alpha_3^2+\alpha_1^2\alpha_{12}^2\alpha_{31}^2+\alpha_2^2\alpha_{23}^2\alpha_{12}^2+\alpha_3^2\alpha_{31}^2\alpha_{23}^2]^{1/2} \ .\end{aligned} \tag{2.5}$$

The $\gamma_k^{(j)}$ are homogeneous third-degree polynomials in the α's:

$$\gamma_0^{(0)} := \mu_0^{(0)}+\mu_1^{(0)}+\mu_2^{(0)}+\mu_3^{(0)} \ , \tag{2.6a}$$
$$\gamma_1^{(0)} := -\mu_0^{(0)}-\mu_1^{(0)}+\mu_2^{(0)}+\mu_3^{(0)} \ , \tag{2.6b}$$
$$\gamma_2^{(0)} := -\mu_0^{(0)}+\mu_1^{(0)}-\mu_2^{(0)}+\mu_3^{(0)} \ , \tag{2.6c}$$
$$\gamma_3^{(0)} := -\mu_0^{(0)}+\mu_1^{(0)}+\mu_2^{(0)}-\mu_3^{(0)} \ , \tag{2.6d}$$

$$\gamma_0^{(1)} := -\mu_0^{(1)}-\mu_1^{(1)}+\mu_2^{(1)}+\mu_3^{(1)} \ , \tag{2.6e}$$
$$\gamma_1^{(1)} := \mu_0^{(1)}+\mu_1^{(1)}+\mu_2^{(1)}+\mu_3^{(1)} \ , \tag{2.6f}$$
$$\gamma_2^{(1)} := \mu_0^{(1)}-\mu_1^{(1)}-\mu_2^{(1)}+\mu_3^{(1)} \ , \tag{2.6g}$$
$$\gamma_3^{(1)} := \mu_0^{(1)}-\mu_1^{(1)}+\mu_2^{(1)}-\mu_3^{(1)} \ , \tag{2.6h}$$

$$\gamma_0^{(2)} := -\mu_0^{(2)}+\mu_1^{(2)}-\mu_2^{(2)}+\mu_3^{(2)} \ , \tag{2.6i}$$
$$\gamma_1^{(2)} := \mu_0^{(2)}-\mu_1^{(2)}-\mu_2^{(2)}+\mu_3^{(2)} \ , \tag{2.6j}$$
$$\gamma_2^{(2)} := \mu_0^{(2)}+\mu_1^{(2)}+\mu_2^{(2)}+\mu_3^{(2)} \ , \tag{2.6k}$$
$$\gamma_3^{(2)} := \mu_0^{(2)}+\mu_1^{(2)}-\mu_2^{(2)}-\mu_3^{(2)} \ , \tag{2.6l}$$

$$\gamma_0^{(3)} := -\mu_0^{(3)}+\mu_1^{(3)}+\mu_2^{(3)}-\mu_3^{(3)} \ , \tag{2.6m}$$
$$\gamma_1^{(3)} := \mu_0^{(3)}-\mu_1^{(3)}+\mu_2^{(3)}-\mu_3^{(3)} \ , \tag{2.6n}$$
$$\gamma_2^{(3)} := \mu_0^{(3)}+\mu_1^{(3)}-\mu_2^{(3)}-\mu_3^{(3)} \ , \tag{2.6o}$$
$$\gamma_3^{(3)} := \mu_0^{(3)}+\mu_1^{(3)}+\mu_2^{(3)}+\mu_3^{(3)} \ , \tag{2.6p}$$

where

$$\mu_0^{(0)} := 2\alpha_{12}\alpha_{23}\alpha_{31} \ , \tag{2.7a}$$
$$\mu_1^{(0)} := \alpha_{23}(-\alpha_1^2+\alpha_{12}^2+\alpha_{31}^2) \tag{2.7b}$$
$$\mu_2^{(0)} := \alpha_{31}(-\alpha_2^2+\alpha_{23}^2+\alpha_{12}^2) \ , \tag{2.7c}$$
$$\mu_3^{(0)} := \alpha_{12}(-\alpha_3^2+\alpha_{31}^2+\alpha_{23}^2) \ , \tag{2.7d}$$

$$\mu_0^{(1)} := \alpha_{23}(-\alpha_1^2+\alpha_2^2+\alpha_3^2) \ , \tag{2.7e}$$
$$\mu_1^{(1)} := 2\alpha_2\alpha_3\alpha_{23} \ , \tag{2.7f}$$
$$\mu_2^{(1)} := \alpha_3(-\alpha_{12}^2+\alpha_{23}^2+\alpha_2^2) \ , \tag{2.7g}$$
$$\mu_3^{(1)} := \alpha_2(-\alpha_{31}^2+\alpha_3^2+\alpha_{23}^2) \ , \tag{2.7h}$$

$$\mu_0^{(2)} := \alpha_{31}(-\alpha_2^2+\alpha_1^2+\alpha_3^2) \ , \tag{2.7i}$$
$$\mu_1^{(2)} := \alpha_3(-\alpha_{12}^2+\alpha_{31}^2+\alpha_1^2) \ , \tag{2.7j}$$
$$\mu_2^{(2)} := 2\alpha_3\alpha_1\alpha_{31} \ , \tag{2.7k}$$
$$\mu_3^{(2)} := \alpha_1(-\alpha_{23}^2+\alpha_3^2+\alpha_{31}^2) \ , \tag{2.7l}$$

$$\mu_0^{(3)} := \alpha_{12}(-\alpha_3^2+\alpha_1^2+\alpha_2^2) \ , \tag{2.7m}$$
$$\mu_1^{(3)} := \alpha_2(-\alpha_{31}^2+\alpha_{12}^2+\alpha_1^2) \ , \tag{2.7n}$$
$$\mu_2^{(3)} := \alpha_i(-\alpha_{23}^2+\alpha_2^2+\alpha_{12}^2) \ , \tag{2.7o}$$
$$\mu_3^{(3)} := 2\alpha_1\alpha_2\alpha_{12} \ . \tag{2.7p}$$

The $\beta_k^{(j)}$, defined by

$$\beta_k^{(j)} := (\sigma-\gamma_k^{(j)})/(\sigma+\gamma_k^{(j)}) \ , \tag{2.8}$$

depend only on the ratio $\gamma_k^{(j)}/\sigma$. The combinations $\beta_0^{(0)}\beta_0^{(j)}$ which appear as arguments of the function u in Eq. (2.1) have four equivalent forms:

$$\beta_0^{(0)}\beta_0^{(1)} = \beta_1^{(1)}\beta_1^{(0)} = \beta_2^{(2)}\beta_2^{(3)} = \beta_3^{(3)}\beta_3^{(2)} \ , \tag{2.9a}$$
$$\beta_0^{(0)}\beta_0^{(2)} = \beta_1^{(1)}\beta_1^{(3)} = \beta_2^{(2)}\beta_2^{(0)} = \beta_3^{(3)}\beta_3^{(1)} \ , \tag{2.9b}$$
$$\beta_0^{(0)}\beta_0^{(3)} = \beta_1^{(1)}\beta_1^{(2)} = \beta_2^{(2)}\beta_2^{(1)} = \beta_3^{(3)}\beta_3^{(0)} \ . \tag{2.9c}$$

B. The symmetry of the generating integral

Symmetry was a major consideration when the generating integral (1.3) was chosen as the fundamental object in the evaluation of the class of integrals (1.2). It is obvious from the definition (1.3) that the value of $I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})$ is unchanged under any permutation of the three indexes 1,2,3. What is less obvious is that I has the permutation group on *four* objects as invariance group: If the index zero is added by replacing $\alpha_1,\alpha_2,\alpha_3$ by $\alpha_{01},\alpha_{02},\alpha_{03}$, and if $\alpha_{ij}=\alpha_{ji}$ by definition, then the value of $I(\alpha_{01},\alpha_{02},\alpha_{03},\alpha_{12},\alpha_{23},\alpha_{31})$ is unchanged under any permutation of the *four* indexes 0,1,2,3. This invariance is present because the nontrivial part of the integration in (1.3) is an integration over the different possible shapes of the tetrahedron whose edges are $\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_1-\mathbf{r}_2$, $\mathbf{r}_2-\mathbf{r}_3$, and $\mathbf{r}_3-\mathbf{r}_1$. Because the group of permutations on the four objects 0,1,2,3 is generated by the interchanges $0\leftrightarrow1$, $1\leftrightarrow2$, and $2\leftrightarrow3$, the fact that I is invariant under the larger symmetry group is equivalent to the relations

$$I(\alpha_{01},\alpha_{02},\alpha_{03},\alpha_{12},\alpha_{23},\alpha_{31})=I(\alpha_{01},\alpha_{12},\alpha_{31},\alpha_{02},\alpha_{23},\alpha_{03})$$
$$=I(\alpha_{02},\alpha_{01},\alpha_{03},\alpha_{12},\alpha_{31},\alpha_{23})$$
$$=I(\alpha_{01},\alpha_{03},\alpha_{02},\alpha_{31},\alpha_{23},\alpha_{12})\ . \qquad (2.10)$$

The relation (2.10) can be easily demonstrated from the definition (1.3) by replacing the dummy variables $\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3$ by $\mathbf{r}_{10},\mathbf{r}_{20},\mathbf{r}_{30}$ and renaming the dummy variables $r_{10},r_{20},r_{30},r_{12},r_{23},r_{31}$ via the same permutation of 0,1,2,3 as was used on the α's. The observation that the Jacobian $\partial(\mathbf{r}_{01},\mathbf{r}_{31},\mathbf{r}_{12})/\partial(\mathbf{r}_{01},\mathbf{r}_{02},\mathbf{r}_{03})$ is 1, which permits replacing the volume element $d^3r_{01}d^3r_{31}d^3r_{12}$ by $d^3r_{01}d^3r_{02}d^3r_{03}$, is needed to complete the proof of the equality in (2.10) which results from the $0\leftrightarrow1$ interchange. The notation introduced via the definitions (2.6) and (2.7) is consistent with the above symmetry: Any permutation of the α's induced by a permutation of (0,1,2,3) induces the same permutation of (0,1,2,3) on the indexes j and k of the $\mu_k^{(j)}$ and $\gamma_k^{(j)}$. Thus a permutation of (0,1,2,3) permutes the $\mu_k^{(j)}$ with $j=k$ among themselves, the $\mu_k^{(j)}$ with $j\neq k$ among themselves, the $\gamma_k^{(j)}$ with $j=k$ among themselves, the $\gamma_k^{(j)}$ with $j\neq k$ among themselves, the $\beta_k^{(j)}$ with $j=k$ among themselves, and the $\beta_k^{(j)}$ with $j\neq k$ among themselves. The quantity σ is invariant under any permutation of 0,1,2,3. The above remarks can be used to verify that the right-hand side of (2.1) is consistent with (2.10). The invariance discussed above was very important in the discovery of the formula (2.1), and should be kept in mind by users of (2.1).

C. The singularities of the generating integral

The functions u and v which appear in the formula (2.1) for the generating integral I are multiple valued, because the logarithms and dilogarithms which appear in their definitions (2.2) and (2.3) are multiple valued. The branches of u and v must be chosen properly if correct numerical values are to be obtained from (2.1). Furthermore, individual terms on the right-hand side of (2.1) have singularities which cancel when all of the terms have been added together to obtain $I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})$. Numerical evaluation of I at or near these singularities requires that the singular u and v be transformed to forms which permit the explicit analytic cancellation of these singularities, as is discussed in more detail in Sec. III F. This subsection will specify the branches of u and v, discuss the location and cancellation of singularities, and provide formulas for the behavior near the singular points.

The first step is the specification of branch cuts for the multiple-valued functions. The complex logarithm has branch points at 0 and at ∞. The branch cut for the logarithm will be taken to run from 0 to ∞ along the negative real axis, with the principal branch chosen so that its value is given by

$$\ln(z)=\ln|z|+i\arg z,\quad -\pi<\arg z<\pi\ . \qquad (2.11)$$

With this convention, the logarithm is an analytic function in the cut plane. The choice (2.11) for the complex logarithm then determines the location of branch cuts, and fixes the branch, for the dilogarithm and for the functions u and v. The dilogarithm function $\mathrm{Li}_2(z)$ has branch points at 1 and ∞; its branch cut then runs from 1 to $+\infty$ along the positive real axis. The function $u(z)$ has branch points at 0, 1, and ∞; its branch cut then runs from 0 to $+\infty$ along the positive real axis. The function $v(z)$ has branch points at 1, -1, and ∞; its branch cuts then run from 1 to $+\infty$ along the positive real axis, and from -1 to $-\infty$ along the negative real axis. Ambiguities in the value of $u(z)$ and/or $v(z)$ when z lies on a branch cut must be removed by specifying whether z approaches the branch cut from the upper half-plane or the lower half-plane. Values on the branch cuts are given by the following formulas, in which x is real and ϵ tends to zero through positive values:

$$\lim_{\epsilon\to0+}\mathrm{Li}_2(x\pm i\epsilon)=\tfrac{1}{3}\pi^2-\mathrm{Li}_2(x^{-1})-\tfrac{1}{2}\ln^2x\pm i\pi\ln x\ ,\quad x>1 \qquad (2.12)$$

$$\lim_{\epsilon\to0+}u(x\pm i\epsilon)=-\tfrac{1}{3}\pi^2+2\mathrm{Li}_2(x)+\tfrac{1}{2}\ln^2x\pm i\pi\ln x\ ,\quad 0<x<1 \qquad (2.13a)$$

$$\lim_{\epsilon\to0+}u(x\pm i\epsilon)=\tfrac{1}{3}\pi^2-2\mathrm{Li}_2(x^{-1})-\tfrac{1}{2}\ln^2x\pm i\pi\ln x\ ,\quad x>1 \qquad (2.13b)$$

$$\lim_{\epsilon\to0+}v(x\pm i\epsilon)=\tfrac{1}{2}\mathrm{Li}_2[2/(1+x)]+\tfrac{1}{2}\ln^2[2/(1+x)]-\tfrac{1}{2}\mathrm{Li}_2[2/(1-x)]-\tfrac{1}{2}\ln^2[2/(x-1)]\pm\tfrac{1}{2}i\pi\ln[(x-1)/(x+1)],\quad x>1 \qquad (2.14a)$$

$$\lim_{\epsilon\to0+}v(x\pm i\epsilon)=\tfrac{1}{2}\mathrm{Li}_2[2/(1+x)]+\tfrac{1}{2}\ln^2[2/(-1-x)]-\tfrac{1}{2}\mathrm{Li}_2[2/(1-x)]-\tfrac{1}{2}\ln^2[2/(1-x)]\mp\tfrac{1}{2}i\pi\ln[(1-x)/(-1-x)]\ ,\quad x<-1\ . \qquad (2.14b)$$

Equations (2.1)–(2.8), with the choices of branch described above for u and v, give correct, unambiguous values of $I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})$ in the neighborhood of the point $\alpha_1=\alpha_2=\alpha_3=\alpha_{12}=\alpha_{23}=\alpha_{31}=1$, which will hereafter be called the standard reference point (SRP). At SRP, σ and all $\gamma_k^{(j)}/\sigma$ are pure imaginary; all $\beta_k^{(j)}$ are on the unit circle in the complex plane. The arguments of u and v are all well removed from the branch cuts at SRP so that no ambiguity can arise. Either choice of branch for the square root σ gives the same numerical value for I; the arbitrary choice $\sigma=+i\sqrt{2}$ at SRP will be made. The proper choice of branch at points other than SRP is determined by keeping track of the branch along a path from SRP to the point in question. The rest of this section records formulas which help with this branch tracking. Examples appear in Secs. II D and II E below.

The following formulas exhibit the behavior of u and v in neighborhoods of their singular points. In these formulas, the functions with the singular point as a subscript are analytic at the singular point, e.g., $u_0(z)$ is analytic at $z=0$:

$$u(z)=\tfrac{1}{2}\ln^2(-z)+u_0(z)\ , \tag{2.15a}$$

where

$$u_0(z):=\tfrac{1}{6}\pi^2+2\mathrm{Li}_2(z),\quad z \text{ near } 0\ ; \tag{2.15b}$$

$$u(z)=-2\ln z\ \ln(1-z)+u_1(z)\ , \tag{2.15c}$$

where

$$u_1(z):=\tfrac{1}{2}\pi^2-2\mathrm{Li}_2(1-z)+\tfrac{1}{2}\ln^2(-z),\quad z \text{ near } 1\ ; \tag{2.15d}$$

$$u(z)=-\tfrac{1}{2}\ln^2(-z)+u_\infty(z)\ , \tag{2.15e}$$

where

$$u_\infty(z):=-\tfrac{1}{6}\pi^2-2\mathrm{Li}_2(z^{-1}),\quad z \text{ near } \infty\ ; \tag{2.15f}$$

$$v(z)=\tfrac{1}{4}\ln^2[(1+z)/(1-z)]+v_{-1}(z)\ , \tag{2.16a}$$

where

$$v_{-1}(z):=\tfrac{1}{12}\pi^2-\mathrm{Li}_2[\tfrac{1}{2}(1+z)]-\tfrac{1}{2}\ln^2[\tfrac{1}{2}(1-z)]\ ,\quad z \text{ near } -1\ ; \tag{2.16b}$$

$$v(z)=-\tfrac{1}{4}\ln^2[(1-z)/(1+z)]+v_1(z)\ , \tag{2.16c}$$

where

$$v_1(z):=-\tfrac{1}{12}\pi^2+\mathrm{Li}_2[\tfrac{1}{2}(1-z)]+\tfrac{1}{2}\ln^2[\tfrac{1}{2}(1+z)]\ ,\quad z \text{ near } 1\ ; \tag{2.16d}$$

$$v(z)=\tfrac{1}{2}\ln(-z^2/4)\ln[(1+z^{-1})/(1-z^{-1})]+v_\infty(z)\ , \tag{2.16e}$$

where

$$v_\infty(z):=\tfrac{1}{2}\{\mathrm{Li}_2[2/(1+z)]-\mathrm{Li}_2[2/(1-z)]+\ln^2(1+z^{-1})-\ln^2(1-z^{-1})\}\ ,\quad z \text{ near } \infty\ . \tag{2.16f}$$

In Eq. (2.16e), the branch with

$$\tfrac{1}{2}\ln(-z^2/4)=\ln(|z|/2)+i(\arg z-\tfrac{1}{2}\pi) \tag{2.17a}$$

should be chosen for z in the upper half-plane. The branch with

$$\tfrac{1}{2}\ln(-z^2/4)=\ln(|z|/2)+i(\arg z+\tfrac{1}{2}\pi) \tag{2.17b}$$

should be chosen for z in the lower half-plane.

The above discussion shows that the $v(\gamma_k^{(j)}/\sigma)$ terms in (2.1) have singularities at $\sigma=0$ and at $\gamma_k^{(j)}=\pm\sigma$, i.e., at $(\gamma_k^{(j)})^2-\sigma^2=0$. The $u(\beta_0^{(0)}\beta_0^{(j)})$ terms have singularities at these points and at some, but not all, of the points where $\gamma_0^{(0)}+\gamma_0^{(j)}=0$. The values of the α's for which σ is zero can be obtained from the definition (2.5) of σ, which can be rewritten in the form

$$\begin{aligned}\sigma^2=&\alpha_{12}^2\{\alpha_3^2+\tfrac{1}{2}\alpha_{12}^{-2}[\alpha_{12}^4-\alpha_{12}^2(\alpha_1^2+\alpha_2^2+\alpha_{23}^2+\alpha_{31}^2)+(\alpha_1^2-\alpha_{31}^2)(\alpha_2^2-\alpha_{23}^2)]\}^2\\&-\tfrac{1}{4}\alpha_{12}^{-2}(\alpha_2+\alpha_{12}+\alpha_{23})(-\alpha_2+\alpha_{12}+\alpha_{23})(\alpha_2-\alpha_{12}+\alpha_{23})\\&\times(\alpha_2+\alpha_{12}-\alpha_{23})(\alpha_1+\alpha_{12}+\alpha_{31})(-\alpha_1+\alpha_{12}+\alpha_{31})(\alpha_1-\alpha_{12}+\alpha_{31})(\alpha_1+\alpha_{12}-\alpha_{31})\ .\end{aligned} \tag{2.18}$$

Equation (2.18), which was obtained from (2.5) by completing the square with respect to α_3^2, can be used to find the zeros of σ regarded as a function of α_3 with the other α's held fixed. Analogs of (2.18), obtained by completing the square with respect to any of the other α's, can be obtained by symmetry. The values of the α's for which the other singularities occur can be read off from the following formulas:

$$(\gamma_0^{(0)})^2-\sigma^2=(\alpha_1+\alpha_{12}+\alpha_{31})(-\alpha_1+\alpha_{12}+\alpha_{31})(\alpha_2+\alpha_{12}+\alpha_{23})(-\alpha_2+\alpha_{12}+\alpha_{23})(\alpha_3+\alpha_{23}+\alpha_{31})(-\alpha_3+\alpha_{23}+\alpha_{31})\ , \tag{2.19a}$$

$$(\gamma_1^{(0)})^2-\sigma^2=(\alpha_1+\alpha_{12}+\alpha_{31})(-\alpha_1+\alpha_{12}+\alpha_{31})(\alpha_2-\alpha_{12}+\alpha_{23})(\alpha_2+\alpha_{12}-\alpha_{23})(\alpha_3+\alpha_{23}-\alpha_{31})(\alpha_3-\alpha_{23}+\alpha_{31})\ , \tag{2.19b}$$

$$(\gamma_2^{(0)})^2-\sigma^2=(\alpha_1+\alpha_{12}-\alpha_{31})(\alpha_1-\alpha_{12}+\alpha_{31})(\alpha_2+\alpha_{12}+\alpha_{23})(-\alpha_2+\alpha_{12}+\alpha_{23})(\alpha_3+\alpha_{23}-\alpha_{31})(\alpha_3-\alpha_{23}+\alpha_{31})\ , \tag{2.19c}$$

$$(\gamma_3^{(0)})^2-\sigma^2=(\alpha_1+\alpha_{12}-\alpha_{31})(\alpha_1-\alpha_{12}+\alpha_{31})(\alpha_2-\alpha_{12}+\alpha_{23})(\alpha_2+\alpha_{12}-\alpha_{23})(\alpha_3+\alpha_{23}+\alpha_{31})(-\alpha_3+\alpha_{23}+\alpha_{31})\ , \tag{2.19d}$$

$$(\gamma_0^{(1)})^2-\sigma^2=(\alpha_1+\alpha_2+\alpha_3)(-\alpha_1+\alpha_2+\alpha_3)(\alpha_2+\alpha_{12}-\alpha_{23})(-\alpha_2+\alpha_{12}+\alpha_{23})(\alpha_3-\alpha_{23}+\alpha_{31})(-\alpha_3+\alpha_{23}+\alpha_{31})\ , \tag{2.19e}$$

$$(\gamma_1^{(1)})^2-\sigma^2=(\alpha_1+\alpha_2+\alpha_3)(-\alpha_1+\alpha_2+\alpha_3)(\alpha_2+\alpha_{12}+\alpha_{23})(\alpha_2-\alpha_{12}+\alpha_{23})(\alpha_3+\alpha_{23}+\alpha_{31})(\alpha_3+\alpha_{23}-\alpha_{31})\ , \tag{2.19f}$$

$$(\gamma_2^{(1)})^2-\sigma^2=(\alpha_1+\alpha_2-\alpha_3)(\alpha_1-\alpha_2+\alpha_3)(\alpha_2+\alpha_{12}+\alpha_{23})(\alpha_2-\alpha_{12}+\alpha_{23})(\alpha_3-\alpha_{23}+\alpha_{31})(-\alpha_3+\alpha_{23}+\alpha_{31})\ , \tag{2.19g}$$

$$(\gamma_3^{(1)})^2-\sigma^2=(\alpha_1+\alpha_2-\alpha_3)(\alpha_1-\alpha_2+\alpha_3)(\alpha_2+\alpha_{12}-\alpha_{23})(-\alpha_2+\alpha_{12}+\alpha_{23})(\alpha_3+\alpha_{23}+\alpha_{31})(\alpha_3+\alpha_{23}-\alpha_{31})\ , \tag{2.19h}$$

$$(\gamma_0^{(2)})^2-\sigma^2=(\alpha_1+\alpha_2+\alpha_3)(\alpha_1-\alpha_2+\alpha_3)(\alpha_1+\alpha_{12}-\alpha_{31})(-\alpha_1+\alpha_{12}+\alpha_{31})(\alpha_3+\alpha_{23}-\alpha_{31})(-\alpha_3+\alpha_{23}+\alpha_{31})\ , \tag{2.19i}$$

$$(\gamma_1^{(2)})^2-\sigma^2=(\alpha_1+\alpha_2-\alpha_3)(-\alpha_1+\alpha_2+\alpha_3)(\alpha_1+\alpha_{12}+\alpha_{31})(\alpha_1-\alpha_{12}+\alpha_{31})(\alpha_3+\alpha_{23}-\alpha_{31})(-\alpha_3+\alpha_{23}+\alpha_{31})\ , \tag{2.19j}$$

$$(\gamma_2^{(2)})^2-\sigma^2=(\alpha_1+\alpha_2+\alpha_3)(\alpha_1-\alpha_2+\alpha_3)(\alpha_1+\alpha_{12}+\alpha_{31})(\alpha_1-\alpha_{12}+\alpha_{31})(\alpha_3+\alpha_{23}+\alpha_{31})(\alpha_3-\alpha_{23}+\alpha_{31})\ , \tag{2.19k}$$

$$(\gamma_3^{(2)})^2-\sigma^2=(\alpha_1+\alpha_2-\alpha_3)(-\alpha_1+\alpha_2+\alpha_3)(\alpha_1+\alpha_{12}-\alpha_{31})(-\alpha_1+\alpha_{12}+\alpha_{31})(\alpha_3+\alpha_{23}+\alpha_{31})(\alpha_3-\alpha_{23}+\alpha_{31})\ , \tag{2.19l}$$

$$(\gamma_0^{(3)})^2-\sigma^2=(\alpha_1+\alpha_2+\alpha_3)(\alpha_1+\alpha_2-\alpha_3)(\alpha_1-\alpha_{12}+\alpha_{31})(-\alpha_1+\alpha_{12}+\alpha_{31})(\alpha_2-\alpha_{12}+\alpha_{23})(-\alpha_2+\alpha_{12}+\alpha_{23}) , \tag{2.19m}$$

$$(\gamma_1^{(3)})^2-\sigma^2=(\alpha_1-\alpha_2+\alpha_3)(-\alpha_1+\alpha_2+\alpha_3)(\alpha_1+\alpha_{12}+\alpha_{31})(\alpha_1+\alpha_{12}-\alpha_{31})(\alpha_2-\alpha_{12}+\alpha_{23})(-\alpha_2+\alpha_{12}+\alpha_{23}) , \tag{2.19n}$$

$$(\gamma_2^{(3)})^2-\sigma^2=(\alpha_1-\alpha_2+\alpha_3)(-\alpha_1+\alpha_2+\alpha_3)(\alpha_1-\alpha_{12}+\alpha_{31})(-\alpha_1+\alpha_{12}+\alpha_{31})(\alpha_2+\alpha_{12}+\alpha_{23})(\alpha_2+\alpha_{12}-\alpha_{23}) , \tag{2.19o}$$

$$(\gamma_3^{(3)})^2-\sigma^2=(\alpha_1+\alpha_2+\alpha_3)(\alpha_1+\alpha_2-\alpha_3)(\alpha_1+\alpha_{12}+\alpha_{31})(\alpha_1+\alpha_{12}-\alpha_{31})(\alpha_2+\alpha_{12}+\alpha_{23})(\alpha_2+\alpha_{12}-\alpha_{23}) , \tag{2.19p}$$

$$\gamma_0^{(0)}+\gamma_0^{(1)}=(-\alpha_2+\alpha_{12}+\alpha_{23}+)(-\alpha_3+\alpha_{23}+\alpha_{31})(\alpha_2+\alpha_3+\alpha_{12}+\alpha_{31}) . \tag{2.20a}$$

$$\gamma_0^{(0)}+\gamma_0^{(2)}=(-\alpha_1+\alpha_{12}+\alpha_{31})(-\alpha_3+\alpha_{23}+\alpha_{31})(\alpha_1+\alpha_3+\alpha_{12}+a_{23}) , \tag{2.20b}$$

$$\gamma_0^{(0)}+\gamma_0^{(3)}=(-\alpha_1+\alpha_{12}+\alpha_{31})(-\alpha_2+\alpha_{12}+\alpha_{23})(\alpha_1+\alpha_2+\alpha_{23}+\alpha_{31}) , \tag{2.20c}$$

$$\gamma_1^{(1)}+\gamma_1^{(0)}=(\alpha_2-\alpha_{12}+\alpha_{23})(\alpha_3+\alpha_{23}-\alpha_{31})(\alpha_2+\alpha_3+\alpha_{12}+\alpha_{31}) , \tag{2.20d}$$

$$\gamma_1^{(1)}+\gamma_1^{(2)}=(-\alpha_1+\alpha_2+\alpha_3)(\alpha_3+\alpha_{23}-\alpha_{31})(\alpha_1+\alpha_2+\alpha_{23}+\alpha_{31}) , \tag{2.20e}$$

$$\gamma_1^{(1)}+\gamma_1^{(3)}=(-\alpha_1+\alpha_2+\alpha_3)(\alpha_2-\alpha_{12}+\alpha_{23})(\alpha_1+\alpha_3+\alpha_{12}+\alpha_{23}) , \tag{2.20f}$$

$$\gamma_2^{(2)}+\gamma_2^{(0)}=(\alpha_1-\alpha_{12}+\alpha_{31})(\alpha_3-\alpha_{23}+\alpha_{31})(\alpha_1+\alpha_3+\alpha_{12}+\alpha_{23}) , \tag{2.20g}$$

$$\gamma_2^{(2)}+\gamma_2^{(1)}=(\alpha_1-\alpha_2+\alpha_3)(\alpha_3-\alpha_{23}+\alpha_{31})(\alpha_1+\alpha_2+\alpha_{23}+\alpha_{31}) , \tag{2.20h}$$

$$\gamma_2^{(2)}+\gamma_2^{(3)}=(\alpha_1-\alpha_{12}+\alpha_{31})(\alpha_1-\alpha_2+\alpha_3)(\alpha_2+\alpha_3+\alpha_{12}+\alpha_{31}) , \tag{2.20i}$$

$$\gamma_3^{(3)}+\gamma_3^{(0)}=(\alpha_1+\alpha_{12}-\alpha_{31})(\alpha_2+\alpha_{12}-\alpha_{23})(\alpha_1+\alpha_2+\alpha_{23}+\alpha_{31}) , \tag{2.20j}$$

$$\gamma_3^{(3)}+\gamma_3^{(1)}=(\alpha_2+\alpha_{12}-\alpha_{23})(\alpha_1+\alpha_2-\alpha_3)(\alpha_1+\alpha_3+\alpha_{12}+\alpha_{23}) , \tag{2.20k}$$

$$\gamma_3^{(3)}+\gamma_3^{(2)}=(\alpha_1+\alpha_{12}-\alpha_{31})(\alpha_1+\alpha_2-\alpha_3)(\alpha_2+\alpha_3+\alpha_{12}+\alpha_{31}) . \tag{2.20l}$$

The singularity at $\sigma=0$, and many of the singularities at zeros of the right-hand sides of Eqs. (2.19) and (2.20) cancel. The only singularities for finite values of the α's which survive in $I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})$ are at

$$\alpha_1+\alpha_2+\alpha_3=0 , \tag{2.21a}$$

$$\alpha_1+\alpha_{12}+\alpha_{31}=0 , \tag{2.21b}$$

$$\alpha_2+\alpha_{12}+\alpha_{23}=0 , \tag{2.21c}$$

$$\alpha_3+\alpha_{23}+\alpha_{31}=0 , \tag{2.21d}$$

$$\alpha_2+\alpha_3+\alpha_{12}+\alpha_{31}=0 , \tag{2.22a}$$

$$\alpha_1+\alpha_3+\alpha_{12}+\alpha_{23}=0 , \tag{2.22b}$$

$$\alpha_1+\alpha_2+\alpha_{23}+\alpha_{31}=0 . \tag{2.22c}$$

The case in which one of the α's tends to infinity with the others near 1 is discussed in Sec. II E. The fact that all of the singularities except (2.21) and (2.22) must cancel can be seen from the original definition (1.3) of $I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})$. The integral in (1.3) is an analytic function of the α's in the interior of the set of α's for which it converges; it can be shown directly that the integral in (1.3) converges at the singular points which cancel. The fact that the singular points (2.21) and (2.22) survive can also be seen from this point of view. Existence of the singularity (2.21b) can be understood from the fact that the condition $\alpha_1+\alpha_{12}+\alpha_{31}>0$ is necessary for exponential decay of the integrand as r_1, r_{12}, and r_{31} get large with r_2, r_3, and r_{23} bounded. Existence of the singularity (2.22c) can be understood from the fact that the condition $\alpha_1+\alpha_2+\alpha_{23}+\alpha_{31}>0$ is necessary for exponential decay of the integrand as r_1, r_2, r_{23}, and r_{31} get large with r_{12} and r_3 bounded. The other singularities which survive can be understood in similar fashion.

The behavior of $I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})$ in the neighborhood of the singularity (2.21a) is given by

$$I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}) =32\pi^3\sigma^{-1}\ln(\alpha_1+\alpha_2+\alpha_3)\ln(-\beta_0^{(0)}) +(\text{analytic function}) . \tag{2.23}$$

The behavior of $I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})$ in the neighborhood of the singularity (2.22c) is given by

$$I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}) =-32\pi^3\sigma^{-1}\ln(\alpha_1+\alpha_2+\alpha_{23}+\alpha_{31})\ln(\beta_0^{(0)}\beta_0^{(3)}) +(\text{analytic function}) . \tag{2.24}$$

The behavior of I at the singularities (2.21b)–(2.21d) and (2.22a)–(2.22b) can be obtained from (2.23) and (2.24) by symmetry.

D. Branch tracking: An example

This subsection will track the branches of $u(\beta_0^{(0)}\beta_0^{(j)})$ and $v(\gamma_k^{(j)}/\sigma)$ along a path from SRP to the point $\alpha_1=\alpha_2=\alpha_3=1$, $\alpha_{12}=\alpha_{23}=\alpha_{31}=0$, which will hereafter be called the auxiliary reference point (ARP). Specifying the path from SRP to ARP is the first step. Let λ be a parameter along the path. Let $\alpha_1=\alpha_2=\alpha_3=1$, $\alpha_{12}=\alpha_{23}=\alpha_{31}=\lambda$. Then SRP is at $\lambda=1$, with ARP at $\lambda=0$. It is convenient to introduce auxiliary functions z_1, z_2, z_3, z_4, and z_5 via

$$z_1(\lambda)=\lambda(8\lambda^2-3)(1-3\lambda^2)^{-1/2}\ , \tag{2.25a}$$

$$z_2(\lambda)=(2+3\lambda)(1-3\lambda^2)^{-1/2}\ , \tag{2.25b}$$

$$z_3(\lambda)=(2-3\lambda)(1-3\lambda^2)^{-1/2}\ , \tag{2.25c}$$

$$z_4(\lambda)=-\lambda(1-3\lambda^2)^{-1/2}\ , \tag{2.25d}$$

$$z_5(\lambda)=[(1-3\lambda^2)^{1/2}-(2+3\lambda)][(1-3\lambda^2)^{1/2}+\lambda]/\{[(1-3\lambda^2)^{1/2}+(2+3\lambda)][(1-3\lambda^2)^{1/2}-\lambda]\}\ . \tag{(2.25e)}$$

Equation (2.5)–(2.8) can be used to show that, on the prescribed path from SRP to ARP,

$$\gamma_0^{(0)}/\sigma=z_1(\lambda)\ , \tag{2.26a}$$

$$\gamma_j^{(j)}/\sigma=z_2(\lambda),\quad j=1,2,3 \tag{2.26b}$$

$$\gamma_0^{(j)}/\sigma=z_3(\lambda),\quad j=1,2,3 \tag{2.26c}$$

$$\gamma_k^{(j)}/\sigma=z_4(\lambda),\quad j\neq k,\quad j=0,1,2,3,\quad k=1,2,3 \tag{2.26d}$$

$$\beta_0^{(0)}\beta_0^{(j)}=z_5(\lambda),\quad j=1,2,3\ . \tag{2.26e}$$

It follows from (2.1) and (2.26) that

$$I(1,1,1,\lambda,\lambda,\lambda)=16\pi^3(1-3\lambda^2)^{-1/2}\times[v(z_1(\lambda))+3v(z_2(\lambda))+3v(z_3(\lambda))+9v(z_4(\lambda))+3u(z_5(\lambda))] \tag{2.27}$$

on the path from SRP to ARP. The discussion of the singularities of u and v in Sec. II C shows that the function u and all of the functions v in (2.27) are singular at $\lambda=1/\sqrt{3}$, where σ is zero, and that u and $v(z_1)$, $v(z_3)$, and $v(z_4)$ are singular at $\lambda=\frac{1}{2}$. These are the only singular points of the functions u and v on the straight-line path along the real axis from $\lambda=1$ to $\lambda=0$. Because $I(1,1,1,\lambda,\lambda,\lambda)$ does not have singularities at $\lambda=1/\sqrt{3}$ and at $\lambda=\frac{1}{2}$, the choice of path in the neighborhood of these singularities of u and v does not affect that value of I. The following path, which avoids the singular points of u and v by passing beneath them, will be used, where δ is a small positive real number:

$$\lambda=x,\quad 1\geq x\geq \frac{1}{\sqrt{3}}+\delta \tag{2.28a}$$

$$\lambda=\frac{1}{\sqrt{3}}+\delta e^{i\theta},\quad -\pi\leq\theta\leq 0 \tag{2.28b}$$

$$\lambda=x,\quad \frac{1}{\sqrt{3}}-\delta\geq x\geq \tfrac{1}{2}+\delta \tag{2.28c}$$

$$\lambda=\tfrac{1}{2}+\delta e^{i\theta},\quad -\pi\leq\theta\leq 0 \tag{2.28d}$$

$$\lambda=x,\quad \tfrac{1}{2}-\delta\geq x\geq 0\ . \tag{2.28e}$$

This path is sketched in Fig. 1(a). With this choice of path, the square root σ is positive imaginary for $1\geq\lambda\geq 1/\sqrt{3}+\delta$, and positive real for $1/\sqrt{3}-\delta\geq\lambda\geq\frac{1}{2}+\delta$ and for $\frac{1}{2}-\delta\geq\lambda\geq 0$. For $1\geq\lambda\geq 1/\sqrt{3}+\delta$, the branches of the function u and the functions v are chosen the same way as at SRP. The appropriate choice of branch for the other straight-line segments of the path is determined by using expansions of the auxiliary functions z_1, z_2, z_3, z_4, and z_5 about the singular points $\lambda=1/\sqrt{3}$ and $\lambda=\frac{1}{2}$ to trace the behavior of the function u and the functions v. These expansions are

$$z_1\left[\frac{1}{\sqrt{3}}+\delta e^{i\theta}\right]=2^{-1/2}3^{-7/4}\delta^{-1/2}\times\exp[i(\pi-\theta)/2]+O(\delta^{1/2})\ , \tag{2.29a}$$

$$z_2\left[\frac{1}{\sqrt{3}}+\delta e^{i\theta}\right]=(2+\sqrt{3})2^{-1/2}3^{-1/4}\delta^{-1/2}\times\exp[-i(\pi+\theta)/2]+O(\delta^{1/2})\ , \tag{2.29b}$$

$$z_3\left[\frac{1}{\sqrt{3}}+\delta e^{i\theta}\right]=(2-\sqrt{3})2^{-1/2}3^{-1/4}\delta^{-1/2}\times\exp[-i(\pi+\theta)/2]+O(\delta^{1/2})\ , \tag{2.29c}$$

$$z_4\left[\frac{1}{\sqrt{3}}+\delta e^{i\theta}\right]=2^{-1/2}3^{-3/4}\delta^{-1/2}\times\exp[i(\pi-\theta)/2]+O(\delta^{1/2})\ , \tag{2.29d}$$

$$z_5\left[\frac{1}{\sqrt{3}}+\delta e^{i\theta}\right]=1+4(\sqrt{3}-1)2^{1/2}3^{1/4}\delta^{1/2}\times\exp[i(\pi+\theta)/2]+O(\delta^{3/2})\ , \tag{2.29e}$$

and

$$z_1(\tfrac{1}{2}+\delta e^{i\theta})=-1-128\delta^3e^{3i\theta}+O(\delta^4)\ , \tag{2.30a}$$

$$z_2(\tfrac{1}{2}+\delta e^{i\theta})=7+O(\delta)\ , \tag{2.30b}$$

$$z_3(\tfrac{1}{2}+\delta e^{i\theta})=1+24\delta^2e^{2i\theta}+O(\delta^3)\ , \tag{2.30c}$$

$$z_4(\tfrac{1}{2}+\delta e^{i\theta})=-1-4\delta e^{i\theta}+O(\delta^2)\ , \tag{2.30d}$$

$$z_5(\tfrac{1}{2}+\delta e^{i\theta})=\tfrac{3}{8}\delta^{-1}e^{-i\theta}+O(1)\ . \tag{2.30e}$$

The paths followed by the $z_i(\lambda)$, which are readily deduced from the definitions (2.25a)–(2.25e) and the expansions (2.29a)–(2.29e) and (2.30a)–(2.30e), are sketched in Figs. 1(b)–1(f). The values of $I(1,1,1,\lambda,\lambda,\lambda)$ on the remaining straight-line segments of the path, which are deduced from Eqs. (2.13a)–(2.17b) with the aid of the sketches in Figs. 1(b)–1(f), are

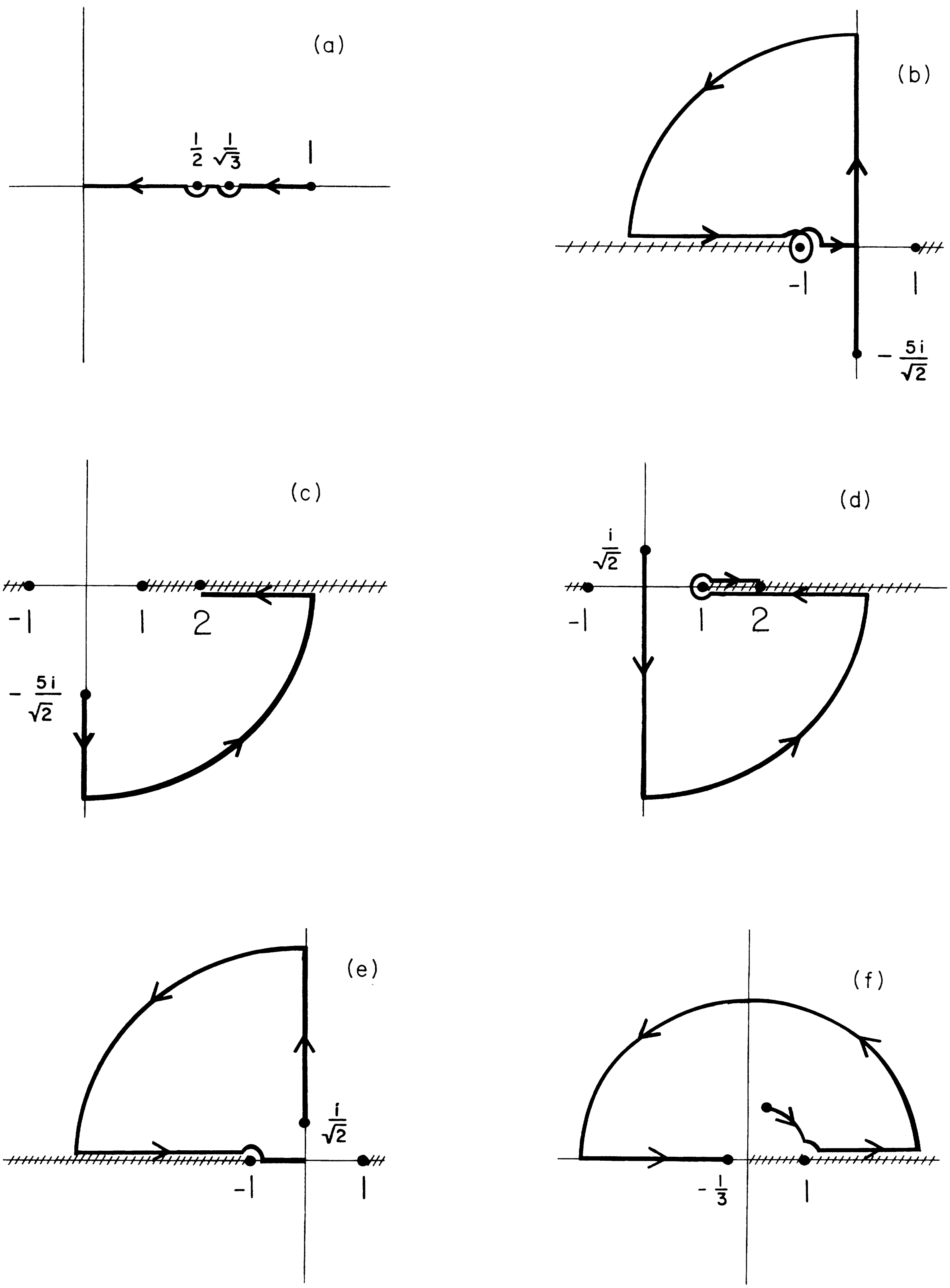

FIG. 1. (a) The path from SRP to ARP in the complex λ plane. (b) The path from SRP to ARP in the complex z_1 plane. (c) The path from SRP to ARP in the complex z_2 plane. (d) The path from SRP to ARP in the complex z_3 plane. (e) The path from SRP to ARP in the complex z_4 plane. (f) The path from SRP to ARP in the complex z_5 plane.

$$I(1,1,1,\lambda,\lambda,\lambda)=16\pi^3(1-3\lambda^2)^{-1/2}\lim_{\epsilon\to 0+}\{v(z_1(\lambda)+i\epsilon)+3v(z_2(\lambda)-i\epsilon)+3v(z_3(\lambda)-i\epsilon)$$
$$+9v(z_4(\lambda)+i\epsilon)+3u(z_5(\lambda)+i\epsilon)\},\quad \frac{1}{\sqrt{3}}-\delta\ge\lambda\ge\tfrac{1}{2}+\delta\ , \tag{2.31}$$

and

$$I(1,1,1,\lambda,\lambda,\lambda)=16\pi^3(1-3\lambda^2)^{-1/2}\lim_{\epsilon\to 0+}\{-\pi^2+v(z_1(\lambda))+3v(z_2(\lambda)-i\epsilon)+3v(z_3(\lambda)+i\epsilon)$$
$$+9v(z_4(\lambda))+3u(z_5(\lambda))\},\quad \tfrac{1}{2}-\delta\ge\lambda\ge 0\ . \tag{2.32}$$

Hence the value of $I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})$ in the neighborhood of ARP is given by

$$I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})=\frac{16\pi^3}{\sigma}\lim_{\epsilon\to 0+}\left[-\pi^2+\sum_{j=1}^{3}u(\beta_0^{(0)}\beta_0^{(j)})+v(\gamma_0^{(0)}/\sigma)+\sum_{j=1}^{3}v((\gamma_j^{(j)}/\sigma)-i\epsilon)\right.$$
$$\left.+\sum_{j=1}^{3}v((\gamma_0^{(j)}/\sigma)+i\epsilon)+\sum_{\substack{j=0\\ j\ne k}}^{3}\sum_{k=1}^{3}v(\gamma_k^{(j)}/\sigma)\right]. \tag{2.33}$$

The term $-\pi^2$ in Eq. (2.33), which is not present in (2.1), is a consequence of the fact that the path for $z_1(\lambda)$ goes around -1, which is a branch point of v, $\frac{3}{2}$ times. By tracking the branches of the functions u and v from ARP, the formula (2.33) can be shown to be valid in the neighborhood of any point where α_1, α_2, and α_3 satisfy the triangle conditions

$$\alpha_1+\alpha_2-\alpha_3>0\ , \tag{2.34a}$$

$$\alpha_1-\alpha_2+\alpha_3>0\ , \tag{2.34b}$$

$$-\alpha_1+\alpha_2+\alpha_3>0\ , \tag{2.34c}$$

with $\alpha_{12}=\alpha_{23}=\alpha_{31}=0$. Values of $I(1,1,1,\lambda,\lambda,\lambda)$ along the path from SRP to ARP are listed in Table I; the smooth change of $I(1,1,1,\lambda,\lambda,\lambda)$ as λ changes confirms the consistency of the choices of branch for the functions u and v.

E. Large α_3

This subsection will track the branches of $u(\beta_0^{(0)}\beta_0^{(j)})$ and $v(\gamma_k^{(j)}/\sigma)$ along a path from SRP to a point with α_3 large and positive and α_1, α_2, α_{12}, α_{23}, and α_{31} all near 1. Expansions about $\alpha_3=\infty$ will be discussed, and $\lim_{\alpha_3\to\infty}\alpha_3^2 I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})$ evaluated.

Specifying the path is the first step. Make the definition

$$\alpha_{3\sigma}:=\tfrac{1}{2}(\{[(\alpha_1+\alpha_{12}+\alpha_{31})(-\alpha_1+\alpha_{12}+\alpha_{31})(\alpha_1-\alpha_{12}+\alpha_{31})(\alpha_1+\alpha_{12}-\alpha_{31})]^{1/2}$$
$$+[(\alpha_2+\alpha_{12}+\alpha_{23})(-\alpha_2+\alpha_{12}+\alpha_{23})(\alpha_2-\alpha_{12}+\alpha_{23})(\alpha_2+\alpha_{12}-\alpha_{23})]^{1/2}\}^2+(\alpha_1^2+\alpha_2^2-\alpha_{23}^2-\alpha_{31}^2)^2)^{1/2}\ . \tag{2.35}$$

Equation (2.18) can be used to verify that $\sigma=0$ at $\alpha_3=\alpha_{3\sigma}$. For $\alpha_1=\alpha_2=\alpha_{12}=\alpha_{23}=\alpha_{31}=1$, $\alpha_{3\sigma}=\sqrt{3}$. There are three branch points on the real axis between $\alpha_3=1$ and large positive α_3, located at $\alpha_3=\alpha_{3\sigma}$, at $\alpha_3=\alpha_1+\alpha_2$, and at $\alpha_3=\alpha_{23}+\alpha_{31}$. It will be assumed that $\alpha_{3\sigma}<\alpha_1+\alpha_2<\alpha_{23}+\alpha_{31}$ (the case $\alpha_{3\sigma}<\alpha_{23}+\alpha_{31}<\alpha_1+\alpha_2$ can be obtained via the interchange $0\leftrightarrow 3$). The following path will be used, where δ is a small positive real number:

$$\alpha_3=x,\quad 1\le x\le\alpha_{3\sigma}-\delta \tag{2.36a}$$

$$\alpha_3=\alpha_{3\sigma}+\delta\exp[i(\pi-\theta)],\quad 0\le\theta\le\pi \tag{2.36b}$$

$$\alpha_3=x,\quad \alpha_{3\sigma}+\delta\le x\le\alpha_1+\alpha_2-\delta \tag{2.36c}$$

$$\alpha_3=\alpha_1+\alpha_2+\delta\exp[i(\pi-\theta)],\quad 0\le\theta\le\pi \tag{2.36d}$$

$$\alpha_3=x,\quad \alpha_1+\alpha_2+\delta\le x\le\alpha_{23}+\alpha_{31}-\delta \tag{2.36e}$$

$$\alpha_3=\alpha_{23}+\alpha_{31}+\delta\exp[i(\pi-\theta)],\quad 0\le\theta\le\pi \tag{2.36f}$$

$$\alpha_3=x,\quad \alpha_{23}+\alpha_{31}+\delta\le x<\infty\ . \tag{2.36g}$$

The square root σ is then positive imaginary for $1\le\alpha_3\le\alpha_{3\sigma}-\delta$, and positive real for $\alpha_{3\sigma}+\delta\le\alpha_3<\infty$. The appropriate choice of branch for the other straight-line segments of the path is determined by using (2.6)–(2.8) to trace the behavior of the arguments of u and v near the branch points, with the signs and relative sizes of σ and the $\gamma_j^{(k)}$ deduced from (2.19) and (2.20). The results are as follows.

For $\alpha_{3\sigma}+\delta\le\alpha_3\le\alpha_1+\alpha_2-\delta$: $\gamma_0^{(0)}/\sigma$, $\gamma_3^{(0)}/\sigma$, $\gamma_1^{(1)}/\sigma$, $\gamma_2^{(1)}/\sigma$, $\gamma_1^{(2)}/\sigma$, $\gamma_2^{(2)}/\sigma$, $\gamma_0^{(3)}/\sigma$, $\gamma_3^{(3)}/\sigma$, $\beta_0^{(0)}\beta_0^{(1)}$, and $\beta_0^{(0)}\beta_0^{(2)}$ are all greater than $+1$; $\gamma_1^{(0)}/\sigma$, $\gamma_2^{(0)}/\sigma$, $\gamma_0^{(1)}/\sigma$, $\gamma_3^{(1)}/\sigma$, $\gamma_0^{(2)}/\sigma$, $\gamma_3^{(2)}/\sigma$, $\gamma_1^{(3)}/\sigma$, and $\gamma_2^{(3)}/\sigma$ are all less than -1; $\beta_0^{(0)}\beta_0^{(3)}$ lies between 0 and 1. The value of I is given by

$$I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})=\frac{16\pi^3}{\sigma}\lim_{\epsilon\to 0+}[u(\beta_0^{(0)}\beta_0^{(1)}+i\epsilon)+u(\beta_0^{(0)}\beta_0^{(2)}+i\epsilon)+u(\beta_0^{(0)}\beta_0^{(3)}-i\epsilon)+v((\gamma_0^{(0)}/\sigma)-i\epsilon)$$
$$+v((\gamma_1^{(0)}/\sigma)+i\epsilon)+v((\gamma_2^{(0)}/\sigma)+i\epsilon)+v((\gamma_3^{(0)}/\sigma)-i\epsilon)$$
$$+v((\gamma_0^{(1)}/\sigma)+i\epsilon)+v((\gamma_1^{(1)}/\sigma)-i\epsilon)+v((\gamma_2^{(1)}/\sigma)-i\epsilon)+v((\gamma_3^{(1)}/\sigma)+i\epsilon)$$
$$+v((\gamma_0^{(2)}/\sigma)+i\epsilon)+v((\gamma_1^{(2)}/\sigma)-i\epsilon)+v((\gamma_2^{(2)}/\sigma)-i\epsilon)+v((\gamma_3^{(2)}/\sigma)+i\epsilon)$$
$$+v((\gamma_0^{(3)}/\sigma)-i\epsilon)+v((\gamma_1^{(3)}/\sigma)+i\epsilon)+v((\gamma_2^{(3)}/\sigma)+i\epsilon)+v((\gamma_3^{(3)}/\sigma)-i\epsilon)]\ . \quad (2.37)$$

The fact that the expression (2.37) for I is real, as of course it must be, can be confirmed with the aid of (2.9), (2.13), (2.14), and the identities

$$\beta_1^{(0)}\beta_2^{(0)}\beta_3^{(0)}=\beta_0^{(0)}\ , \quad (2.38a)$$
$$\beta_0^{(1)}\beta_2^{(1)}\beta_3^{(1)}=\beta_1^{(1)}\ , \quad (2.38b)$$
$$\beta_0^{(2)}\beta_1^{(2)}\beta_3^{(2)}=\beta_2^{(2)}\ , \quad (2.38c)$$

and

$$\beta_0^{(3)}\beta_1^{(3)}\beta_2^{(3)}=\beta_3^{(3)}\ . \quad (2.38d)$$

For $\alpha_1+\alpha_2+\delta\le\alpha_3\le\alpha_{23}+\alpha_{31}-\delta$: $\gamma_0^{(0)}/\sigma$, $\gamma_3^{(0)}/\sigma$, $\gamma_1^{(1)}/\sigma$, $\gamma_2^{(2)}/\sigma$, $\beta_0^{(0)}\beta_0^{(1)}$, and $\beta_0^{(0)}\beta_0^{(2)}$ are all greater than $+1$; $\gamma_2^{(1)}/\sigma$, $\gamma_3^{(1)}/\sigma$, $\gamma_1^{(2)}/\sigma,\gamma_3^{(2)}/\sigma$, $\gamma_0^{(3)}/\sigma$, and $\gamma_3^{(3)}/\sigma$ all lie between -1 and $+1$; $\gamma_1^{(0)}/\sigma$, $\gamma_2^{(0)}/\sigma$, $\gamma_0^{(1)}/\sigma$, $\gamma_0^{(2)}/\sigma$, $\gamma_1^{(3)}/\sigma$, and $\gamma_2^{(3)}/\sigma$ are all less than -1; $\beta_0^{(0)}\beta_0^{(3)}$ is negative. The value of I is given by

$$I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})=\frac{16\pi^3}{\sigma}\lim_{\epsilon\to 0+}[u(\beta_0^{(0)}\beta_0^{(1)}+i\epsilon)+u(\beta_0^{(0)}\beta_0^{(2)}+i\epsilon)+u(\beta_0^{(0)}\beta_0^{(3)})+v((\gamma_0^{(0)}/\sigma)-i\epsilon)$$
$$+v((\gamma_1^{(0)}/\sigma)+i\epsilon)+v((\gamma_2^{(0)}/\sigma)+i\epsilon)+v((\gamma_3^{(0)}/\sigma)-i\epsilon)+v((\gamma_0^{(1)}/\sigma)+i\epsilon)$$
$$+v((\gamma_1^{(1)}/\sigma)-i\epsilon)+v(\gamma_2^{(1)}/\sigma)+v(\gamma_3^{(1)}/\sigma)+v((\gamma_0^{(2)}/\sigma)+i\epsilon)+v(\gamma_1^{(2)}/\sigma)$$
$$+v((\gamma_2^{(2)}/\sigma)-i\epsilon)+v(\gamma_3^{(2)}/\sigma)+v(\gamma_0^{(3)}/\sigma)$$
$$+v((\gamma_1^{(3)}/\sigma)+i\epsilon)+v((\gamma_2^{(3)}/\sigma)+i\epsilon)+v(\gamma_3^{(3)}/\sigma)]\ . \quad (2.39)$$

The fact that (2.39) is real can be confirmed with the aid of (2.9a), (2.9b), (2.13), (2.14), and (2.38a).

For $\alpha_{23}+\alpha_{31}+\delta\le\alpha_3<\infty$; $\gamma_1^{(1)}/\sigma$, $\gamma_2^{(1)}/\sigma$, $\gamma_1^{(2)}/\sigma$, $\gamma_2^{(2)}/\sigma$, $\beta_0^{(0)}\beta_0^{(1)}$, and $\beta_0^{(0)}\beta_0^{(2)}$ are all greater than $+1$; $\gamma_0^{(0)}/\sigma$, $\gamma_3^{(0)}/\sigma$, $\gamma_0^{(1)}/\sigma$, $\gamma_3^{(1)}/\sigma$, $\gamma_0^{(2)}/\sigma$, $\gamma_3^{(2)}/\sigma$, $\gamma_0^{(3)}/\sigma$, and $\gamma_3^{(3)}/\sigma$ all lie between -1 and $+1$; $\gamma_1^{(0)}/\sigma$, $\gamma_2^{(0)}/\sigma$, $\gamma_1^{(3)}/\sigma$, and $\gamma_2^{(3)}/\sigma$ are all less than -1; $\beta_0^{(0)}\beta_0^{(3)}$ lies between 0 and 1. The value of I is given by

$$I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})=\frac{16\pi^3}{\sigma}\lim_{\epsilon\to 0+}[u(\beta_0^{(0)}\beta_0^{(1)}+i\epsilon)+u(\beta_0^{(0)}\beta_0^{(2)}+i\epsilon)+u(\beta_0^{(0)}\beta_0^{(3)}+i\epsilon)+v(\gamma_0^{(0)}/\sigma)+v((\gamma_1^{(0)}/\sigma)+i\epsilon)$$
$$+v((\gamma_2^{(0)}/\sigma)+i\epsilon)+v(\gamma_3^{(0)}/\sigma)+v(\gamma_0^{(1)}/\sigma)+v((\gamma_1^{(1)}/\sigma)-i\epsilon)+v((\gamma_2^{(1)}/\sigma)+i\epsilon)$$
$$+v(\gamma_3^{(1)}/\sigma)+v(\gamma_0^{(2)}/\sigma)+v((\gamma_1^{(2)}/\sigma)+i\epsilon)+v((\gamma_2^{(2)}/\sigma)-i\epsilon)+v(\gamma_3^{(2)}/\sigma)$$
$$+v(\gamma_0^{(3)}/\sigma)+v((\gamma_1^{(3)}/\sigma)+i\epsilon)+v((\gamma_2^{(3)}/\sigma)+i\epsilon)+v(\gamma_3^{(3)}/\sigma)]\ . \quad (2.40)$$

The fact that (2.40) is real can be confirmed with the aid of (2.9), (2.13), and (2.14).

The behavior for $\alpha_3\to+\infty$, with the branches of u and v fixed by (2.40), will be discussed next. By using (2.15) and (2.16) for the terms in (2.40) which have singular points at $\alpha_3=\infty$, it is found that

$$I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})=I_1(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})\ln\alpha_3+I_2(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})\ , \quad (2.41)$$

where the functions I_1 and I_2, which are analytic functions of α_3^{-1} at $\alpha_3^{-1}=0$, are given by

$$I_1(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})=(32\pi^3/\sigma)\ln(\beta_2^{(1)}/\beta_1^{(1)}) \quad (2.42)$$

and

$$
\begin{aligned}
I_2(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}) = \frac{16\pi^3}{\sigma} \lim_{\epsilon\to 0+} \Bigg[& u_\infty(\beta_0^{(0)}\beta_0^{(1)}) + u_\infty(\beta_0^{(0)}\beta_0^{(2)}) + [u(\beta_0^{(0)}\beta_0^{(3)}+i\epsilon) + i\pi\ln(\beta_0^{(0)}\beta_0^{(3)})] + v_{-1}(\gamma_0^{(0)}/\sigma) \\
& + v_{-1}(\gamma_1^{(0)}/\sigma) + v_{-1}(\gamma_2^{(0)}/\sigma) + v_1(\gamma_3^{(0)}/\sigma) + v(\gamma_0^{(1)}/\sigma) \\
& + \left[v((\gamma_1^{(1)}/\sigma) - i\epsilon) + \frac{i\pi}{2}\ln(-\beta_1^{(1)}) \right] + \left[v((\gamma_2^{(1)}/\sigma) + i\epsilon) - \frac{i\pi}{2}\ln(-\beta_2^{(1)}) \right] \\
& + v(\gamma_3^{(1)}/\sigma) + v(\gamma_0^{(2)}/\sigma) + \left[v((\gamma_1^{(2)}/\sigma) + i\epsilon) - \frac{i\pi}{2}\ln(-\beta_1^{(2)}) \right] \\
& + \left[v((\gamma_2^{(2)}/\sigma) - i\epsilon) + \frac{i\pi}{2}\ln(-\beta_2^{(2)}) \right] + v(\gamma_3^{(2)}/\sigma) \\
& + v_1(\gamma_0^{(3)}/\sigma) + v_{-1}(\gamma_1^{(3)}/\sigma) + v_{-1}(\gamma_2^{(3)}/\sigma) + v_{-1}(\gamma_3^{(3)}/\sigma) \\
& + \tfrac{1}{2}\ln[(\beta_0^{(0)}\beta_1^{(1)}\beta_1^{(2)}\beta_3^{(3)})/\alpha_3^4]\ln(\beta_2^{(1)}/\beta_{(1)}^{(1)}) - \ln(-\beta_2^{(1)})\ln(-\beta_1^{(2)}) \Bigg]
\end{aligned}
\tag{2.43}
$$

The combination $\beta_2^{(1)}/\beta_1^{(1)}$ which appears in (2.42) has four equivalent forms:

$$\beta_2^{(1)}/\beta_1^{(1)} = \beta_1^{(2)}/\beta_2^{(2)} = (\beta_0^{(1)}\beta_3^{(1)})^{-1} = (\beta_0^{(2)}\beta_3^{(2)})^{-1} \ . \tag{2.44}$$

Both I_1 and I_2 have power-series expansions in inverse powers of α_3 which converge up to the nearest singularity. Equations (2.19) and (2.22) can be used to show that this singularity occurs at the nearest of the eight points $\alpha_3^{-1}=(\pm\alpha_1\pm\alpha_2)^{-1}$, $(\pm\alpha_{23}\pm\alpha_{31})^{-1}$ for I_1, and at the nearest of the ten points $\alpha_3^{-1}=(\pm\alpha_1\pm\alpha_2)^{-1}$, $(\pm\alpha_{23}\pm\alpha_{31})^{-1}$, $-(\alpha_2+\alpha_{12}+\alpha_{31})^{-1}$, $-(\alpha_1+\alpha_{12}+\alpha_{23})^{-1}$ for I_2. The leading terms of these large α_3 expansions are given by

$$I_1(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}) = -128\pi^3\alpha_3^{-3} + O(\alpha_3^{-4}) \tag{2.45}$$

and

$$
\begin{aligned}
I_2(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}) = \frac{16\pi^3}{\alpha_{12}} \lim_{\epsilon\to 0+} \Bigg[& u\left[\frac{(\alpha_1+\alpha_{31}-\alpha_{12})(\alpha_2+\alpha_{23}-\alpha_{12})}{(\alpha_1+\alpha_{31}+\alpha_{12})(\alpha_2+\alpha_{23}+\alpha_{12})} + i\epsilon \right] \\
& + i\pi\ln\left[\frac{(\alpha_1+\alpha_{31}-\alpha_{12})(\alpha_2+\alpha_{23}-\alpha_{12})}{(\alpha_1+\alpha_{31}+\alpha_{12})(\alpha_2+\alpha_{23}+\alpha_{12})} \right] \\
& + v((\alpha_1+\alpha_{31}+i\epsilon)/\alpha_{12}) + v((\alpha_1+\alpha_{31}-i\epsilon)/\alpha_{12}) \\
& + v((\alpha_2+\alpha_{23}+i\epsilon)/\alpha_{12}) + v((\alpha_2+\alpha_{23}-i\epsilon)/\alpha_{12}) \\
& - \ln\left[\frac{\alpha_1+\alpha_{31}-\alpha_{12}}{\alpha_1+\alpha_{31}+\alpha_{12}} \right] \ln\left[\frac{\alpha_2+\alpha_{23}-\alpha_{12}}{\alpha_2+\alpha_{23}+\alpha_{12}} \right] \Bigg] \alpha_3^{-2} + O(\alpha_3^{-3}) \ .
\end{aligned}
\tag{2.46}
$$

The large α_3 limit can be taken directly on the original integral (1.3) to obtain

$$\int (r_1^2 r_2^2 r_{12})^{-1} \exp[-(\alpha_1+\alpha_{31})r_1 - (\alpha_2+\alpha_{23})r_2 - \alpha_{12}r_{12}]d^3r_1 d^3r_2 = \lim_{\alpha_3\to\infty} \frac{\alpha_3^2}{4\pi} I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}) \ . \tag{2.47}$$

An explicit formula for the integral in (2.47) can be had by using (2.41), (2.45), and (2.46) to evaluate the limit in (2.47). Because the evaluation of limiting cases such as (2.47) provides a useful check on our results, we have sketched a direct evaluation of the integral in (2.47) in an appendix.

Information about the analytic continuation of I to the negative real axis in the complex α_3 plane, where I has a branch cut, will be needed for Sec. II F. This information is most easily obtained by tracking the branches of u and v to the negative real axis along paths with $|\alpha_3|$ large. Formulas for I just above the branch cut can be obtained by starting from (2.40) and tracking the branches along the following path, where δ is a small positive real number:

$$\alpha_3 = \delta^{-1}e^{i\theta}, \quad 0\le\theta\le\pi \tag{2.48a}$$

$$\alpha_3 = x, \quad -\delta^{-1}\le x\le -\alpha_2-\alpha_{12}-\alpha_{31}-\delta \tag{2.48b}$$

$$\alpha_3 = -\alpha_2-\alpha_{12}-\alpha_{31}+\delta\exp[i(\pi-\theta)], \quad 0\le\theta\le\pi \tag{2.48c}$$

$$\alpha_3 = x, \quad -\alpha_2-\alpha_{12}-\alpha_{31}+\delta\le x\le -\alpha_1-\alpha_{12}-\alpha_{23}-\delta \tag{2.48d}$$

$$\alpha_3=-\alpha_1-\alpha_{12}-\alpha_{23}+\delta\exp[i(\pi-\theta)],\quad 0\le\theta\le\pi \tag{2.48e}$$

$$\alpha_3=x,\quad -\alpha_1-\alpha_{12}-\alpha_{23}+\delta\le x\le-\alpha_{23}-\alpha_{31}-\delta \tag{2.48f}$$

$$\alpha_3=-\alpha_{23}-\alpha_{31}+\delta\exp[i(\pi-\theta)],\quad 0\le\theta\le\pi \tag{2.48g}$$

$$\alpha_3=x,\quad -\alpha_{23}-\alpha_{31}+\delta\le x\le-\alpha_1-\alpha_2-\delta \tag{2.48h}$$

$$\alpha_3=-\alpha_1-\alpha_2+\delta\exp[i(\pi-\theta)],\quad 0\le\theta\le\pi \tag{2.48i}$$

$$\alpha_3=x,\quad -\alpha_1-\alpha_2+\delta\le x\le-\alpha_{3\sigma}-\delta\ . \tag{2.48j}$$

Formulas for I just below the branch cut can be obtained by starting from (2.40) with ϵ replaced by $-\epsilon$ (which replacement leaves I unchanged) and tracking the branches along a path which is the reflection of the path (2.48) in the real axis [obtained by replacing i by $-i$ in (2.48)]. The results are as follows.

For $-\infty<\alpha_3\le-\alpha_{23}-\alpha_{31}-\delta$: $\gamma_1^{(1)}/\sigma$, $\gamma_2^{(1)}/\sigma$, $\gamma_1^{(2)}/\sigma$, and $\gamma_2^{(2)}/\sigma$ are all greater than $+1$; $\gamma_0^{(0)}/\sigma$, $\gamma_3^{(0)}/\sigma$, $\gamma_0^{(1)}/\sigma$, $\gamma_3^{(1)}/\sigma$, $\gamma_0^{(2)}/\sigma$, $\gamma_3^{(2)}/\sigma$, $\gamma_0^{(3)}/\sigma$, and $\gamma_3^{(3)}/\sigma$ all lie between -1 and $+1$; $\gamma_1^{(0)}/\sigma$, $\gamma_2^{(0)}/\sigma$, $\gamma_1^{(3)}/\sigma$, and $\gamma_2^{(3)}/\sigma$ are all less than -1; $\beta_0^{(0)}\beta_0^{(3)}$ lies between 0 and 1; $\beta_0^{(0)}\beta_0^{(1)}$ is greater than $+1$ for $\alpha_3\le-\alpha_2-\alpha_{12}-\alpha_{31}-\delta$; $\beta_0^{(0)}\beta_0^{(1)}$ lies between 0 and 1 for $-\alpha_2-\alpha_{12}-\alpha_{31}+\delta\le\alpha_3\le-\alpha_{23}-\alpha_{31}-\delta$; $\beta_0^{(0)}\beta_0^{(2)}$ is greater than $+1$ for $\alpha_3\le-\alpha_1-\alpha_{12}-\alpha_{23}-\delta$; $\beta_0^{(0)}\beta_0^{(2)}$ lies between 0 and 1 for $-\alpha_1-\alpha_{12}-\alpha_{23}+\delta\le\alpha_3\le-\alpha_{23}-\alpha_{31}-\delta$. The values of I above and below the branch cut are given by

TABLE I. Values of $I(1,1,1,\lambda,\lambda,\lambda)$ along the path from ARP to SRP.

λ	$I(\lambda)$	λ	$I(\lambda)$
0.00	4.3822×10^2	0.52	1.0095×10^2
0.02	4.0579×10^2	0.54	9.6802×10
0.04	3.7668×10^2	0.56	9.2892×10
0.06	3.5047×10^2	0.58	8.9200×10
0.08	3.2677×10^2	0.60	8.5712×10
0.10	3.0530×10^2	0.62	8.2412×10
0.12	2.8578×10^2	0.64	7.9289×10
0.14	2.6799×10^2	0.66	7.6329×10
0.16	2.5173×10^2	0.68	7.3522×10
0.18	2.3684×10^2	0.70	7.0858×10
0.20	2.2317×10^2	0.72	6.8328×10
0.22	2.1059×10^2	0.74	6.5923×10
0.24	1.9900×10^2	0.76	6.3635×10
0.26	1.8829×10^2	0.78	6.1457×10
0.28	1.7837×10^2	0.80	5.9382×10
0.30	1.6918×10^2	0.82	5.7404×10
0.32	1.6065×10^2	0.84	5.5518×10
0.34	1.5271×10^2	0.86	5.3717×10
0.36	1.4532×10^2	0.88	5.1997×10
0.38	1.3842×10^2	0.90	5.0353×10
0.40	1.3197×10^2	0.92	4.8781×10
0.42	1.2594×10^2	0.94	4.7277×10
0.44	1.2030×10^2	0.96	4.5837×10
0.46	1.1500×10^2	0.98	4.4458×10
0.48	1.1002×10^2	1.00	4.3136×10
0.50	1.0535×10^2		

$$\begin{aligned}\lim_{\epsilon\to0}I(\alpha_1,\alpha_2,\alpha_3\pm i\epsilon,\alpha_{12},\alpha_{23},\alpha_{31})=\frac{16\pi^3}{\sigma}\lim_{\epsilon\to0}[&u(\beta_0^{(0)}\beta_0^{(1)}\mp i\epsilon)+u(\beta_0^{(0)}\beta_0^{(2)}\mp i\epsilon)+u(\beta_0^{(0)}\beta_0^{(3)}\mp i\epsilon)+v(\gamma_0^{(0)}/\sigma)\\&+v((\gamma_1^{(0)}/\sigma)\mp i\epsilon)+v((\gamma_2^{(0)}/\sigma)\mp i\epsilon)+v(\gamma_3^{(0)}/\sigma)+v(\gamma_0^{(1)}/\sigma)\\&+v((\gamma_1^{(1)}/\sigma)\mp i\epsilon)+v((\gamma_2^{(1)}/\sigma)\pm i\epsilon)+v(\gamma_3^{(1)}/\sigma)+v(\gamma_0^{(2)}/\sigma)\\&+v((\gamma_1^{(2)}/\sigma)\pm i\epsilon)+v((\gamma_2^{(2)}/\sigma)\mp i\epsilon)+v(\gamma_3^{(2)}/\sigma)+v(\gamma_0^{(3)}/\sigma)\\&+v((\gamma_1^{(3)}/\sigma)\mp i\epsilon)+v((\gamma_2^{(3)}/\sigma)\mp i\epsilon)+v(\gamma_3^{(3)}/\sigma)]\ .\end{aligned} \tag{2.49}$$

The $u(\beta_0^{(0)}\beta_0^{(1)}\mp i\epsilon)$ term in (2.49) has a branch point at $\alpha_3=-\alpha_2-\alpha_{12}-\alpha_{31}$; the $u(\beta_0^{(0)}\beta_0^{(2)}\mp i\epsilon)$ term in (2.49) has a branch point at $\alpha_3=-\alpha_1-\alpha_{12}-\alpha_{23}$. Equation (2.49) gives the branch correctly on both sides of these branch points when used with (2.15) and (2.16).

For $-\alpha_{23}-\alpha_{31}+\delta\le\alpha_3\le-\alpha_1-\alpha_2-\delta$: $\gamma_0^{(0)}/\sigma$, $\gamma_3^{(0)}/\sigma$, $\gamma_2^{(1)}/\sigma$, $\gamma_3^{(1)}/\sigma$, $\gamma_1^{(2)}/\sigma$, and $\gamma_3^{(2)}/\sigma$ are all greater than $+1$; $\gamma_0^{(1)}/\sigma$, $\gamma_1^{(1)}/\sigma$, $\gamma_0^{(2)}/\sigma$, $\gamma_2^{(2)}/\sigma$, $\gamma_0^{(3)}/\sigma$, and $\gamma_3^{(3)}/\sigma$ all lie between -1 and 1; $\gamma_1^{(0)}/\sigma$, $\gamma_2^{(0)}/\sigma$, $\gamma_1^{(3)}/\sigma$, and $\gamma_2^{(3)}/\sigma$ are all less than -1; $\beta_0^{(0)}\beta_0^{(1)}$, $\beta_0^{(0)}\beta_0^{(2)}$, and $\beta_0^{(0)}\beta_0^{(3)}$ are all negative. The values of I above and below the branch cut are given by

$$\begin{aligned}\lim_{\epsilon\to0}I(\alpha_1,\alpha_2,\alpha_3\pm i\epsilon,\alpha_{12},\alpha_{23},\alpha_{31})=\frac{16\pi^3}{\sigma}\lim_{\epsilon\to0}[&u(\beta_0^{(0)}\beta_0^{(1)})+u(\beta_0^{(0)}\beta_0^{(2)})+u(\beta_0^{(0)}\beta_0^{(3)})+v((\gamma_0^{(0)}/\sigma)\pm i\epsilon)+v((\gamma_1^{(0)}/\sigma)\mp i\epsilon)\\&+v((\gamma_2^{(0)}/\sigma)\mp i\epsilon)+v((\gamma_3^{(0)}/\sigma)\pm i\epsilon)+v(\gamma_0^{(1)}/\sigma)+v(\gamma_1^{(1)}/\sigma)\\&+v((\gamma_2^{(1)}/\sigma)\pm i\epsilon)+v((\gamma_3^{(1)}/\sigma)\pm i\epsilon)+v(\gamma_0^{(2)}/\sigma)+v((\gamma_1^{(2)}/\sigma)\pm i\epsilon)\\&+v(\gamma_2^{(2)}/\sigma)+v((\gamma_3^{(2)}/\sigma)\pm i\epsilon)+v(\gamma_0^{(3)}/\sigma)+v((\gamma_1^{(3)}/\sigma)\mp i\epsilon)\\&+v((\gamma_2^{(3)}/\sigma)\mp i\epsilon)+v(\gamma_3^{(3)}/\sigma)]\ .\end{aligned} \tag{2.50}$$

For $-\alpha_1-\alpha_2+\delta\le\alpha_3\le-\alpha_{3\sigma}-\delta$: $\gamma_0^{(0)}/\sigma$, $\gamma_3^{(0)}/\sigma$, $\gamma_0^{(1)}/\sigma$, $\gamma_1^{(1)}/\sigma$, $\gamma_2^{(1)}/\sigma$, $\gamma_3^{(1)}/\sigma$, $\gamma_0^{(2)}/\sigma$, $\gamma_1^{(2)}/\sigma$, $\gamma_2^{(2)}/\sigma$, $\gamma_3^{(2)}/\sigma$, $\gamma_0^{(3)}/\sigma$, and $\gamma_3^{(3)}/\sigma$ are all greater than $+1$; $\gamma_1^{(0)}/\sigma$, $\gamma_2^{(0)}/\sigma$, $\gamma_1^{(3)}/\sigma$, and $\gamma_2^{(3)}$ are all less than -1; $\beta_0^{(0)}\beta_0^{(1)}$, $\beta_0^{(0)}\beta_0^{(2)}$, and $\beta_0^{(0)}\beta_0^{(3)}$ all lie between 0 and 1. The value of I is given by

$$I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})=\frac{16\pi^3}{\sigma}\lim_{\epsilon\to 0}[(\beta_0^{(0)}\beta_0^{(1)}+i\epsilon)+u(\beta_0^{(0)}\beta_0^{(2)}+i\epsilon)+u(\beta_0^{(0)}\beta_0^{(3)}+i\epsilon)+v((\gamma_0^{(0)}/\sigma)+i\epsilon)$$
$$+v((\gamma_1^{(0)}/\sigma)-i\epsilon)+v((\gamma_2^{(0)}/\sigma)-i\epsilon)+v((\gamma_3^{(0)}/\sigma)+i\epsilon)$$
$$+v((\gamma_0^{(1)}/\sigma)+i\epsilon)+v((\gamma_1^{(1)}/\sigma)+i\epsilon)+v((\gamma_2^{(1)}/\sigma)+i\epsilon)$$
$$+v((\gamma_3^{(1)}/\sigma)+i\epsilon)+v((\gamma_0^{(2)}/\sigma)+i\epsilon)+v((\gamma_1^{(2)}/\sigma)+i\epsilon)$$
$$+v((\gamma_2^{(2)}/\sigma)+i\epsilon)+v((\gamma_3^{(2)}/\sigma)+i\epsilon)+v((\gamma_0^{(3)}/\sigma)+i\epsilon)$$
$$+v((\gamma_1^{(3)}/\sigma)-i\epsilon)+v((\gamma_2^{(3)}/\sigma)-i\epsilon)+v((\gamma_3^{(3)}/\sigma)+i\epsilon)]\ . \tag{2.51}$$

The fact that (2.51) is real can be confirmed with the aid of (2.9), (2.13a), (2.14a), (2.14b), and (2.38). The jump across the branch cut which runs along the negative real axis from $\alpha_3=-\infty$ to $\alpha_3=-\alpha_1-\alpha_2$ when $\alpha_1+\alpha_2<\alpha_{23}+\alpha_{31}<\alpha_1+\alpha_{12}+\alpha_{23}<\alpha_2+\alpha_{12}+\alpha_{31}$ is given by

$$\frac{\sigma}{64\pi^4 i}\lim_{\epsilon\to 0^+}[I(\alpha_1,\alpha_2,\alpha_3+i\epsilon,\alpha_{12},\alpha_{23},\alpha_{31})-I(\alpha_1,\alpha_2,\alpha_3-i\epsilon,\alpha_{12},\alpha_{23},\alpha_{31})]$$
$$=\begin{cases}\ln(\beta_2^{(1)}/\beta_1^{(1)}), & -\infty<\alpha_3<-\alpha_2-\alpha_{12}-\alpha_{31}\\ \ln(\beta_0^{(0)}/\beta_3^{(1)}), & -\alpha_2-\alpha_{12}-\alpha_{31}<\alpha_3<-\alpha_1-\alpha_{12}-\alpha_{23}\\ \ln(\beta_0^{(0)}\beta_3^{(3)}), & -\alpha_1-\alpha_{12}-\alpha_{23}<\alpha_3<-\alpha_{23}-\alpha_{31}\\ \ln(-\beta_0^{(0)}), & -\alpha_{23}-\alpha_{31}<\alpha_3<-\alpha_1-\alpha_2\ .\end{cases} \tag{2.52}$$

The corresponding formulas for some of the other possible orderings of the branch points $-\alpha_2-\alpha_{12}-\alpha_{31}$, $-\alpha_1-\alpha_{12}-\alpha_{23}$, $-\alpha_{23}-\alpha_{31}$, and $-\alpha_1-\alpha_2$ can be obtained from (2.52) via the interchanges $1\leftrightarrow 2$ and/or $0\leftrightarrow 3$.

F. Relation to molecular matrix element integrals

The three-electron generating integral (1.3) is related to the two-electron two-center generating integral

$$L(\alpha_1,\alpha_2;\alpha_{12},\alpha_{23},\alpha_{31};r_3):=\int(r_1r_2r_{12}r_{23}r_{31})^{-1}\exp(-\alpha_1r_1-\alpha_2r_2-\alpha_{12}r_{12}-\alpha_{23}r_{23}-\alpha_{31}r_{31})d^3\mathbf{r}_1d^3\mathbf{r}_2 \tag{2.53}$$

via the Laplace transform:

$$I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})=4\pi\int_0^\infty r_3L(\alpha_1,\alpha_2;\alpha_{12},\alpha_{23},\alpha_{31};r_3)\times\exp(-\alpha_3r_3)dr_3\ . \tag{2.54}$$

The complex inversion formula for the Laplace transform applied to (2.54) yields a formula for L:

$$L(\alpha_1,\alpha_2;\alpha_{12},\alpha_{23},\alpha_{31};r_3)=\frac{1}{8\pi^2r_3i}\int_{\alpha-i\infty}^{\alpha+i\infty}\exp(\alpha_3r_3)\times I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})d\alpha_3\ , \tag{2.55}$$

where α is chosen to make the path of integration run to the right of all singularities of I regarded as an analytic function of α_3 with α_1, α_2, α_{12}, α_{23}, and α_{31} fixed. The multicenter integrals which arise when Slater orbitals are used for molecular calculations are notoriously difficult;[20] Eq. (2.55) provides an alternative starting point for the evaluation of the two-center integral L and of those integrals which can be obtained from L by taking derivatives with respect to the α's. The rest of this subsection outlines the kind of results which can be obtained for L by starting with (2.55).

Small r_3 expansion. As was shown in Sec. II E, I can be written in the form (2.41) where I_1 and I_2 have power-series expansions of the form

$$I_1(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})=\sum_{n=3}^{\infty}a_n^{(1)}(\alpha_1,\alpha_2;\alpha_{12},\alpha_{23},\alpha_{31})\alpha_3^{-n} \tag{2.56a}$$

and

$$I_2(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})=\sum_{n=2}^{\infty}a_n^{(2)}(\alpha_1,\alpha_2;\alpha_{12},\alpha_{23},\alpha_{31})\alpha_3^{-n} \tag{2.56b}$$

which converge for sufficiently large α_3. Deforming the integration contour in (2.55) until it lies in the interior of the domain of convergence of (2.56a) and (2.56b) makes it possible to insert (2.41), (2.56a), and (2.56b) in (2.55) and integrate term by term. The result is

$$L(\alpha_1,\alpha_2;\alpha_{12},\alpha_{23},\alpha_{31};r_3)=L_1(\alpha_1,\alpha_2;\alpha_{12},\alpha_{23},\alpha_{31};r_3)\ln r_3+L_2(\alpha_1,\alpha_2;\alpha_{12},\alpha_{23},\alpha_{31};r_3)\ , \tag{2.57}$$

where L_1 and L_2 have the power-series expansions

$$L_1(\alpha_1,\alpha_2;\alpha_{12},\alpha_{23},\alpha_{31};r_3)=\sum_{n=1}^{\infty} b_n^{(1)}(\alpha_1,\alpha_2;\alpha_{12},\alpha_{23},\alpha_{31})r_3^n \quad (2.58a)$$

and

$$L_2(\alpha_1,\alpha_2;\alpha_{12},\alpha_{23},\alpha_{31};r_3)=\sum_{n=0}^{\infty} b_n^{(2)}(\alpha_1,\alpha_2;\alpha_{12},\alpha_{23},\alpha_{31})r_3^n \ . \quad (2.58b)$$

The coefficients $b_n^{(1)},b_n^{(2)}$ in (2.58) are related to the coefficients $a_n^{(1)},a_n^{(2)}$ in (2.56) by

$$b_n^{(1)}=-a_{n+2}^{(1)}/[4\pi(n+1)!], \quad n\geq 1 \quad (2.59a)$$

$$b_0^{(2)}=a_2^{(2)}/(4\pi) \ , \quad (2.59b)$$

and

$$b_n^{(2)}=[\psi(n+2)a_{n+2}^{(1)}+a_{n+2}^{(2)}]/[4\pi(n+1)!], \quad n\geq 1 \ , \quad (2.59c)$$

where ψ is the logarithmic derivative of the gamma function:

$$\psi(z)=d\ \ln\Gamma(z)/dz \ . \quad (2.60)$$

The series (2.58a) and (2.58b) converge for all finite r_3. In fact, the results above show that L_1 and L_2, regarded as analytic functions of r_3 with α_1, α_2, α_{12}, α_{23}, and α_{31} fixed, are entire functions of exponential type. Numerical values of the coefficients $a_n^{(1)}$ and $a_n^{(2)}$ which appear in (2.56) and (2.59) are readily computed via methods of the kind outlined in Sec. III following.

An alternative representation for the integral L can be obtained by deforming the integration contour in (2.55) until it surrounds the branch cut of I on the negative real axis in the complex α_3 plane. Let α_0 be the smallest of the four numbers $\alpha_1+\alpha_2$, $\alpha_{23}+\alpha_{31}$, $\alpha_1+\alpha_{12}+\alpha_{23}$, $\alpha_2+\alpha_{12}+\alpha_{31}$. Then

$$L(\alpha_1,\alpha_2;\alpha_{12},\alpha_{23},\alpha_{31};r_3)=\frac{1}{8\pi^2 r_3 i}\exp(-\alpha_0 r_3)\int_0^{\infty}\exp(-xr_3)\lim_{\epsilon\to 0}[I(\alpha_1,\alpha_2,-\alpha_0-x+i\epsilon,\alpha_{12},\alpha_{23},\alpha_{31}) - I(\alpha_1,\alpha_2,-\alpha_0-x-i\epsilon,\alpha_{12},\alpha_{23},\alpha_{31})]dx \ . \quad (2.61)$$

Equation (2.52) gives an explicit formula for the jump across the branch cut needed in (2.61) for one ordering of the four numbers $\alpha_1+\alpha_2$, $\alpha_{23}+\alpha_{31}$, $\alpha_1+\alpha_{12}+\alpha_{23}$, $\alpha_2+\alpha_{12}+\alpha_{31}$. Formulas for some other orderings can be obtained by the interchanges $1\leftrightarrow 2$ and/or $0\leftrightarrow 3$ applied to (2.52); formulas for orderings not obtainable via these interchanges can be obtained via the kind of branch tracking which yielded (2.52). An asymptotic expansion of L for large r_3 can be obtained from (2.61) by expanding the jump across the branch cut in (2.61) for small x and integrating term by term.[21] Equation (2.61) is also a good starting point for the evaluation of L via numerical integration.

G. Integrals which contain spherical harmonics

This subsection shows how certain more general three-electron integrals which contain spherical harmonics can be reduced to integrals of the form (1.2) by averaging over orientations of the coordinate system. Because products of spherical harmonics such as $Y_{l_a,m_a}(\theta,\phi)Y_{l_b,m_b}(\theta,\phi)$ can be written as a sum of spherical harmonics by using[22]

$$Y_{l_a,m_a}(\theta,\phi)Y_{l_b,m_b}(\theta,\phi)=\sum_{l,m}\left[\frac{(2l_a+1)(2l_b+1)(2l+1)}{4\pi}\right]^{1/2}\begin{pmatrix} l_a & l_b & l \\ m_a & m_b & m\end{pmatrix}\begin{pmatrix} l_a & l_b & l \\ 0 & 0 & 0\end{pmatrix}\overline{Y_{l,m}(\theta,\phi)} \ , \quad (2.62)$$

it is sufficient to consider the integral

$$M(l_1,m_1,l_2,m_2,l_3,m_3;n_1,n_2,n_3,n_{12},n_{23},n_{31};\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}) := \int r_1^{l_1+n_1-1} r_2^{l_2+n_2-1} r_3^{l_3+n_3-1} r_{12}^{n_{12}-1} r_{23}^{n_{23}-1} r_{31}^{n_{31}-1} \times\exp(-\alpha_1 r_1-\alpha_2 r_2-\alpha_3 r_3-\alpha_{12}r_{12}-\alpha_{23}r_{23}-\alpha_{31}r_{31})Y_{l_1,m_1}(\theta_1,\phi_1)Y_{l_2,m_2}(\theta_2,\phi_2)Y_{l_3,m_3}(\theta_3,\phi_3)d^3\mathbf{r}_1 d^3\mathbf{r}_2 d^3\mathbf{r}_3 \ . \quad (2.63)$$

The integral (2.63) vanishes if the integrand has odd parity; thus it is necessary to consider only the case where $l_1+l_2+l_3$ is an even integer.

Averaging over orientations of the coordinate system can be done by noting that the rotation of the coordinate system specified by the Euler angles α,β,γ results in the replacement of $Y_{l,m}(\theta,\phi)$ by $Y_{l,m}(\theta',\phi')$ where[23]

$$Y_{l,m}(\theta',\phi')=\sum_{m'=-l}^{l} Y_{l,m'}(\theta,\phi)D_{m'm}^{(l)}(\alpha,\beta,\gamma) \ . \quad (2.64)$$

Here the D's are matrix elements of the rotation operator. If (2.64) is used for each of the three spherical harmonics in (2.63), averaging over orientations can be carried out by integrating over α β, and γ with the aid of the formula for the integral over the product of three D's.[24] The result is

$$M(l_1,m_1,l_2,m_2,l_3,m_3;n_1,n_2,n_3,n_{12},n_{23},n_{31};\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})$$

$$=\begin{bmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{bmatrix}\int r_1^{n_1-1}r_2^{n_2-1}r_3^{n_3-1}r_{12}^{n_{12}-1}r_{23}^{n_{23}-1}r_{31}^{n_{31}-1}R(l_1,l_2,l_3;r_1,r_2,r_3,r_{12},r_{23},r_{31})$$

$$\times\exp(-\alpha_1r_1-\alpha_2r_2-\alpha_3r_3-\alpha_{12}r_{12}-\alpha_{23}r_{23}-\alpha_{31}r_{31})d^3\mathbf{r}_1d^3\mathbf{r}_2d^3\mathbf{r}_3\ , \tag{2.65}$$

where R is given by[25]

$$R(l_1,l_2,l_3;r_1,r_2,r_3,r_{12},r_{23},r_{31}):=r_1^{l_1}r_2^{l_2}r_3^{l_3}\sum_{m_1,m_2,m_3}\begin{bmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{bmatrix}Y_{l_1,m_1}(\theta_1,\phi_1)Y_{l_2,m_2}(\theta_2,\phi_2)Y_{l_3,m_3}(\theta_3,\phi_3)\ . \tag{2.66}$$

R, which is invariant under rotations, is a polynomial in the six variables r_1^2, r_2^2, r_3^2, r_{12}^2, r_{23}^2, and r_{31}^2. Thus the integral in (2.66) is a finite linear combination of integrals of the form (1.2). Explicit expressions for the invariant polynomial R can be worked out on a case-by-case basis by exploiting its rotational invariance to choose the direction of one of the three vectors $\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3$ as the direction of the z axis.

III. NUMERICAL EVALUATION

This section will show how the result (2.1) can be used for the efficient recursive evaluation of a collection of integrals of the form (1.2). The obvious approach to evaluating (1.2) would be to work out a formula for the derivative needed in (1.4) by repeated differentiation of (2.1) with the aid of (2.2)–(2.9). However, such formulas for derivatives grow in complexity at a rapidly increasing rate; thus this approach is to be avoided. Explicit formulas for derivatives are in fact *not needed*, as has been emphasized by Moore;[26] the needed numerical values of derivatives can be obtained by working in efficient recursive fashion with numerical values only. Because these methods deserve to be more widely known, their application to the evaluation of (1.2) via (1.4) will be outlined here.

A. General formulas

This subsection records formulas for the derivatives of a product and for the derivative of a function of a function which are suitable for recursive evaluation. The formula for the derivatives of a product of two functions of n variables $x_1,x_2,\ldots,x_n$ is

$$\left[\prod_{i=1}^{n}\frac{1}{k_i!}\left[\frac{\partial}{\partial x_i}\right]^{k_i}\right]f(x_1,x_2,\ldots,x_n)g(x_1,x_2,\ldots,x_n)$$

$$=\sum_{l_1=0}^{k_1}\sum_{l_2=0}^{k_2}\cdots\sum_{l_n=0}^{k_n}\left\{\left[\prod_{i=1}^{n}\frac{1}{l_i!}\left[\frac{\partial}{\partial x_i}\right]^{l_i}\right]f(x_1,x_2,\ldots,x_n)\right\}\left\{\left[\prod_{j=1}^{n}\frac{1}{(k_j-l_j)!}\left[\frac{\partial}{\partial x_j}\right]^{k_j-l_j}\right]g(x_1,x_2,\ldots,x_n)\right\}\ . \tag{3.1}$$

If the function f depends on the single variable g where g is a function of the n variables $x_1,x_2,\ldots,x_n$, the derivatives are given by

$$\left[\prod_{i=1}^{n}\frac{1}{k_i!}\left[\frac{\partial}{\partial x_i}\right]^{k_i}\right]f(g(x_1,x_2,\ldots,x_n))=\sum_{l=0}^{k}h(k_1,k_2,\ldots,k_n;l;x_1,x_2,\ldots,x_n)\frac{1}{l!}\frac{d^lf(g)}{dg^l}\ , \tag{3.2}$$

where

$$k=\sum_{i=1}^{n}k_i \tag{3.3}$$

with

$$h(0,0,\ldots,0;0;x_1,x_2,\ldots,x_n)=1\ , \tag{3.4}$$

$$h(k_1,k_2,\ldots,k_n;1;x_1,x_2,\ldots,x_n)=\left[\prod_{i=1}^{n}\frac{1}{k_i!}\left[\frac{\partial}{\partial x_i}\right]^{k_i}\right]g(x_1,x_2,\ldots,x_n)\ , \tag{3.5}$$

and

$$h(k_1,k_2,\ldots,k_n;l;x_1,x_2,\ldots,x_n) = \sum_{l_1=0}^{k_1}\sum_{l_2=0}^{k_2}\cdots\sum_{l_n=0}^{k_n} h(l_1,l_2,\ldots,l_n;m;x_1,x_2,\ldots,x_n) \times h(k_1-l_1,k_2-l_2,\ldots,k_n-l_n;l-m;x_1,x_2,\ldots,x_n),\quad 1\le m\le l-1\ . \tag{3.6}$$

Equation (3.1) can be recognized as the rule for constructing the coefficients when two power series in n variables are multiplied; the coefficients are just the Taylor coefficients for functions of n variables. Equations (3.2)–(3.6) can be easily established by expanding $f(g+\Delta g)$ in powers of Δg. Equation (3.6), which is obtained by multiplying the power series for $(\Delta g)^m$ by the power series for $(\Delta g)^{(l-m)}$, is again the rule for constructing the coefficients when two power series in n variables are multiplied; thus the same computer code can be used for (3.1) and (3.6). Equation (3.6) with $m=l-1$ should be used to calculate the coefficients h needed for (3.2) via recursion on l, with starting values provided by (3.5). The code will be more efficient if it is written to work with Taylor coefficients rather than derivatives, because the factorials will then be absent from the product code and the function of a function code.

It is important to realize that these formulas are to be used for the recursive calculation of *numerical* values, and not for the derivation of analytic formulas. Thus (3.1) gives *numerical* values of the derivatives of the product fg assuming that *numerical* values of the derivatives of f and g have already been computed; (3.2) gives *numerical* values of the derivatives of $f(g)$ assuming that *numerical* values of the coefficients h and the derivatives d^lf/dg^l are already available.

B. Evaluation of $u(z)$ and $v(z)$

For $\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}$ all real, two cases must be considered: $\sigma^2>0$ and $\sigma^2<0$.

The case $\sigma^2>0$: The arguments of the dilogarithms which appear in the definitions (2.2) and (2.3) of u and v are real. The transformation theory for the dilogarithm should be used to reduce the problem of evaluating these dilogarithms to the problem of evaluating dilogarithms whose argument lies between $-\frac{1}{2}$ and $\frac{1}{2}$. The identities needed for the different ranges are

$$\mathrm{Li}_2(z)=\mathrm{Li}_2(w)+\tfrac{1}{2}\ln w\,\ln(z^2w)-\frac{\pi^2}{6}\ , \tag{3.7a}$$

where $w=(1-z)^{-1}$ for $z<-1$;

$$\mathrm{Li}_2(z)=-\mathrm{Li}_2(w)-\tfrac{1}{2}\ln^2(-w/z)\ , \tag{3.7b}$$

where $w=z/(z-1)$ for $-1\le z<-\frac{1}{2}$;

$$\mathrm{Li}_2(z)=-\mathrm{Li}_2(w)-\ln z\,\ln w+\frac{\pi^2}{6}\ , \tag{3.7c}$$

where $w=1-z$ for $\frac{1}{2}<z\le 1$;

$$\mathrm{Re}[\mathrm{Li}_2(z)]=\mathrm{Li}_2(w)-\ln z\,\ln w-\tfrac{1}{2}\ln^2 z+\frac{\pi^2}{6}\ , \tag{3.7d}$$

where $w=1-z^{-1}$ for $1<z\le 2$; and

$$\mathrm{Re}[\mathrm{Li}_2(z)]=-\mathrm{Li}_2(w)-\tfrac{1}{2}\ln^2 z+\frac{\pi^2}{3}\ , \tag{3.7e}$$

where $w=1/z$ for $z>2$.

In each case w will lie between $-\frac{1}{2}$ and $\frac{1}{2}$ if z lies in the specified range. $\mathrm{Li}_2(w)$ can be evaluated by using the power series

$$\mathrm{Li}_2(w)=\sum_{n=1}^{N} n^{-2}w^n+R_N(w) \tag{3.8}$$

with the value of N chosen large enough to make the error bound

$$|R_N(w)|\le (N+1)^{-2}(1-|w|)^{-1}|w|^{N+1},\quad |w|<1 \tag{3.9}$$

small enough to guarantee the required accuracy. Because the radius of convergence of the series (3.8) is 1, it is rapidly convergent for w between $-\frac{1}{2}$ and $\frac{1}{2}$.

The case $\sigma^2<0$: The argument of u is on the unit circle in the complex plane, and the argument of v is purely imaginary. The definitions (2.2) and (2.3) of u and v can be brought to the forms

$$u(e^{i\theta})=2i\,\mathrm{Cl}_2(\theta) \tag{3.10}$$

and

$$v(iy)=i\,\mathrm{Cl}_2(\pi+2\phi)\ , \tag{3.11}$$

where $y=\tan\phi$. Clausen's function Cl_2, which is defined by[19]

$$\mathrm{Cl}_2(\omega)=-\int_0^{\omega}\ln|2\sin(t/2)|\,dt\ , \tag{3.12}$$

can be calculated by using the identities

$$\mathrm{Cl}_2(\omega)=\mathrm{Cl}_2(\omega+2\pi)=-\mathrm{Cl}_2(2\pi-\omega)=-\mathrm{Cl}_2(-\omega) \tag{3.13}$$

to reduce the problem of evaluating the Cl_2 to the problem of evaluating a Cl_2 whose argument lies between $-\frac{2}{3}\pi$ and $\frac{4}{3}\pi$. For ω between $-\frac{2}{3}\pi$ and $\frac{2}{3}\pi$, this evaluation is carried out by using the series

$$\mathrm{Cl}_2(\omega)=\omega\left[1-\ln|\omega|+\sum_{n=1}^{N}\frac{(-1)^{n-1}B_{2n}\omega^{2n}}{2n(2n+1)!}+R_N(\omega)\right] \tag{3.14}$$

together with the error bound

$$|R_N(\omega)| \le \frac{2}{(2N+1)(2N+3)}\left[1-\left|\frac{\omega}{2\pi}\right|\right]^{-1}\left|\frac{\omega}{2\pi}\right|^{2N+2}, \quad |\omega|<2\pi . \qquad (3.15)$$

Because the radius of convergence of the series (3.14) is 2π, it is rapidly convergent for ω between $-2\pi/3$ and $2\pi/3$. For ω between $2\pi/3$ and $4\pi/3$, the evaluation is carried out by using the series

$$\mathrm{Cl}_2(\omega)=(\omega-\pi)\left[-\ln 2+\sum_{n=1}^{N}\frac{(-1)^{n-1}B_{2n}}{2n(2n+1)!}(2^{2n}-1)(\omega-\pi)^{2n}+R_n(\omega)\right] \qquad (3.16)$$

together with the error bound

$$|R_N(\omega)| \le \frac{2}{(2N+1)(2N+3)}\left[1-\left|\frac{\omega}{\pi}-1\right|\right]^{-1}\left|\frac{\omega}{\pi}-1\right|^{2N+2}. \qquad (3.17)$$

The series (3.16) can be derived from (3.14) with the aid of the identity $\mathrm{Cl}_2(\omega)=\frac{1}{2}\mathrm{Cl}_2[2(\omega-\pi)]-\mathrm{Cl}_2(\omega-\pi)$. Because the radius of convergence of the series (3.16) is π, it is rapidly convergent for ω between $2\pi/3$ and $4\pi/3$. The series (3.16), rather than the series (3.14), was chosen for ω near π because $\mathrm{Cl}_2(\omega)$ has a zero at π. The B_k which appear in (3.14)–(3.17) are the Bernoulli numbers, defined by

$$z(e^z-1)^{-1}=\sum_{k=0}^{\infty}B_k z^k/k! . \qquad (3.18)$$

The reader should be warned that there are several nonequivalent definitions of the Bernoulli numbers in common use; this can be a pitfall for the unwary.

C. Derivatives of $u(z)$

The case $\sigma^2>0$: The following formulas, which are obtained by differentiating the definition (2.2) of $u(z)$ with the aid of (2.4), can be used for the numerical evaluation of the Taylor coefficients of $u(z)$:

$$\frac{du(z)}{dz}=-\frac{1}{z}\ln[-(1-z)^2/z] , \qquad (3.19)$$

$$\frac{1}{2!}\frac{d^2u(z)}{dz^2}=\frac{1+z}{2z^2(1-z)}-\frac{1}{2z}\frac{du(z)}{dz} , \qquad (3.20)$$

$$\begin{aligned}\frac{1}{n!}\frac{d^nu(z)}{dz^n}=&\frac{1}{6z^2(1-z)}\frac{d^{n-2}(1+z)}{dz^{n-2}}+\frac{(n-3)^2}{n(n-1)z^2(1-z)}\left[\frac{1}{(n-3)!}\frac{d^{n-3}u(z)}{dz^{n-3}}\right]\\&+\frac{(n-2)[(3n-7)z-n+2]}{n(n-1)z^2(1-z)}\left[\frac{1}{(n-2)!}\frac{d^{n-2}u(z)}{dz^{n-2}}\right]\\&+\frac{(3n-5)z-2n+3}{nz(1-z)}\left[\frac{1}{(n-1)!}\frac{d^{n-1}u(z)}{dz^{n-1}}\right], \quad n\ge 3 . \end{aligned} \qquad (3.21)$$

These formulas are to be used recursively, with numerical values of lower Taylor coefficients obtained from previous steps used on the right-hand side of (3.21). Formula (3.21) is derived most easily by multiplying (3.20) by $z^2(1-z)$ and taking $n-2$ derivatives with respect to z.

The case $\sigma^2\le 0$: The following formulas, which are obtained by differentiating the formula (3.10) for $u(e^{i\theta})$ with the aid of (3.12), can be used for the numerical evaluation of the Taylor coefficients of $-iu(e^{i\theta})$.

$$\frac{d}{d\theta}[-iu(e^{i\theta})]=-2\ln|2\sin(\theta/2)| , \qquad (3.22)$$

$$\frac{1}{n!}\frac{d^n}{d\theta^n}[-iu(e^{i\theta})]=\sum_{m=0}^{[(n-1)/2]}b_{m,n}[\cot(\theta/2)]^{n-2m-1} , \quad n\ge 2 \qquad (3.23)$$

$$b_{0,2}=-\tfrac{1}{2} , \qquad (3.24)$$

$$b_{m,n}=-[(n-2m)b_{m-1,n-1}+(n-2m-2)b_{m,n-1}]/(2m) . \qquad (3.25)$$

In formula (3.25), which is to be used with the initial condition (3.24) for the recursive evaluation of the coefficients

$b_{n,m}$ needed for (3.23), the term $(n-2m)b_{m-1,n-1}$ is to be counted as zero for $m=0$, and the term $(n-2m-2)b_{m,n-1}$ is to be counted as zero for $m=[(n-1)/2]$.

D. Derivatives of $v(z)$

The case $\sigma^2 \geq 0$*:* The following formulas, which can be obtained from (2.3) and (2.4), can be used for the numerical evaluation of the Taylor coefficients of $v(z)$.

$$\frac{1}{n!}\frac{d^n v(z)}{dz^n}=\frac{1}{n(1-z^2)^n}\sum_{m=0}^{n-1} v_f(m;z)v_g(n-m-1;z) , \tag{3.26}$$

$$v_f(0;z)=1 , \tag{3.27}$$

$$v_f(1;z)=2z , \tag{3.28}$$

$$v_f(m;z)=2zv_f(m-1;z)+(1-z^2)v_f(m-2;z) , \quad m \geq 2 \tag{3.29}$$

$$v_{ga}(0;z)=1 , \tag{3.30}$$

$$v_{ga}(1;z)=z , \tag{3.31}$$

$$v_{ga}(m;z)=2zv_{ga}(m-1;z)+(1-z^2)v_{ga}(m-2;z) , \quad m \geq 2 \tag{3.32}$$

$$v_g(0,z)=\ln|(1-z^2)/4| , \tag{3.33}$$

$$v_g(m;z)=-2v_{ga}(m;z)/m . \tag{3.34}$$

The polynomials $v_f(m;z)$ and $v_{ga}(m;z)$, which appear in (3.26)–(3.32) and (3.34), are related to the Chebyshev polynomials of the first and second kinds T_m and U_m by

$$v_f(m;z)=(z^2-1)^{m/2}U_m(z(z^2-1)^{-1/2}) , \tag{3.35}$$

$$v_{ga}(m;z)=(z^2-1)^{m/2}T_m(z(z^2-1)^{-1/2}) . \tag{3.36}$$

The recursion relations (3.29) and (3.32) follow directly from the recursion relations

$$U_m(x)=2xU_{m-1}(x)-U_{m-2}(x) , \tag{3.37}$$

$$T_m(x)=2xT_{m-1}(x)-T_{m-2}(x) , \tag{3.38}$$

which are usually used for the computation of Chebyshev polynomials. The recursion relations (3.29) and (3.32) and the formula (3.26) can be shown to be numerically stable.

The case $\sigma^2 \leq 0$*:* Formulas which are suitable for the numerical evaluation of the Taylor coefficients of $-iv(-iz)$ can be obtained from (3.26)–(3.34) by replacing z by $-iz$.

E. Putting it all together

The recursive evaluation of the derivatives in (1.4) can be carried out via the following steps.

Step 1: Multiply the α's by a (positive or negative) power of 2 to obtain rescaled α's which are not unreasonably large or unreasonably small.

Step 2: Check for singularities. Are any of the terms in (2.1) at or near a singular point (see Sec. II C)? If so, the procedure must be modified as outlined in Sec. III F.

Step 3: It is convenient to store numerical values of Taylor coefficients in one-dimensional arrays. Construct pointers which can be used to go back and forth between the single array index and the six indexes $n_1,n_2,n_3,n_{12},n_{23},n_{31}$ which specify a particular Taylor coefficient.

Step 4: Use analytic formulas obtained by squaring (2.5) and differentiating the result to compute numerical values of all needed Taylor coefficients for the Taylor expansion of σ^2 about the point $\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}$.

Step 5: Use analytic formulas obtained by differentiating (2.6) and (2.7) to compute numerical values of all needed Taylor coefficients for the Taylor expansions of the polynomials $\gamma_k^{(j)}$ about the point $\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}$ for $j=0,1,2,3$ and $k=0,1,2,3$.

Step 6: Since the formulas used for σ^2 positive are different from the formulas used for σ^2 negative, the procedure splits into two branches at this point. If σ^2 is positive, use the results of step 4 and the function-of-a-function formulas (3.2)–(3.6) with $f(g)=g^{-1/2}$ and $g=\sigma^2$ to compute numerical values of all needed Taylor coefficients for the Taylor expansion of $1/\sigma$ about the point $\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}$. If σ^2 is negative, use the results of step 4 and the function-of-a-function formulas (3.2)–(3.6) with $f(g)=(-g)^{-1/2}$ and $g=\sigma^2$ to compute numerical values of all needed Taylor coefficients for the Taylor expansion of i/σ.

Step 7: If σ^2 is positive, use Eqs. (2.2), (3.8), (3.9), and (3.19)–(3.21) to compute numerical values of all needed Taylor coefficients for the Taylor expansions of the function u at the three points $\beta_0^{(0)}\beta_0^{(j)}$, $j=1,2,3$. If σ^2 is negative, use Eqs. (3.10), (3.13)–(3.17), and (3.22)–(3.25) to compute numerical values of all needed Taylor coefficients for the Taylor expansions of the function $-iu(e^{i\theta})=2\mathrm{Cl}_2(\theta)$ at the three points $\theta=-i[\ln(\beta_0^{(0)})+\ln(\beta_0^{(j)})]=2[\arctan(i\gamma_0^{(0)}/\sigma)+\arctan(i\gamma_0^{(j)}/\sigma)]$, $j=1,2,3$.

Step 8: If σ^2 is positive, use Eqs. (2.3), (3.8), (3.9), and (3.26)–(3.34) to compute numerical values of all needed Taylor coefficients for the Taylor expansions of the function $v(z)$ about the 16 points $z=\gamma_k^{(j)}/\sigma$, $j=0,1,2,3$, $k=0,1,2,3$. If σ^2 is negative, use Eqs. (3.11), (3.13)–(3.17), and (3.26)–(3.34) as modified by replacing z by $-iz$ to compute numerical values of all needed Taylor coefficients for the Taylor expansions of the function $-iv(-iz)$ about the 16 points $z=i\gamma_k^{(j)}/\sigma$, $j=0,1,2,3$, $k=0,1,2,3$.

Step 9: If σ^2 is positive, use the results of steps 5 and 6 and the product rule (3.1) to compute numerical values of all needed Taylor coefficients for the Taylor expansions of $\gamma_k^{(j)}/\sigma$ about the point $\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}$ for $j=0,1,2,3$ and $k=0,1,2,3$. If σ^2 is negative, use the results of steps 5 and 6 and the product rule (3.1) to compute numerical values of all needed Taylor coefficients for the Taylor expansions of $i\gamma_k^{(j)}/\sigma$.

Step 10: If σ^2 is positive, use the results of steps 8 and 9 and the function-of-a-function formulas (3.2)–(3.6) with $f(g)=v(g)$ and $g=\gamma_k^{(j)}/\sigma$ to compute numerical values of all needed Taylor coefficients for the Taylor expansions of $v(\gamma_k^{(j)}/\sigma)$ about the point $\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}$ for $j=0,1,2,3$ and $k=0,1,2,3$. If σ^2 is negative, use the results of steps 8 and 9 and the function-of-a-function formulas (3.2)–(3.6) with $f(g)=-iv(-ig)$ and $g=i\gamma_k^{(j)}/\sigma$ to compute numerical values of all needed Taylor coefficients for the Taylor expansions of $-iv(\gamma_k^{(j)}/\sigma)$.

Step 11: If σ^2 is positive, use the results of step 9 and the function-of-a-function formulas (3.2)–(3.6) with $f(g)=(1-g)/(1+g)$ and $g=\gamma_k^{(j)}/\sigma$ to compute numerical values of all needed Taylor coefficients for the Taylor expansions of $\beta_0^{(j)}$ about the point $\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}$ for $j=0,1,2,3$. If σ^2 is negative, use the results of step 9 and the function-of-a-function formulas (3.2)–(3.6) with $f(g)=2\arctan(g)$ and $g=\gamma_k^{(j)}/\sigma$ to compute numerical values of all needed Taylor coefficients for the Taylor expansions of $-i\ln(\beta_0^{(j)})=2\arctan(i\gamma_0^{(j)}/\sigma)$.

Step 12: If σ^2 is positive, use the results of step 11 and the product rule (3.1) to compute numerical values of all needed Taylor coefficients for the Taylor expansions of $\beta_0^{(0)}\beta_0^{(j)}$ about the point $\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}$ for $j=1,2,3$. If σ^2 is negative, add the corresponding Taylor coefficients for $2\arctan(i\gamma_0^{(0)}/\sigma)$ and $2\arctan(i\gamma_0^{(j)}/\sigma)$ which were calculated at step 11 to obtain numerical values of all needed Taylor coefficients for the Taylor expansions of $-i\ln(\beta_0^{(0)}\beta_0^{(j)})=2[\arctan(i\gamma_0^{(0)}/\sigma)+\arctan(i\gamma_0^{(j)}/\sigma)]$.

Step 13: If σ^2 is positive, use the results of steps 7 and 12 and the function-of-a-function formulas (3.2)–(3.6) with $f(g)=u(g)$ and $g=\beta_0^{(0)}\beta_0^{(j)}$ to compute numerical values of all needed Taylor coefficients for the Taylor expansions of $u(\beta_0^{(0)}\beta_0^{(j)})$ about the point $\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}$ for $j=1,2,3$. If σ^2 is negative, use the results of steps 7 and 12 and the function-of-a-function formulas (3.2)–(3.6) with $f(g)=-iu(e^{ig})=2\mathrm{Cl}_2(g)$ and

$$g=-i\ln(\beta_0^{(0)}\beta_0^{(j)})=2[\arctan(i\gamma_0^{(0)}/\sigma)+\arctan(i\gamma_0^{(j)}/\sigma)]$$

to compute numerical values of all needed Taylor coefficients for the Taylor expansions of $-iu(\beta_0^{(0)}\beta_0^{(j)})$.

TABLE II. Values of $J(n_1,n_2,n_3,n_{12},n_{23},n_{31};\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})$ at the standard reference point $\alpha_1=\alpha_2=\alpha_3=\alpha_{12}=\alpha_{23}=\alpha_{31}=1$.

n_1	n_2	n_3	n_{12}	n_{23}	n_{31}	J
0	0	0	0	0	0	4.313 608 359 247 323 132 40 × 10
1	0	0	0	0	0	2.156 804 179 623 661 566 20 × 10
2	0	0	0	0	0	1.700 846 212 355 526 103 63 × 10
1	1	0	0	0	0	1.414 143 540 752 485 463 30 × 10
0	0	1	1	0	0	1.269 796 343 129 178 307 95 × 10
3	0	0	0	0	0	1.848 753 666 796 548 493 78 × 10
2	1	0	0	0	0	1.381 285 044 223 778 297 52 × 10
1	1	1	0	0	0	1.196 054 211 143 383 165 86 × 10
1	1	0	1	0	0	1.067 939 764 434 510 620 04 × 10
1	0	1	1	0	0	1.022 076 819 868 488 467 79 × 10
0	0	2	1	0	0	1.130 337 218 085 968 834 30 × 10
4	0	0	0	0	0	2.572 920 829 541 445 519 00 × 10
3	1	0	0	0	0	1.792 270 667 926 595 963 91 × 10
2	2	0	0	0	0	1.620 685 263 846 488 063 36 × 10
2	1	1	0	0	0	1.438 101 395 236 904 542 12 × 10
2	1	0	1	0	0	1.181 872 501 819 159 450 47 × 10
2	0	1	1	0	0	1.174 469 611 543 266 214 74 × 10
1	1	1	1	0	0	9.540 070 270 498 617 896 13
1	0	2	1	0	0	1.080 310 824 970 255 550 55 × 10
0	0	3	1	0	0	1.350 518 499 531 461 588 03 × 10
0	0	2	2	0	0	1.110 261 509 103 329 215 59 × 10
1	0	1	1	1	0	8.893 556 036 274 299 116 51
5	0	0	0	0	0	4.376 590 752 867 569 281 36 × 10
4	1	0	0	0	0	2.901 314 739 016 179 954 21 × 10
3	2	0	0	0	0	2.465 826 611 956 565 607 76 × 10
3	1	1	0	0	0	2.224 981 698 764 935 326 73 × 10
2	2	1	0	0	0	2.064 846 448 745 239 042 65 × 10
3	1	0	1	0	0	1.714 262 898 094 924 412 27 × 10
2	2	0	1	0	0	1.470 822 563 109 573 875 07 × 10
3	0	1	1	0	0	1.743 209 216 821 168 787 08 × 10
2	1	1	1	0	0	1.254 289 852 738 491 732 55 × 10
2	0	2	1	0	0	1.438 737 305 578 736 155 13 × 10
1	1	2	1	0	0	1.203 455 464 925 934 917 68 × 10
1	0	3	1	0	0	1.496 299 510 832 397 659 32 × 10
0	0	4	1	0	0	2.028 596 097 857 829 534 80 × 10
1	1	1	2	0	0	1.108 619 782 943 060 525 78 × 10
1	0	2	2	0	0	1.223 039 963 164 420 655 22 × 10
0	0	3	2	0	0	1.439 835 355 532 810 944 12 × 10
2	0	1	1	1	0	1.092 023 747 347 238 940 71 × 10
1	1	1	1	1	0	9.286 971 180 015 268 093 64

Step 14: If σ^2 is positive, add the corresponding Taylor coefficients for the Taylor expansions of $v(\gamma_k^{(j)}/\sigma)$, $j=0,1,2,3$ and $k=0,1,2,3$ obtained at step 10 and $u(\beta_0^{(0)}\beta_0^{(j)})$, $j=1,2,3$ obtained at step 13. If σ^2 is negative, add the corresponding Taylor coefficients for the Taylor expansions of $-iv(\gamma_k^{(j)}/\sigma)$ and $-iu(\beta_0^{(0)}\beta_0^{(j)})$.

Step 15: If σ^2 is positive, use the results of steps 6 and 14 and the product rule (3.1) to compute numerical values of all needed Taylor coefficients for the Taylor expansion of the sum computed at step 14 multiplied by $1/\sigma$. If σ^2 is negative, use the results of steps 6 and 14 and the product rule (3.1) to compute numerical values of all needed Taylor coefficients for the Taylor expansion of the sum computed at step 14 multiplied by i/σ.

Step 16: Multiply the Taylor coefficients obtained at step 15 by $16\pi^3$, by the factorials needed to convert the Taylor coefficients to derivatives, and by $-(-\nu)^{n_1+n_2+n_3+n_{12}+n_{23}+n_{31}+3}$ where ν is the scale factor

TABLE III. Values of $J(n_1,n_2,n_3,n_{12},n_{23},n_{31};\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})$ at the auxiliary reference point $\alpha_1=\alpha_2=\alpha_3=1$, $\alpha_{12}=\alpha_{23}=\alpha_{31}=0$.

n_1	n_2	n_3	n_{12}	n_{23}	n_{31}	J
0	0	0	0	0	0	$4.382\,174\,441\,144\,904\,256\,32\times10^2$
1	0	0	0	0	0	$4.382\,174\,441\,144\,904\,256\,32\times10^2$
0	0	0	1	0	0	$5.708\,767\,958\,017\,266\,102\,00\times10^2$
2	0	0	0	0	0	$7.260\,097\,789\,286\,319\,204\,61\times10^2$
1	1	0	0	0	0	$5.134\,299\,987\,646\,648\,910\,33\times10^2$
1	0	0	1	0	0	$8.110\,199\,736\,802\,551\,385\,28\times10^2$
0	0	1	1	0	0	$6.614\,672\,358\,463\,961\,637\,43\times10^2$
0	0	0	2	0	0	$1.204\,780\,633\,933\,561\,275\,04\times10^3$
0	0	0	1	1	0	$9.922\,008\,537\,695\,942\,456\,15\times10^2$
3	0	0	0	0	0	$1.747\,012\,312\,662\,465\,058\,98\times10^3$
2	1	0	0	0	0	$9.415\,182\,909\,903\,472\,716\,64\times10^2$
1	1	1	0	0	0	$6.841\,134\,118\,426\,299\,118\,36\times10^2$
2	0	0	1	0	0	$1.826\,714\,954\,848\,235\,598\,82\times10^3$
1	1	0	1	0	0	$1.181\,061\,790\,129\,579\,501\,23\times10^3$
1	0	1	1	0	0	$1.047\,323\,123\,423\,460\,592\,59\times10^3$
0	0	2	1	0	0	$1.212\,689\,932\,385\,059\,633\,53\times10^3$
1	0	0	2	0	0	$2.241\,806\,586\,686\,905\,851\,06\times10^3$
0	0	1	2	0	0	$1.540\,289\,996\,293\,994\,673\,10\times10^3$
0	0	0	3	0	0	$3.574\,813\,512\,644\,218\,635\,98\times10^3$
1	0	0	1	1	0	$1.488\,301\,280\,654\,391\,368\,42\times10^3$
0	1	0	1	1	0	$1.984\,401\,707\,539\,188\,491\,23\times10^3$
0	0	0	2	1	0	$2.630\,054\,872\,257\,844\,588\,82\times10^3$
4	0	0	0	0	0	$5.654\,481\,570\,724\,335\,948\,68\times10^3$
3	1	0	0	0	0	$2.413\,796\,152\,625\,227\,202\,59\times10^3$
2	2	0	0	0	0	$1.867\,086\,769\,631\,596\,603\,73\times10^3$
2	1	1	0	0	0	$1.368\,226\,823\,685\,259\,823\,67\times10^3$
3	0	0	1	0	0	$5.745\,062\,179\,200\,062\,564\,21\times10^3$
2	1	0	1	0	0	$2.697\,977\,235\,696\,121\,183\,34\times10^3$
2	0	1	1	0	0	$2.517\,250\,314\,193\,229\,845\,36\times10^3$
1	1	1	1	0	0	$1.690\,416\,269\,385\,234\,640\,68\times10^3$
1	0	2	1	0	0	$2.076\,272\,156\,962\,299\,069\,53\times10^3$
0	0	3	1	0	0	$3.123\,595\,280\,385\,759\,662\,12\times10^3$
2	0	0	2	0	0	$6.452\,065\,068\,563\,902\,253\,75\times10^3$
1	1	0	2	0	0	$3.900\,864\,887\,089\,675\,738\,18\times10^3$
1	0	1	2	0	0	$3.097\,909\,564\,467\,857\,114\,42\times10^3$
0	0	2	2	0	0	$3.045\,920\,848\,828\,253\,809\,75\times10^3$
1	0	0	3	0	0	$8.275\,566\,545\,764\,150\,426\,21\times10^3$
0	0	1	3	0	0	$4.897\,747\,984\,337\,010\,963\,47\times10^3$
0	0	0	4	0	0	$1.379\,097\,380\,008\,742\,231\,51\times10^4$
2	0	0	1	1	0	$3.472\,702\,988\,193\,579\,859\,65\times10^3$
1	1	0	1	1	0	$2.976\,602\,561\,308\,782\,736\,85\times10^3$
0	2	0	1	1	0	$5.953\,205\,122\,617\,565\,473\,69\times10^3$
1	0	1	1	1	0	$2.480\,502\,134\,423\,985\,614\,04\times10^3$
1	0	0	2	1	0	$4.795\,637\,459\,886\,372\,187\,14\times10^3$
0	1	0	2	1	0	$6.882\,149\,691\,876\,199\,454\,70\times10^3$
0	0	1	2	1	0	$4.102\,542\,081\,784\,495\,891\,09\times10^3$
0	0	0	3	1	0	$9.425\,908\,110\,811\,145\,333\,34\times10^3$
0	0	0	2	2	0	$8.504\,405\,304\,091\,791\,989\,25\times10^3$
1	0	0	1	1	1	$3.968\,803\,415\,078\,376\,982\,46\times10^3$

by which the α's were multiplied at step 1. The result is the collection of integrals J defined in Eq. (1.2).

The steps outlined above have been programmed in FORTRAN 77. Some numerical results obtained by running this program on an IBM 3081 are presented in Tables II and III, which list results for the integrals J at the standard reference point (SRP) and at the auxiliary reference point (ARP). Because these are points of high symmetry, all derivatives through the fifth order at SRP, and all derivatives through the fourth order at ARP, can be obtained from these tabulated results by permutation of the α's.

The FORTRAN program was checked by comparison with the numerical results given by Ho and Page.[10] The results at SRP and at ARP presented in Tables II and III have been checked by computing Taylor series at a sequence of points along a line connecting the point $\alpha_1=\alpha_2=4.72$, $\alpha_3=5.72$, $\alpha_{12}=\alpha_{23}=\alpha_{31}=0$, at which agreement with Ho and Page was obtained, to ARP, and along a line connecting ARP to SRP. The Taylor series at each point was used to compute values of $I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})$ and all of its derivatives through third order at the next point. Because the signs of all derivatives are known, rigorous remainder bounds for the truncated Taylor series could be computed; values obtained from the program were found without exception to lie between the upper and lower bounds obtained from the truncated Taylor series about an adjacent point. All of the results listed in Tables II and III were obtained by running in quadruple precision (about 30 significant digits) and rounding to the number of digits shown. At ARP (Table III), a comparison of these quadruple precision results with the corresponding calculations in double precision showed a loss of one significant digit in the worst case; thus there is no problem with numerical stability at ARP. Such a comparison at SRP (Table II) showed a loss of four significant digits in the worst case; thus there is a mild problem with numerical stability at SRP. In both cases, the tabulated results should be accurate to the number of significant digits shown.

The question of numerical stability for the computational procedure outlined above has not yet been explored in any systematic way. The formulas which are clearly stable at ARP, and mildly unstable at SRP, could turn out to be severely unstable at some other point of interest. However, the many identities known for the dilogarithm function, together with identities such as (2.9a)–(2.9c), (2.19a)–(2.19p), and (2.20a)–(2.20l), should make it possible to find alternate formulas for use at points where numerical stability problems are encountered. Section III F shows how this can be done at and near points where individual terms $u(\beta_0^{(0)}\beta_0^{(j)})$ and $v(\gamma_k^{(j)}/\sigma)$ in (2.1) are singular. In any event, the numerical stability at ARP shows clearly that the Taylor series methods advocated in this section should not themselves be a source of numerical instability.

The amount of computer time required to evaluate a given collection of integrals $J(n_1,n_2,n_3,n_{12},n_{23},n_{31};\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})$ is determined primarily by the time required to compute derivatives of products, which is proportional to the square of the number of derivatives needed, and by the time required to compute derivatives of functions of functions, which is proportional to the square of the number of derivatives needed multiplied by the order of the highest derivatives. Thus the efficiency of the entire program depends primarily on the code which multiplies two Taylor series. This code, and the storage for the Taylor series coefficients, should be constructed to make this multiplication as efficient as possible. In some cases where two or more of the parameters α are equal, the efficiency of the computation can be improved by using symmetry to eliminate unnecessary duplication of effort.

F. Modifications near singularities

Individual terms $u(\beta_0^{(0)}\beta_0^{(j)})$ and $v(\gamma_k^{(j)}/\sigma)$ in (2.1) can be singular at points where their sum is not singular, as was pointed out in Sec. II C. Numerical evaluation at or near such cancelling singularities requires that the cancellations be performed analytically before the numerical evaluation is carried out; this prevents the excessive round off error which would otherwise occur at step 13 of Sec. III E due to near-cancellation between almost equal large positive and negative terms. Since the discussion of this section is meant to be illustrative rather than exhaustive, only two cases will be considered: the points $\alpha_3=\alpha_{3\sigma}+\delta$ and $\alpha_3=\alpha_1+\alpha_2-\delta$ on the path (2.36) from SRP to $\alpha_3=\infty$.

As α_3 approaches $\alpha_{3\sigma}$, all $\gamma_k^{(j)}/\sigma$ approach ∞ and all $\beta_0^{(0)}\beta_0^{(j)}$ approach $+1$. Thus it is appropriate to use (2.15c), (2.15d), (2.16e), (2.16f), and (2.17) for u and v, with branches specified by (2.37). Combining the singular pieces from (2.15c) and (2.16e) with the aid of (2.9) and (2.38) yields

$$I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})=\frac{16\alpha^3}{\sigma}\left\{\sum_{j=1}^{3}\left[\tfrac{1}{2}\ln^2(\beta_0^{(0)}\beta_0^{(j)})-2\ln(\beta_0^{(0)}\beta_0^{(j)})\ln|(1-\beta_0^{(0)}\beta_0^{(j)})/\sigma|-2\mathrm{Li}_2(1-\beta_0^{(0)}\beta_0^{(j)})\right]\right.$$
$$\left.+\sum_{j=0}^{3}\sum_{k=0}^{3}\left[-\ln|\gamma_k^{(j)}|\ln(-\beta_k^{(j)})+v_\infty(\gamma_k^{(j)}/\sigma)\right]\right\}. \quad (3.39)$$

By Taylor expanding the $\beta_k^{(j)}$ in powers of σ, it is easy to verify that each term in the curly bracket { } in (3.39) vanishes linearly with σ as $\sigma\to 0$; such Taylor expansions should be used for the numerical evaluation of (3.39) when σ is very close to zero.

As α_3 approaches $\alpha_1+\alpha_2$, $\gamma_2^{(1)}/\sigma$, $\gamma_1^{(2)}/\sigma$, $\gamma_0^{(3)}/\sigma$, and $\gamma_3^{(3)}/\sigma$ all approach $+1$, $\gamma_3^{(1)}/\sigma$ and $\gamma_3^{(2)}/\sigma$ approach -1, and $\beta_0^{(0)}\beta_0^{(3)}$ approaches 0. Thus it is appropriate to use (2.15a), (2.15b), (2.16a), (2.16b), (2.16c), and (2.16d) for the singular u

and v, with branches specified by (2.37). Combining the singular pieces from (2.15a), (2.16a), and (2.16c) with the aid of (2.9) and (2.38) yields

$$\begin{aligned}I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})=\frac{16\pi^3}{\sigma}\lim_{\epsilon\to 0^+}&[u(\beta_0^{(0)}\beta_0^{(1)}+i\epsilon)-i\pi\ln(\beta_0^{(0)}\beta_0^{(1)})+u(\beta_0^{(0)}\beta_0^{(2)}+i\epsilon)\\&-i\pi\ln(\beta_0^{(0)}\beta_0^{(2)})+u_0(\beta_0^{(0)}\beta_0^{(3)})+v((\gamma_0^{(0)}/\sigma)-i\epsilon)\\&+\tfrac{1}{2}i\pi\ln(-\beta_0^{(0)})+v((\gamma_1^{(0)}/\sigma)+i\epsilon)+\tfrac{1}{2}i\pi\ln(-\beta_1^{(0)})\\&+v((\gamma_2^{(0)}/\sigma)+i\epsilon)+\tfrac{1}{2}i\pi\ln(-\beta_2^{(0)})+v((\gamma_3^{(0)}/\sigma)-i\epsilon)\\&+\tfrac{1}{2}i\pi\ln(-\beta_3^{(0)})+v((\gamma_0^{(1)}/\sigma)+i\epsilon)+\tfrac{1}{2}i\pi\ln(-\beta_0^{(1)})\\&+v((\gamma_1^{(1)}/\sigma)-i\epsilon)+\tfrac{1}{2}i\pi\ln(-\beta_1^{(1)})+v_1(\gamma_2^{(1)}/\sigma)\\&+v_{-1}(\gamma_3^{(1)}/\sigma)+v((\gamma_0^{(2)}/\sigma)+i\epsilon)+\tfrac{1}{2}i\pi\ln(-\beta_0^{(2)})\\&+v_1(\gamma_1^{(2)}/\sigma)+v((\gamma_2^{(2)}/\sigma)-i\epsilon)+\tfrac{1}{2}i\pi\ln(-\beta_2^{(2)})\\&+v_{-1}(\gamma_3^{(2)}/\sigma)+v_1(\gamma_0^{(3)}/\sigma)+v((\gamma_1^{(3)}/\sigma)+i\epsilon)\\&+\tfrac{1}{2}i\pi\ln(-\beta_1^{(3)})+v((\gamma_2^{(3)}/\sigma)+i\epsilon)+\tfrac{1}{2}i\pi\ln(-\beta_2^{(3)})\\&+v_1(\gamma_3^{(3)}/\sigma)+\tfrac{1}{2}\ln(-\beta_1^{(1)})\ln(\beta_1^{(0)}\beta_3^{(0)})\\&+\tfrac{1}{2}\ln(-\beta_2^{(2)})\ln(\beta_2^{(0)}\beta_3^{(0)})-\tfrac{1}{2}\ln(-\beta_1^{(0)})\ln(-\beta_2^{(0)})]\ .\end{aligned}\tag{3.40}$$

The combining of terms at the other cancelling singularities is similar to the combining which yields (3.40).

IV. DERIVATION OF RESULTS

This section will derive the results recorded in Sec. II by using a Fourier integral representation of $r^{-1}\exp(-\alpha r)$ to bring the generating integral (1.3) to the form

$$\begin{aligned}I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})=\frac{8}{\pi^3}\int d^3\mathbf{k}_1 d^3\mathbf{k}_2 d^3\mathbf{k}_3\{&(k_1^2+\alpha_{23}^2)(k_2^2+\alpha_{31}^2)(k_3^2+\alpha_{12}^2)[\alpha_1^2+(\mathbf{k}_2-\mathbf{k}_3)^2][\alpha_2^2+(\mathbf{k}_3-\mathbf{k}_1)^2]\\&\times[\alpha_3^2+(\mathbf{k}_1-\mathbf{k}_2)^2]\}^{-1}\ .\end{aligned}\tag{4.1}$$

Angular integrations over the directions of $\mathbf{k}_1$, $\mathbf{k}_2$, and $\mathbf{k}_3$ are carried out first. Contour integration is then used to integrate over the magnitudes k_1,k_2,k_3 of the vectors $\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3$ and complete the job. The following derivations assume that all the α's are real and non-negative; analytic continuation can be used to extend the result (2.1) to a larger domain.

A. Fourier transformation, coordinates, and notation

The form (4.1) is obtained from (1.3) by using the Fourier integral representation

$$r^{-1}\exp(-\alpha r)=\frac{1}{2\pi^2}\int\frac{\exp(-i\mathbf{k}\cdot\mathbf{r})}{k^2+\alpha^2}d^3\mathbf{k}\tag{4.2}$$

for $r_{12}^{-1}\exp(-\alpha_{12}r_{12})$, for $r_{23}^{-1}\exp(-\alpha_{23}r_{23})$, and for $r_{31}^{-1}\exp(-\alpha_{31}r_{31})$. The expression (4.1) is then obtained by integrating over $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$ with the aid of the formula

$$\int r^{-1}\exp(-\alpha r+i\mathbf{k}\cdot\mathbf{r})d^3\mathbf{r}=4\pi/(k^2+\alpha^2)\ .\tag{4.3}$$

The integrations over $\mathbf{k}_1$, $\mathbf{k}_2$, and $\mathbf{k}_3$ in (4.1) are done by using spherical polar coordinates, with the $\mathbf{k}_1$ direction chosen as the z axis for the $\mathbf{k}_2$ and $\mathbf{k}_3$ integrations, and with the angle ϕ_3 replaced by $\phi=\phi_3-\phi_2$. Then

$$\begin{aligned}d^3\mathbf{k}_1 d^3\mathbf{k}_2 d^3\mathbf{k}_3=&\sin\theta_1 d\theta_1 d\phi_1 d\phi_2\sin\theta_{12}d\theta_{12}\\&\times\sin\theta_{31}d\theta_{31}d\phi k_1^2dk_1k_2^2dk_2k_3^2dk_3\end{aligned}\tag{4.4}$$

and

$$\cos\theta_{23}=\cos\theta_{12}\cos\theta_{31}+\sin\theta_{12}\sin\theta_{31}\cos\phi\ ,\tag{4.5}$$

where θ_{ij} is the angle between $\mathbf{k}_i$ and $\mathbf{k}_j$. With these coordinates, the integrand in (4.1) is independent of θ_1, ϕ_1, and ϕ_2, so that these coordinates can be integrated immediately to obtain $8\pi^2$.

Make the definitions

$$c_1(k_2,k_3;\alpha_1):=(\alpha_1^2+k_2^2+k_3^2)/(2k_2k_3)\ ,\tag{4.6a}$$

$$c_2(k_3,k_1;\alpha_2):=(\alpha_2^2+k_3^2+k_1^2)/(2k_3k_1)\ ,\tag{4.6b}$$

$$c_3(k_1,k_2;\alpha_3):=(\alpha_3^2+k_1^2+k_2^2)/(2k_1k_2)\ , \tag{4.6c}$$

$$D(\theta_{12},\theta_{31};c_1):=\frac{1}{\pi}\int_0^{2\pi}\frac{d\phi}{c_1-\cos\theta_{23}}\ , \tag{4.7}$$

$$E(\theta_{12};c_1,c_2):=\int_0^{\pi}\frac{D(\theta_{12},\theta_{31};c_1)\sin\theta_{31}d\theta_{31}}{c_2-\cos\theta_{31}}\ , \tag{4.8}$$

$$F(c_1,c_2,c_3):=\int_0^{\pi}\frac{E(\theta_{12};c_1,c_2)\sin\theta_{12}d\theta_{12}}{c_3-\cos\theta_{12}}\ , \tag{4.9}$$

$$G(\alpha_1,\alpha_2,\alpha_3,\alpha_{23};k_2,k_3):=2\int_0^{\infty}\frac{dk_1}{k_1^2+\alpha_{23}^2}F(c_1(k_2,k_3;\alpha_1),c_2(k_3,k_1;\alpha_2),c_3(k_1,k_2;\alpha_3))\ , \tag{4.10}$$

and

$$H(\alpha_1,\alpha_2,\alpha_3,\alpha_{23},\alpha_{31};k_3):=2\int_0^{\infty}\frac{dk_2}{k_2^2+\alpha_{31}^2}G(\alpha_1,\alpha_2,\alpha_3,\alpha_{23};k_2,k_3)\ , \tag{4.11}$$

where $\cos\theta_{23}$ in (4.7) is given by (4.5). Then

$$I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})=2\int_0^{\infty}\frac{dk_3}{k_3^2+\alpha_{12}^2}H(\alpha_1,\alpha_2,\alpha_3,\alpha_{23},\alpha_{31};k_3)\ . \tag{4.12}$$

The integrations will now be performed in the order $\phi,\theta_{31},\theta_{12},k_1,k_2,k_3$.

B. Integration over ϕ

The result

$$D(\theta_{12},\theta_{31};c_1)=2\ \mathrm{sgn}(c_1)(\cos^2\theta_{12}+\cos^2\theta_{31}-2c_1\cos\theta_{12}\cos\theta_{31}+c_1^2-1)^{-1/2} \tag{4.13}$$

can be obtained by applying the integration formula

$$\int_0^{2\pi}\frac{d\phi}{a+b\cos\phi}=\frac{2\pi}{a[1-(b/a)^2]^{1/2}} \tag{4.14}$$

to the definition (4.7) with $a=c_1-\cos\theta_{12}\cos\theta_{31}$ and $b=-\sin\theta_{12}\sin\theta_{31}$. The condition $|a|>|b|$, which is necessary for the validity of (4.14), can be established by using $k_2^2+k_3^2-2|k_2k_3|=(|k_2|-|k_3|)^2\geq 0$ to show that $|c_1|>1$ holds for $\alpha_1\neq 0$. The positive square root is to be taken in (4.13); $\mathrm{sgn}(c_1)$ is $+1$ or -1 as c_1 is positive or negative.

C. Integration over θ_{31}

The result

$$E(\theta_{12};c_1,c_2)=2\gamma^{-1/2}\ln\left|\frac{c_1c_2-\cos\theta_{12}+\gamma^{1/2}}{c_1c_2-\cos\theta_{12}-\gamma^{1/2}}\right|\ , \tag{4.15}$$

with

$$\gamma=\cos^2\theta_{12}-2c_1c_2\cos\theta_{12}+c_1^2+c_2^2-1\ , \tag{4.16}$$

can be obtained by using the indefinite integral formula

$$\int\frac{dx}{xX^{1/2}}=\frac{1}{2\gamma^{1/2}}\ln\left|\frac{2(\gamma X)^{1/2}-(\beta x+2\gamma)}{2(\gamma X)^{1/2}+(\beta x+2\gamma)}\right|\ , \tag{4.17}$$

where $X=x^2+\beta x+\gamma$, to evaluate (4.8). Formula (4.17) is applied with $x=\cos\theta_{31}-c_2$ and $\beta=2(c_2-c_1\cos\theta_{12})$. Keeping track of the branch of the logarithm in (4.17) requires a knowledge of the signs of the quantities which appear. These signs can be established as follows. The argument given in Sec. IV B to show that $|c_1|>1$ can be repeated to show that $|c_2|>1$ holds for $\alpha_2\neq 0$. It follows that x has the same sign as $-c_2$ on the entire path of integration. Equation (4.16) can be rearranged to

$$\gamma=(|c_1|-|c_2|)^2+[2|c_1c_2|-1-\mathrm{sgn}(c_1c_2)\cos\theta_{12}]\times[1-\mathrm{sgn}(c_1c_2)\cos\theta_{12}]\ , \tag{4.18}$$

which shows that $\gamma\geq 0$ as a consequence of $|c_1|>1$ and $|c_2|>1$. The definitions of β and γ can be used to obtain $\beta^2-4\gamma=-4(c_1^2-1)\sin^2\theta_{12}$, which shows that

$$\beta^2-4\gamma\leq 0\ . \tag{4.19}$$

Formula (4.19) implies that $X\geq 0$. The easily established identity

$$[2(\gamma X)^{1/2}-(\beta x+2\gamma)][2(\gamma X)^{1/2}+(\beta x+2\gamma)]=(4\gamma-\beta^2)x^2 \tag{4.20}$$

combined with (4.19) now shows that the argument of the logarithm in (4.17) is non-negative on the entire path of integration.

The result of applying (4.17) with integration limits $x_1\leq x\leq x_2$ where

$$x_1:=-1-c_2 \tag{4.21a}$$

and

$$x_2:=1-c_2 \tag{4.21b}$$

can be simplified to the form (4.15) with the aid of the identities

$$2(\gamma X_1)^{1/2}+\beta x_1+2\gamma =2(c_2-1)^{-1}[c_1c_2-\cos\theta_{12}-\gamma^{1/2}\mathrm{sgn}(c_1)] \times[c_1-c_2\cos\theta_{12}+\gamma^{1/2}\mathrm{sgn}(c_1)] , \quad (4.22a)$$

$$2(\gamma X_1)^{1/2}-\beta x_1-2\gamma =2(c_2-1)^{-1}[c_1c_2-\cos\theta_{12}+\gamma^{1/2}\mathrm{sgn}(c_1)] \times[-c_1+c_2\cos\theta_{12}+\gamma^{1/2}\mathrm{sgn}(c_1)] , \quad (4.22b)$$

$$2(\gamma X_2)^{1/2}+\beta x_2+2\gamma =2(c_2+1)^{-1}[c_1c_2-\cos\theta_{12}+\gamma^{1/2}\mathrm{sgn}(c_1)] \times[c_1-c_2\cos\theta_{12}+\gamma^{1/2}\mathrm{sgn}(c_1)] , \quad (4.22c)$$

$$2(\gamma X_2)^{1/2}-\beta x_2-2\gamma =2(c_2+1)^{-1}[c_1c_2-\cos\theta_{12}-\gamma^{1/2}\mathrm{sgn}(c_1)] \times[-c_1+c_2\cos\theta_{12}+\gamma^{1/2}\mathrm{sgn}(c_1)] . \quad (4.22d)$$

In the identities (4.22), X_i stands for X evaluated at x_i. All square roots are non-negative, so that $X_1^{1/2} = |c_1| + \mathrm{sgn}(c_1)\cos\theta_{12}$ and $X_2^{1/2} = |c_1| - \mathrm{sgn}(c_1)\cos\theta_{12}$. The logarithm in (4.15) is to be taken on the principal branch [specified by (2.11)]. Since the logarithm is on the principal branch, the result (4.15) is independent of the branch chosen for the square root $\gamma^{1/2}$.

D. Integration over θ_{12}

The result

$$F(c_1,c_2,c_3)=-4s^{-1}[v((1+c_1+c_2+c_3)/s) +v((1+c_1-c_2-c_3)/s) +v((1-c_1+c_2-c_3)/s) +v((1-c_1-c_2+c_3)/s)] , \quad (4.23)$$

with

$$s:=(c_1^2+c_2^2+c_3^2-2c_1c_2c_3-1)^{1/2} \quad (4.24)$$

and v defined by (2.3), can be obtained via a rationalizing substitution and certain formulas obeyed by the dilogarithm function. The rationalizing substitution changes the dummy integration variable from θ_{12} to ζ via

$$\zeta=-c_1c_2+\cos\theta_{12}+\gamma^{1/2} , \quad (4.25)$$

which implies that

$$\cos\theta_{12}=c_1c_2+(2\zeta)^{-1}[\zeta^2+(c_1^2-1)(c_2^2-1)] \quad (4.26)$$

and

$$\gamma^{1/2}=(2\zeta)^{-1}[\zeta^2-(c_1^2-1)(c_2^2-1)] . \quad (4.27)$$

Using the result (4.15) and the substitution (4.25)–(4.27) in the definition (4.9) of F yields

$$F(c_1,c_2,c_3)=4\int_{\zeta_1}^{\zeta_2}\frac{d\zeta}{\zeta^2+2(c_1c_2-c_3)\zeta+(c_1^2-1)(c_2^2-1)} \times\ln\left[\frac{\zeta^2}{(c_1^2-1)(c_2^2-1)}\right] . \quad (4.28)$$

There are two candidates ζ_{1a} and ζ_{1b} for the lower limit ζ_1 in (4.28), and two candidates ζ_{2a} and ζ_{2b} for the upper limit ζ_2. These are

$$\zeta_{1a}=-(c_1-1)(c_2-1) , \quad (4.29a)$$

$$\zeta_{1b}=-(c_1+1)(c_2+1) , \quad (4.29b)$$

$$\zeta_{2a}=-(c_1-1)(c_2+1) , \quad (4.29c)$$

$$\zeta_{2b}=-(c_1+1)(c_2-1) . \quad (4.29d)$$

The values of $\gamma^{1/2}$ which correspond to these four values of ζ are obtained from (4.27). In an obvious notation they are

$$\gamma_{1a}^{1/2}=c_1+c_2 , \quad (4.30a)$$

$$\gamma_{1b}^{1/2}=-(c_1+c_2) , \quad (4.30b)$$

$$\gamma_{2a}^{1/2}=-(c_1-c_2) , \quad (4.30c)$$

$$\gamma_{2b}^{1/2}=c_1-c_2 . \quad (4.30d)$$

The obvious way to choose between ζ_{1a} and ζ_{1b}, and between ζ_{2a} and ζ_{2b}, is to make the choice which keeps $\gamma^{1/2}$ positive on the entire path of integration. This is awkward because the signs of $\gamma_{1a}^{1/2}$, $\gamma_{1b}^{1/2}$, $\gamma_{2a}^{1/2}$, and $\gamma_{2b}^{1/2}$ depend on the signs and relative magnitudes of c_1 and c_2. Fortunately these choices do not matter; the change of variables

$$\zeta\to\zeta'=(c_1^2-1)(c_2^2-1)/\zeta \quad (4.31)$$

can be used to show that

$$\int_{\zeta_{ia}}^{\zeta_{ib}}\frac{d\zeta}{\zeta^2+2(c_1c_2-c_3)\zeta+(c_1^2-1)(c_2^2-1)} \times\ln\left[\frac{\zeta^2}{(c_1^2-1)(c_2^2-1)}\right]=0 \quad (4.32)$$

for $i=1,2$. Under the change (4.31), the integrand of (4.32) is carried into itself while the path from ζ_{ia} to ζ_{ib} is carried into the same path traversed in the opposite direction from ζ_{ib} to ζ_{ia}. This shows that the integral on the left-hand side of (4.32) equals its negative, and hence must be zero. Thus either ζ_{1a} or ζ_{1b} can be used for ζ_1, and either ζ_{2a} or ζ_{2b} for ζ_2, without changing the numerical value of F as given by (4.28). The partial fraction decomposition

$$[\zeta^2+2(c_1c_2-c_3)\zeta+(c_1^2-1)(c_2^2-1)]^{-1} =(2s)^{-1}[(\zeta+c_1c_2-c_3-s)^{-1} -(\zeta+c_1c_2-c_3+s)^{-1}] \quad (4.33)$$

and the integration formula

$$\int_{\zeta_1}^{\zeta_2}(a+b\zeta)^{-1}\ln(c+e\zeta)d\zeta=\frac{1}{b}\ln\left[\frac{bc-ae}{b}\right]\ln\left[\frac{a+b\zeta_2}{a+b\zeta_1}\right]-\frac{1}{b}\mathrm{Li}_2\left[\frac{e(a+b\zeta_2)}{ae-bc}\right]+\frac{1}{b}\mathrm{Li}_2\left[\frac{e(a+b\zeta_1)}{ae-bc}\right] \quad (4.34)$$

can be used with $\zeta_1=\zeta_{1a}$, $\zeta_2=\zeta_{2a}$ to evaluate the integral in (4.28) and obtain the result

$$F(c_1,c_2,c_3)=\frac{4}{s}\left[\tfrac{1}{2}\ln\left[\frac{c_1c_2-c_3-s}{c_1c_2-c_3+s}\right]\ln\left[\frac{(c_2+1)(c_3-1)}{(c_2-1)(c_3+1)}\right]-\mathrm{Li}_2\left[\frac{1+c_1+c_2+c_3+s}{(c_1+1)(c_2+1)}\right]+\mathrm{Li}_2\left[\frac{1+c_1+c_2+c_3-s}{(c_1+1)(c_2+1)}\right]\right.$$
$$\left.+\mathrm{Li}_2\left[\frac{-1-c_1+c_2+c_3+s}{(c_1+1)(c_2-1)}\right]-\mathrm{Li}_2\left[\frac{-1-c_1+c_2+c_3-s}{(c_1+1)(c_2-1)}\right]\right]. \tag{4.35}$$

The integration formula (4.34) can be verified by differentiating with respect to the upper limit ζ_2 and using the definition (2.4) of the dilogarithm to show that

$$d\mathrm{Li}_2(z)/dz=-z^{-1}\ln(1-z)\ . \tag{4.36}$$

The result (4.35) for F can be brought to the form (4.23) with the aid of the identities

$$\mathrm{Li}_2(z)-\mathrm{Li}_2(w)=v\left[\frac{z+w}{z-w}\right]+v\left[\frac{2zw-z-w}{z-w}\right]-\mathrm{Li}_2\left[\frac{w-z}{1-z}\right]-\tfrac{1}{4}\ln^2\left[\frac{1-z}{1-w}\right]$$
$$-\tfrac{1}{2}\ln\left[\frac{1-z}{1-w}\right]\left[\ln\left[\frac{z}{z-w}\right]+\ln\left[\frac{-w}{z-w}\right]+\ln(1-z)+\ln(1-w)\right], \tag{4.37}$$

$$\mathrm{Li}_2(z)+\mathrm{Li}_2[-z/(1-z)]+\tfrac{1}{2}\ln^2(1-z)=0\ , \tag{4.38}$$

$$(1+c_1+c_2+c_3-s)(c_1c_2-c_3-s)=-(c_1+1)(c_2+1)(1-c_1-c_2+c_3+s)\ , \tag{4.39}$$

$$(1+c_1+c_2+c_3)^2-s^2=2(c_1+1)(c_2+1)(c_3+1)\ . \tag{4.40}$$

The dilogarithm identities (4.37) and (4.38) can be established by differentiation: The derivatives with respect to z of the two sides of (4.37) can be shown to be equal with the aid of (4.36). The derivatives with respect to w of the two sides of (4.37) can be proven equal in similar fashion. Hence the two sides of (4.37) can differ by at most a constant. By setting $z=2w$, taking a limit as $w\to 0$, and using $\mathrm{Li}_2(0)=0$ and $v(-3)=-v(3)$, it can be shown that this constant is zero. A similar argument establishes (4.38). The identities (4.39) and (4.40) follow from the definition (4.24) of s. The identity (4.37) is used with

$$w=(1+c_1+c_2+c_3+s)/[(c_1+1)(c_2+1)]$$

and

$$z=(1+c_1+c_2+c_3-s)/[(c_1+1)(c_2+1)]\ ,$$

and the expression $z(1-w)/(z-w)$ simplified with the aid of (4.39), to obtain

$$-\mathrm{Li}_2\left[\frac{1+c_1+c_2+c_3+s}{(c_1+1)(c_2+1)}\right]+\mathrm{Li}_2\left[\frac{1+c_1+c_2+c_3-s}{(c_1+1)(c_2+1)}\right]$$
$$=-v((1+c_1+c_2+c_3)/s)-v((1-c_1-c_2+c_3)/s)-\mathrm{Li}_2\left[\frac{2s}{c_1c_2-c_3+s}\right]-\tfrac{1}{4}\ln^2\left[\frac{c_1c_2-c_3-s}{c_1c_2-c_3+s}\right]$$
$$+\tfrac{1}{2}\ln\left[\frac{c_1c_2-c_3-s}{c_1c_2-c_3+s}\right]\left[\ln\left[\frac{1+c_1+c_2+c_3+s}{2s}\right]+\ln\left[\frac{1+c_1+c_2+c_3-s}{-2s}\right]\right.$$
$$\left.+\ln\left[\frac{c_1c_2-c_3-s}{(c_1+1)(c_2+1)}\right]+\ln\left[\frac{c_1c_2-c_3+s}{(c_1+1)(c_2+1)}\right]\right]. \tag{4.41}$$

Replacing c_2 and c_3 in (4.41) by $-c_2$ and $-c_3$ yields

$$\mathrm{Li}_2\left[\frac{-1-c_1+c_2+c_3+s}{(c_1+1)(c_2-1)}\right]-\mathrm{Li}_2\left[\frac{-1-c_1+c_2+c_3-s}{(c_1+1)(c_2-1)}\right]$$
$$=-v((1+c_1-c_2-c_3)/s)-v((1-c_1+c_2-c_3)/s)-\mathrm{Li}_2\left[\frac{-2s}{c_1c_2-c_3-s}\right]-\tfrac{1}{4}\ln^2\left[\frac{c_1c_2-c_3-s}{c_1c_2-c_3+s}\right]$$
$$-\tfrac{1}{2}\ln\left[\frac{c_1c_2-c_3-s}{c_1c_2-c_3+s}\right]\left[\ln\left[\frac{1+c_1-c_2-c_3+s}{2s}\right]+\ln\left[\frac{1+c_1-c_2-c_3-s}{-2s}\right]\right.$$
$$\left.+\ln\left[\frac{c_1c_2-c_3-s}{(c_1+1)(c_2-1)}\right]+\ln\left[\frac{c_1c_2-c_3+s}{(c_1+1)(c_2-1)}\right]\right]. \tag{4.42}$$

The identity (4.38) is used with $z=2s/(c_1c_2-c_3-s)$ to obtain

$$\mathrm{Li}_2\left[\frac{2s}{c_1c_2-c_3+s}\right]+\mathrm{Li}_2\left[\frac{-2s}{c_1c_2-c_3-s}\right]+\tfrac{1}{2}\ln^2\left[\frac{c_1c_2-c_3-s}{c_1c_2-c_3+s}\right]=0\ . \tag{4.43}$$

Adding (4.41), (4.42), and (4.43) and simplifying the result with the aid of (4.40) yields the identity needed to bring (4.35) to the form (4.23). The branches of the multiple-valued logarithms and dilogarithms which appear in the manipulations described above can be kept track of by doing the calculations for c_1,c_2,c_3 all large compared to 1; in this limit $F(c_1,c_2,c_3)\cong 8/(c_1c_2c_3)$, as can be seen directly by neglecting the cosines in the denominators of (4.7)–(4.9). The result (4.23) can then be extended to a wider domain via analytic continuation.

The fact that $F(c_1,c_2,c_3)$ is invariant under any permutation of 1,2,3 is obvious from (4.23) and (4.24), which also show that

$$\begin{aligned}F(-c_1,-c_2,c_3)&=F(c_1,-c_2,-c_3)\\&=F(-c_1,c_2,-c_3)\\&=F(c_1,c_2,c_3)\ .\end{aligned} \tag{4.44}$$

The property (4.44) implies that $F(c_1,c_2,c_3)$ is even in k_1, k_2, and k_3 when the c_i are given by (4.6). The fact that $v(-z)=-v(z)$, which is obvious from (2.3), shows that (4.23) is independent of the branch chosen for the square root s when the branch for $v(z)$ is chosen as described in Sec. II C.

E. Additional notation

In order to clarify the relationship of the final result (2.1) for the generating integral I to the results for the intermediate integrals F, G, and H defined by Eqs. (4.9)–(4.11), it is convenient to introduce the following notation. The symbols σ_F, $\gamma_{Fk}^{(j)}$, $\mu_{Fk}^{(j)}$, $\beta_{Fk}^{(j)}$ stand, respectively, for the quantities $\sigma,\gamma_k^{(j)}$, $\mu_k^{(j)}$, $\beta_k^{(j)}$ defined by (2.5)–(2.8) evaluated at $\alpha_{12}=-ik_3$, $\alpha_{23}=-ik_1$, $\alpha_{31}=-ik_2$. The symbols σ_G, $\gamma_{Gk}^{(j)}$, $\mu_{Gk}^{(j)}$, $\beta_{Gk}^{(j)}$ stand, respectively, for the quantities σ, $\gamma_k^{(j)}$, $\mu_k^{(j)}$, $\beta_k^{(j)}$ evaluated at $\alpha_{12}=-ik_3$, $\alpha_{31}=-ik_2$. The symbols σ_H, $\gamma_{Hk}^{(j)}$, $\mu_{Hk}^{(j)}$, $\beta_{Hk}^{(j)}$ stand, respectively, for the quantities σ, $\gamma_k^{(j)}$, $\mu_k^{(j)}$, $\beta_k^{(j)}$ evaluated at $\alpha_{12}=-ik_3$. With this notation, $\sigma_F=-\mu_{F0}^{(0)}s$ and $\mu_{Fk}^{(0)}=\mu_{F0}^{(0)}c_k$ when the c_k are given by (4.6), so that the result (4.23) for F can be written in the equivalent form

$$F(c_1(k_2,k_3;\alpha_1),c_2(k_3,k_1;\alpha_2),c_3(k_1,k_2;\alpha_3))=4\mu_{F0}^{(0)}\sigma_F^{-1}\left[-v(\gamma_{F0}^{(0)}/\sigma_F)+\sum_{k=1}^{3}v(\gamma_{Fk}^{(0)}/\sigma_F)\right]. \tag{4.45}$$

F. Integration over k_1

The result

$$G(\alpha_1,\alpha_2,\alpha_3,\alpha_{23};k_2,k_3)=\pi\alpha_{23}^{-1}[F(c_1(k_2,k_3;\alpha_1),c_2(k_3,k_1;\alpha_2),c_3(k_1,k_2;\alpha_3))+\tilde{F}(\alpha_1,\alpha_2,\alpha_3;k_1,k_2,k_3)]_{k_1=i\alpha_{23}}\ , \tag{4.46}$$

with $\tilde{F}$ defined by

$$\tilde{F}(\alpha_1,\alpha_2,\alpha_3;k_1,k_2,k_3)=4\mu_{F0}^{(0)}\sigma_F^{-1}[u(\beta_{F1}^{(0)}/\beta_{F0}^{(0)})+u(B_{F1}^{(1)}\beta_{F1}^{(0)})-u(\beta_{F1}^{(1)}/\beta_{F2}^{(0)})-u(\beta_{F1}^{(1)}/\beta_{F3}^{(0)})]\ , \tag{4.47}$$

can be obtained via complex integration. The combinations $\beta_{F1}^{(1)}/\beta_{Fi}^{(0)}$ and $\beta_{F1}^{(1)}\beta_{F1}^{(0)}$ which appear as arguments of the function u in Eq. (4.47) have four equivalent forms:

$$\beta_1^{(1)}/\beta_0^{(0)}=\beta_0^{(1)}/\beta_1^{(0)}=\beta_0^{(3)}/\beta_1^{(2)}=\beta_0^{(2)}/\beta_1^{(3)}\ , \tag{4.48a}$$

$$\beta_1^{(1)}\beta_1^{(0)}=\beta_0^{(1)}\beta_0^{(0)}=\beta_3^{(3)}\beta_3^{(2)}=\beta_2^{(2)}\beta_2^{(3)}\ , \tag{4.48b}$$

$$\beta_1^{(1)}/\beta_2^{(0)}=\beta_0^{(1)}\beta_3^{(0)}=\beta_0^{(3)}\beta_3^{(2)}=\beta_2^{(2)}/\beta_1^{(3)}\ , \tag{4.48c}$$

$$\beta_1^{(1)}/\beta_3^{(0)}=\beta_0^{(1)}\beta_2^{(0)}=\beta_3^{(3)}/\beta_1^{(2)}=\beta_0^{(2)}\beta_2^{(3)}\ . \tag{4.48d}$$

The derivation of (4.46) and (4.47) begins by using the fact that the function F in the integrand of (4.10) is even in k_1. Thus (4.10) can be replaced by

$$G(\alpha_1,\alpha_2,\alpha_3,\alpha_{23};k_2,k_3)=\int_{-\infty}^{\infty}\frac{dk_1}{k_1^2+\alpha_{23}^2}F(c_1(k_2,k_3;\alpha_1),c_2(k_3,k_1;\alpha_2),c_3(k_1,k_2;\alpha_3))\ . \tag{4.49}$$

The function F is analytic in k_1 except for branch points at $k_1=\pm k_2\pm i\alpha_3$ and at $k_1=\pm k_3\pm i\alpha_2$. The behavior of F in the neighborhood of these branch points can be deduced from (4.6), (4.24), (4.35), and the fact that $F(c_1,c_2,c_3)$ is invariant under any permutation of 1,2,3. The dilogarithm (Li_2) terms in (4.35) are not singular at $c_3=\pm 1$; only the logarithm term is singular at $c_3=\pm 1$. Hence the behavior of F at the $k_1=\pm k_2\pm i\alpha_3$ branch points is given by

$$F(c_1(k_2,k_3;\alpha_1),c_2(k_3,k_1;\alpha_2),c_3(k_1,k_2;\alpha_3))=\frac{2}{s}\ln\left[\frac{c_1c_2-c_3-s}{c_1c_2-c_3+s}\right]\ln\left[\frac{(k_1-k_2-i\alpha_3)(k_1-k_2+i\alpha_3)}{(k_1+k_2-i\alpha_3)(k_1+k_2+i\alpha_3)}\right]$$

$$+\text{analytic function},\ k_1 \text{ near } \pm k_2 \pm i\alpha_3\ , \tag{4.50}$$

with the understanding that the c_i are given by (4.6). The behavior of F at the $k_1=\pm k_3 \pm i\alpha_2$ branch points is obtained by interchanging 2 and 3 in (4.50). It follows that the branch cuts associated with these branch points can be taken to connect $-k_2+i\alpha_3$ to $k_2+i\alpha_3$ and $-k_3+i\alpha_2$ to $k_3+i\alpha_2$ in the upper half-plane, and to connect $-k_2-i\alpha_3$ to $k_2-i\alpha_3$ and $-k_3-i\alpha_2$ to $k_3-i\alpha_2$ in the lower half-plane. These branch points, and the poles at $k_1=\pm i\alpha_{23}$, are the only singularities of the integrand in (4.49). Thus the integration contour can be closed over the upper half-plane to obtain G as the sum of three terms: a contribution G_{23} from the pole at $k_1=i\alpha_{23}$, a contribution G_2 from the branch cut which runs from $-k_3+i\alpha_2$ to $k_3+i\alpha_2$, and a contribution G_3 from the branch cut which run from $-k_2+i\alpha_3$ to $k_2+i\alpha_3$. Explicitly

$$G(\alpha_1,\alpha_2,\alpha_3,\alpha_{23};k_2,k_3)=G_{23}+G_2+G_3\ , \tag{4.51}$$

where

$$G_{23}=\frac{\pi}{\alpha_{23}}F(c_1(k_2,k_3;\alpha_1),c_2(k_3,k_1;\alpha_2),c_3(k_1,k_2;\alpha_3))_{k_1=i\alpha_{23}}\ , \tag{4.52}$$

$$G_2=-4\pi i\int_{-k_3+i\alpha_2}^{k_3+i\alpha_2}\frac{dk_1}{(k_1^2+\alpha_{23}^2)s}\ln\left[\frac{c_3c_1-c_2-s}{c_3c_1-c_2+s}\right]\ , \tag{4.53}$$

$$G_3=-4\pi i\int_{-k_2+i\alpha_3}^{k_2+i\alpha_3}\frac{dk_1}{(k_1^2+\alpha_{23}^2)s}\ln\left[\frac{c_1c_2-c_3-s}{c_1c_2-c_3+s}\right]\ . \tag{4.54}$$

The jump across the branch cut needed for (4.54) is obtained from (4.50); (4.53) is obtained from (4.54) by interchanging 2 and 3. It can now be seen that the first (F) term in (4.46) comes from G_{23}. The second ($\tilde{F}$) term will come from G_2+G_3.

G_3 will now be computed via a rationalizing substitution and certain formulas obeyed by the dilogarithm function. The rationalizing substitution changes the dummy integration variable from k_1 to η via

$$\eta=\alpha_1(k_1^2+\alpha_{23}^2)+\sigma_F\ , \tag{4.55}$$

which implies that

$$k_1^2=-\alpha_{23}^2+(\eta^2-\sigma_G^2)/[2\alpha_1(\eta-B)] \tag{4.56}$$

and

$$\sigma_F=(\eta^2-2\eta B+\sigma_G^2)/[2(\eta-B)]\ , \tag{4.57}$$

where

$$B=\tfrac{1}{2}\alpha_1(2\alpha_{23}^2+\alpha_1^2-\alpha_2^2-\alpha_3^2)+\tfrac{1}{2}\alpha_1^{-1}[(\alpha_1^2+\alpha_2^2-\alpha_3^2)k_2^2+(\alpha_1^2-\alpha_2^2+\alpha_3^2)k_3^2]\ . \tag{4.58}$$

Using (4.55)–(4.58) in (4.54) yields

$$G_3=8\pi k_2k_3\int_{-\gamma_{G1}^{(2)}}^{\gamma_{G3}^{(2)}}\frac{d\eta}{\eta^2-\sigma_G^2}\ln\left[\frac{(B+\gamma_{G0}^{(3)})(\eta+\gamma_{G1}^{(3)})(\eta+\gamma_{G3}^{(3)})}{(B+\gamma_{G3}^{(3)})(\eta-\gamma_{G2}^{(3)})(\eta+\gamma_{G0}^{(3)})}\right]\ . \tag{4.59}$$

Remark: The integrand in (4.59) is invariant under the transformation $\eta\to\eta' := (B\eta-\sigma_G^2)/(\eta-B)$. This transformation carries the lower limit $-\gamma_{G1}^{(2)}$ into $-\gamma_{G0}^{(2)}$, the upper limit $\gamma_{G3}^{(2)}$ into $-\gamma_{G2}^{(2)}$, k_1^2 into k_1^2, and σ_F into $-\sigma_F$. Thus the limits $-\gamma_{G1}^{(2)}$ and $\gamma_{G3}^{(2)}$ could be replaced by $-\gamma_{G0}^{(2)}$ and $-\gamma_{G2}^{(2)}$ if desired; this is just the fact that either branch of the square root could be chosen for s and σ_F. This transformation appears to show that the integrand in (4.59) integrated from $-\gamma_{G1}^{(2)}$ to $-\gamma_{G0}^{(2)}$ is zero. This conclusion is, however, not correct because the image under the transformation of the original path from $-\gamma_{G1}^{(2)}$ to $-\gamma_{G0}^{(2)}$ is not the original path (traversed in the opposite direction), and cannot be deformed to coincide with the original path without crossing singular points of the integrand.

The integral (4.59) can be evaluated by performing a partial fraction decomposition of $(\eta^2-\sigma_G^2)^{-1}$ and using the integration formula (4.34). The result is

$$G_3=4\pi k_2k_3\sigma_G^{-1}\left[\ln\left[\frac{\sigma_G^2-(\gamma_{G1}^{(2)})^2}{\sigma_G^2-(\gamma_{G3}^{(2)})^2}\right]\ln(\beta_{G1}^{(3)}\beta_{G2}^{(3)})+\mathrm{Li}_2\left[\frac{\sigma_G-\gamma_{G1}^{(2)}}{\sigma_G-\gamma_{G0}^{(3)}}\right]-\mathrm{Li}_2\left[\frac{\sigma_G+\gamma_{G1}^{(2)}}{\sigma_G+\gamma_{G0}^{(3)}}\right]-\mathrm{Li}_2\left[\frac{\sigma_G+\gamma_{G3}^{(2)}}{\sigma_G-\gamma_{G0}^{(3)}}\right]+\mathrm{Li}_2\left[\frac{\sigma_G-\gamma_{G3}^{(2)}}{\sigma_G+\gamma_{G0}^{(3)}}\right]\right.$$

$$-\mathrm{Li}_2\left[\frac{\sigma_G-\gamma_{G1}^{(2)}}{\sigma_G-\gamma_{G1}^{(3)}}\right]+\mathrm{Li}_2\left[\frac{\sigma_G+\gamma_{G1}^{(2)}}{\sigma_G+\gamma_{G1}^{(3)}}\right]+\mathrm{Li}_2\left[\frac{\sigma_G+\gamma_{G3}^{(2)}}{\sigma_G-\gamma_{G1}^{(3)}}\right]-\mathrm{Li}_2\left[\frac{\sigma_G-\gamma_{G3}^{(2)}}{\sigma_G+\gamma_{G1}^{(3)}}\right]$$

$$+\mathrm{Li}_2\left[\frac{\sigma_G-\gamma_{G1}^{(2)}}{\sigma_G+\gamma_{G2}^{(3)}}\right]-\mathrm{Li}_2\left[\frac{\sigma_G+\gamma_{G1}^{(2)}}{\sigma_G-\gamma_{G2}^{(3)}}\right]-\mathrm{Li}_2\left[\frac{\sigma_G+\gamma_{G3}^{(2)}}{\sigma_G+\gamma_{G2}^{(3)}}\right]+\mathrm{Li}_2\left[\frac{\sigma_G-\gamma_{G3}^{(2)}}{\sigma_G-\gamma_{G2}^{(3)}}\right]$$

$$\left.-\mathrm{Li}_2\left[\frac{\sigma_G-\gamma_{G1}^{(2)}}{\sigma_G-\gamma_{G3}^{(3)}}\right]+\mathrm{Li}_2\left[\frac{\sigma_G+\gamma_{G1}^{(2)}}{\sigma_G+\gamma_{G3}^{(3)}}\right]+\mathrm{Li}_2\left[\frac{\sigma_G+\gamma_{G3}^{(2)}}{\sigma_G-\gamma_{G3}^{(3)}}\right]-\mathrm{Li}_2\left[\frac{\sigma_G-\gamma_{G3}^{(2)}}{\sigma_G+\gamma_{G3}^{(3)}}\right]\right]. \tag{4.60}$$

The result (4.60) can be rewritten in terms of the function u with the aid of the identities

$$\mathrm{Li}_2\left[\frac{1+x}{1+y}\right]-\mathrm{Li}_2\left[\frac{1-x}{1-y}\right]=-u\left[\frac{(1-x)(1+y)}{(1+x)(1-y)}\right]-v(x)+v(y\pm i\epsilon)$$

$$\mp\tfrac{1}{2}i\pi\ln[(1-|y|^{-1})/(1+|y|^{-1})]+\tfrac{1}{2}\ln[(y-1)/(y+1)]\ln[(y^2-1)/(1-x^2)],$$

$$|x|<1,\quad |y|>1,\quad \epsilon\to 0^+, \tag{4.61}$$

$$\mathrm{Li}_2\left[\frac{1+x}{1+y\pm i\epsilon}\right]-\mathrm{Li}_2\left[\frac{1-x}{1-y\mp i\epsilon}\right]=-u\left[\frac{(1-x)(1+y\pm i\epsilon)}{(1+x)(1-y\mp i\epsilon)}\right]-v(x)+v(y)\pm\tfrac{1}{2}i\pi\ln[(1-y^2)/(1-x^2)]$$

$$+\tfrac{1}{2}\ln[(1-y)/(1+y)]\ln[(1-y^2)/(1-x^2)],\quad |x|<1,\quad |y|<1,\quad \epsilon\to 0^+, \tag{4.62}$$

and (2.28d). The identities (4.61) and (4.62), in which it is assumed that x and y are real, can be established by differentiation. The branches of the multiple-valued functions can be kept track of by keeping $\alpha_1,\alpha_2,\alpha_3$ all near 1 with α_{23}, k_2, and k_3 all near 0. σ_G is then near 1, $\gamma_{G1}^{(2)}$, $\gamma_{G3}^{(2)}$, $\gamma_{G1}^{(3)}$, $\gamma_{G2}^{(3)}$ are near 0, and $\gamma_{G0}^{(2)}$, $\gamma_{G2}^{(2)}$, $\gamma_{G0}^{(3)}$, $\gamma_{G3}^{(3)}$ are near 2. Identity (4.61) is applied with $x=-\gamma_{G1}^{(2)}/\sigma_G$, $y=-\gamma_{G0}^{(3)}/\sigma_G$, with $x=\gamma_{G3}^{(2)}/\sigma_G$, $y=-\gamma_{G0}^{(3)}/\sigma_G$, with $x=\gamma_{G1}^{(2)}/\sigma_G$, $y=\gamma_{G3}^{(3)}/\sigma_G$, and with $x=-\gamma_{G3}^{(2)}/\sigma_G$, $y=\gamma_{G3}^{(3)}/\sigma_G$. Identity (4.62) is applied with $x=-\gamma_{G1}^{(2)}/\sigma_G$, $y=-\gamma_{G1}^{(3)}/\sigma_G$, with $x=\gamma_{G3}^{(2)}/\sigma_G$, $y=-\gamma_{G1}^{(3)}/\sigma_G$, with $x=\gamma_{G1}^{(2)}/\sigma_G$, $y=-\gamma_{G2}^{(3)}/\sigma_G$, and with $x=-\gamma_{G3}^{(2)}/\sigma_G$, $y=-\gamma_{G2}^{(3)}/\sigma_G$. The logarithm terms can be shown to cancel with the aid of (2.28d). The result is

$$G_3=4\pi k_2k_3\sigma_G^{-1}(-u(\beta_{G0}^{(3)}/\beta_{G1}^{(2)})-u(\beta_{G3}^{(3)}\beta_{G3}^{(2)})+u(\beta_{G0}^{(3)}\beta_{G3}^{(2)})+u(\beta_{G3}^{(3)}/\beta_{G1}^{(2)})$$

$$+u(\beta_{G2}^{(3)}\beta_{G1}^{(2)})-u(\beta_{G1}^{(3)}\beta_{G3}^{(2)})-u(\beta_{G2}^{(3)}/\beta_{G3}^{(2)})+u(\beta_{G1}^{(3)}/\beta_{G1}^{(2)}))\,. \tag{4.63}$$

A consistent choice of branch at $\alpha_1=\alpha_2=\alpha_3=1$, $\alpha_{23}=k_2=k_3=0$ can be had by giving small positive imaginary parts to $\gamma_{G1}^{(3)}$ and to $\gamma_{G2}^{(3)}$ when they appear in $\beta_{G1}^{(3)}$ and $\beta_{G2}^{(3)}$. The arguments of the functions u which appear in (4.64) each have four equivalent forms, provided by the identities (4.48) for the first four, and by the identities

$$\beta_0^{(0)}/\beta_3^{(1)}=\beta_1^{(0)}\beta_2^{(1)}=\beta_2^{(3)}\beta_1^{(2)}=\beta_3^{(3)}/\beta_0^{(2)}, \tag{4.64a}$$

$$\beta_1^{(0)}\beta_3^{(1)}=\beta_0^{(0)}/\beta_2^{(1)}=\beta_1^{(3)}\beta_3^{(2)}=\beta_2^{(2)}/\beta_0^{(3)}, \tag{4.64b}$$

$$\beta_2^{(0)}/\beta_3^{(1)}=\beta_2^{(1)}/\beta_3^{(0)}=\beta_2^{(3)}/\beta_3^{(2)}=\beta_3^{(3)}/\beta_2^{(2)}, \tag{4.64c}$$

$$\beta_3^{(1)}/\beta_3^{(0)}=\beta_2^{(0)}/\beta_2^{(1)}=\beta_1^{(3)}/\beta_1^{(2)}=\beta_0^{(2)}/\beta_0^{(3)} \tag{4.64d}$$

for the last four.

The verification of identities such as (2.9), (2.38), (4.48), and (4.64) from the definitions (2.5)–(2.8) becomes tedious very quickly. Fortunately there is an easier way. The definitions (2.5)–(2.8) are used to show that $\beta_0^{(1)}\beta_0^{(0)}=\beta_3^{(2)}\beta_3^{(3)}$, which is the second equality in (2.9a). Interchanging 0 and 1 then yields the first equality in (2.9a); interchanging 2 and 3 yields the third equality in (2.9a). With (2.9a) verified, (2.9b) can be obtained from (2.9a) by interchanging 1 and 2; (2.9c) can be obtained from (2.9a) by interchanging 1 and 3. Formula (4.48a) can be obtained from (2.9a) by replacing α_2 and α_3, respectively, by $-\alpha_2$ and $-\alpha_3$. Formula (4.48b) is (2.9a). Formula (4.48c) can be obtained from (2.9a) by replacing α_{12} by $-\alpha_{12}$. Formula (4.48d) can be obtained from (2.9a) by replacing α_{31} by $-\alpha_{31}$. Formulas (4.64a)–(4.64d) can be obtained from (4.48a)–(4.48d) by replacing α_2 by $-\alpha_2$. Formula (2.38a) follows from the first equalities in (4.64b) and (4.64c). Finally, (2.38b)–(2.38d) follow from (2.38a) by symmetry.

A formula for G_2 analogous to (4.64) can be obtained from (4.64) by interchanging 2 and 3. This formula is

$$G_2=4\pi k_2 k_3 \sigma_G^{-1}[-u(\beta_{G0}^{(2)}/\beta_{G1}^{(3)})-u(\beta_{G3}^{(2)}\beta_{G3}^{(3)})+u(\beta_{G0}^{(2)}\beta_{G2}^{(3)})+u(\beta_{G2}^{(2)}/\beta_{G1}^{(3)})$$
$$+u(\beta_{G3}^{(2)}\beta_{G1}^{(3)})-u(\beta_{G1}^{(2)}\beta_{G2}^{(3)})-u(\beta_{G3}^{(2)}/\beta_{G2}^{(3)})+u(\beta_{G1}^{(2)}/\beta_{G1}^{(3)})] \ . \tag{4.65}$$

The identities (4.48) and the relation $u(z)=-u(z^{-1})$ can be used to show that the first four terms add and the last four terms cancel when (4.63) and (4.65) are added to form G_2+G_3. Comparing the result with (4.47) and using the definition (2.7a) of $\mu_0^{(0)}$ then shows that

$$G_2+G_3=\pi\alpha_{23}^{-1}\tilde{F}(\alpha_1,\alpha_2,\alpha_3;i\alpha_{23},k_2,k_3) \ . \tag{4.66}$$

The result (4.46) now follows from (4.51), (4.52), and (4.66).

Extended remark: An alternative route to the result (4.46) begins with the observation that $\tilde{F}(\alpha_1,\alpha_2,\alpha_3;k_1,k_2,k_3)$ is an odd function of k_1. This implies that (4.49) can be replaced by

$$G(\alpha_1,\alpha_2,\alpha_3,\alpha_{23};k_2,k_3)=\int_{-\infty}^{\infty}\frac{dk_1}{k_1^2+\alpha_{23}^2}[F(c_1(k_2,k_3;\alpha_1),c_2(k_3,k_1;\alpha_2),c_3(k_1,k_2;\alpha_3))+\tilde{F}(\alpha_1,\alpha_2,\alpha_3;k_1,k_2,k_3)] \ . \tag{4.67}$$

It can be shown that the sum $F+\tilde{F}$ has no singularities in the upper half-plane. Hence a pole at $k_1=i\alpha_{23}$ is the only singularity of the integrand of (4.67) in the upper half-plane. The result (4.46) then follows from closing the contour over the upper half-plane and extracting the residue at $k_1=i\alpha_{23}$. This route to (4.46) can, of course, only be used after the function $\tilde{F}$ has been obtained.

G. Integration over k_2

The result

$$H(\alpha_1,\alpha_2,\alpha_3,\alpha_{23},\alpha_{31};k_3)=16\pi^2 i k_3 \sigma_H^{-1}[-u(\beta_{H0}^{(0)}\beta_{H0}^{(1)})-u(\beta_{H0}^{(0)}\beta_{H0}^{(2)})+u(\beta_{H1}^{(1)}/\beta_{H2}^{(0)})$$
$$+u(\beta_{H2}^{(2)}/\beta_{H1}^{(0)})-v(\gamma_{H1}^{(0)}/\sigma_H)-v(\gamma_{H2}^{(0)}/\sigma_H)-v(\gamma_{H1}^{(3)}/\sigma_H)-v(\gamma_{H2}^{(3)}/\sigma_H)] \tag{4.68}$$

can be obtained via complex integration. The arguments of the functions u which appear in (4.68) each have four equivalent forms, as can be seen from (2.9a), (2.9b), (4.48), and

$$\beta_2^{(2)}/\beta_1^{(0)}=\beta_3^{(0)}\beta_0^{(2)}=\beta_1^{(1)}/\beta_2^{(3)}=\beta_0^{(3)}\beta_3^{(1)} \ . \tag{4.69}$$

The identity (4.69) can be obtained from (2.9b) by replacing α_{12} by $-\alpha_{12}$.

The derivation of (4.68) begins by using the fact that the function G in the integrand of (4.11) is even in k_2. Thus (4.11) can be replaced by

$$H(\alpha_1,\alpha_2,\alpha_3,\alpha_{23},\alpha_{31};k_3)=\int_{-\infty}^{\infty}\frac{dk_2}{k_2^2+\alpha_{31}^2}G(\alpha_1,\alpha_2,\alpha_3,\alpha_{23};k_2,k_3) \ . \tag{4.70}$$

The function G is analytic in k_2 except for branch points at $k_2=\pm i(\alpha_3+\alpha_{23})$, at $k_2=\pm k_3 \pm i\alpha_1$, and at $k_2=\pm k_3 \pm i(\alpha_2+\alpha_3)$. The most obvious route to follow in evaluating (4.70) is the one used to compute G in Sec. IV F. H can be written as the sum of a term from the pole at $k_2=i\alpha_{31}$ plus contributions from the jumps across the branch cuts of G in the upper half-plane. Unfortunately this approach fails; the branch cut jumps associated with the branch points at $k_2=\pm k_3+i(\alpha_2+\alpha_3)$ lead to intractable integrals.

The method which succeeds is based on the extended remark at the end of Sec. IV F. A function $\tilde{G}(\alpha_1,\alpha_2,\alpha_3,\alpha_{23};k_2,k_3)$ is sought which is odd in k_2 and which has the property that $G+\tilde{G}$ has no singularities in the upper half-plane. Then (4.70) can be replaced by

$$H(\alpha_1,\alpha_2,\alpha_3,\alpha_{23},\alpha_{31};k_3)=\int_{-\infty}^{\infty}\frac{dk_2}{k_2^2+\alpha_{31}^2}[G(\alpha_1,\alpha_2,\alpha_3,\alpha_{23};k_2,k_3)+\tilde{G}(\alpha_1,\alpha_2,\alpha_3,\alpha_{23};k_2,k_3)] \ . \tag{4.71}$$

The integral (4.71) can be evaluated by closing the contour over the upper half-plane and extracting the residue at $k_2=i\alpha_{31}$. The result is

$$H(\alpha_1,\alpha_2,\alpha_3,\alpha_{23},\alpha_{31};k_3)=\pi\alpha_{31}^{-1}[G(\alpha_1,\alpha_2,\alpha_3,\alpha_{23};i\alpha_{31},k_3)+\tilde{G}(\alpha_1,\alpha_2,\alpha_3,\alpha_{23};i\alpha_{31},k_3)] \ . \tag{4.72}$$

The difficult part of this method is finding $\tilde{G}$ and verifying that it has the desired properties. The symmetry of the problem makes this task much easier. Because only the integration over k_3 remains to be done once H has been obtained, H is invariant under interchange of 1 and 2 *and* under interchange of 0 and 3. This invariance indicates what functions should be considered when searching for $\tilde{G}$. The required $\tilde{G}$ is

$$\tilde{G}(\alpha_1,\alpha_2,\alpha_3,\alpha_{23};k_2,k_3)=8\pi k_2 k_3 \sigma_G^{-1}[-u(\beta_{G0}^{(0)}\beta_{G0}^{(1)})-2u(\beta_{G0}^{(0)}\beta_{G0}^{(2)})+u(\beta_{G1}^{(1)}/\beta_{G2}^{(0)})$$
$$+2u(\beta_{G2}^{(2)}/\beta_{G1}^{(0)})+u(\beta_{G1}^{(1)}/\beta_{G0}^{(0)})-u(\beta_{G1}^{(1)}/\beta_{G3}^{(0)})$$
$$-v(\gamma_{G0}^{(0)}/\sigma_G)-v(\gamma_{G1}^{(0)}/\sigma_G)-v(\gamma_{G2}^{(0)}/\sigma_G)+v(\gamma_{G3}^{(0)}/\sigma_G)$$
$$-2v(\gamma_{G1}^{(3)}/\sigma_G)-2v(\gamma_{G2}^{(3)}/\sigma_G)] \ . \tag{4.73}$$

The result (4.68) follows from (2.7a), (4.45)–(4.47), (4.72), and (4.73).

H. Integration over k_3

The result (2.1) for I is also obtained via complex integration. The derivation of (2.1) begins by using the fact that the function H in the integrand of (4.12) is even in k_3. Thus (4.12) can be replaced by

$$I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})=\int_{-\infty}^{\infty}\frac{dk_3}{k_3^2+\alpha_{12}^2}H(\alpha_1,\alpha_2,\alpha_3,\alpha_{23},\alpha_{31};k_3) \ . \tag{4.74}$$

The function H is analytic in k_3 except for branch points at $k_3=\pm i(\alpha_1+\alpha_{31})$, at $k_3=\pm i(\alpha_2+\alpha_{23})$, at $k_3=\pm i(\alpha_1+\alpha_3+\alpha_{23})$, and at $k_3=\pm i(\alpha_2+\alpha_3+\alpha_{31})$. Thus I could be written as the sum of a term from the pole at $k_3=i\alpha_{12}$ plus contributions from the jumps across the branch cuts of H in the upper half-plane. Unfortunately this approach fails just as it did in Sec. IV G; the branch cut jumps associated with the branch points at $k_3=i(\alpha_1+\alpha_3+\alpha_{23})$ and at $k_3=i(\alpha_2+\alpha_3+\alpha_{31})$ lead to intractable integrals. This difficulty is circumvented in the same way as in Sec. IV G. A function $\tilde{H}(\alpha_1,\alpha_2,\alpha_3,\alpha_{23},\alpha_{31};k_3)$ is sought which is odd in k_3 and which has the property that $H+\tilde{H}$ has no singularities in the upper half-plane. Then (4.74) can be replaced by

$$I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})=\int_{-\infty}^{\infty}\frac{dk_3}{k_3^2+\alpha_{12}^2}[H(\alpha_1,\alpha_2,\alpha_3,\alpha_{23},\alpha_{31};k_3)+\tilde{H}(\alpha_1,\alpha_2,\alpha_3,\alpha_{23},\alpha_{31};k_3)] \ , \tag{4.75}$$

which is evaluated by extracting the residue at $k_3=i\alpha_{12}$ to obtain

$$I(\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31})=\pi\alpha_{12}^{-1}[H(\alpha_1,\alpha_2,\alpha_3,\alpha_{23},\alpha_{31};i\alpha_{12})+\tilde{H}(\alpha_1,\alpha_2,\alpha_3,\alpha_{23},\alpha_{31};i\alpha_{12})] \ . \tag{4.76}$$

The hard part is finding $\tilde{H}$. Again symmetry comes to the rescue; I is invariant under the permutation group on the four indexes 0,1,2,3 as was discussed in detail in Sec. II B. This invariance indicates what functions should be considered when searching for $\tilde{H}$. The required $\tilde{H}$ is

$$\tilde{H}(\alpha_1,\alpha_2,\alpha_3,\alpha_{23},\alpha_{31};k_3)=16\pi^2 ik_3\sigma_H^{-1}\Bigg\{-u(\beta_{H0}^{(0)}\beta_{H0}^{(1)})-u(\beta_{H0}^{(0)}\beta_{H0}^{(2)})-2u(\beta_{H0}^{(0)}\beta_{H0}^{(3)})$$
$$-u(\beta_{H1}^{(1)}/\beta_{H2}^{(0)})-u(\beta_{H2}^{(2)}/\beta_{H1}^{(0)})-v(\gamma_{H0}^{(0)}/\sigma_H)$$
$$-v(\gamma_{H3}^{(0)}/\sigma_H)-v(\gamma_{H0}^{(3)}/\sigma_H)-v(\gamma_{H3}^{(3)}/\sigma_H)-\sum_{j=0}^{3}[v(\gamma_{Hj}^{(1)}/\sigma_H)+v(\gamma_{Hj}^{(2)}/\sigma_H)]\Bigg\} \ . \tag{4.77}$$

The result (2.1) follows from (4.68), (4.76), and (4.77).

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APPENDIX: DIRECT EVALUATION OF A LIMITING CASE

This Appendix will sketch a direct evaluation of the integral $K(\beta_1,\beta_2,\beta_{12})$ defined by

$$K(\beta_1,\beta_2,\beta_{12}) := \int (r_1^2 r_2^2 r_{12})^{-1}\exp[-\beta_1 r_1-\beta_2 r_2-\beta_{12}r_{12}]d^3r_1 d^3r_2 \ . \tag{A1}$$

Equation (2.47) shows how K can be obtained as a limiting case of the integral I. To facilitate comparison with (2.47), the evaluation will be carried out for β_{12} near $+1$ and β_1,β_2 both near $+2$. If $r_{12}^{-1}\exp(-\beta_{12}r_{12})$ is represented by the

Fourier integral (4.2), the integration over $\mathbf{r}_1$ and $\mathbf{r}_2$ can be carried out, followed by integration over the direction of $\mathbf{k}$. The result is

$$K(\beta_1,\beta_2,\beta_{12})=-8\pi\int_0^\infty \frac{dk}{k^2+\beta_{12}^2}\ln\left[\frac{\beta_1+ik}{\beta_1-ik}\right]\ln\left[\frac{\beta_2+ik}{\beta_2-ik}\right] . \tag{A2}$$

In (A2) the branch of the logarithm which makes the logarithm zero when $k=0$ is to be chosen. Branch cuts for the logarithms run from $+i\beta_1$ to $+i\infty$ and from $+i\beta_2$ to $+i\infty$ in the upper half-plane, and from $-i\beta_1$ to $-i\infty$ and from $-i\beta_2$ to $-i\infty$ in the lower half-plane. With this choice of branch, the integrand in (A2) is an even function of k, so that the integral in (A2) can be replaced by half of the same integrand integrated from $-\infty$ to ∞. The integration contour can then be closed in the upper half-plane to obtain

$$K(\beta_1,\beta_2,\beta_{12})=K_{12}(\beta_1,\beta_2,\beta_{12})+K_1(\beta_1,\beta_2,\beta_{12})+K_2(\beta_1,\beta_2,\beta_{12}) , \tag{A3}$$

where K_{12} is the contribution from the pole at $k=i\beta_{12}$, K_1 is the contribution from the jump across the branch cut which runs from $+i\beta_1$ to $+i\infty$, and K_2 is the contribution from the jump across the branch cut which runs from $+i\beta_2$ to $+i\infty$. It is convenient to separate the branch cuts and the pole by assuming $\beta_1>\beta_2>\beta_{12}$ and adding $+i\epsilon$ to β_1 and $-i\epsilon$ to β_2. Then it is found that

$$K_{12}(\beta_1,\beta_2,\beta_{12})=-\frac{4\pi^2}{\beta_{12}}\ln\left[\frac{\beta_1-\beta_{12}}{\beta_1+\beta_{12}}\right]\ln\left[\frac{\beta_2-\beta_{12}}{\beta_2+\beta_{12}}\right] , \tag{A4}$$

$$\begin{aligned}\lim_{\epsilon\to 0+}K_1(\beta_1+i\epsilon,\beta_2-i\epsilon,\beta_{12})&=-8\pi^2\int_0^\infty[\ln(\beta_1-\beta_2+y)-\ln(\beta_1+\beta_2+y)-i\pi][(\beta_1+y)^2-\beta_{12}^2]^{-1}dy\\&=\frac{4\pi^2}{\beta_{12}}\left[\mathrm{Li}_2\left[-\frac{\beta_2-\beta_{12}}{\beta_1+\beta_{12}}\right]-\mathrm{Li}_2\left[-\frac{\beta_2+\beta_{12}}{\beta_1-\beta_{12}}\right]+\mathrm{Li}_2\left[\frac{\beta_2-\beta_{12}}{\beta_1-\beta_{12}}\right]\right.\\&\qquad\left.-\mathrm{Li}_2\left[\frac{\beta_2+\beta_{12}}{\beta_1+\beta_{12}}\right]+i\pi\ln\left[\frac{\beta_1+\beta_{12}}{\beta_1-\beta_{12}}\right]\right] ,\end{aligned} \tag{A5}$$

$$\begin{aligned}\lim_{\epsilon\to 0+}K_2(\beta_1+i\epsilon,\beta_2-i\epsilon,\beta_{12})&=-8\pi^2\int_0^\infty[\ln|\beta_2-\beta_1+y|-\ln(\beta_1+\beta_2+y)][(\beta_2+y)^2-\beta_{12}^2]^{-1}dy\\&\quad-8i\pi^3\int_{\beta_1-\beta_2}^\infty[(\beta_2+y)^2-\beta_{12}^2]^{-1}dy\\&=\frac{4\pi^2}{\beta_{12}}\left[-\mathrm{Li}_2\left[-\frac{\beta_1+\beta_{12}}{\beta_2-\beta_{12}}\right]+\mathrm{Li}_2\left[-\frac{\beta_1-\beta_{12}}{\beta_2+\beta_{12}}\right]-\mathrm{Li}_2\left[\frac{\beta_2-\beta_{12}}{\beta_1-\beta_{12}}\right]\right.\\&\qquad\left.+\mathrm{Li}_2\left[\frac{\beta_2+\beta_{12}}{\beta_1+\beta_{12}}\right]+\tfrac{1}{2}\ln^2\left[\frac{\beta_2+\beta_{12}}{\beta_1+\beta_{12}}\right]-\tfrac{1}{2}\ln^2\left[\frac{\beta_2-\beta_{12}}{\beta_1-\beta_{12}}\right]-i\pi\ln\left[\frac{\beta_1+\beta_{12}}{\beta_1-\beta_{12}}\right]\right] .\end{aligned} \tag{A6}$$

The integrations in (A5) and (A6) have been performed with the aid of (4.34) and the dilogarithm identity

$$\mathrm{Li}_2(-z^{-1})=-\mathrm{Li}_2(-z)-\tfrac{1}{2}\ln^2(z)-\frac{\pi^2}{6} . \tag{A7}$$

The result for K which is obtained by inserting (A4)–(A6) in (A3) is not immediately comparable with the result obtained from (2.47), but can be transformed into it with the aid of dilogarithm identities. Equation (A7) and the identity

$$\mathrm{Li}_2(z)+\mathrm{Li}_2(1-z)=-\ln z\,\ln(1-z)+\frac{\pi^2}{6} \tag{A8}$$

can be used to show that

$$\lim_{\epsilon\to 0}[v((\beta+i\epsilon)/\beta_{12})+v((\beta-i\epsilon)/\beta_{12})]=-2\mathrm{Li}_2\left[\frac{\beta-\beta_{12}}{\beta+\beta_{12}}\right]-\tfrac{1}{2}\ln^2\left[\frac{\beta-\beta_{12}}{\beta+\beta_{12}}\right]+\tfrac{1}{3}\pi^2 \tag{A9}$$

holds for $\beta>\beta_{12}$. Identities (A7), (A8), and

$$\mathrm{Li}_2(zw)=\mathrm{Li}_2(z)+\mathrm{Li}_2(w)-\mathrm{Li}_2[z(1-w)/(1-zw)]-\mathrm{Li}_2[w(1-z)/(1-zw)]-\ln[(1-z)/(1-zw)]\ln[(1-w)/(1-zw)] \tag{A10}$$

with $z=(\beta_1-\beta_{12})/(\beta_1+\beta_{12})$ and $w=(\beta_2-\beta_{12})/(\beta_2+\beta_{12})$ can be used to show that

$$\lim_{\epsilon\to 0+}\left[u\left[\frac{(\beta_1-\beta_{12})(\beta_2-\beta_{12})}{(\beta_1+\beta_{12})(\beta_2+\beta_{12})}+i\epsilon\right]+i\pi\ln\left[\frac{(\beta_1-\beta_{12})(\beta_2-\beta_{12})}{(\beta_1+\beta_{12})(\beta_2+\beta_{12})}\right]\right]$$
$$=2\mathrm{Li}_2\left[\frac{\beta_1-\beta_{12}}{\beta_1+\beta_{12}}\right]+2\mathrm{Li}_2\left[\frac{\beta_2-\beta_{12}}{\beta_2+\beta_{12}}\right]+\mathrm{Li}_2\left[-\frac{\beta_2-\beta_{12}}{\beta_1+\beta_{12}}\right]-\mathrm{Li}_2\left[-\frac{\beta_2+\beta_{12}}{\beta_1-\beta_{12}}\right]$$
$$-\mathrm{Li}_2\left[-\frac{\beta_1+\beta_{12}}{\beta_2-\beta_{12}}\right]+\mathrm{Li}_2\left[-\frac{\beta_1-\beta_{12}}{\beta_2+\beta_{12}}\right]+\tfrac{1}{2}\ln^2\left[\frac{\beta_2+\beta_{12}}{\beta_1+\beta_{12}}\right]-\tfrac{1}{2}\ln^2\left[-\frac{\beta_2-\beta_{12}}{\beta_1-\beta_{12}}\right]$$
$$+\tfrac{1}{2}\ln^2\left[\frac{\beta_1-\beta_{12}}{\beta_1+\beta_{12}}\right]+\tfrac{1}{2}\ln^2\left[\frac{\beta_2-\beta_{12}}{\beta_2+\beta_{12}}\right]-\tfrac{2}{3}\pi^2\ . \qquad \text{(A11)}$$

Identities (A9) and (A11) can be used to show that the result for the integral K obtained from (2.41) and (2.45)–(2.47) agrees with the result obtained from (A3)–(A6).

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[1]T. Kato, Commun. Pure Appl. Math. **10**, 151 (1957).
[2]C. Schwartz, Methods Comput. Phys. **2**, 241 (1963).
[3]W. Lakin, J. Chem. Phys. **43**, 2954 (1965).
[4]B. Klahn and J. D. Morgan III, J. Chem. Phys. **81**, 410 (1984).
[5]R. N. Hill, J. Chem. Phys. **83**, 1173 (1985).
[6]W. Kutzelnigg, Theor. Chim. Acta **68**, 445 (1985).
[7]H. M. James and A. S. Coolidge, Phys. Rev. **49**, 688 (1936).
[8]E. A. Burke, Phys. Rev. **130**, 1871 (1963).
[9]S. Larsson, Phys. Rev. **169**, 49 (1968).
[10]Y. K. Ho and B. A. P. Page, J. Comput. Phys. **17**, 122 (1975).
[11]Y. K. Ho, Int. J. Quantum Chem. **20**, 1077 (1981).
[12]J. F. Perkins, J. Chem. Phys. **48**, 1985 (1968).
[13]J. F. Perkins, J. Chem. Phys. **50**, 2819 (1969).
[14]Y. Ohrn and J. Nordling, J. Chem. Phys. **39**, 1864 (1963).
[15]J. Hinze and K. S. Pitzer, J. Chem. Phys. **41**, 3484 (1964).
[16]R. A. Sack, J. Math. Phys. **5**, 245 (1964).
[17]C. L. Pekeris and K. Frankowski, Proc. Nat. Acad. Sci. U.S.A. **82**, 1299 (1985).
[18]R. A. Bonham, J. Mol. Spectrosc. **15**, 112 (1965); **20**, 197 (1966).
[19]The standard reference on the dilogarithm function is L. Lewin, *Polylogarithms and Associated Functions* (North-Holland, Amsterdam, 1981). Other useful references are K. S. Kolbig, J. A. Mignaco, and E. Remiddi, B.I.T., Nord. Tidskr. Infbehandl. **10**, 38 (1970); R. Barbieri, J. A. Mignaco, and E. Remiddi, Nuovo Cimento **11A**, 824 (1972); A. Devoto and D. W. Duke, Riv. Nuovo Cimento **7** (6), 1 (1984).
[20]The multicenter integrals which arise when Slater orbitals are used for molecular calculations have been discussed extensively in a series of recent papers by Steinborn and his collaborators. A representative selection from which the earlier literature can be traced includes E. J. Weniger and E. O. Steinborn, Phys. Rev. A **28**, 2026 (1983); **29**, 2268 (1984); J. Chem. Phys. **78**, 6121 (1983); J. Math. Phys. **24**, 2553 (1983); H. P. Trivedi and E. O. Steinborn, Phys. Rev. A **25**, 113 (1982); **27**, 670 (1983); H. H. Kranz and E. O. Steinborn, Phys. Rev. A **25**, 66 (1982); E. Filter and E. O. Steinborn, Theor. Chim. Acta **52**, 189 (1979); J. Math. Phys. **21**, 2725 (1980). Other earlier references can be traced from the recent paper of Herbert W. Jones, Int. J. Quantum Chem. **29**, 177 (1986).
[21]This works because $\exp(-xr_3)$ cuts off the integral so quickly for large r_3 that only small x matters. The rigorous justification for the suggested procedure is provided by Watson's lemma, for which see G. N. Watson, Proc. London Math. Soc. **27** (2) 113 (1918) or E. T. Copson, *An Introduction to the Theory of Functions of a Complex Variable* (Oxford University Press, London, 1935), pp. 218–219. A collection of theorems on the asymptotics of the Laplace transform can be found in J. Lavoine, Ann. Inst. Henri Poincaré A **4**, 49 (1966). An elementary discussion of this kind of procedure appears in R. N. Hill, Am. J. Phys. **38**, 1440 (970).
[22]A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University, Princeton, 1960), Eq. (4.6.5), p. 63.
[23]Reference 21, Eq. (4.1.4), p. 54 and Eq. (4.1.10), p. 55.
[24]Reference 21, Eq. (4.6.2), p. 62.
[25]See L. C. Biedenharn and J. D. Louck, *Angular Momentum in Quantum Physics Theory and Application* (Addison-Wesley, Reading, MA, 1981), pp. 307–311. R differs from the invariant $I_{(l_1 l_2 l_3)}(\mathbf{x}^1,\mathbf{x}^2,\mathbf{x}^3)$ defined in Eq. (6.153) by a constant factor.
[26]Ramon E. Moore, *Methods and Applications of Interval Analysis* (Society for Industrial and Applied Mathematics, Philadelphia, 1979), pp. 24–29 and 31.