Analytical Evaluation of Multicenter Integrals of r_{12}^{-1} with Slater-Type Atomic Orbitals. V. Four-Center Integrals by Fourier-Transform Method*

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The four-center integral of r_{12}^{-1} with Slater-type atomic orbitals is evaluated analytically. The Fourier-transform convolution theorem is used to express the integral as an infinite sum in which the internuclear angles appear in spherical harmonics, and the internuclear distances in integrals over spherical Bessel functions and exponential-type integrals. These "radial" integrals are evaluated as convergent infinite expansions by contour integration techniques. The formulas are valid for general values of the n, l, m, ζ parameters of the orbitals and for general nonzero values of the internuclear distance vectors.

I. INTRODUCTION

Analytical formulas for the four-center integral of r_{12}^{-1} with Slater-type atomic orbitals are derived by Fourier transform methods. The approach is similar to that of Papers I–III of this series,[1–3] to which the reader is referred for much of the detail. The Fourier-transform approach, and the resulting formulas, differ considerably from the Taylor-series approach of Paper IV.[4] The Taylor series method is much easier to grapple with analytically, but it yields inflexible, slowly convergent formulas. The Fourier transform technique is more complicated analytically, but it yields more rapidly convergent formulas, with some flexibility in how the answers are represented.

The technique used in this paper readily expresses the four-center integral as a double infinite sum of one-dimensional integrals over the radial Fourier-transform coordinate k. In the three-center cases discussed in Papers I–III, this final integration could be carried out in closed form by contour integration techniques. In the general four-center case, we have been unable to carry out this final integration in closed form. The most important mathematical difference between the final integrands of the three- and four-center cases is the appearance of two logarithmic branch points in the four-center case vs one in the three-center case. Our main purpose in this paper is to carry out the final integration in terms of convergent infinite expansions.

The formulas given for the four-center integral involve Condon–Shortley coefficients[5] [Eq. (14) of Paper I], various versions of the exponential-type integral,[6] $E_n(x)$, $\tilde{E}_n(x)$, $\alpha_n(x)$, $\hat{\alpha}_n(x)$ [Eqs. (21)–(25) of Paper I], and modified spherical Bessel functions,[6] $\mathcal{I}_l(x)$ and $\mathcal{K}_l(x)$ [Eqs. (15) and (16) of Paper I]. The formulas hold for integer-n Slater-type orbitals with general values of the l and m quantum numbers, with general values of the orbital exponents, and with arbitrary nuclear geometry, except that all four centers must be distinct.

II. SPECIAL FUNCTIONS, NOTATION, ETC.

To simplify the derivations in succeeding sections, we define in this section most of the special functions and symbols that are used.

We denote a Slater-type atomic orbital by

$$\Psi_{nlm\zeta}(\mathbf{r})=Nr^{n-1}\exp(-\zeta r)Y_l^m(\theta,\varphi). \qquad (2.1)$$

The $Y_l^m(\theta,\varphi)$ is a spherical harmonic, (r,θ,φ) are the spherical polar coordinates of $\mathbf{r}$, the ζ is called the orbital exponent, and N is a normalization constant. The n and l are integers which satisfy

$$n\geq l+1. \qquad (2.2)$$

We use the following standard mathematical functions[6]: spherical Bessel functions,

$$j_l(x)=(-x)^l(x^{-1}d/dx)^lx^{-1}\sin(x), \qquad (2.3)$$

$$\mathcal{I}_l(x)=x^l(x^{-1}d/dx)^lx^{-1}\sinh(x) \qquad (2.4)$$

$$=\sum_{s=0}^{\infty}\frac{x^{l+2s}}{(2s)!!(2l+2s+1)!!} \qquad (2.5)$$

$$=-\tfrac{1}{2}[\mathcal{K}_l(-x)+(-1)^l\mathcal{K}_l(x)], \qquad (2.6)$$

$$\mathcal{K}_l(x)=(-x)^l(x^{-1}d/dx)^lx^{-1}\exp(-x) \qquad (2.7)$$

$$=\sum_{s=0}^{\infty}\frac{x^{s-l-1}(-1)^{s+l}}{s!!(s-2l-1)!!} \qquad (2.8)$$

$$\sim x^{-1}\exp(-x) \qquad (\text{as } x\to\infty); \qquad (2.9)$$

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the double factorial function,

$$(2N)!!=2^N N! \qquad (N\geq 0), \qquad (2.10)$$

$$(2N-1)!!=(2N)!/(2N)!! \qquad (2.11)$$

$$=(-1)^N/(-2N-1)!!, \qquad (2.12)$$

$$1/(2N)!!=0 \qquad (N<0); \qquad (2.13)$$

various versions of exponential-type integrals,

$$E_n(x)=\int_1^\infty dt\, t^{-n}\exp(-xt) \qquad (2.14)$$

$$=(-d/dx)E_{n+1}(x) \qquad (2.15)$$

$$=\alpha_{-n}(x) \qquad (2.16)$$

$$=\tilde{E}_n(x)-(-x)^{n-1}[\log x-\psi(n)]/(n-1)! \qquad (n>0) \qquad (2.17)$$

$$=\hat{\alpha}_{-n}(x)+(-n)!x^{n-1} \qquad (n\leq 0) \qquad (2.18)$$

$$\sim x^{-1}\exp(-x) \qquad (\text{as } x\rightarrow\infty), \qquad (2.19)$$

$$E_n(x+y)=\sum_{s=0}^{\infty}\frac{(-y)^s E_{n-s}(x)}{s!} \qquad (|y|<|x|), \qquad (2.20)$$

$$\tilde{E}_n(x)=-\sum_{s=0;\,(s\neq n-1)}^{\infty}\frac{(-x)^s}{s!(s-n+1)} \qquad (n>0) \qquad (2.21)$$

$$=(-d/dx)\tilde{E}_{n+1}(x), \qquad (2.22)$$

$$\hat{\alpha}_n(x)=-\int_0^1 dt\, t^n\exp(-xt) \qquad (n\geq 0) \qquad (2.23)$$

$$=-\sum_{s=0}^{\infty}\frac{(-x)^s}{s!(s+n+1)} \qquad (2.24)$$

$$=(-d/dx)\hat{\alpha}_{n-1}(x), \qquad (2.25)$$

$$\hat{\alpha}_0(x)=(-d/dx)\tilde{E}_1(x), \qquad (2.26)$$

$$\hat{\alpha}_n(x)=\tilde{E}_{-n}(x)\ (\text{by convention}), \qquad (2.27)$$

$$\tilde{E}_n(x+y)=\sum_{s=0}^{\infty}\frac{(-y)^s\tilde{E}_{n-s}(x)}{s!} \qquad (|y|<\infty); \qquad (2.28)$$

the logarithmic derivative of the gamma function,

$$\psi(n)=(d/dn)\log\Gamma(n); \qquad (2.29)$$

the Condon–Shortley coefficients,[5]

$$c^\lambda(l_1m_1;l_2m_2)=[4\pi/(2\lambda+1)]^{1/2}\times\int d\Omega\, Y_{l_1}^{m_1 *}Y_{l_2}^{m_2}Y_{\lambda}^{m_1-m_2}, \qquad (2.30)$$

which are nonzero only when

$$l_1+l_2+\lambda \text{ is even} \qquad (2.31)$$

and

$$|l_1-l_2|\leq\lambda\leq l_1+l_2; \qquad (2.32)$$

and the standard expansion,

$$\exp(i\mathbf{k}\cdot\mathbf{r})=4\pi\sum_{l=0}^{\infty}i^l j_l(kr)\sum_{m=-l}^{l}Y_l^{m*}(\theta,\varphi)Y_l^m(\theta_k,\varphi_k). \qquad (2.33)$$

Often we use both Cartesian and spherical polar coordinates for the same vector, e.g., $\mathbf{r}$, $\mathbf{k}$, $\mathbf{R}$, etc., correspond to (r,θ,φ), (k,θ_k,φ_k), (R,θ_R,φ_R), etc.

We often meet the expression, $(x^{-1}d/dx)^l x^{-1}$, which has the expansion

$$\left(x^{-1}\frac{d}{dx}\right)^l x^{-1}=\sum_{\mu=0}^{l}\begin{bmatrix} l\\ \mu\end{bmatrix}(-1)^\mu x^{-l-\mu-1}\left(\frac{d}{dx}\right)^{l-\mu}, \qquad (2.34)$$

where

$$\begin{bmatrix} l\\ \mu\end{bmatrix}=\frac{(l+\mu)!}{(l-\mu)!(2\mu)!!}. \qquad (2.35)$$

In addition to

$$\begin{bmatrix} l\\ \mu\end{bmatrix},$$

we define several special symbols which appear repeatedly: the 3-Λ symbol,

$$\begin{pmatrix}\Lambda_1\\ \Lambda_2\Lambda_3\end{pmatrix}=\frac{(2\Lambda_1-1)!!}{(2\Lambda_2+1)!!(2\Lambda_3+1)!!}; \qquad (2.36)$$

the symbol $\{\cdots F_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}$,

$$\{\cdots F_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\equiv\left[\left(-\frac{d}{d\zeta_b}\right)^{n_b-l_b}\left(\zeta_b^{-1}\frac{d}{d\zeta_b}\right)^{l_b}\zeta_b^{l_1+l_b+1}F_{\lambda_1}(\zeta_b\mathcal{R}_1)\left(\zeta_b^{-1}\frac{d}{d\zeta_b}\right)^{l_1}\zeta_b^{-1}\left(-\frac{d}{d\zeta_a}\right)^{n_a+\Delta_1-l_1}\mathcal{R}_1^{-2\Delta_1}\right], \qquad (2.37)$$

$$\doteq[\cdots F_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots]\mathcal{R}_1^{-n_a-\Delta_1+l_1}(-d/d\zeta_a)^{n_a+\Delta_1-l_1}, \qquad (2.38)$$

where F will be either $\mathcal{I}$ or $\mathcal{K}$, and where the $[\cdots F\cdots]$ was used in Paper III. The $\{\cdots F\cdots\}$ will also be used with subscripts 2, c, d instead of 1, a, b.

We define via integrals certain special functions, in terms of which the four-center integral will be expressed. The evaluation of these special functions in terms of simpler functions is postponed to Sec. V;

$$\mathfrak{A}(\Lambda_3, R; \Lambda_2, \zeta_2, \mathfrak{R}_2; \Lambda_1, \zeta_1, \mathfrak{R}_1) \equiv (2\pi i)^{-1} \int_{\infty}^{(\zeta_1^+)} dx \mathcal{K}_{\Lambda_3}(xR) x^{\Lambda_1+\Lambda_2}$$

$$\times\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_2} x^{-1}\{E_{2\Lambda_2+1}[(\zeta_2-x)\mathfrak{R}_2]-\mathfrak{R}_2^{2\Lambda_2}(R-\mathfrak{R}_1)^{-2\Lambda_2}E_{2\Lambda_2+1}[(\zeta_2-x)(R-\mathfrak{R}_1)]\}$$

$$\times\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_1} x^{-1}\mathfrak{R}_1^{2\Lambda_1}(\zeta_1-x)^{2\Lambda_1}\frac{\log(\zeta_1-x)}{(2\Lambda_1)!}, \quad (2.39)$$

$$A_2(\Lambda_3, R; \Lambda_1, \zeta_a\pm\zeta_b, \mathfrak{R}_1; \Lambda_2, \zeta_2, \mathfrak{R}_2) \equiv (2\pi i)^{-1} \int_{\infty}^{(\zeta_2^+)} dx \mathcal{K}_{\Lambda_3}(xR) x^{\Lambda_1+\Lambda_2}\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_1} x^{-1}$$

$$\times\{\tilde{E}_{2\Lambda_1+1}[(\zeta_a+\zeta_b+x)\mathfrak{R}_1]-\tilde{E}_{2\Lambda_1+1}[(\zeta_a+\zeta_b-x)\mathfrak{R}_1]-\tilde{E}_{2\Lambda_1+1}[(\zeta_a-\zeta_b+x)\mathfrak{R}_1]+\tilde{E}_{2\Lambda_1+1}[(\zeta_a-\zeta_b-x)\mathfrak{R}_1]\}$$

$$\times\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_2} x^{-1}\mathfrak{R}_2^{2\Lambda_2}(\zeta_2-x)^{2\Lambda_2}\frac{\log(\zeta_2-x)}{(2\Lambda_2)!}, \quad (2.40)$$

$$\hat{A}_4(\Lambda_3, R; \Lambda_1, \zeta_a\pm\zeta_b, \mathfrak{R}_1; \Lambda_2, \zeta_c\pm\zeta_d, \mathfrak{R}_2) \equiv (2\pi i)^{-1} \int_{\infty}^{[(-\zeta_c-\zeta_d)^+]} dx \mathcal{K}_{\Lambda_3}(xR) x^{\Lambda_1+\Lambda_2}$$

$$\times\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_1} x^{-1}\{\tilde{E}_{2\Lambda_1+1}[(\zeta_a+\zeta_b+x)\mathfrak{R}_1]-\tilde{E}_{2\Lambda_1+1}[(\zeta_a+\zeta_b-x)\mathfrak{R}_1]-\tilde{E}_{2\Lambda_1+1}[(\zeta_a-\zeta_b+x)\mathfrak{R}_1]+\tilde{E}_{2\Lambda_1+1}[(\zeta_a-\zeta_b-x)\mathfrak{R}_1]\}$$

$$\times\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_2} x^{-1}\mathfrak{R}_2^{2\Lambda_2}[(2\Lambda_2)!]^{-1}\{(\zeta_c+\zeta_d-x)^{2\Lambda_2}\log(\zeta_c+\zeta_d-x)-(\zeta_c-\zeta_d-x)^{2\Lambda_2}\log(\zeta_c-\zeta_d-x)\}, \quad (2.41)$$

$$\mathfrak{B}(\Lambda_3, R; \Lambda_1, \zeta_1, \mathfrak{R}_1; \Lambda_2, \zeta_2, \mathfrak{R}_2) \equiv (2\pi i)^{-1}(-1)^{\Lambda_3+1}\mathfrak{R}_1^{2\Lambda_1}(R+\mathfrak{R}_2)^{-2\Lambda_1} \int_{\infty}^{(\zeta_2^+)} dx \mathcal{K}_{\Lambda_3}(-xR) x^{\Lambda_1+\Lambda_2}\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_1} x^{-1}$$

$$\times E_{2\Lambda_1+1}[(\zeta_1+x)(R+\mathfrak{R}_2)]\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_2} x^{-1}\mathfrak{R}_2^{2\Lambda_2}(\zeta_2-x)^{2\Lambda_2}\frac{\log(\zeta_2-x)}{(2\Lambda_2)!}, \quad (2.42)$$

$$B(\Lambda_3, R; \Lambda_1, \zeta_1, \mathfrak{R}_1; \Lambda_2, \zeta_2, \mathfrak{R}_2) \equiv (2\pi i)^{-1} \int_{\infty}^{(\zeta_2^+)} dx \mathcal{I}_{\Lambda_3}(xR) x^{\Lambda_1+\Lambda_2}\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_1} x^{-1}E_{2\Lambda_1+1}[(\zeta_1+x)\mathfrak{R}_1]$$

$$\times\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_2} x^{-1}\mathfrak{R}_2^{2\Lambda_2}(\zeta_2-x)^{2\Lambda_2}\frac{\log(\zeta_2-x)}{(2\Lambda_2)!}, \quad (2.43)$$

$$C_2(\Lambda_3, R; \Lambda_1, \zeta_a\pm\zeta_b, \mathfrak{R}_1; \Lambda_2, \zeta_2, \mathfrak{R}_2) \equiv (2\pi i)^{-1} \int_{\infty}^{[(-\zeta_a-\zeta_b-\zeta_c-\zeta_d)^+]} dx \mathcal{K}_{\Lambda_3}(xR)$$

$$\times x^{\Lambda_1+\Lambda_2}\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_1} x^{-1}\{E_{2\Lambda_1+1}[(\zeta_2+\zeta_b+x)\mathfrak{R}_1]-E_{2\Lambda_1+1}[(\zeta_a-\zeta_b+x)\mathfrak{R}_1]\}\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_2} x^{-1}E_{2\Lambda_2+1}[(\zeta_2-x)\mathfrak{R}_2], \quad (2.44)$$

$$\tilde{C}_2(\Lambda_3, R; \Lambda_1, \zeta_a\pm\zeta_b, \mathfrak{R}_1; \Lambda_2, \zeta_2, \mathfrak{R}_2) \equiv (2\pi i)^{-1} \int_{\infty}^{[(-\zeta_a-\zeta_b-\zeta_c-\zeta_d)^+]} dx \mathcal{K}_{\Lambda_3}(xR)$$

$$\times x^{\Lambda_1+\Lambda_2}\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_1} x^{-1}\{\tilde{E}_{2\Lambda_1+1}[(\zeta_a+\zeta_b+x)\mathfrak{R}_1]-\tilde{E}_{2\Lambda_1+1}[(\zeta_a-\zeta_b+x)\mathfrak{R}_1]\}\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_2} x^{-1}E_{2\Lambda_2+1}[(\zeta_2-x)\mathfrak{R}_2], \quad (2.45)$$

$$C_2{}^l(\Lambda_3, R; \Lambda_1, \zeta_a\pm\zeta_b, \mathcal{R}_1; \Lambda_2, \zeta_2, \mathcal{R}_2) = (2\pi i)^{-1}\int_\infty^{[(-\zeta_a-\zeta_b-\zeta_c-\zeta_d)^+]} dx\mathcal{K}_{\Lambda_3}(xR)$$

$$\times x^{\Lambda_1+\Lambda_2}\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_1} x^{-1}\mathcal{R}_1{}^{2\Lambda_1}\frac{\{(\zeta_a+\zeta_b+x)^{2\Lambda_1}\log(\zeta_a+\zeta_b+x)-(\zeta_a-\zeta_b+x)^{2\Lambda_1}\log(\zeta_a-\zeta_b+x)\}}{(2\Lambda_1)!}$$

$$\times\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_2} x^{-1}E_{2\Lambda_2+1}[(\zeta_2-x)\mathcal{R}_2], \quad (2.46)$$

$$\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}C_2{}^l(\Lambda_3, R; \Lambda_1, \zeta_a\pm\zeta_b, \mathcal{R}_1; \Lambda_2, \zeta_2, \mathcal{R}_2) = \{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}$$

$$\times\{\tilde{C}_2(\Lambda_3, R; \Lambda_1, \zeta_a\pm\zeta_b, \mathcal{R}_1; \Lambda_2, \zeta_2, \mathcal{R}_2) - C_2(\Lambda_3, R; \Lambda_1, \zeta_a\pm\zeta_b, \mathcal{R}_1; \Lambda_2, \zeta_2, \mathcal{R}_2)\}, \quad (2.47)$$

$$C_4(\Lambda_3 R; \Lambda_1, \zeta_a\pm\zeta_b, \mathcal{R}_1; \Lambda_2, \zeta_c\pm\zeta_d, \mathcal{R}_2) = C_2(\Lambda_3 R; \Lambda_1, \zeta_a\pm\zeta_b, \mathcal{R}_1; \Lambda_2, \zeta_c+\zeta_d, \mathcal{R}_2)$$

$$-C_2(\Lambda_3 R; \Lambda_1, \zeta_a\pm\zeta_b, \mathcal{R}_1; \Lambda_2, \zeta_c-\zeta_d, \mathcal{R}_2), \quad (2.48)$$

$$\tilde{C}_4(\Lambda_3 R; \Lambda_1, \zeta_a\pm\zeta_b, \mathcal{R}_1; \Lambda_2, \zeta_c\pm\zeta_d, \mathcal{R}_2) = \tilde{C}_2(\cdots, \zeta_c+\zeta_d, \mathcal{R}_2) - \tilde{C}_2(\cdots, \zeta_c-\zeta_d, \mathcal{R}_2), \quad (2.49)$$

$$C_4{}^l(\Lambda_3, R; \Lambda_1, \zeta_a\pm\zeta_b, \mathcal{R}_1; \Lambda_2, \zeta_c\pm\zeta_d, \mathcal{R}_2) = C_2{}^l(\cdots, \zeta_c+\zeta_d, \mathcal{R}_2) - C_2{}^l(\cdots, \zeta_c-\zeta_d, \mathcal{R}_2). \quad (2.50)$$

III. FORMULATION

The four-center integral is defined by

$$I_{n_c l_c m_c \zeta_c, n_d l_d m_d \zeta_d; n_a l_a m_a \zeta_a, n_b l_b m_b \zeta_b}(\boldsymbol{\mathcal{R}}_1, \boldsymbol{\mathcal{R}}_2, \mathbf{R}) \equiv (N_a N_b N_c N_d)^{-1}\int dV_1 \int dV_2 r_{12}^{-1}[\Psi_{n_c l_c m_c \zeta_c}{}^*(\mathbf{r}_2)\Psi_{n_d l_d m_d \zeta_d}(\mathbf{r}_2-\boldsymbol{\mathcal{R}}_2)]^*$$

$$\times[\Psi_{n_a l_a m_a \zeta_a}{}^*(\mathbf{r}_1-\mathbf{R})\Psi_{n_b l_b m_b \zeta_b}(\mathbf{r}_1-\mathbf{R}-\boldsymbol{\mathcal{R}}_1)], \quad (3.1)$$

$$= I_{cd;ab}(\boldsymbol{\mathcal{R}}_1, \boldsymbol{\mathcal{R}}_2, \mathbf{R}). \quad (3.2)$$

Following the approach developed in Papers I–III, we use simultaneously the Fourier-transform convolution theorem, the expression for the Fourier-transform of a two-center charge distribution obtained by expanding one Slater-type orbital about the origin of the other, and the expression for $\exp(i\mathbf{k}\cdot\boldsymbol{\mathcal{R}})$ [Eq. (2.33)] to obtain

$$I_{cd;ab}(\boldsymbol{\mathcal{R}}_1, \boldsymbol{\mathcal{R}}_2, \mathbf{R}) = \sum_{l_1=0}^{\infty}\sum_{l_2=0}^{\infty}\sum_{m_1=-l_1}^{l_1}\sum_{m_2=-l_2}^{l_2}\sum_{\lambda_1=|l_1-l_b|}^{l_1+l_b}\sum_{\lambda_2=|l_2-l_d|}^{l_2+l_d}\sum_{\Lambda_1=|l_1-l_a|}^{l_1+l_a}\sum_{\Lambda_2=|l_2-l_c|}^{l_2+l_c}\sum_{\Lambda_3=|\Lambda_1-\Lambda_2|}^{\Lambda_1+\Lambda_2}[(2\lambda_1+1)(2\lambda_2+1)$$

$$\times(2\Lambda_1+1)(2\Lambda_2+1)(2\Lambda_3+1)4\pi^3]^{1/2}c^{\lambda_1}(l_b m_b; l_1 m_1)c^{\lambda_2}(l_d m_d; l_2 m_2)c^{\Lambda_1}(l_1 m_1; l_a m_a)c^{\Lambda_2}(l_2 m_2; l_c m_c)$$

$$\times c^{\Lambda_3}(\Lambda_1, m_1-m_a; \Lambda_2, m_2-m_c)Y_{\lambda_1}{}^{m_b-m_1}(\theta_{\mathcal{R}_1}, \varphi_{\mathcal{R}_1})Y_{\lambda_2}{}^{m_d-m_2}\gamma^*(\theta_{\mathcal{R}_2}, \varphi_{\mathcal{R}_2})Y_{\Lambda_3}{}^{m_1-m_2-m_a+m_c}(\theta_R, \varphi_R)$$

$$\times I_{cd;ab}{}^{l_1\lambda_1; l_2\lambda_2; \Lambda_1\Lambda_2; \Lambda_3}(\mathcal{R}_1, \mathcal{R}_2, R), \quad (3.3)$$

where the "radial function" is defined by

$$I_{cd;ab}{}^{l_1\lambda_1; l_2\lambda_2; \Lambda_1\Lambda_2; \Lambda_3}(\mathcal{R}_1, \mathcal{R}_2, R) = I_{cd;ab}{}^{\text{rad}} \quad (3.4)$$

$$= \tfrac{1}{4}\pi^{-3}(-1)^{\Lambda_2}i^{\Lambda_3}\int_{-\infty}^{\infty} dk j_{\Lambda_3}(kR)G_{l_1\lambda_1 l_b\Lambda_1}{}^{n_a\zeta_a n_b\zeta_b}(k, \mathcal{R}_1)G_{l_2\lambda_2 l_d\Lambda_2}{}^{n_c\zeta_c n_d\zeta_d}(k, \mathcal{R}_2), \quad (3.5)$$

and the G's are the "radial part" of the Fourier transform of the two-center charge distributions,

$$G_{l\lambda l_b\Lambda}{}^{n_a\zeta_a n_b\zeta_b}(k, \mathcal{R}) = 2\pi i^{\Lambda-1}(-1)^{\Lambda+\lambda}\{\cdots\mathcal{I}_\lambda(\zeta_b\mathcal{R})\cdots\}k^\Lambda(k^{-1}\,d/dk)^\Lambda k^{-1}\{E_{2\Lambda+1}[(\zeta_a+\zeta_b-ik)\mathcal{R}]$$

$$-E_{2\Lambda+1}[(\zeta_a+\zeta_b+ik)\mathcal{R}]\} + \pi i^{\Lambda-1}(-1)^\Lambda\{\cdots\mathcal{K}_\lambda(\zeta_b\mathcal{R})\cdots\}k^\Lambda(k^{-1}\,d/dk)^\Lambda k^{-1}\{\tilde{E}_{2\Lambda+1}[(\zeta_a+\zeta_b-ik)\mathcal{R}]$$

$$-\tilde{E}_{2\Lambda+1}[(\zeta_a+\zeta_b+ik)\mathcal{R}] - \tilde{E}_{2\Lambda+1}[(\zeta_a-\zeta_b-ik)\mathcal{R}] + \tilde{E}_{2\Lambda+1}[(\zeta_a-\zeta_b+ik)\mathcal{R}]\}. \quad (3.6)$$

Note that in Eq. (3.3) summations over l's, λ's, and Λ's have restrictions like Eqs. (2.31) and (2.32). The main difficulty in evaluating $I_{cd;ab}(\boldsymbol{\mathcal{R}}_1, \boldsymbol{\mathcal{R}}_2, \mathbf{R})$ is in evaluating the one-dimensional integral $I_{cd;ab}{}^{\text{rad}}$.

It is convenient to break $I_{cd;ab}{}^{\text{rad}}$ into four parts:

$$I_{cd;ab}{}^{\text{rad}} = I^{(1)} + I^{(2)} + I^{(3)} + I^{(4)}, \quad (3.7)$$

where

$$I^{(1)}\equiv(\pi i)^{-1}(-1)^{\Lambda_1+\lambda_1+\lambda_2}\mathcal{P}\int_{i\infty}^{-i\infty}dx\mathcal{K}_{\Lambda_3}(xR)\{\cdots\mathcal{I}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{I}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}$$
$$\times\left[x^{\Lambda_1}\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_1}x^{-1}\{E_{2\Lambda_1+1}[(\zeta_a+\zeta_b+x)\mathcal{R}_1]-E_{2\Lambda_1+1}[(\zeta_a+\zeta_b-x)\mathcal{R}_1]\}\right]$$
$$\times\left[x^{\Lambda_2}\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_2}x^{-1}\{E_{2\Lambda_2+1}[(\zeta_c+\zeta_d+x)\mathcal{R}_2]-E_{2\Lambda_2+1}[(\zeta_c+\zeta_d-x)\mathcal{R}_2]\}\right],\quad(3.8)$$

$$I^{(2)}\equiv(2\pi i)^{-1}(-1)^{\Lambda_1+\lambda_1}\mathcal{P}\int_{i\infty}^{-i\infty}dx\mathcal{K}_{\Lambda_3}(xR)\{\cdots\mathcal{I}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}$$
$$\times\left[x^{\Lambda_1}\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_1}x^{-1}\{E_{2\Lambda_1+1}[(\zeta_a+\zeta_b+x)\mathcal{R}_1]-E_{2\Lambda_1+1}[(\zeta_a+\zeta_b-x)\mathcal{R}_1]\}\right]$$
$$\times\left[x^{\Lambda_2}\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_2}x^{-1}\{\tilde{E}_{2\Lambda_2+1}[(\zeta_c+\zeta_d+x)\mathcal{R}_2]-\tilde{E}_{2\Lambda_2+1}[(\zeta_c+\zeta_d-x)\mathcal{R}_2]\right.$$
$$\left.-\tilde{E}_{2\Lambda_2+1}[(\zeta_c-\zeta_d+x)\mathcal{R}_2]+\tilde{E}_{2\Lambda_2+1}[(\zeta_c-\zeta_d-x)\mathcal{R}_2]\}\right],\quad(3.9)$$

$$I^{(3)}\equiv(2\pi i)^{-1}(-1)^{\Lambda_1+\lambda_2}\mathcal{P}\int_{i\infty}^{-i\infty}dx\mathcal{K}_{\Lambda_3}(xR)\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{I}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}$$
$$\times\left[x^{\Lambda_1}\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_1}x^{-1}\{\tilde{E}_{2\Lambda_1+1}[(\zeta_a+\zeta_b+x)\mathcal{R}_1]-\tilde{E}_{2\Lambda_1+1}[(\zeta_a+\zeta_b-x)\mathcal{R}_1]\right.$$
$$\left.-\tilde{E}_{2\Lambda_1+1}[(\zeta_a-\zeta_b+x)\mathcal{R}_1]+\tilde{E}_{2\Lambda_1+1}[(\zeta_a-\zeta_b-x)\mathcal{R}_1]\}\right]$$
$$\times\left[x^{\Lambda_2}\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_2}x^{-1}\{E_{2\Lambda_2+1}[(\zeta_c+\zeta_d+x)\mathcal{R}_2]-E_{2\Lambda_2+1}[(\zeta_c+\zeta_d-x)\mathcal{R}_2]\}\right],\quad(3.10)$$

$$I^{(4)}\equiv(4\pi i)^{-1}(-1)^{\Lambda_1}\mathcal{P}\int_{i\infty}^{-i\infty}dx\mathcal{K}_{\Lambda_3}(xR)\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}$$
$$\times\left[x^{\Lambda_1}\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_1}x^{-1}\{\tilde{E}_{2\Lambda_1+1}[(\zeta_a+\zeta_b+x)\mathcal{R}_1]-\tilde{E}_{2\Lambda_1+1}[(\zeta_a+\zeta_b-x)\mathcal{R}_1]\right.$$
$$\left.-\tilde{E}_{2\Lambda_1+1}[(\zeta_a-\zeta_b+x)\mathcal{R}_1]+\tilde{E}_{2\Lambda_1+1}[(\zeta_a-\zeta_b-x)\mathcal{R}_1]\}\right]$$
$$\times\left[x^{\Lambda_2}\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_2}x^{-1}\{\tilde{E}_{2\Lambda_2+1}[(\zeta_c+\zeta_b+x)\mathcal{R}_2]-\tilde{E}_{2\Lambda_2+1}[(\zeta_c+\zeta_d-x)\mathcal{R}_2]\right.$$
$$\left.-\tilde{E}_{2\Lambda_2+1}[(\zeta_c-\zeta_d+x)\mathcal{R}_2]-\tilde{E}_{2\Lambda_2+1}[(\zeta_c-\zeta_d-x)\mathcal{R}_2]\}\right],\quad(3.11)$$

and where $\mathcal{P}$ denotes the principal value (cf. I). Note that we have made the substitution

$$k=ix\quad(3.12)$$

and used the identity Eq. (2.6).

Evaluation of $I_{cd;ab}{}^{\text{rad}}$ is complicated by two considerations: the relative values of $\mathcal{R}_1$, $\mathcal{R}_2$, and R, which eventually determine the behavior of the integrand at infinity, and the logarithmic branch points in the integrand. Equations (3.8)–(3.11) represent a convenient starting point for discussion of these complications and resolution of the final integration in $I_{cd;ab}{}^{\text{rad}}$.

IV. EVALUATION OF $I_{cd;ab}{}^{\text{rad}}$

Our approach to the evaluation of $I_{cd;ab}{}^{\text{rad}}$, i.e., of the $I^{(i)}$ [Eqs. (3.8)–(3.11)] is to exploit as fully as possible contour integration techniques. In the three-

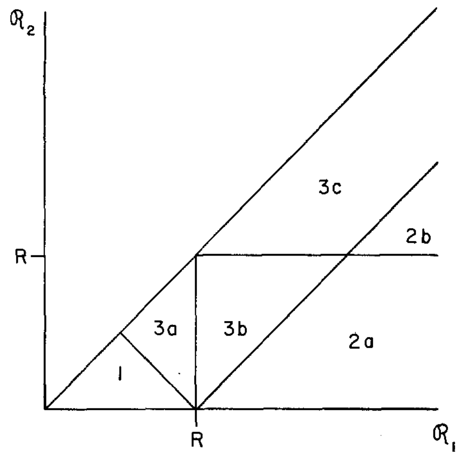

FIG. 1. The cases and subcases for which the various formulas for $I_{cd;ab}{}^{\rm rad}$ are valid.

center cases, Papers I–III, it was always possible to arrange for the integrands to vanish at infinity in a half-plane containing no singularity worse than a pole (i.e., no branch points). The contour was then closed at infinity and the integral evaluated by the residue theorem. In the four-center case, it does not seem possible in general[7] to use the residue theorem alone. There are always terms, no matter how the contours are deformed, which involve integrating around logarithmic branch cuts. These terms we have evaluated by convergent infinite expansions.

We note that the $I^{(i)}$ are functions of many variables. There is a great deal of flexibility in the choice of expansion variable, and we report here only selected choices.

We assume that the reader is familiar with Papers I and III, which discuss the method in detail. In this paper only a brief sketch outlines the path from the integration of Eq. (3.5) to the expression of $I_{cd;ab}{}^{\rm rad}$ in terms of simple functions.

A. Cases and Subcase Classified by Relative Values of $\mathcal{R}_1$, $\mathcal{R}_2$, and R

The manipulation of contours in Eqs. (3.8)–(3.11) requires knowledge of the behavior of the integrands at infinity. The building blocks of the integrands are E_n, $\tilde{E}_n$, and $\mathcal{K}_n$ functions, whose asymptotic behavior is given by Eqs. (2.19), (2.17), and (2.9). The behavior of the $I^{(i)}$ integrands depends on the relative values of $\mathcal{R}_1$, $\mathcal{R}_2$, and R. Without loss of generality, we assume $\mathcal{R}_1 \geq \mathcal{R}_2$; the identity [cf. Eqs. (3.4) and (3.5)]

$$I_{cd;ab}{}^{l_1\lambda_1;l_2\lambda_2;\Lambda_1\Lambda_2;\Lambda_3}(\mathcal{R}_1,\mathcal{R}_2,R) =(-1)^{\Lambda_3} I_{ab;cd}{}^{l_2\lambda_2;l_1\lambda_1;\Lambda_2\Lambda_1;\Lambda_3}(\mathcal{R}_2,\mathcal{R}_1,R) \quad (4.1)$$

can be used to reverse the roles of $\mathcal{R}_1$ and $\mathcal{R}_2$. Then, the way the various terms in the integrand vanish at infinity delineate the following three cases with five subcases (which are illustrated in Fig. 1):

Case 1. $R \geq \mathcal{R}_1+\mathcal{R}_2$,

Case 2. $\mathcal{R}_1 \geq R+\mathcal{R}_2$,

Subcases (a): $\mathcal{R}_1 \geq R \geq \mathcal{R}_2$,

(b): $\mathcal{R}_1 \geq \mathcal{R}_2 \geq R$,

Case 3. $\mathcal{R}_1-\mathcal{R}_2 \leq R \leq \mathcal{R}_1+\mathcal{R}_2$,

Subcases (a): $R \geq \mathcal{R}_1 \geq \mathcal{R}_2$,

(b): $\mathcal{R}_1 \geq R \geq \mathcal{R}_2$,

(c): $\mathcal{R}_1 \geq \mathcal{R}_2 \geq R$.

We treat the integration of $I_{cd;ab}{}^{\rm rad}$ case by case.

B. Case 1. $\mathcal{R}_1+\mathcal{R}_2 \leq R$

For Case 1, the integrands of all four $I^{(i)}$ are dominated at ∞ by $\mathcal{K}_{\Lambda_3}(xR)$. We deform the integration path to run from $\infty+i\epsilon$ to 0 to $\infty-i\epsilon$. We now treat each $I^{(i)}$ separately, reducing it to a linear combination of the functions given in Sec. II.

1. $I^{(1)}$

Regard $I^{(1)}$[Eq. (3.8)] as consisting of four terms. The term involving

$$\cdots E_{2\Lambda_1+1}[(\zeta_a+\zeta_b+x)\mathcal{R}_1]\cdots E_{2\Lambda_2+1}[(\zeta_c+\zeta_d+x)\mathcal{R}_2] \quad (4.2)$$

has no singularities in the right half-plane, where the integration contour can be closed, and contributes just a residue at $x=0$ to $I^{(1)}$. The term involving

$$\cdots E_{2\Lambda_1+1}[(\zeta_a+\zeta_b-x)\mathcal{R}_1]\cdots E_{2\Lambda_2+1}[(\zeta_c+\zeta_d-x)\mathcal{R}_2] \quad (4.3)$$

has two logarithmic branch cuts inside the integration contour. We use the identity

$$\int dx\mathcal{K}_{\Lambda_3}(xR)\cdots E_{2\Lambda_1+1}[(\zeta_a+\zeta_b-x)\mathcal{R}_1]\cdots E_{2\Lambda_2+1}[(\zeta_c+\zeta_d-x)\mathcal{R}_2]$$

$$= \int dx\mathcal{K}_{\Lambda_3}(xR)\cdots E_{2\Lambda_1+1}[(\zeta_a+\zeta_b-x)\mathcal{R}_1]\cdots\{E_{2\Lambda_2+1}[(\zeta_c+\zeta_d-x)\mathcal{R}_2] -\mathcal{R}_2{}^{2\Lambda_2}(R-\mathcal{R}_1)^{-2\Lambda_2}E_{2\Lambda_2+1}[(\zeta_c+\zeta_d-x)(R-\mathcal{R}_1)]\}+\int dx\mathcal{K}_{\Lambda_3}(xR)\cdots E_{2\Lambda_1+1}[(\zeta_a+\zeta_b-x)\mathcal{R}_1]\cdots\mathcal{R}_2{}^{2\Lambda_2}(R-\mathcal{R}_1)^{-2\Lambda_2} \times E_{2\Lambda_2+1}[(\zeta_c+\zeta_d-x)(R-\mathcal{R}_1)], \quad (4.4)$$

[7] For certain values of the parameters a few of the $I_{cd;ab}{}^{\rm rad}$ can be expressed in closed form via the residue theorem.

to cast the double logarithmic branch cut in a form [second term on right-hand side of Eq. (4.4)] which can be closed in the left half-plane, which has no singularities. The first term on the right in Eq. (4.4) is essentially an $\mathfrak{A}$ [Eq. (2.39)], and both terms give contributions from residues at $x=0$.

The term involving

$$\cdots E_{2\Lambda_1+1}[(\zeta_a+\zeta_b+x)\mathcal{R}_1]\cdots E_{2\Lambda_2+1}[(\zeta_c+\zeta_d-x)\mathcal{R}_2] \tag{4.5}$$

has one logarithmic branch cut enclosed by the contour and one outside. We use the identity

$$\int dx\mathcal{K}_{\Lambda_3}(xR)\cdots E_{2\Lambda_1+1}[(\zeta_a+\zeta_b+x)\mathcal{R}_1]\cdots E_{2\Lambda_2+1}[(\zeta_c+\zeta_d-x)\mathcal{R}_2]=\int dx\mathcal{K}_{\Lambda_3}(xR)\cdots E_{2\Lambda_1+1}[(\zeta_a+\zeta_b+x)\mathcal{R}_1]\cdots$$
$$\times\{E_{2\Lambda_2+1}[(\zeta_c+\zeta_d-x)\mathcal{R}_2]-\mathcal{R}_2^{2\Lambda_2}(R+\mathcal{R}_1)^{-2\Lambda_2}E_{2\Lambda_2+1}[(\zeta_c+\zeta_d-x)(R+\mathcal{R}_1)]\}$$
$$+\int dx\mathcal{K}_{\Lambda_3}(xR)\cdots E_{2\Lambda_1+1}[(\zeta_a+\zeta_b+x)\mathcal{R}_1]\cdots\mathcal{R}_2^{2\Lambda_2}(R+\mathcal{R}_1)^{-2\Lambda_2}E_{2\Lambda_2+1}[(\zeta_c+\zeta_d-x)(R+\mathcal{R}_1)]. \tag{4.6}$$

The first term on the right in Eq. (4.6) has no singularities in the right half-plane and contributes only a residue at $x=0$. The second term can be closed in the left half-plane, yielding (after letting $x\rightarrow -x$) a $\mathfrak{B}$ [Eq. (2.42)] plus a residue at $x=0$. The remaining term in $I^{(1)}$ which involves

$$\cdots E_{2\Lambda_1+1}[(\zeta_a+\zeta_b-x)\mathcal{R}_1]\cdots E_{2\Lambda_2+1}[(\zeta_c+\zeta_d+x)\mathcal{R}_2] \tag{4.7}$$

is treated the same way as the term in Eq. (4.5), *mutatis mutandis.*

With these considerations, $I^{(1)}$ is

$$I^{(1)}=2(-1)^{\Lambda_1+\lambda_1+\lambda_2}\{\cdots g_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots g_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}$$
$$\times\Bigg[\delta_{\Lambda_3,\Lambda_1+\Lambda_2}\binom{\Lambda_3}{\Lambda_1\Lambda_2}\mathcal{R}_1^{2\Lambda_1}\mathcal{R}_2^{2\Lambda_2}R^{-\Lambda_3-1}\{2\mathcal{R}_1\alpha_0[(\zeta_a+\zeta_b)\mathcal{R}_1]\mathcal{R}_2\alpha_0[(\zeta_c+\zeta_d)\mathcal{R}_2]-\mathcal{R}_1\alpha_0[(\zeta_a+\zeta_b)\mathcal{R}_1]$$
$$\times(R+\mathcal{R}_1)\alpha_0[(\zeta_c+\zeta_d)(R+\mathcal{R}_1)]-(R+\mathcal{R}_2)\alpha_0[(\zeta_a+\zeta_b)(R+\mathcal{R}_2)]\mathcal{R}_2\alpha_0[(\zeta_c+\zeta_d)\mathcal{R}_2]$$
$$-\mathcal{R}_1\alpha_0[(\zeta_a+\zeta_b)\mathcal{R}_1](R-\mathcal{R}_1)\alpha_0[(\zeta_c+\zeta_d)(R-\mathcal{R}_1)]\}+\delta_{\Lambda_3,\Lambda_1-\Lambda_2}(-1)^{\Lambda_2}\binom{\Lambda_1}{\Lambda_2\Lambda_3}\mathcal{R}_2^{2\Lambda_2}R^{\Lambda_3}$$
$$\times\big(-E_{2\Lambda_1+1}[(\zeta_a+\zeta_b)\mathcal{R}_1]\{(R+\mathcal{R}_1)\alpha_0[(\zeta_c+\zeta_d)(R+\mathcal{R}_1)]-(R-\mathcal{R}_1)\alpha_0[(\zeta_c+\zeta_d)(R-\mathcal{R}_1)]\}$$
$$+\mathcal{R}_1^{2\Lambda_1}(R+\mathcal{R}_2)^{-2\Lambda_1}E_{2\Lambda_1+1}[(\zeta_a+\zeta_b)(R+\mathcal{R}_2)]\mathcal{R}_2\alpha_0[(\zeta_c+\zeta_d)\mathcal{R}_2]\big)$$
$$+\delta_{\Lambda_3,\Lambda_2-\Lambda_1}(-1)^{\Lambda_1}\binom{\Lambda_2}{\Lambda_1\Lambda_3}\mathcal{R}_1^{2\Lambda_1}R^{\Lambda_3}\big(\mathcal{R}_1\alpha_0[(\zeta_a+\zeta_b)\mathcal{R}_1]\mathcal{R}_2^{2\Lambda_2}\{(R+\mathcal{R}_1)^{-2\Lambda_2}E_{2\Lambda_2+1}[(\zeta_c+\zeta_d)(R+\mathcal{R}_1)]$$
$$+(R-\mathcal{R}_1)^{-2\Lambda_2}E_{2\Lambda_2+1}[(\zeta_c+\zeta_d)(R-\mathcal{R}_1)]\}-(R+\mathcal{R}_2)\alpha_0[(\zeta_a+\zeta_b)(R+\mathcal{R}_2)]E_{2\Lambda_2+1}[(\zeta_c+\zeta_d)\mathcal{R}_2]\big)$$
$$+(-1)^{\Lambda_3}\sum_{\substack{\nu_1\geq 0}}\sum_{\nu_2\geq 0}\sum_{\nu_3\geq 0}{}_{[\nu_1+\nu_2+\nu_3=(\Lambda_1+\Lambda_2+\Lambda_3+2)/2]}R^{2\nu_3-\Lambda_3-1}[(2\nu_1)!!(2\nu_1-2\Lambda_1-1)!!(2\nu_2)!!(2\nu_2-2\Lambda_2-1)!!(2\nu_3)!!(2\nu_3-2\Lambda_3-1)!!]^{-1}$$
$$\times\{\mathcal{R}_1^{2\nu_1}E_{2\Lambda_1-2\nu_1+1}[(\zeta_a+\zeta_b)\mathcal{R}_1]\mathcal{R}_2^{2\Lambda_2}(R+\mathcal{R}_1)^{2\nu_2-2\Lambda_2}E_{2\Lambda_2-2\nu_2+1}[(\zeta_c+\zeta_d)(R+\mathcal{R}_1)]$$
$$-\mathcal{R}_1^{2\nu_1}E_{2\Lambda_1-2\nu_1+1}[(\zeta_a+\zeta_b)\mathcal{R}_1]\mathcal{R}_2^{2\Lambda_2}(R-\mathcal{R}_1)^{2\nu_2-2\Lambda_2}E_{2\Lambda_2-2\nu_2+1}[(\zeta_c+\zeta_d)(R-\mathcal{R}_1)]$$
$$+\mathcal{R}_1^{2\Lambda_1}(R+\mathcal{R}_2)^{2\nu_1-2\Lambda_1}E_{2\Lambda_1-2\nu_1+1}[(\zeta_a+\zeta_b)(R+\mathcal{R}_2)]\mathcal{R}_2^{2\nu_2}E_{2\Lambda_2-2\nu_2+1}[(\zeta_c+\zeta_d)\mathcal{R}_2]\}$$
$$-\mathfrak{A}(\Lambda_3,R;\Lambda_1,\zeta_a+\zeta_b,\mathcal{R}_1;\Lambda_2,\zeta_c+\zeta_d,\mathcal{R}_2)-\mathfrak{B}(\Lambda_3,R;\Lambda_1,\zeta_a+\zeta_b,\mathcal{R}_1;\Lambda_2,\zeta_c+\zeta_d,\mathcal{R}_2)$$
$$-\mathfrak{B}(\Lambda_3,R;\Lambda_2,\zeta_c+\zeta_d,\mathcal{R}_2;\Lambda_1,\zeta_a+\zeta_b,\mathcal{R}_1)\Bigg]\quad\text{(Case 1)}. \tag{4.8}$$

2. $I^{(2)}$ and $I^{(3)}$

In $I^{(2)}$, as well as $I^{(3)}$, there is only one logarithmic branch cut enclosed within the contour. Without further manipulation, they can be written as A_2's [Eq. (2.40)] plus residues for $x=0$:

$$I^{(2)}=(-1)^{\Lambda_1+\lambda_1}\{\cdots\mathcal{J}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}$$
$$\times\Big[2\delta_{\Lambda_3,\Lambda_1+\Lambda_2}\binom{\Lambda_3}{\Lambda_1\Lambda_2}\mathcal{R}_1^{2\Lambda_1+1}\mathcal{R}_2^{2\Lambda_2+1}R^{-\Lambda_3-1}\alpha_0[(\zeta_a+\zeta_b)\mathcal{R}_1]\{\hat{\alpha}_0[(\zeta_c+\zeta_d)\mathcal{R}_2]-\hat{\alpha}_0[(\zeta_c-\zeta_d)\mathcal{R}_2]\}$$
$$+A_2(\Lambda_3,R;\Lambda_2,\zeta_c\pm\zeta_d,\mathcal{R}_2;\zeta_a+\zeta_b,\mathcal{R}_1)\Big]\quad\text{(Case 1)},\qquad(4.9)$$

$$I^{(3)}=(-1)^{\Lambda_1+\lambda_2}\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{J}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}$$
$$\times\Big[2\delta_{\Lambda_3,\Lambda_1+\Lambda_2}\binom{\Lambda_3}{\Lambda_1\Lambda_2}\mathcal{R}_1^{2\Lambda_1+1}\mathcal{R}_2^{2\Lambda_2+1}R^{-\Lambda_3-1}\{\hat{\alpha}_0[(\zeta_a+\zeta_b)\mathcal{R}_1]-\hat{\alpha}_0[(\zeta_a-\zeta_b)\mathcal{R}_1]\}\alpha_0[(\zeta_c+\zeta_d)\mathcal{R}_2]$$
$$+A_2(\Lambda_3,R;\Lambda_1,\zeta_a\pm\zeta_b,\mathcal{R}_1;\Lambda_2,\zeta_c+\zeta_d,\mathcal{R}_2)\Big]\quad\text{(Case 1)}.\qquad(4.10)$$

3. $I^{(4)}$

The integrand of $I^{(4)}$ has no logarithmic singularities. The only contribution to $I^{(4)}$ in this case is from the residue at $x=0$:

$$I^{(4)}=(-1)^{\Lambda_1}\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}$$
$$\times\delta_{\Lambda_3,\Lambda_1+\Lambda_2}\binom{\Lambda_3}{\Lambda_1\Lambda_2}\mathcal{R}_1^{2\Lambda_1+1}\mathcal{R}_2^{2\Lambda_2+1}R^{-\Lambda_3-1}(\hat{\alpha}_0[(\zeta_a+\zeta_b)\mathcal{R}_1]-\hat{\alpha}_0[(\zeta_a-\zeta_b)\mathcal{R}_1])$$
$$\times(\hat{\alpha}_0[(\zeta_c+\zeta_d)\mathcal{R}_2]-\hat{\alpha}_0[(\zeta_c-\zeta_d)\mathcal{R}_2])\quad\text{(Case 1)}.\qquad(4.11)$$

C. Case 2. $R+\mathcal{R}_2\leq\mathcal{R}_1$

1. $I^{(1)}$

The integrand of $I^{(1)}$ [Eq. (3.8)] is dominated at ∞ by $E_{2\Lambda_1+1}[(\zeta_a+\zeta_b\pm x)\mathcal{R}_1]$. For the $(+x)$ term, the contour can be deformed to be $(\infty+i\epsilon, 0, \infty-i\epsilon)$, and for the $(-x)$ term, to be $(-\infty+i\epsilon, 0, -\infty-i\epsilon)$. After substitution of $-x$ for x, the latter term can be combined with the former by using Eq. (2.6) to yield a B [Eq. (2.43)] plus a residue at the origin:

$$I^{(1)}=4(-1)^{\Lambda_1+\lambda_1+\lambda_2}\{\cdots\mathcal{J}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{J}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}$$
$$\times\Big[\delta_{\Lambda_3,\Lambda_1-\Lambda_2}(-1)^{\Lambda_2}\binom{\Lambda_1}{\Lambda_2\Lambda_3}\mathcal{R}_2^{2\Lambda_2+1}R^{\Lambda_3}E_{2\Lambda_1+1}[(\zeta_a+\zeta_b)\mathcal{R}_1]\alpha_0[(\zeta_c+\zeta_d)\mathcal{R}_2]$$
$$-(-1)^{\Lambda_3}B(\Lambda_3,R;\Lambda_1,\zeta_a+\zeta_b,\mathcal{R}_1;\Lambda_2,\zeta_c+\zeta_d,\mathcal{R}_2)\Big]\quad\text{(Case 2)}.\qquad(4.12)$$

2. $I^{(2)}$

The integrand of $I^{(2)}$ is also dominated at ∞ by $E_{2\Lambda_1+1}[(\zeta_a+\zeta_b\pm x)\mathcal{R}_1]$, and the contour can be deformed accordingly, as for $I^{(1)}$. In this case, however, there are no logarithmic branch cuts enclosed by the contour, and the only contribution to the integral is from the residue at the origin. The result is

$$I^{(2)}=2(-1)^{\Lambda_1+\lambda_1}\{\cdots\mathcal{J}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}$$
$$\times\delta_{\Lambda_3,\Lambda_1-\Lambda_2}(-1)^{\Lambda_2}\binom{\Lambda_1}{\Lambda_2\Lambda_3}\mathcal{R}_2^{2\Lambda_2+1}R^{\Lambda_3}E_{2\Lambda_1+1}[(\zeta_a+\zeta_b)\mathcal{R}_1]\{\hat{\alpha}_0[(\zeta_c+\zeta_d)\mathcal{R}_2]-\hat{\alpha}_0[(\zeta_c-\zeta_d)\mathcal{R}_2]\}\quad\text{(Case 2)}.\qquad(4.13)$$

3. $I^{(3)}$

$I^{(3)}$ is slightly more complicated than $I^{(2)}$ for Case 2, because the $\tilde{E}_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b\pm x)\mathcal{R}_1]$, which contains the largest $\mathcal{R}$, has "mixed" asymptotic behavior [cf. Eqs. (2.19) and (2.17)]. The consequence is that Case 2 has two subcases, depending on the sign of $R-\mathcal{R}_2$. The contour for the term involving

$$\cdots\tilde{E}_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b+x)\mathcal{R}_1]\cdots E_{2\Lambda_2+1}[(\zeta_c+\zeta_d+x)\mathcal{R}_2] \tag{4.14}$$

for both subcases can be closed at $+\infty$ and contributes only a residue from $x=0$. To treat the term involving

$$\cdots\tilde{E}_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b-x)\mathcal{R}_1]\cdots E_{2\Lambda_2+1}[(\zeta_c+\zeta_d+x)\mathcal{R}_2], \tag{4.15}$$

first pull the contour to the right of $x=\zeta_a+\zeta_b$ [picking up a residue at $x=0$], then use

$$\tilde{E}_{2\Lambda_1+1}=E_{2\Lambda_1+1}+(\tilde{E}_{2\Lambda_1+1}-E_{2\Lambda_1+1}). \tag{4.16}$$

Note that the deformed contour passes to the right of the logarithmic branch cuts at $x=\zeta_a\pm\zeta_b$. The contour for the term in $I^{(3)}$ involving $E_{2\Lambda_1+1}$ in Eq. (4.16) can be deformed into $[-\infty+i\epsilon,\ (\zeta_a+\zeta_b)^-,\ -\infty-i\epsilon]$, which, after letting $x\rightarrow-x$, becomes a C_2 [Eq. (2.44)] plus a contribution from the residue at $x=0$. The contour for the integral containing the last term in Eq. (4.16) can be closed in the right half-plane, where there are no singularities to the right of the contour.

The term involving

$$\cdots\tilde{E}_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b+x)\mathcal{R}_1]\cdots E_{2\Lambda_2+1}[(\zeta_c+\zeta_d-x)\mathcal{R}_2] \tag{4.17}$$

must be treated differently for the two subcases. For Subcase 2a, $\mathcal{R}_2\leq R$, the contour can be deformed into $(\infty+i\epsilon,\ 0,\ \infty-i\epsilon)$, which is seen to be a $\tilde{C}_2$ [Eq. (2.45)] plus a residue at the origin. For Subcase 2b, first pull the contour to the left of $x=-(\zeta_a+\zeta_b)$ picking up a residue from $x=0$, then use Eq. (4.16), the net effect of which is to change $\tilde{E}_{2\Lambda_1+1}$ into $E_{2\Lambda_1+1}$ with the logarithmic branch cut to the right of the contour, then deform the contour into $[\infty+i\epsilon,\ (-\zeta_a-\zeta_b)^+,\ \infty-i\epsilon]$. The result is a C_2 [Eq. (2.44)].

Finally, the term involving

$$\cdots\tilde{E}_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b-x)\mathcal{R}_1]\cdots E_{2\Lambda_2+1}[(\zeta_c+\zeta_d-x)\mathcal{R}_2] \tag{4.18}$$

can be similarly treated. It gives a contribution from the residue at $x=0$ for both subcases, and in addition, a $C_2{}^l$ [Eq. (2.46)] for Subcase 2a.

The results are

$$\begin{aligned}I^{(3)}=(-1)^{\Lambda_1+\lambda_2}&\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{I}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}\\&\times\Bigg[2\delta_{\Lambda_3,\Lambda_2-\Lambda_1}(-1)^{\Lambda_1}\binom{\Lambda_2}{\Lambda_1\Lambda_3}\mathcal{R}_1{}^{2\Lambda_1+1}R^{\Lambda_3}(\hat{\alpha}_0[(\zeta_a+\zeta_b)\mathcal{R}_1]-\hat{\alpha}_0[(\zeta_a-\zeta_b)\mathcal{R}_1])E_{2\Lambda_2+1}[(\zeta_c+\zeta_d)\mathcal{R}_2]\\&-(-1)^{\Lambda_3}C_2(\Lambda_3,-R;\Lambda_1,\zeta_a\pm\zeta_b,\mathcal{R}_1;\Lambda_2,\zeta_c+\zeta_d,\mathcal{R}_2)-\tilde{C}_2(\Lambda_3,R;\Lambda_1,\zeta_a\pm\zeta_b,\mathcal{R}_1;\Lambda_2,\zeta_c+\zeta_d,\mathcal{R}_2)\\&+C_2{}^l(\Lambda_3,R;\Lambda_1,-\zeta_a\mp\zeta_b,\mathcal{R}_1;\Lambda_2,\zeta_c+\zeta_d,\mathcal{R}_2)\Bigg]\quad(\text{Subcase 2a, }\mathcal{R}_2\leq R),\end{aligned} \tag{4.19}$$

$$\begin{aligned}I^{(3)}=(-1)^{\Lambda_1+\lambda_2}&\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{I}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}\Bigg[2\delta_{\Lambda_3,\Lambda_2-\Lambda_1}(-1)^{\Lambda_1}\binom{\Lambda_2}{\Lambda_1\Lambda_3}\mathcal{R}_1{}^{2\Lambda_1+1}R^{\Lambda_3}\\&\times\{\hat{\alpha}_0[(\zeta_a+\zeta_b)\mathcal{R}_1]-\hat{\alpha}_0[(\zeta_a-\zeta_b)\mathcal{R}_1]\}E_{2\Lambda_2+1}[(\zeta_c+\zeta_d)\mathcal{R}_2]\\&-(-1)^{\Lambda_3}C_2(\Lambda_3,-R;\Lambda_1,\zeta_a\pm\zeta_b,\mathcal{R}_1;\Lambda_2,\zeta_c+\zeta_d,\mathcal{R}_2)\\&-C_2(\Lambda_3,R;\Lambda_1,\zeta_a\pm\zeta_b,\mathcal{R}_1;\Lambda_2,\zeta_c+\zeta_d,\mathcal{R}_2)\Bigg]\quad(\text{Subcase 2b, }\mathcal{R}_2\geq R).\end{aligned} \tag{4.20}$$

4. $I^{(4)}$

Subcase 2a is straightforward. The contour for all terms involving $\tilde{E}_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b+x)\mathcal{R}_1]$ can be closed at $x=+\infty$, and only residues from $x=0$ contribute to the integral. For the remaining terms, one uses Eq. (2.17) for $\tilde{E}_{2\Lambda_1+1}$. The contour for the "$E_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b-x)\mathcal{R}_1]$" terms can be closed at $x=-\infty$, yielding only a residue at $x=0$, and the "$\log(\zeta_a\pm\zeta_b-x)$" terms give essentially an $\hat{A}_4$ [Eq. (2.41)] plus a residue at $x=0$.

The treatment of Case 2b, $R\leq\mathcal{R}_2$, involves the following maneuvers: For the

$$\cdots\tilde{E}_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b+x)\mathcal{R}_1]\cdots\tilde{E}_{2\Lambda_2+1}[(\zeta_c\pm\zeta_d+x)\mathcal{R}_2] \tag{4.21}$$

term, close contour at $x=+\infty$ to obtain the residue contribution from $x=0$. For the $(+x\mathcal{R}_1)(-x\mathcal{R}_2)$ terms, pull the contour to the right of $x=\zeta_c+\zeta_d$ [picking up a residue from $x=0$], then use

$$\begin{aligned}\cdots\tilde{E}_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b+x)\mathcal{R}_1]\cdots\tilde{E}_{2\Lambda_2+1}[(\zeta_c\pm\zeta_d-x)\mathcal{R}_2]\\=\cdots\mathcal{R}_1^{2\Lambda_1}(\zeta_a\pm\zeta_b+x)^{2\Lambda_1}\log(\zeta_a\pm\zeta_b+x)/(2\Lambda_1)!\cdots E_{2\Lambda_2+1}[(\zeta_c\pm\zeta_d-x)\mathcal{R}_2]\\+\{\cdots\tilde{E}_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b+x)\mathcal{R}_1]\cdots\tilde{E}_{2\Lambda_2+1}[(\zeta_c\pm\zeta_d-x)\mathcal{R}_2]\\-\cdots\mathcal{R}_1^{2\Lambda_1}(\zeta_a\pm\zeta_b+x)^{2\Lambda_1}\log(\zeta_a\pm\zeta_b+x)/(2\Lambda_1)!\cdots E_{2\Lambda_2+1}[(\zeta_c\pm\zeta_d-x)\mathcal{R}_2]\}.\qquad(4.22)\end{aligned}$$

The integral over the bracketed terms in Eq. (4.22) vanishes, because the contour can be closed at $x=\infty$ and does not enclose any singularities. The contour for the integral over the first term on the right of Eq. (4.22) can be deformed to $[-\infty+i\epsilon,\ (\zeta_c+\zeta_d)^-,\ -\infty-i\epsilon]$, which, after letting $x\to-x$, is seen to be a $C_4{}^l$ [Eq. (2.46)].

Finally, we consider the remaining terms together. By virtue of the derivatives $(x^{-1}d/dx)^{\Lambda_2}x^{-1}$, in the integrand of $I^{(4)}$ [Eq. (3.11)], there is an identity [cf. I, Eq. (48)],

$$\begin{aligned}\mathcal{P}\int dx\mathcal{K}_{\Lambda_3}(xR)\cdots\tilde{E}_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b-x)\mathcal{R}_1](x^{-1}d/dx)^{\Lambda_2}x^{-1}\{\tilde{E}_{2\Lambda_2+1}[(\zeta_c\pm\zeta_d+x)\mathcal{R}_2]-\tilde{E}_{2\Lambda+1}[(\zeta_c\pm\zeta_d-x)\mathcal{R}_2]\}\\=\mathcal{P}\int dx\mathcal{K}_{\Lambda_3}(xR)\cdots\tilde{E}_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b-x)\mathcal{R}_1](x^{-1}d/dx)^{\Lambda_2}x^{-1}\\\times\mathcal{R}_2^{2\Lambda_2}R^{-2\Lambda_2}\{\tilde{E}_{2\Lambda_2+1}[(\zeta_c\pm\zeta_d+x)R]-\tilde{E}_{2\Lambda_2+1}[(\zeta_c\pm\zeta_d-x)R]\}\\+\mathcal{P}\int dx\mathcal{K}_{\Lambda_3}(xR)\cdots\tilde{E}_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b-x)\mathcal{R}_1](x^{-1}d/dx)^{\Lambda_2}x^{-1}\\\times\{E_{2\Lambda_2+1}[(\zeta_c\pm\zeta_d+x)\mathcal{R}_2]-\mathcal{R}_2^{2\Lambda_2}R^{-2\Lambda_2}E_{2\Lambda_2+1}[(\zeta_c\pm\zeta_d+x)R]\}\\-\mathcal{P}\int dx\mathcal{K}_{\Lambda_3}(xR)\cdots\tilde{E}_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b-x)\mathcal{R}_1](x^{-1}d/dx)^{\Lambda_2}x^{-1}\\\times\{E_{2\Lambda_2+1}[(\zeta_c\pm\zeta_d-x)\mathcal{R}_2]-\mathcal{R}_2^{2\Lambda_2}R^{-2\Lambda_2}E_{2\Lambda_2+1}[(\zeta_c\pm\zeta_d-x)R]\}.\qquad(4.23)\end{aligned}$$

The first integral on the right in Eq. (4.23) is treated as in Case 2a, and yields an $\hat{A}_4$ plus a residue at $x=0$. The second integral on the right in Eq. (4.23) is treated by substituting Eq. (2.17) for $\tilde{E}_{2\Lambda_1+1}$, closing the contour for $E_{2\Lambda_1+1}$ on the left, and deforming the contour for the "log" part to $[\infty+i\epsilon,\ (-\zeta_c-\zeta_d)^+,\ \infty-i\epsilon]$, yielding contributions from residues at $x=0$ and the difference of two $C_4{}^l$'s [Eq. (2.46)]. The contour for the last integral in (4.23) is closed at $x=-\infty$ and yields just a contribution from $x=0$:

$$\begin{aligned}I^{(4)}=\tfrac{1}{2}(-1)^{\Lambda_1}\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}\\\times\bigg[2\delta_{\Lambda_3,\Lambda_1-\Lambda_2}(-1)^{\Lambda_2}\begin{pmatrix}\Lambda_1\\\Lambda_2\Lambda_3\end{pmatrix}\mathcal{R}_2^{2\Lambda_2+1}R^{\Lambda_3}\{\tilde{E}_{2\Lambda_1+1}[(\zeta_a+\zeta_b)\mathcal{R}_1]-\tilde{E}_{2\Lambda_1+1}[(\zeta_a-\zeta_b)\mathcal{R}_1]\}\{\hat{\alpha}_0[(\zeta_c+\zeta_d)\mathcal{R}_2]-\hat{\alpha}_0[(\zeta_c-\zeta_d)\mathcal{R}_2]\}\\-\hat{A}_4(\Lambda_3,R;\Lambda_2,\zeta_c\pm\zeta_d,\mathcal{R}_2;\Lambda_1,\zeta_a\pm\zeta_b,\mathcal{R}_1)\bigg]\quad(\text{Subcase 2a, }\mathcal{R}_2\leq R),\qquad(4.24)\end{aligned}$$

$$\begin{aligned}I^{(4)}=\tfrac{1}{2}(-1)^{\Lambda_1}\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}\\\times\bigg[2\delta_{\Lambda_3,\Lambda_1-\Lambda_2}(-1)^{\Lambda_2}\begin{pmatrix}\Lambda_1\\\Lambda_2\Lambda_3\end{pmatrix}\mathcal{R}_2^{2\Lambda_2+1}R^{\Lambda_3}\{\tilde{E}_{2\Lambda_1+1}[(\zeta_a+\zeta_b)\mathcal{R}_1]-\tilde{E}_{2\Lambda_1+1}[(\zeta_a-\zeta_b)\mathcal{R}_1]\}\{\hat{\alpha}_0[(\zeta_c+\zeta_d)\mathcal{R}_2]-\hat{\alpha}_0[(\zeta_c-\zeta_d)\mathcal{R}_2]\}\\-\mathcal{R}_2^{2\Lambda_2}R^{-2\Lambda_2}\hat{A}_4(\Lambda_3,R;\Lambda_2,\zeta_c\pm\zeta_d,R;\Lambda_1,\zeta_a\pm\zeta_b,\mathcal{R}_1)\\-C_4{}^l(\Lambda_3,R;\Lambda_1,-\zeta_a\mp\zeta_b,\mathcal{R}_1;\Lambda_2,-\zeta_c\mp\zeta_d,-\mathcal{R}_2)\\+\mathcal{R}_2^{2\Lambda_2}R^{-2\Lambda_2}C_4{}^l(\Lambda_3,R;\Lambda_1,-\zeta_a\mp\zeta_b,\mathcal{R}_1;\Lambda_2,-\zeta_c\mp\zeta_d,-R)\\-(-1)^{\Lambda_3}C_4{}^l(\Lambda_3,-R;\Lambda_1,-\zeta_a\mp\zeta_b,\mathcal{R}_1;\Lambda_2,-\zeta_c\mp\zeta_d,-\mathcal{R}_2)\bigg]\quad(\text{Subcase 2b, }\mathcal{R}_2\geq R).\qquad(4.25)\end{aligned}$$

D. Case 3

1. $I^{(1)}$

The treatment of $I^{(1)}$ is exactly the same for Case 3 as for Case 1, except that the contour for the term involving

$$\cdots E_{2\Lambda_1+1}[(\zeta_a+\zeta_b-x)\mathcal{R}_1]\cdots E_{2\Lambda_2+1}[(\zeta_c+\zeta_d-x)\mathcal{R}_2] \tag{4.26}$$

can be closed at $x=-\infty$, yielding only a residue at the origin and no $\mathfrak{A}$. The result is:

$$I^{(1)}=2(-1)^{\Lambda_1+\lambda_1+\lambda_2}\{\cdots\mathcal{J}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{J}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}$$
$$\times\Big[\delta_{\Lambda_3,\Lambda_1+\Lambda_2}\binom{\Lambda_3}{\Lambda_1\Lambda_2}R_1^{2\Lambda_1}\mathcal{R}_2^{2\Lambda_2}R^{-\Lambda_3-1}\big(\mathcal{R}_1\alpha_0[(\zeta_a+\zeta_b)\mathcal{R}_1]\{\mathcal{R}_2\alpha_0[(\zeta_c+\zeta_d)\mathcal{R}_2]-(R+\mathcal{R}_1)\alpha_0[(\zeta_c+\zeta_d)(R+\mathcal{R}_1)]\}$$
$$-(R+\mathcal{R}_2)\alpha_0[(\zeta_a+\zeta_b)(R+\mathcal{R}_2)]\mathcal{R}_2\alpha_0[(\zeta_c+\zeta_d)\mathcal{R}_2]\big)+\delta_{\Lambda_3,\Lambda_1-\Lambda_2}(-1)^{\Lambda_2}\binom{\Lambda_1}{\Lambda_2\Lambda_3}\mathcal{R}_2^{2\Lambda_2}R^{\Lambda_3}$$
$$\times\big(E_{2\Lambda_1+1}[(\zeta_a+\zeta_b)\mathcal{R}_1]\{\mathcal{R}_2\alpha_0[(\zeta_c+\zeta_d)\mathcal{R}_2]-(R+\mathcal{R}_1)\alpha_0[(\zeta_c+\zeta_d)(R+\mathcal{R}_1)]\}$$
$$+\mathcal{R}_1^{2\Lambda_1}(R+\mathcal{R}_2)^{-2\Lambda_1}E_{2\Lambda_1+1}[(\zeta_a+\zeta_b)(R+\mathcal{R}_2)]\mathcal{R}_2\alpha_0[(\zeta_c+\zeta_d)\mathcal{R}_2]\big)+\delta_{\Lambda_3,\Lambda_2-\Lambda_1}(-1)^{\Lambda_1}\binom{\Lambda_2}{\Lambda_1\Lambda_3}\mathcal{R}_1^{2\Lambda_1}R^{\Lambda_3}$$
$$\times\big(\mathcal{R}_1\alpha_0[(\zeta_a+\zeta_b)\mathcal{R}_1]\{E_{2\Lambda_2+1}[(\zeta_c+\zeta_d)\mathcal{R}_2]+\mathcal{R}_2^{2\Lambda_2}(R+\mathcal{R}_1)^{-2\Lambda_2}E_{2\Lambda_2+1}[(\zeta_c+\zeta_d)(R+\mathcal{R}_1)]\}$$
$$-(R+\mathcal{R}_2)\alpha_0[(\zeta_a+\zeta_b)(R-\mathcal{R}_2)]E_{2\Lambda_2+1}[(\zeta_c+\zeta_d)\mathcal{R}_2]\big)$$
$$-(-1)^{\Lambda_3}\sum_{\substack{\nu_1\geq0\\ [\nu_1+\nu_2+\nu_3=(\Lambda_1+\Lambda_2+\Lambda_3+2)/2]}}\sum_{\nu_2\geq0}\sum_{\nu_3\geq0}R^{2\nu_3-\Lambda_3-1}[(2\nu_1)!!(2\nu_1-2\Lambda_1-1)!!(2\nu_2)!!(2\nu_2-2\Lambda_2-1)!!(2\nu_3)!!(2\nu_3-2\Lambda_3-1)!!]^{-1}$$
$$\times\{\mathcal{R}_1^{2\nu_1}E_{2\Lambda_1-2\nu_1+1}[(\zeta_a+\zeta_b)\mathcal{R}_1]\mathcal{R}_2^{2\nu_2}E_{2\Lambda_2-2\nu_2+1}[(\zeta_c+\zeta_d)\mathcal{R}_2]$$
$$-\mathcal{R}_1^{2\nu_1}E_{2\Lambda_1-2\nu_1+1}[(\zeta_a+\zeta_b)\mathcal{R}_1]\mathcal{R}_2^{2\Lambda_2}(R+\mathcal{R}_1)^{2\nu_2-2\Lambda_2}E_{2\Lambda_2-2\nu_2+1}[(\zeta_c+\zeta_d)(R+\mathcal{R}_1)]$$
$$-\mathcal{R}_1^{2\Lambda_1}(R+\mathcal{R}_2)^{2\nu_1-2\Lambda_1}E_{2\Lambda_1-2\nu_1+1}[(\zeta_a+\zeta_b)(R+\mathcal{R}_2)]\mathcal{R}_2^{2\nu_2}E_{2\Lambda_2-2\nu_2+1}[(\zeta_c+\zeta_d)\mathcal{R}_2]\}$$
$$-\mathfrak{B}(\Lambda_3,R;\Lambda_1,\zeta_a+\zeta_b,\mathcal{R}_1;\Lambda_2,\zeta_c+\zeta_d,\mathcal{R}_2)$$
$$-\mathfrak{B}(\Lambda_3,R;\Lambda_2,\zeta_c+\zeta_d,\mathcal{R}_2;\Lambda_1,\zeta_a+\zeta_b,\mathcal{R}_1)\Big]\quad\text{(Case 3).} \tag{4.27}$$

2. $I^{(2)}$ and $I^{(3)}$

Both $I^{(2)}$ and $I^{(3)}$ can be treated in the same manner. Consider first $I^{(3)}$. The treatment for Cases 3a and 3b is exactly the same as for Case 2a, except for the term involving

$$\cdots\tilde{E}_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b-x)\mathcal{R}_1]\cdots E_{2\Lambda_2+1}[(\zeta_c+\zeta_d+x)\mathcal{R}_2]. \tag{4.28}$$

In the present case, the contour for this term can be closed at $x=+\infty$, yielding just a residue at $x=0$, whereas in Case 2a, part of this term led to a C_2. Precisely the same considerations hold for $I^{(3)}$ in Case 3c versus Case 2b.

Next consider $I^{(2)}$. It is easily seen that $I^{(2)}$ in Case 3a behaves like $I^{(3)}$ in Cases 3a and 3b, and $I^{(2)}$ in Cases 3b and 3c, like $I^{(3)}$ in Case 3c. Also, ζ_a, $\mathcal{R}_1$, etc., are interchanged with ζ_c, $\mathcal{R}_2$, etc.

The results are:

$$I^{(2)}=(-1)^{\Lambda_1+\lambda_1}\{\cdots\mathcal{J}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}$$
$$\times\Big[2\delta_{\Lambda_3,\Lambda_1-\Lambda_2}(-1)^{\Lambda_2}\binom{\Lambda_1}{\Lambda_2\Lambda_3}\mathcal{R}_2^{2\Lambda_2+1}R^{\Lambda_3}E_{2\Lambda_1+1}[(\zeta_a+\zeta_b)\mathcal{R}_1]\{\hat{\alpha}_0[(\zeta_c+\zeta_d)\mathcal{R}_2]-\hat{\alpha}_0[(\zeta_c-\zeta_d)\mathcal{R}_2]\}$$
$$-\tilde{C}_2(\Lambda_3R;\Lambda_2,\zeta_c\pm\zeta_d,\mathcal{R}_2;\Lambda_1,\zeta_a+\zeta_b,\mathcal{R}_1)$$
$$+C_2^{l}(\Lambda_3,R;\Lambda_2,-\zeta_c\mp\zeta_d,\mathcal{R}_2;\Lambda_1,\zeta_a+\zeta_b,\mathcal{R}_1)\Big]\quad\text{(Subcase 3a, }R\geq\mathcal{R}_1\text{),} \tag{4.29}$$

$$I^{(2)}=(-1)^{\Lambda_1+\lambda_1}\{\cdots\mathcal{G}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}$$

$$\times\bigg[2\delta_{\Lambda_3,\Lambda_1-\Lambda_2}(-1)^{\Lambda_2}\binom{\Lambda_1}{\Lambda_2\Lambda_3}\mathcal{R}_2^{2\Lambda_2+1}R^{\Lambda_3}E_{2\Lambda_1+1}[(\zeta_a+\zeta_b)\mathcal{R}_1]\{\hat{\alpha}_0[(\zeta_c+\zeta_d)\mathcal{R}_2]-\hat{\alpha}_0[(\zeta_c-\zeta_d)\mathcal{R}_2]\}$$

$$-C_2(\Lambda_3,R;\Lambda_2,\zeta_c\pm\zeta_d,\mathcal{R}_2;\Lambda_1,\zeta_a+\zeta_b,\mathcal{R}_1)\bigg]\quad(\text{Subcases 3b and 3c, } R\leq\mathcal{R}_1),\quad(4.30)$$

$$I^{(3)}=(-1)^{\Lambda_1+\lambda_2}\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{G}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}$$

$$\times\bigg[2\delta_{\Lambda_3,\Lambda_2-\Lambda_1}(-1)^{\Lambda_1}\binom{\Lambda_2}{\Lambda_1\Lambda_3}\mathcal{R}_1^{2\Lambda_1+1}R^{\Lambda_3}\{\hat{\alpha}_0[(\zeta_a+\zeta_b)\mathcal{R}_1]-\hat{\alpha}_0[(\zeta_a-\zeta_b)\mathcal{R}_1]\}$$

$$\times E_{2\Lambda_2+1}[(\zeta_c+\zeta_d)\mathcal{R}_2]-\tilde{C}_2(\Lambda_3,R;\Lambda_1,\zeta_a\pm\zeta_b,\mathcal{R}_1;\Lambda_2,\zeta_c+\zeta_d,\mathcal{R}_2)$$

$$+C_2{}^l(\Lambda_3,R;\Lambda_1,-\zeta_a\mp\zeta_b,\mathcal{R}_1;\Lambda_2,\zeta_c+\zeta_d,\mathcal{R}_2)\bigg]\quad(\text{Subcases 3a and 3b, } R\geq\mathcal{R}_2),\quad(4.31)$$

$$I^{(3)}=(-1)^{\Lambda_1+\lambda_2}\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{G}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}$$

$$\times\bigg[2\delta_{\Lambda_3,\Lambda_2-\Lambda_1}(-1)^{\Lambda_1}\binom{\Lambda_2}{\Lambda_1\Lambda_3}\mathcal{R}_1^{2\Lambda_1+1}R^{\Lambda_3}\{\hat{\alpha}_0[(\zeta_a+\zeta_b)\mathcal{R}_1]-\hat{\alpha}_0[(\zeta_a-\zeta_b)\mathcal{R}_1]\}E_{2\Lambda_2+1}[(\zeta_c+\zeta_d)\mathcal{R}_2]$$

$$-C_2(\Lambda_3,R;\Lambda_1,\zeta_a\pm\zeta_b,\mathcal{R}_1;\Lambda_2,\zeta_c+\zeta_d,\mathcal{R}_2)\bigg]\quad(\text{Subcase 3c, } R\leq\mathcal{R}_2).\quad(4.32)$$

3. $I^{(4)}$

For Cases 3b and 3c, $I^{(4)}$ is very similar to Cases 2a and 2b, respectively. The difference concerns the term

$$\int dx\mathcal{K}_{\Lambda_3}(xR)\cdots E_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b-x)\mathcal{R}_1]\cdots\tilde{E}_{2\Lambda_2+1}[(\zeta_c\pm\zeta_d+x)\mathcal{R}_2].\quad(4.33)$$

In Case 2, the contour for this term could be closed at $x=-\infty$, and only a residue from $x=0$ survived. In Cases 3b and 3c $[\mathcal{R}_1\geq R]$, an additional part of (4.33) survives

$$\int_{\infty}^{[(-\zeta_c-\zeta_d)^+]} dx\mathcal{K}_{\Lambda_3}(xR)\cdots E_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b-x)\mathcal{R}_1]\cdots E_{2\Lambda_2+1}[(\zeta_c\pm\zeta_d+x)\mathcal{R}_2],\quad(4.34)$$

which is essentially C_4 [Eq. (2.48)].

For Case 3a, the contour for those terms in $I^{(4)}$ which involve $\tilde{E}_{2\Lambda_2+1}[(\zeta_c\pm\zeta_d+x)\mathcal{R}_2]$ can be closed at $x=\infty$ in the right half-plane and contributes only a residue at $x=0$. The remaining terms can be written [after taking into account the effect of the $\{\cdots\mathcal{K}_\lambda(xR)\cdots\}$ operators]

$$\int dx\mathcal{K}_{\Lambda_3}(xR)\cdots\{\tilde{E}_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b+x)\mathcal{R}_1]-\tilde{E}_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b-x)\mathcal{R}_1]\}\cdots\tilde{E}_{2\Lambda_2+1}[(\zeta_c\pm\zeta_d-x)\mathcal{R}_2]$$

$$=\int dx\mathcal{K}_{\Lambda_3}(xR)\cdots\{\tilde{E}_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b+x)\mathcal{R}_1]-\tilde{E}_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b-x)\mathcal{R}_1]\}\cdots\mathcal{R}_2^{2\Lambda_2}(\zeta_c\pm\zeta_d-x)^{2\Lambda_2}\frac{\log(\zeta_c\pm\zeta_d-x)}{(2\Lambda_2)!}$$

$$+\int dx\mathcal{K}_{\Lambda_3}(xR)\cdots\tilde{E}_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b+x)\mathcal{R}_1]\cdots E_{2\Lambda_2+1}[(\zeta_c\pm\zeta_d-x)\mathcal{R}_2]$$

$$-\int dx\mathcal{K}_{\Lambda_3}(xR)\cdots\mathcal{R}_1^{2\Lambda_1}(\zeta_a\pm\zeta_b-x)^{2\Lambda_1}\frac{\log(\zeta_a\pm\zeta_b-x)}{(2\Lambda_1)!}\cdots E_{2\Lambda_2+1}[(\zeta_c\pm\zeta_d-x)\mathcal{R}_2]$$

$$-\int dx\mathcal{K}_{\Lambda_3}(xR)\cdots E_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b-x)\mathcal{R}_1]\cdots E_{2\Lambda_2+1}[(\zeta_c\pm\zeta_d-x)\mathcal{R}_2].\quad(4.35)$$

The four terms on the right-hand side of Eq. (4.35) go to zero, respectively, at $x=+\infty$, $+\infty$, $+\infty$, and $-\infty$, and, in addition to residues at $x=0$, yield an $\hat{A}_4$ [Eq. (2.41)], $\tilde{C}_4$ [Eq. (2.49)], $C_4{}^l$ [Eq. (2.50)], and zero, respectively.

The results are:

$$I^{(4)}=\tfrac{1}{2}(-1)^{\Lambda_1}\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}$$
$$\times\Big[2\delta_{\Lambda_3,\Lambda_2-\Lambda_1}(-1)^{\Lambda_1}\begin{pmatrix}\Lambda_2\\ \Lambda_1\Lambda_3\end{pmatrix}\mathcal{R}_1^{2\Lambda_1}R^{\Lambda_3}(\hat{\alpha}_0[(\zeta_a+\zeta_b)\mathcal{R}_1]-\hat{\alpha}_0[(\zeta_a-\zeta_b)\mathcal{R}_1])(\tilde{E}_{2\Lambda_2+1}[(\zeta_c+\zeta_d)\mathcal{R}_2]-\tilde{E}_{2\Lambda_2+1}[(\zeta_c-\zeta_d)\mathcal{R}_2])$$
$$-\hat{A}_4(\Lambda_3,R;\Lambda_1;\zeta_a\pm\zeta_b,\mathcal{R}_1;\Lambda_2,\zeta_c\pm\zeta_d,\mathcal{R}_2)-\tilde{C}_4(\Lambda_3,R;\Lambda_1,\zeta_a\pm\zeta_b,\mathcal{R}_1;\Lambda_2,\zeta_c\pm\zeta_d,\mathcal{R}_2)$$
$$+C_4^l(\Lambda_3,R;\Lambda_1,-\zeta_a\mp\zeta_b,\mathcal{R}_1;\Lambda_2,\zeta_c\pm\zeta_d,\mathcal{R}_2)\Big]\quad(\text{Subcase 3a, }R\geq\mathcal{R}_1),\qquad(4.36)$$

$$I^{(4)}=\tfrac{1}{2}(-1)^{\Lambda_1}\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}$$
$$\times\Big[2\delta_{\Lambda_3,\Lambda_1-\Lambda_2}(-1)^{\Lambda_2}\begin{pmatrix}\Lambda_1\\ \Lambda_2\Lambda_3\end{pmatrix}\mathcal{R}_2^{2\Lambda_2+1}R^{\Lambda_3}(\tilde{E}_{2\Lambda_1+1}[(\zeta_a+\zeta_b)\mathcal{R}_1]-\tilde{E}_{2\Lambda_1+1}[(\zeta_a-\zeta_b)\mathcal{R}_1])\{\hat{\alpha}_0[(\zeta_c+\zeta_d)\mathcal{R}_2]-\hat{\alpha}_0[(\zeta_c-\zeta_d)\mathcal{R}_2]\}$$
$$-\hat{A}_4(\Lambda_3,R;\Lambda_2,\zeta_c\pm\zeta_d,\mathcal{R}_2;\Lambda_1,\zeta_a\pm\zeta_b,\mathcal{R}_1)$$
$$-C_4(\Lambda_3,R;\Lambda_2,\zeta_c\pm\zeta_d,\mathcal{R}_2;\Lambda_1,\zeta_a\pm\zeta_b,\mathcal{R}_1)\Big]\quad(\text{Subcase 3b, }\mathcal{R}_1\geq R\geq\mathcal{R}_2),\qquad(4.37)$$

$$I^{(4)}=\tfrac{1}{2}(-1)^{\Lambda_1}\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}$$
$$\times\Big[2\delta_{\Lambda_3,\Lambda_1-\Lambda_2}(-1)^{\Lambda_2}\begin{pmatrix}\Lambda_1\\ \Lambda_2\Lambda_3\end{pmatrix}\mathcal{R}_2^{2\Lambda_2+1}R^{\Lambda_3}\{\tilde{E}_{2\Lambda_1+1}[(\zeta_a+\zeta_b)\mathcal{R}_1]-\tilde{E}_{2\Lambda_1+1}[(\zeta_a-\zeta_b)\mathcal{R}_1]\}\{\hat{\alpha}_0[(\zeta_c+\zeta_d)\mathcal{R}_2]-\hat{\alpha}_0[(\zeta_c-\zeta_d)\mathcal{R}_2]\}$$
$$-\mathcal{R}_2^{2\Lambda_2}R^{-2\Lambda_2}\hat{A}_4(\Lambda_3,R;\Lambda_2,\zeta_c\pm\zeta_d,R;\Lambda_1,\zeta_a\pm\zeta_b,\mathcal{R}_1)$$
$$-C_4^l(\Lambda_3,R;\Lambda_1,-\zeta_a\mp\zeta_b,\mathcal{R}_1;\Lambda_2,-\zeta_c\mp\zeta_d,-\mathcal{R}_2)$$
$$+\mathcal{R}_2^{2\Lambda_2}R^{-2\Lambda_2}C_4^l(\Lambda_3,R;\Lambda_1,-\zeta_a\mp\zeta_b,\mathcal{R}_1;\Lambda_2,-\zeta_c\mp\zeta_d,-R)$$
$$-(-1)^{\Lambda_3}C_4^l(\Lambda_3,-R;\Lambda_1,-\zeta_a\mp\zeta_b,\mathcal{R}_1;\Lambda_2,-\zeta_c\mp\zeta_d,-\mathcal{R}_2)$$
$$-C_4(\Lambda_3,R;\Lambda_2,\zeta_c\pm\zeta_d,\mathcal{R}_2;\Lambda_1,\zeta_a\pm\zeta_b,\mathcal{R}_1)\Big]\quad(\text{Subcase 3c, }\mathcal{R}_2\geq R).\qquad(4.38)$$

V. EVALUATION OF CERTAIN SPECIAL FUNCTIONS

In this section we give formulas for the special functions defined in Eqs. (2.39)–(2.50). It should be noted that the breakdown of $I_{cd;ab}{}^{\mathrm{rad}}$ into special functions is not unique. After exploring several alternative choices, we decided on the formulation given here, with the following aims in mind:

(1) All infinite expansions should be convergent in the appropriate regions of Fig. 1, i.e., convergence should not depend on the relative magnitudes of the ζ's.

(2) There should be no "canceling" singularities in the final formulas when certain combinations of ζ's vanish.

(3) The number of infinite summations should be as few as possible (believe it or not!).

A. $\mathfrak{A}$

The $\mathfrak{A}$ [Eq. (2.39)], which appears only in $I^{(1)}$, Case 1, is designed so that the $\mathcal{K}_{\Lambda_3}(xR)$ dominates the integrand at ∞. The only singularity in the right half-plane is a logarithmic branch point at $x=\zeta_1$ (the logarithmic singularities in the two $E_{2\Lambda_2+1}$'s cancel). We use

$$(2\pi i)^{-1}\int_{\infty}^{(\zeta^+)}dx\mathcal{K}_{\Lambda_3}(xR)\cdots\left(x^{-1}\frac{d}{dx}\right)^{\Lambda}x^{-1}(\zeta-x)^{2\Lambda}\frac{\log(\zeta-x)}{(2\Lambda)!}=\int_{\zeta}^{\infty}dx\mathcal{K}_{\Lambda_3}(xR)\cdots\left(x^{-1}\frac{d}{dx}\right)^{\Lambda}x^{-1}\frac{(\zeta-x)^{2\Lambda}}{(2\Lambda)!},\qquad(5.1)$$

$$=\sum_{\mu=0}^{\Lambda}\zeta^{2\mu}(-1)^{\mu}[(2\Lambda-2\mu)!!(2\mu)!!]^{-1}$$
$$\times\int_{\zeta}^{\infty}dx\mathcal{K}_{\Lambda_3}(xR)\cdots x^{-2\mu-1},\qquad(5.2)$$

the definitions of $\mathcal{K}_{\Lambda_3}(xR)$ [Eq. (2.7)] and α_n [Eq. (2.16)], and the expansion for $E_n(x+y)$ [Eq. (2.20)]. The result is

$$\mathfrak{A}(\Lambda_3, R; \Lambda_2, \zeta_2, \mathcal{R}_2; \Lambda_1, \zeta_1, \mathcal{R}_1) = (-1)^{\Lambda_3}\zeta_1^{\Lambda_1-\Lambda_2-\Lambda_3-2}\mathcal{R}_1^{2\Lambda_1}\mathcal{R}_2^{2\Lambda_2}\sum_{s=0}^{\infty}\zeta_1^s[s!!(s-2\Lambda_2-1)!!]^{-1}$$
$$\times\{\mathcal{R}_2^{s-2\Lambda_2}\hat{\alpha}_{s-2\Lambda_2-1}(\zeta_2\mathcal{R}_2)-(R-\mathcal{R}_1)^{s-2\Lambda_2}\hat{\alpha}_{s-2\Lambda_2-1}[\zeta_2(R-\mathcal{R}_1)]\}$$
$$\times\sum_{\mu_1=0}^{\Lambda_1}(-1)^{\mu_1}[(2\Lambda_1-2\mu_1)!!(2\mu_1)!!]^{-1}R^{\Lambda_3}\left(R^{-1}\frac{d}{dR}\right)^{\Lambda_3}R^{-1}\alpha_{s+\Lambda_1-\Lambda_2-\Lambda_3-2\mu_1-2}(\zeta_1 R). \quad (5.3)$$

The expansion (5.3) converges everywhere in Region 1, except at the single point $\mathcal{R}_1=\mathcal{R}_2=0$, where the four-center integral reduces to an ordinary two-center Coulomb integral.

B. A_2

Evaluation of A_2 is similar to that of $\mathfrak{A}$ [cf. Eqs. (2.39) and (2.40)] except that the expansion (2.28) for $\tilde{E}_n(x+y)$ is used instead of the expansion for $E_n(x+y)$. The result is

$$A_2(\Lambda_3, R; \Lambda_1, \zeta_a\pm\zeta_b, \mathcal{R}_1; \Lambda_2, \zeta_2, \mathcal{R}_2)$$
$$=-2(-1)^{\Lambda_3}\zeta_2^{\Lambda_1+\Lambda_2-\Lambda_3-1}\mathcal{R}_1^{2\Lambda_1+1}\mathcal{R}_2^{2\Lambda_2}\sum_{s=0}^{\infty}(\zeta_2\mathcal{R}_1)^{2s}[(2s+2\Lambda_1+1)!!(2s)!!]^{-1}$$
$$\times\{\hat{\alpha}_{2s}[(\zeta_a+\zeta_b)\mathcal{R}_1]-\hat{\alpha}_{2s}[(\zeta_a-\zeta_b)\mathcal{R}_1]\}\sum_{\mu_2=0}^{\Lambda_2}(-1)^{\mu_2}[(2\Lambda_2-2\mu_2)!!(2\mu_2)!!]^{-1}$$
$$\times R^{\Lambda_3}\left(R^{-1}\frac{d}{dR}\right)^{\Lambda_3}R^{-1}\alpha_{\Lambda_1+\Lambda_2-\Lambda_3+2s-2\mu_2-2}(\zeta_2 R). \quad (5.4)$$

The expansion (5.4) for A_2 converges everywhere in Region 1 except at the point $(\mathcal{R}_1=R, \mathcal{R}_2=0)$, in which case the four-center integral reduces to a (1–2)-type three-center integral [see Paper I].

C. $\hat{A}_4$

To evaluate $\hat{A}_4$ [Eq. (2.41)] note that $\hat{A}_4$ is the difference of two A_2's plus a residue at $x=0$. After some minor manipulations to exorcise negative powers of $(\zeta_c\pm\zeta_d)$, and noting that $(\zeta_d^{-1}d/d\zeta_d)^{l_2}\zeta_d^{-1}(-d/d\zeta_c)^{n_c+\Lambda_2-l_2}$ from $\{\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}$ always acts on $\hat{A}_4$, one obtains

$$\{\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}\hat{A}_4(\Lambda_3, R; \Lambda_1, \zeta_a\pm\zeta_b, \mathcal{R}_1; \Lambda_2, \zeta_c\pm\zeta_d, \mathcal{R}_2)$$
$$=\{\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}[-2(-1)^{\Lambda_3}\mathcal{R}_1^{2\Lambda_1+1}\mathcal{R}_2^{2\Lambda_2}\sum_{s=0;\,(\Lambda_1+\Lambda_2-\Lambda_3+2s-2\geq 0)}^{\infty}\mathcal{R}_1^{2s}[(2s+2\Lambda_1+1)!!(2s)!!]^{-1}$$
$$\times\{\hat{\alpha}_{2s}[(\zeta_a+\zeta_b)\mathcal{R}_1]-\hat{\alpha}_{2s}[(\zeta_a-\zeta_b)\mathcal{R}_1]\}\sum_{\mu_2=0}^{\Lambda_2}(-1)^{\mu_2}[(2\Lambda_2-2\mu_2)!!(2\mu_2)!!]^{-1}$$
$$\times R^{\Lambda_3}(R^{-1}d/dR)^{\Lambda_3}R^{-1}\{[\zeta_c+\zeta_d]^{\Lambda_1+\Lambda_2-\Lambda_3+2s-1}\hat{\alpha}_{\Lambda_1+\Lambda_2-\Lambda_3+2s-2\mu_2-2}[(\zeta_c+\zeta_d)R]$$
$$-[\zeta_c-\zeta_d]^{\Lambda_1+\Lambda_2-\Lambda_3+2s-1}\hat{\alpha}_{\Lambda_1+\Lambda_2-\Lambda_3+2s-2\mu_2-2}[(\zeta_c-\zeta_d)R]\}$$
$$+2(-1)^{\Lambda_3}\delta_{\Lambda_3,\Lambda_1+\Lambda_2}\mathcal{R}_1^{2\Lambda_1+1}\mathcal{R}_2^{2\Lambda_2}\{\hat{\alpha}_0[(\zeta_a+\zeta_b)\mathcal{R}_1]-\hat{\alpha}_0[(\zeta_a-\zeta_b)\mathcal{R}_1]\}[(2\Lambda_1+1)!!]^{-1}$$
$$\times R^{\Lambda_3}(R^{-1}d/dR)^{\Lambda_3}\Big(\sum_{\mu_2=0}^{\Lambda_2}(-1)^{\mu_2}\{\tilde{E}_{2\mu_2+1}[(\zeta_c+\zeta_d)R]-\tilde{E}_{2\mu_2+1}[(\zeta_c-\zeta_d)R]\}$$
$$\times[(2\Lambda_2-2\mu_2)!!(2\mu_2)!!(2\mu_2+1)]^{-1}-\{\hat{\alpha}_0[(\zeta_c+\zeta_d)R]-\hat{\alpha}_0[(\zeta_c-\zeta_d)R]\}[(2\Lambda_2+1)!!]^{-1}\Big)]. \quad (5.5)$$

The expansion for $\hat{A}_4$[(5.5)] converges everywhere.

D. $\mathfrak{B}$

In evaluating $\mathfrak{B}$ [Eq. (2.42)], we use Eq. (5.2), the expansion for $\mathcal{K}_{\Lambda_3}$ [Eq. (2.8)], and Eqs. (2.34) and (2.35) to expand $(x^{-1}d/dx)^{\Lambda_1}x^{-1}$, to obtain,

$$\mathfrak{B}(\Lambda_3, R; \Lambda_1, \zeta_1, \mathfrak{R}_1; \Lambda_2, \zeta_2, \mathfrak{R}_2) = (-1)^{\Lambda_2}\mathfrak{R}_1^{2\Lambda_1}\mathfrak{R}_2^{2\Lambda_2} \sum_{\mu_1=0}^{\Lambda_1} \sum_{\mu_2=0}^{\Lambda_2} \begin{bmatrix}\Lambda_1\\ \mu_1\end{bmatrix} [(2\Lambda_2-2\mu_2)!!(2\mu_2)!!]^{-1}$$

$$\times (R+\mathfrak{R}_2)^{-\Lambda_1-\mu_1}(-1)^{\mu_2}\zeta_2^{2\mu_2} \sum_{s=0}^{\infty} [s!!(s-2\Lambda_3-1)!!]^{-1}R^{s-\Lambda_3-1}$$

$$\times \aleph(s+\Lambda_2-\Lambda_3-\mu_1-2\mu_2-3; \Lambda_1+\mu_1, \zeta_1, R+\mathfrak{R}_2; 0, \zeta_2, 1). \quad (5.6)$$

The $\aleph$ is defined by

$$\aleph(n; \nu_1, \zeta_1, \mathfrak{R}_1; \nu_2, \zeta_2, \mathfrak{R}_2) = (2\pi i)^{-1}(-\mathfrak{R}_2)^{\nu_2} \int_{\infty}^{(\zeta_2^+)} dx x^n E_{\nu_1+1}[(\zeta_1+x)\mathfrak{R}_1](\zeta_2-x)^{\nu_2} \frac{\log(\zeta_2-x)}{(\nu_2!)}. \quad (5.7)$$

We evaluate $\aleph$ for $\nu_2 \geq 0$ when $n \geq 0$, since these cases are required for B [see Eq. (5.20)]. For $n<0$, we need only $\nu_2=0$. First, when $n \geq 0$, use

$$x^n = \sum_{t=0}^{n} \binom{n}{t} \zeta_2^{n-t}(x-\zeta_2)^t \quad (5.8)$$

in Eq. (5.7), then integrate by parts (ν_2+t) times, to obtain

$$\aleph(n; \nu_1, \zeta_1, \mathfrak{R}_1; \nu_2, \zeta_2, \mathfrak{R}_2) = \sum_{t=0}^{n} \binom{n}{t} \frac{(\nu_2+t)!}{\nu_2!} \zeta_2^{n-t}\mathfrak{R}_2^{\nu_2}\mathfrak{R}_1^{-\nu_2-t-1}E_{\nu_1+\nu_2+t+2}[(\zeta_1+\zeta_2)\mathfrak{R}_1]. \quad (5.9)$$

When $n=-N-1<0$, we take the following approach:

$$\aleph(-N-1; \nu_1, \zeta_1, \mathfrak{R}_1; 0, \zeta_2, 1) = \int_{\zeta_2}^{\infty} dx x^{-N-1} E_{\nu_1+1}[(\zeta_1+x)\mathfrak{R}_1] \quad (5.10)$$

$$= (\zeta_1+\zeta_2)^{-N} \int_1^{\infty} dt \left(t - \frac{\zeta_1}{\zeta_1+\zeta_2}\right)^{-N-1} E_{\nu_1+1}[(\zeta_1+\zeta_2)\mathfrak{R}_1 t] \quad (5.11)$$

$$= (\zeta_1+\zeta_2)^{-N} \int_1^{\infty} dt\, t^{-\nu_1-1} \exp[-(\zeta_1+\zeta_2)\mathfrak{R}_1 t] \int_1^t dx\, x^{\nu_1} \left(x - \frac{\zeta_1}{(\zeta_1+\zeta_2)}\right)^{-N-1}. \quad (5.12)$$

Expand $[x-\zeta_1/(\zeta_1+\zeta_2)]^{-N-1}$ in a Laurent series and integrate term by term to obtain

$$\aleph(-N-1; \nu_1, \zeta_1, \mathfrak{R}_1; 0, \zeta_2, 1) = (\zeta_1+\zeta_2)^{-N} \sum_{k=0}^{\infty} \binom{N+k}{k} \left(\frac{\zeta_1}{\zeta_1+\zeta_2}\right)^k$$

$$\times \left((1-\delta_{k,\nu_1-N}) \frac{E_{N+k+1}[(\zeta_1+\zeta_2)\mathfrak{R}_1] - E_{\nu_1+1}[(\zeta_1+\zeta_2)\mathfrak{R}_1]}{\nu_1-N-k} - \delta_{k,\nu_1-N} E_{\nu_1+1}'[(\zeta_1+\zeta_2)\mathfrak{R}_1] \right). \quad (5.13)$$

The series (5.13) for $\aleph$ is convergent whenever $|\zeta_1/(\zeta_1+\zeta_2)|<1$.

In Eq. (5.13) we have introduced the special function $E_n'(x)$. This function is closely related to the exponential integral function [cf. Eqs. (2.14), (2.17), and (2.21)] and is defined by

$$E_n'(x) = -\int_1^{\infty} dt t^{-n} \log t \exp(-xt), \quad (5.14)$$

$$= (d/dn)E_n(x), \quad (5.15)$$

$$= -\sum_{s=0, (s\neq n-1)}^{\infty} (-1)^s x^s [s!(s-n+1)^2]^{-1} - (-x)^{n-1} \frac{\frac{1}{2}[\log x - \psi(n)]^2 - \frac{1}{2}\psi^{(1)}(n) + \frac{1}{6}\pi^2}{(n-1)!}, \quad (5.16)$$

where

$$\psi^{(1)}(n) = (d/dn)\psi(n) \quad (5.17)$$

and $\psi(n)$ is defined in Eq. (2.29).

Note that only a finite number of terms in Eq. (5.6) for $\mathfrak{B}$ have $(s+\Lambda_2-\Lambda_3-2\mu_2-\mu_1-3)<0$, and require the representation of $\aleph$ given in Eq. (5.13).

Expansion (5.6) for $\mathfrak{B}$ converges whenever $|R/(R+\mathcal{R}_2)|<1$.

E. B

Insertion of the series expansion for $\mathcal{J}_{\Lambda_3}(xR)$ [Eq. (2.5)] into Eq. (2.43) for B focuses attention on terms of the type

$$\int dx\left[\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_1}x^{-1}f\right]x^{\Lambda_1+\Lambda_2+\Lambda_3+2s}\left[\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_2}x^{-1}g\right]. \tag{5.18}$$

Close inspection reveals that if the integrand of (5.18) is rewritten as (derivatives of f)$\times$(derivatives of g)$\times$(powers of x), the only negative power of x which occurs is x^{-1}, in the special case $\Lambda_3=|\Lambda_1-\Lambda_2|$ and $s=0$. Thus, with the aid of Eqs. (2.34) and (2.35), terms like (5.18) can be written[8]:

$$\begin{aligned}\int dx&\left[\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_1}x^{-1}E_{2\Lambda_1+1}[(\zeta_1+x)\mathcal{R}_1]\right]x^{\Lambda_3+\Lambda_1+\Lambda_2+2s}\left[\left(x^{-1}\frac{d}{dx}\right)^{\Lambda_2}x^{-1}[(\zeta_2-x)^{2\Lambda_2}\log(\zeta_2-x)]\right]\\
&=\sum_{\substack{\mu_1=0\\(\Lambda_3+2s-\mu_1-\mu_2-2\geq 0)}}^{\Lambda_1}\sum_{\mu_2=0}^{\Lambda_2}\begin{bmatrix}\Lambda_1\\ \mu_1\end{bmatrix}\begin{bmatrix}\Lambda_2\\ \mu_2\end{bmatrix}(-1)^{\mu_1+\mu_2}\int dx\,x^{\Lambda_3+2s-\mu_1-\mu_2-2}\left[\left(\frac{d}{dx}\right)^{\Lambda_1-\mu_1}E_{2\Lambda_1+1}[(\zeta_1+x)\mathcal{R}_1]\right]\\
&\times\left[\left(\frac{d}{dx}\right)^{\Lambda_2-\mu_2}[(\zeta_2-x)^{2\Lambda_2}\log(\zeta_2-x)]\right]+(-1)^{\Lambda_1}\delta_{\Lambda_3,\Lambda_1-\Lambda_2}\delta_{s,0}\frac{(2\Lambda_1-1)!!}{(2\Lambda_2+1)!!}\int dx\{E_{2\Lambda_1+1}[(\zeta_1+x)\mathcal{R}_1]\}\\
&\times x^{-1}\left[\left(\frac{d}{dx}\right)^{2\Lambda_2+1}[(\zeta_2-x)^{2\Lambda_2}\log(\zeta_2-x)]\right]+(-1)^{\Lambda_2}\delta_{\Lambda_3,\Lambda_2-\Lambda_1}\delta_{s,0}\frac{(2\Lambda_2-1)!!}{(2\Lambda_1+1)!!}\int dx\{[(\zeta_2-x)^{2\Lambda_2}\log(\zeta_2-x)]\}\\
&\times x^{-1}\left[\left(\frac{d}{dx}\right)^{2\Lambda_1+1}E_{2\Lambda_1+1}[(\zeta_1+x)\mathcal{R}_1]\right].\end{aligned} \tag{5.19}$$

The first term on the right term in Eq. (5.19) is essentially an $\aleph$ of the kind evaluated in Eq. (5.9). The integrands of the $\delta_{\Lambda_3,|\Lambda_1-\Lambda_2|}$ terms each contain only one logarithmic branch cut (the other has been differentiated into a pole), and these integrals can be evaluated by manipulations which permit their contours to be closed in the half-plane containing only poles. The result is

$$\begin{aligned}B(\Lambda_3,R;\Lambda_1,\zeta_1,\mathcal{R}_1;\Lambda_2,\zeta_2,\mathcal{R}_2)&=(-1)^{\Lambda_1}\sum_{\substack{s=0\\(\Lambda_3+2s-\mu_1-\mu_2-2\geq 0)}}^{\infty}\sum_{\mu_1=0}^{\Lambda_1}\sum_{\mu_2=0}^{\Lambda_2}\begin{bmatrix}\Lambda_1\\ \mu_1\end{bmatrix}\begin{bmatrix}\Lambda_2\\ \mu_2\end{bmatrix}(-1)^{\mu_2}\mathcal{R}_1^{\Lambda_1-\mu_1}\mathcal{R}_2^{\Lambda_2-\mu_2}\\
&\times R^{\Lambda_3+2s}[(2\Lambda_3+2s+1)!!(2s)!!]^{-1}\aleph(\Lambda_3+2s-\mu_1-\mu_2-2;\Lambda_1+\mu_1,\zeta_1,\mathcal{R}_1;\Lambda_2+\mu_2,\zeta_2,\mathcal{R}_2)\\
&+\delta_{\Lambda_3,\Lambda_1-\Lambda_2}(-1)^{\Lambda_1}\begin{pmatrix}\Lambda_1\\ \Lambda_2\Lambda_3\end{pmatrix}R^{\Lambda_3}\mathcal{R}_2^{2\Lambda_2}\zeta_2^{-1}E_{2\Lambda_1+1}[(\zeta_1+\zeta_2)\mathcal{R}_1]+\delta_{\Lambda_3,\Lambda_2-\Lambda_1}(-1)^{\Lambda_2}\begin{pmatrix}\Lambda_2\\ \Lambda_1\Lambda_3\end{pmatrix}R^{\Lambda_3}\mathcal{R}_1^{2\Lambda_1-2\Lambda_2}\mathcal{R}_2^{2\Lambda_2}\\
&\times\{\zeta_1^{-1}E_{2\Lambda_2+1}[(\zeta_1+\zeta_2)\mathcal{R}_1]-\mathcal{R}_1\alpha_0(\zeta_1\mathcal{R}_1)E_{2\Lambda_2+1}(\zeta_2\mathcal{R}_1)\}.\end{aligned} \tag{5.20}$$

Equation (5.20) for B converges whenever $|R/\mathcal{R}_1|<1$.

F. C-Type Functions

Consider first C_2 [Eq. (2.44)]. Since it is possible to deform the integration path so that always $|x|>|\zeta_a+\zeta_b|$, we can use Eq. (2.20) to expand the $E_{2\Lambda_1+1}[(\zeta_a\pm\zeta_b+x)\mathcal{R}_1]$ in powers of $(\zeta_a\pm\zeta_b)$. We note that C_2 is always operated on by $\{\cdots\mathcal{K}_{\Lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}$ which contains derivatives [see Eq. (2.37)] that make at least the first $2\Lambda_1$ terms of the expansion vanish, and that, therefore, each surviving term in the expansion contains only a pole [see Eq.

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[8] For a more complete discussion of the arguments leading to the $\delta_{\Lambda_3,|\Lambda_1-\Lambda_2|}$ terms in Eq. (5.19), see H. J. Silverstone, J. Chem. Phys. **46**, 4377 (1967), Eqs. (12)–(15).

(2.18)]. We use Eqs. (2.34) and (2.35) to expand $(x^{-1}d/dx)^{\Lambda_2}x^{-1}$, Eq. (2.7) for $\mathcal{K}_{\Lambda_3}(xR)$, and

$$(x^{-1}d/dx)^{\Lambda_1}x^{-1}\alpha_s(x\mathcal{R}_1)=\mathcal{R}_1^{2\Lambda_1+1}(\mathcal{R}_1^{-1}d/d\mathcal{R}_1)^{\Lambda_1}\mathcal{R}_1^{-1}(-d/d\mathcal{R}_1)^s\mathcal{R}_1^{-1}\exp(-x\mathcal{R}_1)x^{-2\Lambda_1-s-2}, \quad (5.21)$$

which follows from Eq. (2.15), to obtain

$$\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}C_2(\Lambda_3, R; \Lambda_1, \zeta_a\pm\zeta_b, \mathcal{R}_1; \Lambda_2, \zeta_2, \mathcal{R}_2)=\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\mathcal{R}_1^{2\Lambda_1+1}\mathcal{R}_2^{2\Lambda_2}(-R)^{\Lambda_3}\left(R^{-1}\frac{d}{dR}\right)^{\Lambda_3}R^{-1}$$
$$\times\sum_{s=0}^{\infty}(-\mathcal{R}_1)^{2\Lambda_1+s+1}[(\zeta_a+\zeta_b)^{2\Lambda_1+s+1}-(\zeta_a-\zeta_b)^{2\Lambda_1+s+1}][(2\Lambda_1+s+1)!]^{-1}$$
$$\times\left(\mathcal{R}_1^{-1}\frac{d}{d\mathcal{R}_1}\right)^{\Lambda_1}\mathcal{R}_1^{-1}\left(-\frac{d}{d\mathcal{R}_1}\right)^{s}\mathcal{R}_1^{-1}\sum_{\mu_2=0}^{\Lambda_2}\begin{bmatrix}\Lambda_2\\ \mu_2\end{bmatrix}(-1)^{\mu_2}\int_{\infty}^{[-(\zeta_a+\zeta_b)^+]}dx\,x^{-\Lambda_1-\mu_2-\Lambda_3-s-4}$$
$$\times\exp[-x(R+\mathcal{R}_1)]\mathcal{R}_2^{-\Lambda_2-\mu_2}E_{\Lambda_2+\mu_2+1}[(\zeta_2-x)\mathcal{R}_2]. \quad (5.22)$$

We use the following identity:

$$\int dx\cdots\mathcal{R}_2^{-\Lambda_2-\mu_2}E_{\Lambda_2+\mu_2+1}[(\zeta_2-x)\mathcal{R}_2]$$
$$=\int dx\cdots\{\mathcal{R}_2^{-\Lambda_2-\mu_2}E_{\Lambda_2+\mu_2+1}[(\zeta_2-x)\mathcal{R}_2]-(R+\mathcal{R}_1)^{-\Lambda_2-\mu_2}E_{\Lambda_2+\mu_2+1}[(\zeta_2-x)(R+\mathcal{R}_1)]\}$$
$$+\int dx\cdots(R+\mathcal{R}_1)^{-\Lambda_2-\mu_2}E_{\Lambda_2+\mu_2+1}[(\zeta_2-x)(R+\mathcal{R}_1)]. \quad (5.23)$$

The contour for the second term on the right in Eq. (5.23) can be closed at $-\infty$ in the left half-plane where the integrand has no singularities. The only singularities enclosed by the contour of the first integral on the right in Eq. (5.23) are poles at $x=0$, and this integral can be evaluated by the residue theorem. The result is

$$\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}C_2(\Lambda_3, R; \Lambda_1, \zeta_a\pm\zeta_b, \mathcal{R}_1; \Lambda_2, \zeta_2, \mathcal{R}_2)=\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}(-1)^{\Lambda_3}\mathcal{R}_1^{2\Lambda_1+1}\mathcal{R}_2^{2\Lambda_2}R^{\Lambda_3}\left(R^{-1}\frac{d}{dR}\right)^{\Lambda_3}R^{-1}$$
$$\times\sum_{s=0}^{\infty}\mathcal{R}_1^{2\Lambda_1+s+1}[(\zeta_a+\zeta_b)^{2\Lambda_1+s+1}-(\zeta_a-\zeta_b)^{2\Lambda_1+s+1}][(2\Lambda_1+s+1)!]^{-1}$$
$$\times\left(\mathcal{R}_1^{-1}\frac{d}{d\mathcal{R}_1}\right)^{\Lambda_1}\mathcal{R}_1^{-1}\left(\frac{d}{d\mathcal{R}_1}\right)^{s}\mathcal{R}_1^{-1}\sum_{\mu_2=0}^{\Lambda_2}\begin{bmatrix}\Lambda_2\\ \mu_2\end{bmatrix}(-1)^{\mu_2}[(\Lambda_1+\mu_2+\Lambda_3+s+3)!]^{-1}$$
$$\times\exp[-\zeta_2(R+\mathcal{R}_1)]\left(-\frac{d}{d\zeta_1}\right)^{\Lambda_1+\mu_2+\Lambda_3+s+3}\exp[\zeta_2(R+\mathcal{R}_1)]$$
$$\times\{(R+\mathcal{R}_1)^{-\Lambda_2-\mu_2}E_{\Lambda_2+\mu_2+1}[\zeta_2(R+\mathcal{R}_1)]-\mathcal{R}_2^{-\Lambda_2-\mu_2}E_{\Lambda_2+\mu_2+1}(\zeta_2\mathcal{R}_2)\}. \quad (5.24)$$

$\tilde{C}_2$ [Eq. (2.45)] and C_2^l [Eq. (2.46)] are evaluated in an almost identical way, except that $\tilde{E}_{2\Lambda_1+1}[(\zeta_1+x)\mathcal{R}_1]$ and $(\zeta_1+x)^{2\Lambda_1}\log(\zeta_1+x)$, respectively, are expanded instead of $E_{2\Lambda_1+1}$, and that in the C_2^l case, Eq. (5.21) is not used. The results are

$$\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}C_2^l(\Lambda_3, R; \Lambda_1, \zeta_a\pm\zeta_b, \mathcal{R}_1; \Lambda_2, \zeta_2, \mathcal{R}_2)=\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}(-1)^{\Lambda_2}\mathcal{R}_1^{2\Lambda_1}\mathcal{R}_2^{2\Lambda_2}R^{\Lambda_3}\left(R^{-1}\frac{d}{dR}\right)^{\Lambda_3}R^{-1}$$
$$\times\sum_{s=0}^{\infty}(-1)^s[(\zeta_a+\zeta_b)^{2\Lambda_1+s+1}-(\zeta_a-\zeta_b)^{2\Lambda_1+s+1}]\frac{(s-1)!!}{(2\Lambda_1+s+1)!!}\sum_{\mu_2=0}^{\Lambda_2}\begin{bmatrix}\Lambda_2\\ \mu_2\end{bmatrix}(-1)^{\mu_2}[(\Lambda_1+\mu_2+\Lambda_3+s+3)!]^{-1}$$
$$\times\exp(-\zeta_2R)\left(-\frac{d}{d\zeta_2}\right)^{\Lambda_1+\mu_2+\Lambda_3+s+3}\exp(\zeta_2R)\{\mathcal{R}_2^{-\Lambda_2-\mu_2}E_{\Lambda_2+\mu_2+1}(\zeta_2\mathcal{R}_2)-R^{-\Lambda_2-\mu_2}E_{\Lambda_2+\mu_2+1}(\zeta_2R)\}, \quad (5.25)$$

$$\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\tilde{C}_2(\Lambda_3, R; \Lambda_1, \zeta_a\pm\zeta_b, \mathcal{R}_1; \Lambda_2, \zeta_2, \mathcal{R}_2)=\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{C_2(\Lambda_3, R; \Lambda_1, \zeta_a\pm\zeta_b, \mathcal{R}_1; \Lambda_2, \zeta_2, \mathcal{R}_2)$$
$$+C_2^l(\Lambda_3, R; \Lambda_1, \zeta_a\pm\zeta_b, \mathcal{R}_1; \Lambda_2, \zeta_2, \mathcal{R}_2)\}. \quad (5.26)$$

C_4, $\tilde{C}_4$, and $C_4{}^l$ are evaluated from the formulas derived above for C_2, $\tilde{C}_2$, and $C_2{}^l$, [Eqs. (5.24)–(5.26)], respectively, via Eqs. (2.48)–(2.50). The results are

$$\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}C_4(\Lambda_3, R;\Lambda_1,\zeta_a\pm\zeta_b,\mathcal{R}_1;\Lambda_2,\zeta_c\pm\zeta_d,\mathcal{R}_2)$$

$$=\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}(-1)^{\Lambda_3}\mathcal{R}_1{}^{2\Lambda_1+1}\mathcal{R}_2{}^{2\Lambda_2}R^{\Lambda_3}\left(R^{-1}\frac{d}{dR}\right)^{\Lambda_3}R^{-1}$$

$$\times\sum_{s=0}^{\infty}\mathcal{R}_1{}^{2\Lambda_1+s+1}[(\zeta_a+\zeta_b)^{2\Lambda_1+s+1}-(\zeta_a-\zeta_b)^{2\Lambda_1+s+1}][(2\Lambda_1+s+1)!]^{-1}$$

$$\times\left(\mathcal{R}_1{}^{-1}\frac{d}{d\mathcal{R}_1}\right)^{\Lambda_1}\mathcal{R}_1{}^{-1}\left(\frac{d}{d\mathcal{R}_1}\right)^{s}\mathcal{R}_1{}^{-1}\sum_{\mu_2=0}^{\Lambda_2}\begin{bmatrix}\Lambda_2\\ \mu_2\end{bmatrix}(-1)^{\mu_2}[(\Lambda_1+\mu_2+\Lambda_3+s+3)!]^{-1}$$

$$\times\exp[-\zeta_c(R+\mathcal{R}_1)]\left(-\frac{d}{d\zeta_c}\right)^{\Lambda_1+\mu_2+\Lambda_3+s+3}\exp[\zeta_c(R+\mathcal{R}_1)]$$

$$\times\big((R+\mathcal{R}_1)^{-\Lambda_2-\mu_2}\{\tilde{E}_{\Lambda_2+\mu_2+1}[(\zeta_c+\zeta_d)(R+\mathcal{R}_1)]-\tilde{E}_{\Lambda_2+\mu_2+1}[(\zeta_c-\zeta_d)(R+\mathcal{R}_1)]\}$$

$$-\mathcal{R}_2{}^{-\Lambda_2-\mu_2}\{\tilde{E}_{\Lambda_2+\mu_2+1}[(\zeta_c+\zeta_d)\mathcal{R}_2]-\tilde{E}_{\Lambda_2+\mu_2+1}[(\zeta_c-\zeta_d)\mathcal{R}_2]\}\big),\quad(5.27)$$

$$\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}C_4{}^l(\Lambda_3, R;\Lambda_1,\zeta_a\pm\zeta_b,\mathcal{R}_1;\Lambda_2,\zeta_c\pm\zeta_d,\mathcal{R}_2)$$

$$=\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}(-1)^{\Lambda_2}\mathcal{R}_1{}^{2\Lambda_1}\mathcal{R}_2{}^{2\Lambda_2}R^{\Lambda_3}\left(R^{-1}\frac{d}{dR}\right)^{\Lambda_3}R^{-1}$$

$$\times\sum_{s=0}^{\infty}(-1)^s[(\zeta_a+\zeta_b)^{2\Lambda_1+s+1}-(\zeta_a-\zeta_b)^{2\Lambda_1+s+1}]\frac{(s-1)!!}{(2\Lambda_1+s+1)!!}\sum_{\mu_2=0}^{\Lambda_2}\begin{bmatrix}\Lambda_2\\ \mu_2\end{bmatrix}(-1)^{\mu_2}[(\Lambda_1+\mu_2+\Lambda_3+s+3)!]^{-1}$$

$$\times\exp(-\zeta_cR)\left(-\frac{d}{d\zeta_c}\right)^{\Lambda_1+\mu_2+\Lambda_3+s+3}\exp(\zeta_cR)\big(\mathcal{R}_2{}^{-\Lambda_2-\mu_2}\{\tilde{E}_{\Lambda_2+\mu_2+1}[(\zeta_c+\zeta_d)\mathcal{R}_2]-\tilde{E}_{\Lambda_2+\mu_2+1}[(\zeta_c-\zeta_d)\mathcal{R}_2]\}$$

$$-R^{-\Lambda_2-\mu_2}\{\tilde{E}_{\Lambda_2+\mu_2+1}[(\zeta_c+\zeta_d)R]-\tilde{E}_{\Lambda_2+\mu_2+1}[(\zeta_c-\zeta_d)R]\}\big),\quad(5.28)$$

$$\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\tilde{C}_4(\Lambda_3, R;\Lambda_1,\zeta_a\pm\zeta_b,\mathcal{R}_1;\Lambda_2,\zeta_c\pm\zeta_d,\mathcal{R}_2)$$

$$=\{\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots\}\{C_4(\Lambda_3, R;\Lambda_1,\zeta_a\pm\zeta_b,\mathcal{R}_1;\Lambda_2,\zeta_c\pm\zeta_d,\mathcal{R}_2)$$

$$+C_4{}^l(\Lambda_3, R;\Lambda_1,\zeta_a\pm\zeta_b,\mathcal{R}_1;\Lambda_2,\zeta_c\pm\zeta_d,\mathcal{R}_2)\}.\quad(5.29)$$

In Eqs. (5.27)–(5.29) we have used the presence of derivatives in $\{\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots\}$ [see Eq. (2.37)] to express what were combinations of $E_{\Lambda_2+\mu_2+1}$'s in the C_2 formulas as combinations of $\tilde{E}_{\Lambda_2+\mu_2+1}$'s in the C_4 formulas. All C-type function formulas converge for all values of R, $\mathcal{R}_1$, and $\mathcal{R}_2$.

VI. SUMMARY

The four-center integral of $r_{12}{}^{-1}$ with Slater-type atomic orbitals has been evaluated analytically. Equations (3.3) and (3.4) express the integral as an infinite sum over spherical harmonics of the internuclear angles multiplied by the "radial" integral, $I_{cd;ab}{}^{\text{rad}}$. Equations (3.7)–(3.11) decompose $I_{cd;ab}{}^{\text{rad}}$ into four terms: $I^{(1)}$, $I^{(2)}$, $I^{(3)}$, and $I^{(4)}$. Equations (4.8)–(4.13), (4.19), (4.20), (4.24), (4.25), (4.27), (4.29)–(4.32), and (4.36)–(4.38) express these $I^{(i)}$ in terms of special functions defined in Eq. (2.39)–(2.50). Finally, Eqs. (5.3)–(5.6), (5.9), (5.13), (5.20), and (5.24)–(5.29) represent the special functions as convergent infinite expansions involving various versions of the exponential-type integral [Eqs. (2.14), (2.16)–(2.18), and (5.14)]. The formulas given are valid for all integer-n-type Slater-type orbitals ($n\geq l+1$) with general values of the l and m quantum numbers and general values for the orbital exponents. In addition, the formulas are valid for arbitrary nuclear geometry, provided that all four centers are distinct.

This paper completes a first goal of the series—the development of purely analytical formulas for two-electron multicenter integrals of $r_{12}{}^{-1}$ with Slater-type atomic orbitals. Subsequent work will deal with asymptotic expansions for large internuclear distances, recursion formulas, and the practical details of obtaining numbers.