so that

$$\lim_{\zeta_c\to\infty} \zeta_c^3 I_{c;a,b}{}^{\Lambda l\lambda\Lambda} = \zeta_c^3 \times \{\delta_{t,\Lambda\pm l_c} \text{ terms in } I_{c;a,b}{}^{\Lambda l\lambda\Lambda}\}, \qquad (n_c=1,\ l_c=0). \tag{11}$$

The result then follows immediately from Eqs. (59) and (60) of I and Eq. (11), that

$$\begin{aligned} I_{ab}{}^{l\lambda\Lambda} = {} & \left(-\frac{d}{d\zeta_b}\right)^{n_b-l_b}\left(\zeta_b^{-1}\frac{d}{d\zeta_b}\right)^{l_b}\zeta_b{}^{l_b+1}\mathcal{G}_\lambda(\zeta_b\mathcal{R})\zeta_b{}^{l}\left(\zeta_b^{-1}\frac{d}{d\zeta_b}\right)^{l}\zeta_b{}^{-1} \\ & \times 16(-1)^{\Lambda+l+l_b}(2\Lambda+1)^{-1}R^{-1-\Lambda}\{R^{n_a+\Lambda-l+1}E_{\Lambda+l+1-n_a}[(\zeta_a+\zeta_b)R] \\ & +\mathcal{R}^{n_a+\Lambda-l+1}\hat{\alpha}_{n_a+\Lambda-l}[(\zeta_a+\zeta_b)\mathcal{R}]-R^{n_a+\Lambda-l+1}\hat{\alpha}_{n_a+\Lambda-l}[(\zeta_a+\zeta_b)R]\} \\ & +\left(-\frac{d}{d\zeta_b}\right)^{n_b-l_b}\left(\zeta_b^{-1}\frac{d}{d\zeta_b}\right)^{l_b}\zeta_b{}^{l_b+1}\mathcal{K}_\lambda(\zeta_b\mathcal{R})\zeta_b{}^{l}\left(\zeta_b^{-1}\frac{d}{d\zeta_b}\right)^{l}\zeta_b{}^{-1}8(-1)^{\Lambda}(2\Lambda+1)^{-1} \\ & \times R^{-1-\Lambda}\mathcal{R}^{n_a+\Lambda-l+1}\{\hat{\alpha}_{n_a+\Lambda-l}[(\zeta_a+\zeta_b)\mathcal{R}]-\hat{\alpha}_{n_a+\Lambda-l}[(\zeta_a-\zeta_b)\mathcal{R}]\}, \qquad (\mathcal{R}<R), \end{aligned} \tag{12}$$

and

$$\begin{aligned} I_{ab}{}^{l\lambda\Lambda} = {} & \left(-\frac{d}{d\zeta_b}\right)^{n_b-l_b}\left(\zeta_b^{-1}\frac{d}{d\zeta_b}\right)^{l_b}\zeta_b{}^{l_b+1}\mathcal{G}_\lambda(\zeta_b\mathcal{R})\zeta_b{}^{l}\left(\zeta_b^{-1}\frac{d}{d\zeta_b}\right)^{l}\zeta_b{}^{-1} \\ & \times 16(-1)^{\Lambda+l+l_b}(2\Lambda+1)^{-1}R^{\Lambda}\mathcal{R}^{n_a-\Lambda-l}E_{\Lambda+l+1-n_a}[(\zeta_a+\zeta_b)\mathcal{R}] \\ & +\left(-\frac{d}{d\zeta_b}\right)^{n_b-l_b}\left(\zeta_b^{-1}\frac{d}{d\zeta_b}\right)^{l_b}\zeta_b{}^{l_b+1}\mathcal{K}_\lambda(\zeta_b\mathcal{R})\zeta_b{}^{l}\left(\zeta_b^{-1}\frac{d}{d\zeta_b}\right)^{l}\zeta_b{}^{-1}8(-1)^{\Lambda}(2\Lambda+1)^{-1}R^{\Lambda} \\ & \times(\mathcal{R}^{n_a-\Lambda-l}\{\tilde{E}_{\Lambda+l+1-n_a}[(\zeta_a+\zeta_b)\mathcal{R}]-\tilde{E}_{\Lambda+l+1-n_a}[(\zeta_a-\zeta_b)\mathcal{R}\} \\ & +R^{n_a-\Lambda-l}\{-\tilde{E}_{\Lambda+l+1-n_a}[(\zeta_a+\zeta_b)R]+\tilde{E}_{\Lambda+l+1-n_a}[(\zeta_a-\zeta_b)R] \\ & +\hat{\alpha}_{n_a+\Lambda-l}[(\zeta_a+\zeta_b)R]-\hat{\alpha}_{n_a+\Lambda-l}[(\zeta_a-\zeta_b)R]\}), \qquad (\mathcal{R}>R). \end{aligned} \tag{13}$$

The functions $\mathcal{G}_\lambda$, $\mathcal{K}_\lambda$, E_n, $\tilde{E}_n$, α_n and $\hat{\alpha}_n$ are defined by Eqs. (15), (16), and (21)–(25) of I.

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Analytical Evaluation of Multicenter Integrals of r_{12}^{-1} with Slater-Type Atomic Orbitals. III. (2–2)-Type Three-Center Integrals*

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The three-center integral of r_{12}^{-1}, with each electron described by a two-center product of integer-n Slater-type orbitals, is evaluated analytically. The result, obtained via the Fourier-transform convolution theorem, is an infinite sum involving spherical harmonics for the internuclear angular coordinates and exponential integral and spherical Bessel-type functions for the internuclear distances. The two-center exchange integral is evaluated as a special case. All results given are for general values of the n, l, m, and ζ parameters of the Slater-type orbitals.

INTRODUCTION

In this third paper of a series[1] on multicenter integrals, analytical formulas are derived for the general (2–2)-type three-center two-electron integral of the Coulomb interaction r_{12}^{-1} with Slater-type atomic orbitals (STO's). The basic techniques used in evaluating the integral are the Fourier-transform convolution theorem, expansion of an STO on one center about another, evaluation of products of three spherical harmonics in terms of Condon–Shortley coefficients, contour integration, and the residue theorem. The reader is referred to paper I for a discussion of how these techniques relate to the multicenter integral problem and for appropriate references to the literature.

The most complicated functions which appear in the formulas are Condon–Shortley coefficients, $c^\lambda(l_1m_1;l_2m_2)$

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[1] The first two papers in this series, hereafter referred to as I and II, are H. J. Silverstone, J. Chem. Phys. **48**, 4098, 4106 (1968) (preceding papers).

[Eq. (14) of I]; various versions of the exponential-type integral, $E_n(x)$, $\tilde{E}_n(x)$, $\alpha_n(x)$, $\hat{\alpha}_n(x)$ [Eqs. (21)–(25) of I]; and modified spherical Bessel functions, $\mathcal{I}_l(x)$ and $\mathcal{K}_l(x)$ [Eqs. (15) and (16) of I].

The formulas are derived for general values of the quantum numbers and orbital exponents of the STO's involved. Analytical formulas for the two-center exchange integral, which is a special case of the three-center integral, are obtained gratis[2] at the end. The reader interested only in the final results is referred to Eqs. (1), (2), (7), (11), (16), (17)–(20), (21)–(23), (42), and (43).

FORMULATION

The (2–2)-type three-center integral is first defined and then formulated as an infinite sum of one-dimensional integrals in this section.

The (2–2)-type three-center integral of r_{12}^{-1} is defined by

$$I_{n_cl_cm_c\zeta_c,n_dl_dm_d\zeta_d;n_al_am_a\zeta_a,n_bl_bm_b\zeta_b}(\boldsymbol{\mathcal{R}}_1,\boldsymbol{\mathcal{R}}_2)$$

$$=(N_aN_bN_cN_d)^{-1}\int dV_1dV_2r_{12}^{-1}$$

$$\times[\Psi^*_{n_cl_cm_c\zeta_c}(\mathbf{r}_2)\Psi_{n_dl_dm_d\zeta_d}(\mathbf{r}_2-\boldsymbol{\mathcal{R}}_2)]^*$$

$$\times[\Psi^*_{n_al_am_a\zeta_a}(\mathbf{r}_1)\Psi_{n_bl_bm_b\zeta_b}(\mathbf{r}_1-\boldsymbol{\mathcal{R}}_1)], \quad (1)$$

$$=I_{cd;ab}(\boldsymbol{\mathcal{R}}_1,\boldsymbol{\mathcal{R}}_2), \quad (2)$$

where the STO $\Psi_{nlm\zeta}(\mathbf{r})$ is defined by

$$\Psi_{nlm\zeta}(\mathbf{r})=Nr^{n-1}\exp(-\zeta r)Y_l^m(\theta,\phi). \quad (3)$$

The N is a normalization constant factored out in Eq. (1), the n is an integer which satisfies

$$n\geq l+1, \quad (4)$$

the $Y_l^m(\theta,\phi)$ is a spherical harmonic, and (r,θ,ϕ) are the usual spherical coordinates of $\mathbf{r}$.

Note that in Eq. (1), electron 1 is described by a product of STO's centered at the origin and at $\boldsymbol{\mathcal{R}}_1$, while the STO's of electron 2 are centered at the origin and at $\boldsymbol{\mathcal{R}}_2$ [thus the name (2–2)-type three-center integral].

As in I, the integral $I_{cd;ab}$ can be replaced by a three-dimensional integral over Fourier-transform variables [cf. Eq. (5) of I],

$$I_{cd;ab}(\boldsymbol{\mathcal{R}}_1,\boldsymbol{\mathcal{R}}_2)=(2\pi)^{-3}\int d^3\mathbf{k}(4\pi k^{-2})$$

$$\times G^*_{n_cl_cm_c\zeta_c;n_dl_dm_d\zeta_d}(\mathbf{k},\boldsymbol{\mathcal{R}}_2)$$

$$\times G_{n_al_am_a\zeta_a;n_bl_bm_b\zeta_b}(\mathbf{k},\boldsymbol{\mathcal{R}}_1). \quad (5)$$

Here $\mathbf{k}$ denotes the Fourier-transform variables, $(4\pi k^{-2})$ the Fourier-transform of r_{12}^{-1}, and

$$G_{n_al_am_a\zeta_a;n_bl_bm_b\zeta_b}(\mathbf{k},\boldsymbol{\mathcal{R}}_1)\equiv(N_aN_b)^{-1}\int dV$$

$$\times\exp(i\mathbf{k}\cdot\mathbf{r})\Psi^*_{n_al_am_a\zeta_a}(\mathbf{r})\Psi_{n_bl_bm_b\zeta_b}(\mathbf{r}-\boldsymbol{\mathcal{R}}_1). \quad (6)$$

In Eqs. (19) and (30) of I, the two-center Fourier-transform $G_{n_al_am_a\zeta_a;n_bl_bm_b\zeta_b}(\mathbf{k},\boldsymbol{\mathcal{R}}_1)$ is expanded in terms of spherical harmonics of the angular variables, θ_k and ϕ_k of $\mathbf{k}$, and "radial" functions of $k=|\mathbf{k}|$. With this expansion substituted for each of the G's in Eq. (5), and with the angular integration over θ_k and ϕ_k carried out, $I_{cd;ab}$ becomes

$$I_{cd;ab}(\boldsymbol{\mathcal{R}}_1,\boldsymbol{\mathcal{R}}_2)=\sum_{l_1=0}^{\infty}\sum_{\lambda_1=|l_1-l_b|}^{l_1+l_b}\sum_{l_2=0}^{l_1+l_a+l_c}\sum_{\lambda_2=|l_2-l_d|}^{l_2+l_d}\sum_{m_1=-l_1}^{l_1}\sum_{\Lambda=\max\{|l_1-l_a|,|l_2-l_c|\}}^{\min\{l_1+l_a,l_2+l_c\}}\pi[(2\lambda_1+1)(2\lambda_2+1)]^{1/2}c^{\lambda_1}(l_bm_b;l_1m_1)$$

$$\times c^{\lambda_2}(l_dm_d;l_2,m_1+m_c-m_a)c^{\Lambda}(l_1m_1;l_am_a)c^{\Lambda}(l_2,m_1+m_c-m_a;l_cm_c)$$

$$\times Y_{\lambda_1}^{m_b-m_1}(\theta_{\mathcal{R}_1},\phi_{\mathcal{R}_1})Y_{\lambda_2}^{m_d-m_c+m_a-m_1*}(\theta_{\mathcal{R}_2},\phi_{\mathcal{R}_2})I_{cd;ab}^{l_1\lambda_1;l_2\lambda_2;\Lambda}(\mathcal{R}_1,\mathcal{R}_2). \quad (7)$$

Here $(\mathcal{R},\theta_{\mathcal{R}},\phi_{\mathcal{R}})$ denote the spherical coordinates of $\boldsymbol{\mathcal{R}}$, and

$$I_{cd;ab}^{l_1\lambda_1;l_2\lambda_2;\Lambda}(\mathcal{R}_1,\mathcal{R}_2)=\tfrac{1}{4}(-1)^{\Lambda}(2\Lambda+1)\pi^{-3}$$

$$\times\int_{-\infty}^{\infty}dkG_{l_1\lambda_1l_b\Lambda}^{n_a\zeta_an_b\zeta_b}(k,\mathcal{R}_1)G_{l_2\lambda_2l_d\Lambda}^{n_c\zeta_cn_d\zeta_d}(k,\mathcal{R}_2), \quad (8)$$

where $G_{l_1\lambda_1l_b\Lambda}^{n_a\zeta_an_b\zeta_b}(k,\mathcal{R}_1)$ is defined by Eqs. (20) and (30) of I. In obtaining Eq. (8), we have also used the relation, valid for real k,

$$[G_{l_2\lambda_2l_d\Lambda}^{n_c\zeta_cn_d\zeta_d}(k,\mathcal{R}_2)]^*=(-1)^{\Lambda}G_{l_2\lambda_2l_d\Lambda}^{n_c\zeta_cn_d\zeta_d}(k,\mathcal{R}_2),$$

$$(k\text{ real}), \quad (9)$$

and that the integrand in (8) is even. In Eq. (7), the following restrictions on the summation indices are implicit:

$$\left.\begin{array}{l} l_1+\lambda_1+l_b\quad\text{is even,}\\ l_2+\lambda_2+l_d\quad\text{is even,}\\ l_1+l_2+l_a+l_c\quad\text{is even,}\\ l_1+l_a+\Lambda\quad\text{is even,}\\ |l_1-l_a|\leq l_2+l_c,\\ |l_2-l_c|\leq l_1+l_a. \end{array}\right\} \quad (10)$$

Examination of Eq. (30) of I for $G_{l_1\lambda_1l_b\Lambda}^{n_a\zeta_an_b\zeta_b}(k,\mathcal{R}_1)$ shows that $I_{cd;ab}^{l_1\lambda_1;l_2\lambda_2;\Lambda}(\mathcal{R}_1,\mathcal{R}_2)$ [Eq. (8)] decomposes

[2] Courtesy of the National Science Foundation, which is paying the page charges.

naturally into four terms,

$$I_{cd;ab}{}^{l_1\lambda_1;l_2;\Lambda}(\mathfrak{R}_1,\mathfrak{R}_2)=I^{(1)}+I^{(2)}+I^{(3)}+I^{(4)}. \tag{11}$$

The $I^{(i)}$ are defined by

$$\begin{aligned}I^{(1)}=&-(2\Lambda+1)(-1)^{l_1+l_b+l_2+l_d}\pi^{-1}\int_{-\infty}^{\infty}dk\left[\left(-\frac{d}{d\zeta_b}\right)^{n_b-l_b}\left(\zeta_b^{-1}\frac{d}{d\zeta_b}\right)^{l_b}\zeta_b^{l_b+1}\mathcal{G}_{\lambda_1}(\zeta_b\mathfrak{R}_1)\zeta_b^{l_1}\left(\zeta_b^{-1}\frac{d}{d\zeta_b}\right)^{l_1}\zeta_b^{-1}\mathfrak{R}_1^{n_a-\Lambda-l_1}\right]\\&\times\left[\left(-\frac{d}{d\zeta_d}\right)^{n_d-l_d}\left(\zeta_d^{-1}\frac{d}{d\zeta_d}\right)^{l_d}\zeta_d^{l_d+1}\mathcal{G}_{\lambda_2}(\zeta_d\mathfrak{R}_2)\zeta_d^{l_2}\left(\zeta_d^{-1}\frac{d}{d\zeta_d}\right)^{l_2}\zeta_d^{-1}\mathfrak{R}_2^{n_c-\Lambda-l_2}\right]\\&\times(k^\Lambda(k^{-1}d/dk)^\Lambda k^{-1}\{E_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b-ik)\mathfrak{R}_1]-E_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+ik)\mathfrak{R}_1]\})\\&\times(k^\Lambda(k^{-1}d/dk)^\Lambda k^{-1}\{E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d-ik)\mathfrak{R}_2]-E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d+ik)\mathfrak{R}_2]\}),\end{aligned} \tag{12}$$

$$\begin{aligned}I^{(2)}=&-\tfrac{1}{2}(2\Lambda+1)(-1)^{l_1+l_b}\pi^{-1}\int_{-\infty}^{\infty}dk[\cdots\mathcal{G}_{\lambda_1}(\zeta_b\mathfrak{R}_1)\cdots][\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathfrak{R}_2)\cdots]\\&\times(k^\Lambda(k^{-1}d/dk)^\Lambda k^{-1}\{E_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b-ik)\mathfrak{R}_1]-E_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+ik)\mathfrak{R}_1]\})\\&\times(k^\Lambda(k^{-1}d/dk)^\Lambda k^{-1}\{\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d-ik)\mathfrak{R}_2]-\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d+ik)\mathfrak{R}_2]\\&\qquad-\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c-\zeta_d-ik)\mathfrak{R}_2]+\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c-\zeta_d+ik)\mathfrak{R}_2]\}),\end{aligned} \tag{13}$$

where in, say, $[\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathfrak{R}_2)\cdots]$ the dots stand for $\mathfrak{R}^{n-\Lambda-l}$ and the derivatives, etc., with respect to the ζ's which are present in the corresponding factor of Eq. (12),

$$\begin{aligned}I^{(3)}=&-\tfrac{1}{2}(2\Lambda+1)(-1)^{l_2+l_d}\pi^{-1}\int_{-\infty}^{\infty}dk[\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathfrak{R}_1)\cdots][\cdots\mathcal{G}_{\lambda_2}(\zeta_d\mathfrak{R}_2)\cdots]\\&\times(k^\Lambda(k^{-1}d/dk)^\Lambda k^{-1}\{\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b-ik)\mathfrak{R}_1]-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+ik)\mathfrak{R}_1]\\&-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b-ik)\mathfrak{R}_1]+\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b+ik)\mathfrak{R}_1]\})\\&\times(k^\Lambda(k^{-1}d/dk)^\Lambda k^{-1}\{E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d-ik)\mathfrak{R}_2]-E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d+ik)\mathfrak{R}_2]\}),\end{aligned} \tag{14}$$

and

$$\begin{aligned}I^{(4)}=&-\tfrac{1}{4}(2\Lambda+1)\pi^{-1}\int_{-\infty}^{\infty}dk[\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathfrak{R}_1)\cdots][\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathfrak{R}_2)\cdots]\\&\times(k^\Lambda(k^{-1}d/dk)^\Lambda k^{-1}\{\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b-ik)\mathfrak{R}_1]-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+ik)\mathfrak{R}_1]\\&-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b-ik)\mathfrak{R}_1]+\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b+ik)\mathfrak{R}_1]\})\\&\times(k^\Lambda(k^{-1}d/dk)^\Lambda k^{-1}\{\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d-ik)\mathfrak{R}_2]-\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d+ik)\mathfrak{R}_2]\\&\qquad-\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c-\zeta_d-ik)\mathfrak{R}_2]+\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c-\zeta_d+ik)\mathfrak{R}_2]\}).\end{aligned} \tag{15}$$

The problem of evaluating the integral of Eq. (1) has thus been reduced via Eqs. (7) and (11) to the evaluation of four one-dimensional integrals, Eqs. (12)–(15). These final integrations are carried out, after considerable manipulation, by the residue theorem. The results are stated in the next section.

RESULTS

So as not to lose the cart behind a herd of horses, we first give the results of integrating Eqs. (12)–(15) and postpone the tedious details to the following section.

Restriction: The formulas given are valid only when $\mathfrak{R}_1\geq\mathfrak{R}_2$. This is no loss of generality, because from Eqs. (8) it is clear that

$$I_{cd;ab}{}^{l_1\lambda_1;l_2\lambda_2;\Lambda}(\mathfrak{R}_1,\mathfrak{R}_2)=I_{ab;cd}{}^{l_2\lambda_2;l_1\lambda_1;\Lambda}(\mathfrak{R}_2,\mathfrak{R}_1), \tag{16}$$

which can be used to interchange the roles of $\mathfrak{R}_1$ and $\mathfrak{R}_2$.

The results are

$$I^{(1)}=4(-1)^{l_1+l_b+l_2+l_d}[(-d/d\zeta_b)^{n_b-l_b}(\zeta_b^{-1}d/d\zeta_b)^{l_b}\zeta_b^{l_b+1}\mathcal{G}_{\lambda_1}(\zeta_b\mathcal{R}_1)\zeta_b^{l_1}(\zeta_b^{-1}d/d\zeta_b)^{l_1}\zeta_b^{-1}\mathcal{R}_1^{n_a-\Lambda-l_1}]$$
$$\times[(-d/d\zeta_d)^{n_d-l_d}(\zeta_d^{-1}d/d\zeta_d)^{l_d}\zeta_d^{l_d+1}\mathcal{G}_{\lambda_2}(\zeta_d\mathcal{R}_2)\zeta_d^{l_2}(\zeta_d^{-1}d/d\zeta_d)^{l_2}\zeta_d^{-1}\mathcal{R}_2^{n_c-\Lambda-l_2}]$$
$$\times(\mathcal{R}_1^{2\Lambda+1}(\mathcal{R}_2/\mathcal{R}_1)^{\Lambda+l_2-n_c}\{\alpha_{n_a+\Lambda-l_1}[(\zeta_a+\zeta_b)\mathcal{R}_1]E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d)\mathcal{R}_1]-\mathcal{R}_1^{l_1-\Lambda-n_a-1}(-d/d\zeta_a)^{n_a+\Lambda-l_1}$$
$$\times(\zeta_a+\zeta_b)^{-1}E_{\Lambda+l_2+1-n_c}[(\zeta_a+\zeta_b+\zeta_c+\zeta_d)\mathcal{R}_1]\}+\mathcal{R}_2^{2\Lambda+1}\{\alpha_{n_c+\Lambda-l_2}[(\zeta_c+\zeta_d)\mathcal{R}_2]E_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b)\mathcal{R}_1]$$
$$-\mathcal{R}_2^{l_2-\Lambda-n_c-1}(-d/d\zeta_c)^{n_c+\Lambda-l_2}(\zeta_c+\zeta_d)^{-1}E_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+\zeta_c+\zeta_d)\mathcal{R}_1]\}),\quad(\mathcal{R}_1\geq\mathcal{R}_2),\quad(17)$$

$$I^{(2)}=2(-1)^{l_1+l_b}[(-d/d\zeta_b)^{n_b-l_b}(\zeta_b^{-1}d/d\zeta_b)^{l_b}\zeta_b^{l_b+1}\mathcal{G}_{\lambda_1}(\zeta_b\mathcal{R}_1)\zeta_b^{l_1}(\zeta_b^{-1}d/d\zeta_b)^{l_1}\zeta_b^{-1}\mathcal{R}_1^{n_a-\Lambda-l_1}]$$
$$\times[(-d/d\zeta_d)^{n_d-l_d}(\zeta_d^{-1}d/d\zeta_d)^{l_d}\zeta_d^{l_d+1}\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\zeta_d^{l_2}(\zeta_d^{-1}d/d\zeta_d)^{l_2}\zeta_d^{-1}\mathcal{R}_2^{n_c-\Lambda-l_2}]$$
$$\times\mathcal{R}_2^{2\Lambda+1}E_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b)\mathcal{R}_1]\{\hat{\alpha}_{n_c+\Lambda-l_2}[(\zeta_c+\zeta_d)\mathcal{R}_2]-\hat{\alpha}_{n_c+\Lambda-l_2}[(\zeta_c-\zeta_d)\mathcal{R}_2]\},\quad(\mathcal{R}_1\geq\mathcal{R}_2),\quad(18)$$

$$I^{(3)}=2(-1)^{l_2+l_d}[(-d/d\zeta_b)^{n_b-l_b}(\zeta_b^{-1}d/d\zeta_b)^{l_b}\zeta_b^{l_b+1}\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\zeta_b^{l_1}(\zeta_b^{-1}d/d\zeta_b)^{l_1}\zeta_b^{-1}\mathcal{R}_1^{n_a-\Lambda-l_1}]$$
$$\times[(-d/d\zeta_d)^{n_d-l_d}(\zeta_d^{-1}d/d\zeta_d)^{l_d}\zeta_d^{l_d+1}\mathcal{G}_{\lambda_2}(\zeta_d\mathcal{R}_2)\zeta_d^{l_2}(\zeta_d^{-1}d/d\zeta_d)^{l_2}\zeta_d^{-1}\mathcal{R}_2^{n_c-\Lambda-l_2}]$$
$$\times\{\mathcal{R}_1^{\Lambda-l_2+1+n_c}\mathcal{R}_2^{\Lambda+l_2-n_c}E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d)\mathcal{R}_1]\{\hat{\alpha}_{n_a+\Lambda-l_1}[(\zeta_a+\zeta_b)\mathcal{R}_1]-\hat{\alpha}_{n_a+\Lambda-l_1}[(\zeta_a-\zeta_b)\mathcal{R}_1]\}$$
$$+\mathcal{R}_2^{2\Lambda+1}\alpha_{n_c+\Lambda-l_2}[(\zeta_c+\zeta_d)\mathcal{R}_2][\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b)\mathcal{R}_1]-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b)\mathcal{R}_1]$$
$$-(\mathcal{R}_1/\mathcal{R}_2)^{\Lambda+l_1-n_a}\{\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b)\mathcal{R}_2]-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b)\mathcal{R}_2]\}]$$
$$-\mathcal{R}_2^{\Lambda+l_2-n_c}(-d/d\zeta_c)^{n_c+\Lambda-l_2}(\zeta_c+\zeta_d)^{-1}$$
$$\times[\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+\zeta_c+\zeta_d)\mathcal{R}_1]-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b+\zeta_c+\zeta_d)\mathcal{R}_1]$$
$$-(\mathcal{R}_1/\mathcal{R}_2)^{\Lambda+l_1-n_a}\{\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+\zeta_c+\zeta_d)\mathcal{R}_2]-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b+\zeta_c+\zeta_d)\mathcal{R}_2]\}]$$
$$+\mathcal{R}_1^{\Lambda+l_1-n_a}(-d/d\zeta)^{n_a+\Lambda-l_1}[(\zeta_a+\zeta_b)^{-1}(E_{\Lambda+l_2+1-n_c}[(\zeta_a+\zeta_b+\zeta_c+\zeta_d)\mathcal{R}_2]-E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d)\mathcal{R}_2]$$
$$-(\mathcal{R}_2/\mathcal{R}_1)^{\Lambda+l_2-n_c}\{E_{\Lambda+l_2+1-n_c}[(\zeta_a+\zeta_b+\zeta_c+\zeta_d)\mathcal{R}_1]-E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d)\mathcal{R}_1]\})$$
$$-(\zeta_a-\zeta_b)^{-1}(E_{\Lambda+l_2+1-n_c}[(\zeta_a-\zeta_b+\zeta_c+\zeta_d)\mathcal{R}_2]-E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_c)\mathcal{R}_2]$$
$$-(\mathcal{R}_2/\mathcal{R}_1)^{\Lambda+l_2-n_c}\{E_{\Lambda+l_2+1-n_c}[(\zeta_a-\zeta_b+\zeta_c+\zeta_d)\mathcal{R}_1]-E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d)\mathcal{R}_1]\})]\},\quad(\mathcal{R}_1\geq\mathcal{R}_2),\quad(19)$$

and

$$I^{(4)}=[(-d/d\zeta_b)^{n_b-l_b}(\zeta_b^{-1}d/d\zeta_b)^{l_b}\zeta_b^{l_b+1}\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\zeta_b^{l_1}(\zeta_b^{-1}d/d\zeta_b)^{l_1}\zeta_b^{-1}\mathcal{R}_1^{n_a-\Lambda-l_1}]$$
$$\times[(-d/d\zeta_d)^{n_d-l_d}(\zeta_d^{-1}d/d\zeta_d)^{l_d}\zeta_d^{l_d+1}\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\zeta_d^{l_2}(\zeta_d^{-1}d/d\zeta_d)^{l_2}\zeta_d^{-1}\mathcal{R}_2^{n_c-\Lambda-l_2}]$$
$$\times\{\mathcal{R}_2^{2\Lambda+1}\{\hat{\alpha}_{n_c+\Lambda-l_2}[(\zeta_c+\zeta_d)\mathcal{R}_2]-\hat{\alpha}_{n_c+\Lambda-l_2}[(\zeta_c-\zeta_d)\mathcal{R}_2]\}$$
$$\times[\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b)\mathcal{R}_1]-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b)\mathcal{R}_1]$$
$$-(\mathcal{R}_1/\mathcal{R}_2)^{\Lambda+l_1-n_a}\{\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b)\mathcal{R}_2]-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b)\mathcal{R}_2]\}]+\mathcal{R}_1^{\Lambda+l_1-n_a}(-d/d\zeta_a)^{n_a+\Lambda-l_1}$$
$$\times((\zeta_a+\zeta_b)^{-1}\{\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_a+\zeta_b+\zeta_c+\zeta_d)\mathcal{R}_2]-\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d)\mathcal{R}_2]$$
$$-\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_a+\zeta_b+\zeta_c-\zeta_d)\mathcal{R}_2]+\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c-\zeta_d)\mathcal{R}_2]\}$$
$$-(\zeta_a-\zeta_b)^{-1}\{\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_a-\zeta_b+\zeta_c+\zeta_d)\mathcal{R}_2]-\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d)\mathcal{R}_2]$$
$$-\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_a-\zeta_b+\zeta_c-\zeta_d)\mathcal{R}_2]+\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c-\zeta_d)\mathcal{R}_2]\})$$
$$+\mathcal{R}_2^{\Lambda+l_2-n_c}(\mathcal{R}_1/\mathcal{R}_2)^{\Lambda+l_1-n_a}(-d/d\zeta_c)^{n_c+\Lambda-l_2}$$
$$\times((\zeta_c+\zeta_d)^{-1}\{\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+\zeta_c+\zeta_d)\mathcal{R}_2]-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b)\mathcal{R}_2]$$
$$-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b+\zeta_c+\zeta_d)\mathcal{R}_2]+\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b)\mathcal{R}_2]\}$$
$$-(\zeta_c-\zeta_d)^{-1}\{\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+\zeta_c-\zeta_d)\mathcal{R}_2]-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b)\mathcal{R}_2]$$
$$-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b+\zeta_c-\zeta_d)\mathcal{R}_2]+\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b)\mathcal{R}_2]\})\},\quad(\mathcal{R}_1\geq\mathcal{R}_2).\quad(20)$$

Note that in any one of the expressions enclosed by the bold-face brackets in Eqs. (19) and (20) all the E_n functions can be replaced by $\tilde{E}_n$ functions, and vice versa. Conceivably there are computational situations favoring use of one function over the other. Note also that Eqs. (17)–(20) presuppose that $\mathcal{R}_1\neq 0\neq\mathcal{R}_2$.

A cursory examination of Eqs. (19) and (20) might indicate trouble from the factors $(\zeta_a-\zeta_b)^{-1}$ and $(\zeta_c-\zeta_d)^{-1}$ whenever $\zeta_a-\zeta_b$ or $\zeta_c-\zeta_d$ is close to zero. A closer examination reveals that such factors multiply other factors which go to zero at the same time. Explicitly, one can use the expansions [cf. Eqs. (27), (28), (22), and (25) of I],

$$E_n(x+y)=\sum_{m=0}^{\infty}(-y)^m E_{n-m}(x)/m!, \tag{21}$$

and

$$\tilde{E}_n(x+y)=\sum_{m=0}^{\infty}(-y)^m \tilde{E}_{n-m}(x)/m!, \tag{22}$$

to write, for instance,

$$(\zeta_a-\zeta_b)^{-1}\{E_{\Lambda+l_2+1-n_c}[(\zeta_a-\zeta_b+\zeta_c+\zeta_d)\mathcal{R}_2]-E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d)\mathcal{R}_2]\}=\sum_{m=1}^{\infty}\mathcal{R}_2[(\zeta_b-\zeta_a)\mathcal{R}_2]^{m-1}\frac{E_{\Lambda+l_2+1-n_c-m}[(\zeta_c+\zeta_d)\mathcal{R}_2]}{m!}, \tag{23}$$

which is most useful when $\zeta_a-\zeta_b\sim 0$. [Note that when $\zeta_a=\zeta_b$, first use Eq. (23) in Eq. (19), next take all the derivatives, then set $\zeta_a=\zeta_b$. The infinite expansion (23) will always reduce to a single term. Similar considerations apply to Eq. (20), *mutatis mutandis*.]

For simplifying the derivatives, Eqs. (61)–(65) of I are useful.

DETAILS

The integration of Eqs. (12)–(15) for $I^{(1)}-I^{(4)}$ to obtain Eqs. (17)–(20) is similar to the integration of Eqs. (45) and (46) of I. One manipulates the contour and the integrand of each $I^{(i)}$ until the residue theorem can be used. A new difficulty here, not encountered with the (1–2)-type integral, is the possibility of two logarithmic branch points in the integrand. [Only one logarithmic branch point occurs in the (1–2)-type integral.] In this section we first show how to eliminate one of the branch points, and then we manipulate each integral until every term can be evaluated by the residue theorem.

The device which greatly simplifies evaluation of $I^{(i)}$ involves manipulation of the $[k^\Lambda(k^{-1}d/dk)^\Lambda k^{-1}]$ parts of the integrands. The basic structure of the integrals $I^{(i)}$ is

$$I=\int_{-\infty}^{\infty}dk\left[k^\Lambda\left(k^{-1}\frac{d}{dk}\right)^\Lambda k^{-1}A\right]\left[k^\Lambda\left(k^{-1}\frac{d}{dk}\right)^\Lambda k^{-1}B\right], \tag{24}$$

where A and B are linear combinations of $\tilde{E}_{\Lambda+l+1-n}$ or $E_{\Lambda+l+1-n}$ functions. Integrating by parts Λ times and assuming that A and B vanish sufficiently fast at $k=\pm\infty$, one obtains

$$I=(-1)^\Lambda\int dkA\left(k^{-1}\frac{d}{dk}\right)^\Lambda k^{2\Lambda-1}\left(k^{-1}\frac{d}{dk}\right)^\Lambda k^{-1}B, \tag{25}$$

which is obviously [cf. Eq. (73) of I]

$$=(-1)^\Lambda\int dkAk^{-1}\left(\frac{d}{dk}\right)^{2\Lambda}k^{-1}B, \tag{26}$$

which also [cf. Eq. (74) of I]

$$=(-1)^\Lambda(2\Lambda+1)^{-1}\int dkA\left[k^{-1}\left(\frac{d}{dk}\right)^{2\Lambda+1}-\left(\frac{d}{dk}\right)^{2\Lambda+1}k^{-1}\right]B, \tag{27}$$

which becomes, after integrating half of Eq. (27) by parts $2\Lambda+1$ times,

$$=(-1)^\Lambda(2\Lambda+1)^{-1}\times\int dk\left[Ak^{-1}\left(\frac{d}{dk}\right)^{2\Lambda+1}B+Bk^{-1}\left(\frac{d}{dk}\right)^{2\Lambda+1}A\right]. \tag{28}$$

But

$$(d/dx)^{2\Lambda+1}E_{\Lambda+l_1+1-n_a}(x)=-\alpha_{n_a+\Lambda-l_1}(x), \tag{29}$$

and

$$n_a+\Lambda-l_1\geq n_a+|l_1-l_a|-l_1, \tag{30}$$

$$\geq n_a-l_a, \tag{31}$$

$$\geq 1. \tag{32}$$

[Similar considerations apply to $E_{\Lambda+l_2+1-n_c}(x)$.] Since $\alpha_{n+\Lambda-l}(x)$ has only a pole of order $n+\Lambda-l+1$ at $x=0$, in each of the terms in Eq. (28) a logarithmic branch point has been changed into a pole.

Now consider $I^{(1)}$, Eq. (12). We simultaneously set $k=ix$, use Eqs. (28) and (29), and use [the integrands of Eqs. (12)–(15) are all even functions of k]

$$\int_{-\infty}^{\infty}\cdots(E_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b-ik)\mathcal{R}_1]-E_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+ik)\mathcal{R}_1])\cdots dk$$

$$=2\mathcal{P}\int_{-\infty}^{\infty}\cdots E_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b-ik)\mathcal{R}_1]\cdots dk, \tag{33}$$

where $\mathcal{P}$ denotes the principal value (see I), to obtain

$$I^{(1)}=-2i\pi^{-1}(-1)^{l_1+l_b+l_2+l_d}\mathcal{P}\int_{i\infty}^{-i\infty}dx[\cdots\mathcal{J}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots][\cdots\mathcal{J}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots]$$
$$\times(\mathcal{R}_1^{2\Lambda+1}\alpha_{n_a+\Lambda-l_1}[(\zeta_a+\zeta_b+x)\mathcal{R}_1]x^{-1}\{E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d+x)\mathcal{R}_2]-E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d-x)\mathcal{R}_2]\}$$
$$+\mathcal{R}_2^{2\Lambda+1}\{\alpha_{n_c+\Lambda-l_2}[(\zeta_c+\zeta_d+x)\mathcal{R}_2]+\alpha_{n_c+\Lambda-l_2}[(\zeta_c+\zeta_d-x)\mathcal{R}_2]\}x^{-1}E_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+x)\mathcal{R}_1]).\quad(34)$$

Assume $\mathcal{R}_1\geq\mathcal{R}_2$. Then all terms in Eq. (34) can be evaluated by "closing the contour" at infinity in the right half-plane [cf. Eqs. (29) and (22) of I] and using the residue theorem except the term involving $E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d-x)\mathcal{R}_2]$, which has a branch cut running from $x=\zeta_c+\zeta_d$ to ∞. As discussed in I, the logarithmic part of $E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d-x)\mathcal{R}_2]$ can be clothed in such a way as to permit closure of this part of the integral in the left-hand plane, where there are no branch points. The relevant maneuver is [cf. Eq. (23) and (38) of I]

$$\mathcal{P}\int_{i\infty}^{-i\infty}dx\,x^{-1}\alpha_{n_a+\Lambda-l_1}[(\zeta_a+\zeta_b+x)\mathcal{R}_1]E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d-x)\mathcal{R}_2]=\pi i\alpha_{n_a+\Lambda-l_1}[(\zeta_a+\zeta_b)\mathcal{R}_1]E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d)\mathcal{R}_2]$$
$$+\left(\frac{\mathcal{R}_2}{\mathcal{R}_1}\right)^{\Lambda+l_2-n_c}\int_{i\infty+\epsilon}^{-i\infty+\epsilon}dx\,x^{-1}\alpha_{n_a+\Lambda-l_1}[(\zeta_a+\zeta_b+x)\mathcal{R}_1]E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_b-x)\mathcal{R}_1],\quad(\mathcal{R}_1\geq\mathcal{R}_2),\quad(35)$$

where ϵ is a small positive number. Equation (34), modified by Eq. (35), can be directly evaluated by the residue theorem to give Eq. (17).

By the same logic which leads to Eq. (34) for $I^{(1)}$, one can obtain from Eq. (13) for $I^{(2)}$,

$$I^{(2)}=-i\pi^{-1}(-1)^{l_1+l_b}\mathcal{P}\int_{i\infty}^{-i\infty}dx[\cdots\mathcal{J}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots][\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots]$$
$$\times(\mathcal{R}_1^{2\Lambda+1}\alpha_{n_a+\Lambda-l_1}[(\zeta_a+\zeta_b+x)\mathcal{R}_1]x^{-1}\{\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d+x)\mathcal{R}_2]-\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d-x)\mathcal{R}_2]$$
$$-\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c-\zeta_d+x)\mathcal{R}_2]+\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c-\zeta_d-x)\mathcal{R}_2]\}+\mathcal{R}_2^{2\Lambda+1}E_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+x)\mathcal{R}_1]x^{-1}$$
$$\times\{\hat{\alpha}_{n_c+\Lambda-l_2}[(\zeta_c+\zeta_d+x)\mathcal{R}_2]+\hat{\alpha}_{n_c+\Lambda-l_2}[(\zeta_c+\zeta_d-x)\mathcal{R}_2]-\hat{\alpha}_{n_c+\Lambda-l_2}[(\zeta_c-\zeta_d+x)\mathcal{R}_2]$$
$$-\hat{\alpha}_{n_c+\Lambda-l_2}[(\zeta_c-\zeta_d-x)\mathcal{R}_2]\}).\quad(36)$$

Equation (36) can be evaluated without further manipulation (there are no singularities in the right-hand plane) when $\mathcal{R}_1\geq\mathcal{R}_2$ by closing the contour to right and using the residue theorem. The result is Eq. (18).

After taking the steps which led to Eqs. (34) and (36), we obtain for $I^{(3)}$ from Eq. (14),

$$I^{(3)}=-i\pi^{-1}(-1)^{l_2+l_d}\mathcal{P}\int_{i\infty}^{-i\infty}dx[\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R}_1)\cdots][\cdots\mathcal{J}_{\lambda_2}(\zeta_d\mathcal{R}_2)\cdots]$$
$$\times(\mathcal{R}_1^{2\Lambda+1}\{\hat{\alpha}_{n_a+\Lambda-l_1}[(\zeta_a+\zeta_b+x)\mathcal{R}_1]-\hat{\alpha}_{n_a+\Lambda-l_1}[(\zeta_a-\zeta_b+x)\mathcal{R}_1]\}x^{-1}$$
$$\times\{E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d+x)\mathcal{R}_2]-E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d-x)\mathcal{R}_2]\}$$
$$+\mathcal{R}_2^{2\Lambda+1}\{\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+x)\mathcal{R}_1]-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b+x)\mathcal{R}_1]\}x^{-1}$$
$$\times\{\alpha_{n_c+\Lambda-l_2}[(\zeta_c+\zeta_d+x)\mathcal{R}_2]+\alpha_{n_c+\Lambda-l_2}[(\zeta_c+\zeta_d-x)\mathcal{R}_2]\}).\quad(37)$$

Unlike the integrands of $I^{(1)}$ and $I^{(2)}$ [Eqs. (34) and (36)], the integrand of $I^{(3)}$ [Eq. (37)] contains terms which do not vanish at either $x=\pm\infty$. All terms containing only "$+x$" vanish at $x=+\infty$, contain no singularity for

$\Re e x>0$, and donate a residue only at $x=0$. To handle the "$-x$" terms, we make use of [cf. Eqs. (22)-(25) of I]

$$\hat{\alpha}_{n_a+\Lambda-l_1}[(\zeta_a\pm\zeta_b+x)\Re_1]=\alpha_{n_a+\Lambda-l_1}[(\zeta_a\pm\zeta_b+x)\Re_1]-(n_a+\Lambda-l_1)!([\zeta_a\pm\zeta_b+x)\Re_1]^{l_1-\Lambda-n_a-1}, \quad (38)$$

a relation similar to Eq. (35), and Eq. (56) of I to cast $I^{(3)}$ in the form,

$$I^{(3)}=-i\pi^{-1}(-1)^{l_2+l_d}\int_{i\infty+\epsilon}^{-i\infty+\epsilon}dx[\cdots\mathcal{K}_{\lambda_1}(\zeta_b\Re_1)\cdots][\cdots\mathcal{I}_{\lambda_2}(\zeta_d\Re_2)\cdots]$$
$$\times\Re_1^{2\Lambda+1}(\{\hat{\alpha}_{n_a+\Lambda-l_1}[(\zeta_a+\zeta_b+x)\Re_1]-\hat{\alpha}_{n_a+\Lambda-l_1}[(\zeta_a-\zeta_b+x)\Re_1]\}x^{-1}$$
$$\times\{-(\Re_2/\Re_1)^{\Lambda+l_2-n_c}E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d-x)\Re_1]\}$$
$$+(n_a+\Lambda-l_1)!\Re_1^{l_1-\Lambda-n_a-1}\{(\zeta_a+\zeta_b+x)^{l_1-\Lambda-n_a-1}-(\zeta_a-\zeta_b+x)^{l_1-\Lambda-n_a-1}\}x^{-1}$$
$$\times\{E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d-x)\Re_2]-(\Re_2/\Re_1)^{\Lambda+l_2-n_c}E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d-x)\Re_1]\})$$
$$-i\pi^{-1}(-1)^{l_2+l_d}\left\{\oint^{[0^+]}dx+\oint^{[(\zeta_c+\zeta_d)^+]}dx\right\}[\cdots\mathcal{K}_{\lambda_1}(\zeta_b\Re_1)\cdots][\cdots\mathcal{I}_{\lambda_2}(\zeta_d\Re_2)\cdots]$$
$$\times\Re_2^{2\Lambda+1}(\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+x)\Re_1]-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b+x)\Re_1]$$
$$-(\Re_1/\Re_2)^{\Lambda+l_1-n_a}\{\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+x)\Re_2]-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b+x)\Re_2]\})$$
$$\times x^{-1}\alpha_{n_c+\Lambda-l_2}[(\zeta_c+\zeta_d-x)\Re_2],\qquad(\zeta_a>\zeta_b,\ \Re_1\geq\Re_2). \quad (39)$$

Equation (39) now leads directly to Eq. (19). Note that in Eq. (39) we tacitly took ζ_a to be greater than ζ_b. The reverse case requires a slightly modified approach, but the end result [Eq. (19)] is the same.

Equation (15) for $I^{(4)}$ is readily transformed into

$$I^{(4)}=-i(2\pi)^{-1}\mathcal{P}\int_{i\infty}^{-i\infty}dx[\cdots\mathcal{K}_{\lambda_1}(\zeta_b\Re_1)\cdots][\cdots\mathcal{K}_{\lambda_2}(\zeta_d\Re_2)\cdots]$$
$$\times(\Re_1^{2\Lambda+1}\{\hat{\alpha}_{n_a+\Lambda-l_1}[(\zeta_a+\zeta_b+x)\Re_1]-\hat{\alpha}_{n_a+\Lambda-l_1}[(\zeta_a-\zeta_b+x)\Re_1]\}x^{-1}\{\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d+x)\Re_2]$$
$$-\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d-x)\Re_2]-\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c-\zeta_d+x)\Re_2]+\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c-\zeta_d-x)\Re_2]\}$$
$$+\Re_2^{2\Lambda+1}\{\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+x)\Re_1]-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b+x)\Re_1]\}x^{-1}$$
$$\times\{\hat{\alpha}_{n_c+\Lambda-l_2}[(\zeta_c+\zeta_d+x)\Re_2]+\hat{\alpha}_{n_c+\Lambda-l_2}[(\zeta_c+\zeta_d-x)\Re_2]$$
$$-\hat{\alpha}_{n_c+\Lambda-l_2}[(\zeta_c-\zeta_d+x)\Re_2]-\hat{\alpha}_{n_c+\Lambda-l_2}[(\zeta_c-\zeta_d-x)\Re_2]\}). \quad (40)$$

Assume that $\zeta_a>\zeta_b$ and $\zeta_c>\zeta_d$. (The other cases require slightly different treatments but the end result is the same.) By arguments similar to those leading to Eq. (39), $I^{(4)}$ can be recast as

$$I^{(4)}=-i(2\pi)^{-1}\int_{i\infty+\epsilon}^{-i\infty+\epsilon}dx[\cdots\mathcal{K}_{\lambda_1}(\zeta_b\Re_1)\cdots][\cdots\mathcal{K}_{\lambda_2}(\zeta_d\Re_2)\cdots]$$
$$\times\Re_1^{\Lambda+l_1-n_a}(n_a+\Lambda-l_1)![(\zeta_a+\zeta_b+x)^{l_1-\Lambda-n_a-1}-(\zeta_a-\zeta_b+x)^{l_1-\Lambda-n_a-1}]x^{-1}$$
$$\times\{\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d-x)\Re_2]-\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c-\zeta_d-x)\Re_2]\}$$
$$+i(2\pi)^{-1}\oint^{[0^+,(\zeta_c+\zeta_d)^+]}dx[\cdots\mathcal{K}_{\lambda_1}(\zeta_b\Re_1)\cdots][\cdots\mathcal{K}_{\lambda_2}(\zeta_d\Re_2)\cdots]$$
$$\times\Re_2^{2\Lambda+1}(\Re_1/\Re_2)^{\Lambda+l_1-n_a}\{\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+x)\Re_2]-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b+x)\Re_2]\}x^{-1}$$
$$\times(n_c+\Lambda-l_2)!\Re_2^{l_2-\Lambda-n_c-1}[(\zeta_c+\zeta_d-x)^{l_2-\Lambda-n_c-1}-(\zeta_c-\zeta_d-x)^{l_2-\Lambda-n_c-1}]$$
$$-i(2\pi)^{-1}\oint^{[0^+]}dx[\cdots\mathcal{K}_{\lambda_1}(\zeta_b\Re_1)\cdots][\cdots\mathcal{K}_{\lambda_2}(\zeta_d\Re_2)\cdots]$$
$$\times\Re_2^{2\Lambda+1}\{\hat{\alpha}_{n_c+\Lambda-l_2}[(\zeta_c+\zeta_d-x)\Re_1]-\hat{\alpha}_{n_c+\Lambda-l_2}[(\zeta_c-\zeta_d-x)\Re_2]\}x^{-1}$$
$$\times(\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+x)\Re_1]-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b+x)\Re_1]-(\Re_1/\Re_2)^{\Lambda+l_1-n_a}\{\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+x)\Re_2]$$
$$-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b+x)\Re_2]\}),\qquad(\Re_1\geq\Re_2,\ \zeta_a>\zeta_b,\ \zeta_c>\zeta_d), \quad (41)$$

which then leads directly to Eq. (20).

TWO-CENTER EXCHANGE INTEGRAL

The two-center exchange integral results from setting $\mathbf{R}_1=\mathbf{R}_2=\mathbf{R}$. Note that the angular dependence in Eq. (7) can be simplified via

$$\begin{aligned}Y_{\lambda_1}{}^{m_b-m_1}(\theta_{\mathcal{R}},\phi_{\mathcal{R}})Y_{\lambda_2}{}^{m_d-m_c+m_a-m_1*}(\theta_{\mathcal{R}},\phi_{\mathcal{R}})=&\sum_{t=|\lambda_1-\lambda_2|}^{\lambda_1+\lambda_2}\left(\frac{2t+1}{4\pi}\right)^{1/2}c^t(\lambda_1,m_b-m_1;\lambda_2,m_d-m_c+m_a-m_1)\\&\times Y_t{}^{m_b-m_a-m_d+m_c}(\theta_{\mathcal{R}},\phi_{\mathcal{R}}).\end{aligned}\tag{42}$$

When $\mathcal{R}_1$ and $\mathcal{R}_2$ are set equal to $\mathcal{R}$ in $I_{cd;ab}{}^{l_1\lambda_1;l_2\lambda_2;\Lambda}(\mathcal{R}_1,\mathcal{R}_2)$, one finds, via Eqs. (11) and (17)–(20),

$$\begin{aligned}I_{cd;ab}{}^{l_1\lambda;l_2\lambda_2;\Lambda}(\mathcal{R},\mathcal{R})=&4\mathcal{R}^{2\Lambda+1}(-1)^{l_1+l_b+l_2+l_d}[(-d/d\zeta_b)^{n_b-l_b}(\zeta_b^{-1}d/d\zeta_b)^{l_b}\zeta_b^{l_b+1}\mathcal{I}_{\lambda_1}(\zeta_b\mathcal{R})\zeta_b^{l_1}(\zeta_b^{-1}d/d\zeta_b)^{l_1}\zeta_b^{-1}\mathcal{R}^{n_a-\Lambda-l_1}]\\
&\times[(-d/d\zeta_d)^{n_d-l_d}(\zeta_d^{-1}d/d\zeta_d)^{l_d}\zeta_d^{l_d+1}\mathcal{I}_{\lambda_2}(\zeta_d\mathcal{R})\zeta_d^{l_2}(\zeta_d^{-1}d/d\zeta_d)^{l_2}\zeta_d^{-1}\mathcal{R}^{n_c-\Lambda-l_2}]\\
&\times\{\alpha_{n_a+\Lambda-l_1}[(\zeta_a+\zeta_b)\mathcal{R}]E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d)\mathcal{R}]\\
&\quad+\alpha_{n_c+\Lambda-l_2}[(\zeta_c+\zeta_d)\mathcal{R}]E_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b)\mathcal{R}]\\
&\quad-\mathcal{R}^{l_1-\Lambda-n_a-1}(-d/d\zeta_a)^{n_a+\Lambda-l_1}(\zeta_a+\zeta_b)^{-1}E_{\Lambda+l_2+1-n_c}[(\zeta_a+\zeta_b+\zeta_c+\zeta_d)\mathcal{R}]\\
&\quad-\mathcal{R}^{l_2-\Lambda-n_c-1}(-d/d\zeta_c)^{n_c+\Lambda-l_2}(\zeta_c+\zeta_d)^{-1}E_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+\zeta_c+\zeta_d)\mathcal{R}]\}\\
&\quad+2\mathcal{R}^{2\Lambda+1}(-1)^{l_1+l_b}[\cdots\mathcal{I}_{\lambda_1}(\zeta_b\mathcal{R})\cdots][\cdots\mathcal{K}_{\lambda_2}\zeta_d\mathcal{R})\cdots]\\
&\times E_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b)\mathcal{R}]\{\hat{\alpha}_{n_c+\Lambda-l_2}[(\zeta_c+\zeta_d)\mathcal{R}]-\hat{\alpha}_{n_c+\Lambda-l_2}[(\zeta_c-\zeta_d)\mathcal{R}]\}\\
&\quad+2\mathcal{R}^{2\Lambda+1}(-1)^{l_2+l_d}[\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R})\cdots][\cdots\mathcal{I}_{\lambda_2}(\zeta_d\mathcal{R})\cdots]\\
&\times E_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d)\mathcal{R}]\{\hat{\alpha}_{n_a+\Lambda-l_1}[(\zeta_a+\zeta_b)\mathcal{R}]-\hat{\alpha}_{n_a+\Lambda-l_1}[(\zeta_a-\zeta_b)\mathcal{R}]\}\\
&\quad+\mathcal{R}^{2\Lambda+1}[\cdots\mathcal{K}_{\lambda_1}(\zeta_b\mathcal{R})\cdots][\cdots\mathcal{K}_{\lambda_2}(\zeta_d\mathcal{R})\cdots][\mathcal{R}^{l_1-\Lambda-n_a-1}(-d/d\zeta_a)^{n_a+\Lambda-l_1}\\
&\times((\zeta_a+\zeta_b)^{-1}\{\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_a+\zeta_b+\zeta_c+\zeta_d)\mathcal{R}]-\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d)\mathcal{R}]\\
&\quad-\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_a+\zeta_b+\zeta_c-\zeta_d)\mathcal{R}]+\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c-\zeta_d)\mathcal{R}]\\
&\quad-(\zeta_a-\zeta_b)^{-1}\{\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_a-\zeta_b+\zeta_c+\zeta_d)\mathcal{R}]-\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c+\zeta_d)\mathcal{R}]\\
&\quad-\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_a-\zeta_b+\zeta_c-\zeta_d)\mathcal{R}]+\tilde{E}_{\Lambda+l_2+1-n_c}[(\zeta_c-\zeta_d)\mathcal{R}]\})\\
&\quad+\mathcal{R}^{l_2-\Lambda-n_c-1}(-d/d\zeta_c)^{n_c+\Lambda-l_2}((\zeta_c+\zeta_d)^{-1}\{\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+\zeta_c+\zeta_d)\mathcal{R}]\\
&\quad-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b)\mathcal{R}]-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b+\zeta_c+\zeta_d)\mathcal{R}]\\
&\quad+\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b)\mathcal{R}]\}-(\zeta_c-\zeta_d)^{-1}\{\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b+\zeta_c-\zeta_d)\mathcal{R}]\\
&\quad-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a+\zeta_b)\mathcal{R}]-\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b+\zeta_c-\zeta_d)\mathcal{R}]\\
&\qquad+\tilde{E}_{\Lambda+l_1+1-n_a}[(\zeta_a-\zeta_b)\mathcal{R}]\})].\end{aligned}\tag{43}$$

As discussed above, when $\zeta_a=\zeta_b$ and/or $\zeta_c=\zeta_d$, Eqs. (21)–(23), etc., must be used to modify Eq. (43) to avoid singularities.

SUMMARY

An analytical formula has been derived for (2–2)-type three-center integrals of r_{12}^{-1} with integer-n Slater-type orbitals. The derivation is similar to the one given in Paper I on (1–2)-type three-center integrals and involves the Fourier-transform convolution theorem, expansion of a STO about another center, Condon–Shortley coefficients, and contour integration techniques. The main additional difficulty of (2–2)-type integrals—two logarithmic branch cuts in the integrand—is circumvented by differentiating away a logarithm. Then the resulting expressions are cast in a form which permits evaluation by techniques developed in I. The integral (1) ends up as an infinite expansion (7) involving spherical harmonics and radial functions [Eqs. (11) and (17)–(20)]. The radial functions given are valid only for $\mathcal{R}_1\geq\mathcal{R}_2>0$, but it is trivial [Eq. (16)] to obtain the $\mathcal{R}_1<\mathcal{R}_2$ case. The radial functions involve the same functions which occur in (1–2)-type integrals, spherical Bessel-type and exponential integral-type functions, and are valid for general values of the parameters of the STO's, except that some care is required when $\zeta_a\sim\zeta_b$ and $\zeta_c\sim\zeta_d$ [Eqs. (21)–(23)]. A formula for two-center exchange integrals is obtained from the three-center integral by setting $\mathbf{R}_1=\mathbf{R}_2=\mathbf{R}$ [Eqs. (1), (7), (42), and (43)].