geometric series. Therefore $e_1(S_N)>S_N$ and the e_1 transformation makes the approximation

$$\epsilon_N \doteq (N+1)^{-n} \sum_{j=0}^{\infty} \left[\left(\frac{N}{N+1}\right)^n\right]^j \qquad \text{(B3)}$$

for the truncation error of the Riemann zeta function. The exact truncation error is

$$\epsilon_N = \sum_{j=0}^{\infty} (N+j+1)^{-n}. \qquad \text{(B4)}$$

To compare Eq. (B3) with Eq. (B4) we multiply the numerator and denominator of the terms in Eq. (B4) by N^{jn}. This gives

$$(N+j+1)^{-n} = \{N^j/[N^{j+1}+(j+1)N^j]\}^n, \qquad \text{(B5)}$$

where the denominator is the first two terms in the expansion of $(N+1)^{j+1}$. This leads us to the approximation

$$(N+j+1)^{-n} = \{N^j/[(N+1)^{j+1}]\}^n[1+O(j^2/N^2)], \qquad \text{(B6)}$$

where the term $O(j^2/N^2)$ is positive. Therefore

$$(N+j+1)^{-n} = (N+1)^{-n}\{[N/(N+1)]^n\}^j[1+O(j^2/N^2)] \qquad \text{(B7)}$$

which is the desired connection between Eqs. (B3) and (B4). The approximation of the truncation error given by Eq. (B3) is asymptotically correct. The transformed sequence increases monotonically to the limit $\zeta(n)$, and

$$S_N < e_1(S_N) < \zeta(N). \qquad \text{(B8)}$$

We shall find the approximation, Eq. (B7), especially useful.

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Series Expansion for Two-Center Noninteger-n Overlap Integrals*

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A series in the internuclear distance R is derived for the two-center overlap integral between noninteger-n Slater-type orbitals. There are in general two types of terms: $R^{2N+\lambda}$ and $R^{n_1+n_2+1+N}$, $(N=0,1,2,\cdots;$ $\lambda=|l_1-l_2|, |l_1-l_2|+1, \cdots, l_1+l_2)$. When n_1+n_2 is an integer while n_1 and n_2 are not integers, logarithmic terms arise. The series is for general values of n_1, n_2, l_1, l_2, m_1, m_2, ζ_1, and ζ_2, and it converges absolutely for $R<\infty$.

INTRODUCTION

TWO-CENTER overlap integrals with noninteger-n Slater-type atomic orbitals (STO) were reduced to a one-dimensional integration by the Fourier-transform convolution theorem in an earlier paper.[1] In this paper the final integration is expressed as a series in the internuclear distance R. The series is valid for general values of n_1, n_2, l_1, l_2, m_1, m_2, ζ_1, ζ_2, and $\mathbf{R}$. When n_1+n_2 is nonintegral, the series consists of two types of terms: a power series and $R^{n_1+n_2}$ times a power series. The series becomes an ordinary power series when both n_1 and n_2 are integers. When neither n_1 nor n_2 is an integer while n_1+n_2 is, there are logarithmic terms.

For the reader interested only in the working results, see Eqs. (7), (32), (33), (37), and (41).

FORMULATION

The overlap integral between a STO at the origin, characterized by the parameters n_1, l_1, m_1, ζ_1, and a STO at $\mathbf{R}$ with parameters n_2, l_2, m_2, ζ_2, is given by [Eq. (16) of I]

$$S_{n_1l_1m_1\zeta_1;n_2l_2m_2\zeta_2}(\mathbf{R}) = N_{n_1\zeta_1}N_{n_2\zeta_2}(2\pi^2)^{-1}\sum_{\lambda=|l_1-l_2|}^{l_1+l_2} c^\lambda(l_2, m_2; l_1, m_1)(2\lambda+1)^{1/2}(4\pi)^{-1/2}Y_\lambda^{m_2-m_1}(\theta_R, \phi_R)i^\lambda \times\int_0^\infty dk\, k^2 f^*_{n_1l_1\zeta_1}(k) f_{n_2l_2\zeta_2}(k) j_\lambda(kR). \qquad (1)$$

(A complete explanation of the symbols and conventions can be found in I.) Briefly, the $N_{n\zeta}$ are normalization

* Supported by a National Science Foundation Grant.
[1] H. J. Silverstone, J. Chem. Phys. **45**, 4337 (1966), hereafter referred to as I.

constants, the $c^\lambda(l_2, m_2; l_1, m_1)$ Condon–Shortley coefficients,[2] the Y_l^m spherical harmonics, the $f_{nl\zeta}(k)$ the radial part of the Fourier transform of a STO, [Eq. (13) of I],

$$f_{nl\zeta}(k) = 2\pi i^l \Gamma(n-l+1)(-k)^l[(1/k)(d/dk)]^l(ik)^{-1}[(\zeta-ik)^{l-n-1}-(\zeta+ik)^{l-n-1}], \tag{2}$$

and the $j_\lambda(kR)$ are spherical Bessel functions,[3a]

$$j_\lambda(kR) = k^{-1-\lambda}(-R)^\lambda[R^{-1}(d/dR)]^\lambda R^{-1}\sin kR. \tag{3}$$

NATURE OF THE EXPANSION

One approach to expanding $S(\mathbf{R})$ in powers of R is to substitute[3b]

$$j_\lambda(kR) = \sum_{N=0}^{\infty}(kR)^{2N+\lambda}(-1)^N 2^\lambda(N+\lambda)![N!(2N+2\lambda+1)!]^{-1} \tag{4}$$

into Eq. (1). This attempt is doomed by the divergence of

$$\int_0^\infty dk\, k^{2N+\lambda+2} f^*_{n_1l_1\zeta_1}(k) f_{n_2l_2\zeta_2}(k)$$

when $2N+\lambda \geq n_1+n_2+1$. A second approach is to expand $f_{nl\zeta}(k)$ in (ζ/k). The resulting integrals are like

$$\int_{-\infty}^{\infty} dk e^{ikR} k^{-n_1-n_2-2-N} \sim \frac{R^{n_1+n_2+1+N}}{\Gamma(n_1+n_2+2+N)}, \tag{5}$$

where $\Gamma(x)$ is the gamma function. Although all these integrals are finite, the rub is that the expansion of $f_{nl\zeta}(k)$ in (ζ/k) is invalid when $|k/\zeta|<1$.

The first approach fails because terms in the expansion of the integrand are too big on part of the integration path, the second because the expansion of the integrand is invalid on another part of the path. The successful compromise is to manipulate the integration path in the complex plane so as to be able to use the (ζ/k) expansion on part of the path, which yields terms of the type $R^{n_1+n_2+1+N}$, and to use Eq. (4) on the remainder of the path, which yields terms of the type $R^{2N+\lambda}$.

REFORMULATION

To facilitate these manipulations, we reformulate Eq. (1). Define $\mathcal{S}^\lambda_{n_1l_1\zeta_1;n_2l_2\zeta_2}(R)$ by

$$\mathcal{S}^\lambda_{n_1l_1\zeta_1;n_2l_2\zeta_2}(R) \equiv (16\pi^3)^{-1}(-1)^{l_1} i^\lambda \int_{-\infty}^{\infty} dk\, k^2 f_{n_1l_1\zeta_1}(k) f_{n_2l_2\zeta_2}(k) j_\lambda(kR). \tag{6}$$

Then,

$$S_{n_1l_1m_1\zeta_1;n_2l_2m_2\zeta_2}(\mathbf{R}) = N_{n_1\zeta_1}N_{n_2\zeta_2} \sum_{\lambda=|l_1-l_2|}^{l_1+l_2} (4\pi)^{1/2}(2\lambda+1)^{1/2} c^\lambda(l_2, m_2; l_1, m_1) Y_\lambda^{m_2-m_1}(\theta_R, \phi_R) \mathcal{S}^\lambda_{n_1l_1\zeta_1;n_2l_2\zeta_2}(R). \tag{7}$$

The integrand of $\mathcal{S}^\lambda(R)$ is an even function of k ($\lambda+l_1+l_2$ must be even), so that

$$\tfrac{1}{2}\int_{-\infty}^{\infty} dk = \int_0^\infty dk.$$

Also, for real k, $f^*_{n_1l_1\zeta_1}(k) = (-1)^{l_1} f_{n_1l_1\zeta_1}(k)$. Use Eq. (2) for $f_{nl\zeta}(k)$, Eq. (3) for j_λ, replace $\sin kR$ by $-ie^{ikR}$, and substitute $k=ix$ to obtain

$$\begin{aligned}\mathcal{S}^\lambda(R) = {} & i(4\pi)^{-1}(-1)^{l_1}\Gamma(n_1-l_1+1)\Gamma(n_2-l_2+1)R^\lambda\left(R^{-1}\frac{d}{dR}\right)^\lambda R^{-1} \\ & \times\int_{i\infty}^{-i\infty} dx e^{-xR} x^{1-\lambda+l_1+l_2}\left[\left(x^{-1}\frac{d}{dx}\right)^{l_1} x^{-1}[(\zeta_1+x)^{l_1-n_1-1}-(\zeta_1-x)^{l_1-n_1-1}]\right] \\ & \times\left[\left(x^{-1}\frac{d}{dx}\right)^{l_2} x^{-1}[(\zeta_2+x)^{l_2-n_2-1}-(\zeta_2-x)^{l_2-n_2-1}]\right].\end{aligned} \tag{8}$$

(When there is no danger of confusion, long lists of subscripts are suppressed.) We break $\mathcal{S}^\lambda(R)$ into four parts,

[2] E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, London, 1935), p. 175, Eq. (6).
[3] *Handbook of Mathematical Functions*, M. Abramowitz and I. A. Stegun, Eds. (National Bureau of Standards, Washington, D.C., Appl. Math. Ser. No. 55, 1964); (a) p. 439, Eq. (10.1.25); (b) p. 437, Eq. (10.1.2); (c) p. 258, Eq. (6.2.1); (d) p. 561, Eq. (15.4.1).

depending upon the location of the *branch points* of the integrand:

$$\mathcal{S}^\lambda(R)=\mathcal{S}^\lambda\{+\zeta_1,+\zeta_2\}+\mathcal{S}^\lambda\{+\zeta_1,-\zeta_2\}+\mathcal{S}^\lambda\{-\zeta_1,+\zeta_2\}+\mathcal{S}^\lambda\{-\zeta_1,-\zeta_2\}, \tag{9}$$

where

$$\mathcal{S}^\lambda\{+\zeta_1,+\zeta_2\}=i(4\pi)^{-1}(-1)^{l_1}\Gamma(n_1-l_1+1)\Gamma(n_2-l_2+1)R^\lambda\left(R^{-1}\frac{d}{dR}\right)^\lambda R^{-1}$$
$$\times\int_\Lambda dxe^{-xR}x^{1-\lambda+l_1+l_2}\left[\left(x^{-1}\frac{d}{dx}\right)^{l_1}x^{-1}(\zeta_1-x)^{l_1-n_1-1}\right]\left[\left(x^{-1}\frac{d}{dx}\right)^{l_2}x^{-1}(\zeta_2-x)^{l_2-n_2-1}\right], \tag{10}$$

$$\mathcal{S}^\lambda\{+\zeta_1,-\zeta_2\}=-i(4\pi)^{-1}(-1)^{l_1}\Gamma(n_1-l_1+1)\Gamma(n_2-l_2+1)R^\lambda\left(R^{-1}\frac{d}{dR}\right)^\lambda R^{-1}$$
$$\times\int_\Lambda dxe^{-xR}x^{1-\lambda+l_1+l_2}\left[\left(x^{-1}\frac{d}{dx}\right)^{l_1}x^{-1}(\zeta_1-x)^{l_1-n_1-1}\right]\left[\left(x^{-1}\frac{d}{dx}\right)^{l_2}x^{-1}(\zeta_2+x)^{l_2-n_2-1}\right], \tag{11}$$

and similarly for $\mathcal{S}^\lambda\{-\zeta_1,+\zeta_2\}$ and $\mathcal{S}^\lambda\{-\zeta_1,-\zeta_2\}$. The integration path, denoted by Λ and illustrated in Fig. 1, has been indented to the right at the origin. The origin is not a singular point in the integrand of $S^\lambda(R)$, but it is in each of the four $S^\lambda\{\pm\zeta_1,\pm\zeta_2\}$.

SERIES FOR $\mathcal{S}^\lambda\{+\zeta_1,+\zeta_2\}$ AND $\mathcal{S}^\lambda\{-\zeta_1,-\zeta_2\}$

The $\mathcal{S}^\lambda\{-\zeta_1,-\zeta_2\}$ is trivial to calculate. The e^{-xR} permits closure of the path Λ at ∞ in the right-hand plane. Since the only singularities of the $\mathcal{S}^\lambda\{-\zeta_1,-\zeta_2\}$ integrand lie at $x=0$, $-\zeta_1$, and $-\zeta_2$,

$$\mathcal{S}^\lambda\{-\zeta_1,-\zeta_2\}=0 \tag{12}$$

by Cauchy's integral theorem.[4]

The integrand of $\mathcal{S}^\lambda\{+\zeta_1,+\zeta_2\}$ has branch points at $x=+\zeta_1$, $+\zeta_2$. First wrap the integration path around the branch cuts, then blow up the loop around the branch points (see Λ_1, Fig. 2) so that on Λ_1, $|x|$ is $>\zeta_1$ and $>\zeta_2$:

$$S^\lambda\{+\zeta_1,+\zeta_2\}=\left(-\oint^{(0^+)}dx+\int_{\Lambda_1}dx\right)i(4\pi)^{-1}(-1)^{l_1}\Gamma(n_1-l_1+1)\Gamma(n_2-l_2+1)R^\lambda\left(R^{-1}\frac{d}{dR}\right)^\lambda R^{-1}e^{-xR}x^{1-\lambda+l_1+l_2}$$
$$\times\left[\left(x^{-1}\frac{d}{dx}\right)^{l_1}x^{-1}(\zeta_1-x)^{l_1-n_1-1}\right]\left[\left(x^{-1}\frac{d}{dx}\right)^{l_2}x^{-1}(\zeta_2-x)^{l_2-n_2-1}\right]. \tag{13}$$

On Λ_1 the (ζ/x) expansion can be used. Thus, with

$$\left(x^{-1}\frac{d}{dx}\right)^l x^{-1}=\sum_{\mu=0}^{l}2^{-\mu}(l+\mu)![(l-\mu)!\mu!]^{-1}(-1)^\mu x^{-l-\mu-1}\left(\frac{d}{dx}\right)^{l-\mu}, \tag{14}$$

$$(\zeta-x)^{\mu-n-1}=\exp[-i\pi(\mu-n-1)]x^{\mu-n-1}\sum_{m=0}^{\infty}\frac{\Gamma(\mu-n)(-1)^m}{\Gamma(\mu-n-m)m!}\zeta^m x^{-m}, \tag{15}$$

$$\frac{R^{q-1}}{\Gamma(q)}=\tfrac{1}{2}i\pi^{-1}e^{\pi iq}\int_{\Lambda_1}dxe^{-xR}x^{-q}, \tag{16}$$

$$\Gamma(q)\Gamma(1-q)\sin\pi q=\pi, \tag{17}$$

and

$$R^\lambda\left(R^{-1}\frac{d}{dR}\right)^\lambda R^{n_1+n_2+1+\lambda+N}=R^{n_1+n_2+1+N}\frac{2^\lambda\Gamma[\frac{1}{2}(n_1+n_2+1+N+\lambda)+1]}{\Gamma[\frac{1}{2}(n_1+n_2+1+N-\lambda)+1]}, \tag{18}$$

the Λ_1 part of $\mathcal{S}^\lambda\{+\zeta_1,+\zeta_2\}$ becomes

$$\mathcal{S}^\lambda\{+\zeta_1,+\zeta_2\}(\Lambda_1\text{ part})=-\tfrac{1}{2}(-1)^{l_2}R^{n_1+n_2+1}$$
$$\times\sum_{\mu_1=0}^{l_1}\sum_{\mu_2=0}^{l_2}\sum_{N=0}^{\infty}(-R)^N\frac{(l_1+\mu_1)!(l_2+\mu_2)!}{2^{\mu_1+\mu_2}(l_1-\mu_1)!(l_2-\mu_2)!\mu_1!\mu_2!}\frac{2^\lambda\Gamma[\frac{1}{2}(n_1+n_2+1+N+\lambda)+1]}{\Gamma[\frac{1}{2}(n_1+n_2+1+N-\lambda)+1]\Gamma(n_1+n_2+3+N+\lambda)}$$
$$\times\sum_{M=0}^{N}\zeta_1^M\zeta_2^{N-M}[M!(N-M)!]^{-1}\Gamma(n_1-\mu_1+1+M)\Gamma(n_2-\mu_2+1+N-M). \tag{19}$$

[The $\oint dx$ part of Eq. (13) is discussed later.]

[4] See, e.g., G. F. Carrier, M. Krook, and C. E. Pearson, *Functions of a Complex Variable* (McGraw-Hill Book Co., New York, 1966).

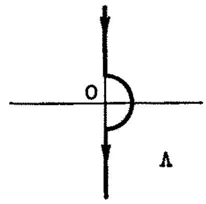


FIG. 1. Contour for Eqs. (9)–(11).

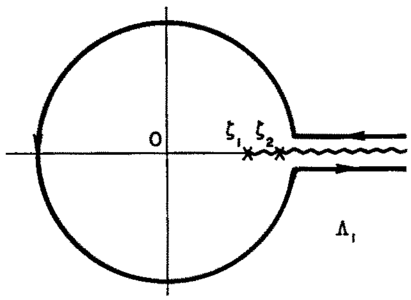


FIG. 2. Contour for Eq. (13). The arguments of (ζ_1-x) and (ζ_2-x) are both $-\pi$ at the beginning of the contour. (It is irrelevant that ζ_1 is shown $<\zeta_2$.)

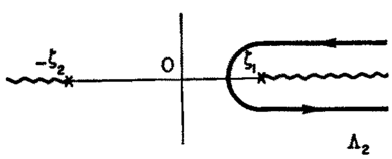


FIG. 3. Contour for $\mathcal{S}^\lambda\{+\zeta_1, -\zeta_2\}$.

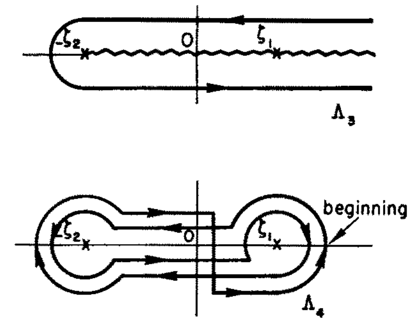


FIG. 4. Contours for Eq. (20).

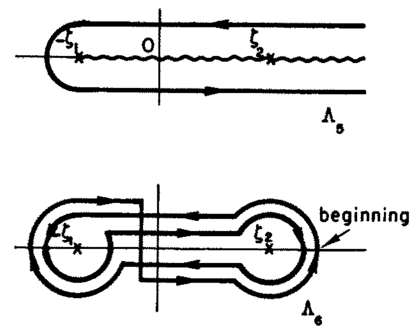
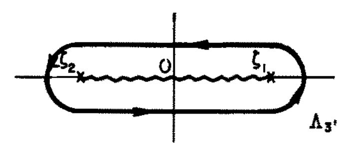


FIG. 5. Contours for Eq. (21).

FIG. 6. $\Lambda_{3'}$ (Λ_3 when n_1+n_2 is an integer).



SERIES FOR $\mathcal{S}^\lambda\{+\zeta_1, -\zeta_2\}+\mathcal{S}^\lambda\{-\zeta_1, +\zeta_2\}$

The $\mathcal{S}^\lambda\{+\zeta_1, -\zeta_2\}$ and $\mathcal{S}^\lambda\{-\zeta_1, +\zeta_2\}$ are more difficult to evaluate because Λ separates the branch cuts. Consider first $\mathcal{S}^\lambda\{+\zeta_1, -\zeta_2\}$. Wrap Λ about the branch cut which runs from ζ_1 to ∞ [Λ_2, Fig. 3]. We slip the second branch cut inside the contour (and get essentially the $\mathcal{S}^\lambda\{+\zeta_1, +\zeta_2\}$ case) by a manipulation analogous to

$$\int_{\zeta_1}^{\infty} dx=\int_{-\zeta_2}^{\infty} dx+\int_{\zeta_1}^{-\zeta_2} dx,$$

but which (because ζ_1 and $-\zeta_2$ are singularities) involves the esoteric, decorative Pochhammer contours (Λ_3 and Λ_4, Fig. 4):

$$\begin{aligned}\mathcal{S}^\lambda\{+\zeta_1, -\zeta_2\}=&\{1-\exp[-2\pi i(n_1+n_2)]\}^{-1}\\ &\times\left([1-\exp(-2\pi i n_1)]\int_{\Lambda_3} dx+\exp(-2\pi i n_1)\int_{\Lambda_4} dx\right)(-i)(4\pi)^{-1}(-1)^{l_1}\Gamma(n_1-l_1+1)\Gamma(n_2-l_2+1)R^\lambda\\ &\times\left(R^{-1}\frac{d}{dR}\right)^\lambda R^{-1}\exp(-xR_x1-\lambda+l_1+l_2)\left[\left(x^{-1}\frac{d}{dx}\right)^{l_1}x^{-1}(\zeta_1-x)^{l_1-n_1-1}\right]\left[\left(x^{-1}\frac{d}{dx}\right)^{l_2}x^{-1}(\zeta_2+x)^{l_2-n_2-1}\right].\end{aligned}\tag{20}$$

Similarly, for $\mathcal{S}^\lambda\{-\zeta_1, +\zeta_2\}$ we write (see Fig. 5 for Λ_5 and Λ_6)

$$\begin{aligned}\mathcal{S}^\lambda\{-\zeta_1, +\zeta_2\}=&\left[\{1-\exp[-2\pi i(n_1+n_2)]\}^{-1}\left([1-\exp(-2\pi i n_2)]\int_{\Lambda_5} dx+\exp(-2\pi i n_2)\int_{\Lambda_6} dx\right)-\oint^{(0^+)} dx\right]\\ &\times(-i)(4\pi)^{-1}(-1)^{l_1}\Gamma(n_1-l_1+1)\Gamma(n_2-l_2+1)R^\lambda\left(R^{-1}\frac{d}{dR}\right)^\lambda R^{-1}\exp(-xR_x1\cdots\lambda+l_1+l_2)\\ &\times\left[\left(x^{-1}\frac{d}{dx}\right)^{l_1}x^{-1}(\zeta_1+x)^{l_1-n_1-1}\right]\left[\left(x^{-1}\frac{d}{dx}\right)^{l_2}x^{-1}(\zeta_2-x)^{l_2-n_2-1}\right].\end{aligned}\tag{21}$$

[The arguments of (ζ_1+x) and (ζ_2+x) are 0, and the arguments of (ζ_1-x) and (ζ_2-x) are $-\pi$, at the beginning of Λ_3, Λ_4, Λ_5, and Λ_6.] Equations (20) and (21) hold only when n_1+n_2 is not an integer.

The Λ_3 and Λ_5 integrations proceed as for $\mathcal{S}^\lambda\{+\zeta_1, +\zeta_2\}$ and give essentially Eq. (19) with

$$(-1)^{l_2+N-M}\sin\pi n_1/\sin\pi(n_1+n_2) \quad \text{and} \quad (-1)^{l_1+M}\sin\pi n_2/\sin\pi(n_1+n_2)$$

inserted just after the $\sum_M$. Together with Eq. (19) these constitute all the terms in $\mathcal{S}^\lambda(R)$ proportional to $R^{n_1+n_2}$:

$$\{\text{total } R^{n_1+n_2} \text{ contribution to } \mathcal{S}^\lambda(R)\} = -\tfrac{1}{2}(-1)^{l_2}R^{n_1+n_2+1}\sum_{\mu_1=0}^{l_1}\sum_{\mu_2=0}^{l_2}\sum_{N=0}^{\infty}(-R)^N$$
$$\times\frac{(l_1+\mu_1)!(l_2+\mu_2)!}{2^{\mu_1+\mu_2}(l_1-\mu_1)!(l_2-\mu_2)!\mu_1!\mu_2!}\frac{2^\lambda\Gamma[\frac{1}{2}(n_1+n_2+1+N+\lambda)+1]}{\Gamma[\frac{1}{2}(n_1+n_2+1+N-\lambda)+1]\Gamma(n_1+n_2+3+N+\lambda)}$$
$$\times\sum_{M=0}^{N}\left(1+(-1)^{l_2+N-M}\frac{\sin\pi n_1}{\sin\pi(n_1+n_2)}+(-1)^{l_1+M}\frac{\sin\pi n_2}{\sin\pi(n_1+n_2)}\right)$$
$$\times\zeta_1^M\zeta_2^{N-M}[M!(N-M)!]^{-1}\Gamma(n_1-\mu_1+1+M)\Gamma(n_2-\mu_2+1+N-M). \tag{22}$$

The Λ_6 integration in Eq. (21) can be manipulated into an integration over Λ_4 by substituting $-x$ for x and redefining the starting point of the contour [if proper attention is paid to the arguments of $(\zeta_1\pm x)$ and $(\zeta_2\pm x)$ and to the direction of travel on the contour]:

$$\int_{\Lambda_6} dx e^{-xR}x^{1-\lambda+l_1+l_2}\cdots(\zeta_1+x)^{l_1-n_1-1}\cdots(\zeta_2-x)^{l_2-n_2-1} = -\exp[2\pi i(n_2-n_1)]$$
$$\times\int_{\Lambda_4} dx e^{+xR}x^{1-\lambda+l_1+l_2}\cdots(\zeta_1-x)^{l_1-n_1-1}\cdots(\zeta_2+x)^{l_2-n_2-1}. \tag{23}$$

Thus,

$\mathcal{S}^\lambda\{\Lambda_4 \text{ and } \Lambda_6 \text{ contributions}\}$

$$= i(2\pi)^{-1}(-1)^{l_1}\Gamma(n_1-l_1+1)\Gamma(n_2-l_2+1)R^\lambda\left(R^{-1}\frac{d}{dR}\right)^\lambda R^{-1}\{1-\exp[-2\pi i(n_1+n_2)]\}^{-1}$$
$$\times\exp(-2\pi i n_1)\int_{\Lambda_4} dx\,\sinh(xR)\,x^{1-\lambda+l_1+l_2}\left[\left(x^{-1}\frac{d}{dx}\right)^{l_1}x^{-1}(\zeta_1-x)^{l_1-n_1-1}\right]\left[\left(x^{-1}\frac{d}{dx}\right)^{l_2}x^{-1}(\zeta_2+x)^{l_2-n_2-1}\right]. \tag{24}$$

Since Λ_4 does not run off to ∞, one may expand $R^\lambda[(1/R)(d/dR)]^\lambda R^{-1}\sinh(xR)$ in R [cf. Eq. (4)] and expand $[x^{-1}(d/dx)]^l x^{-1}$ as in Eq. (14), to obtain

$$\mathcal{S}^\lambda\{\Lambda_4,\Lambda_6\} = \tfrac{1}{2}i\pi(-1)^{l_1+l_2}[\sin\pi n_1\sin\pi n_2]^{-1}\{1-\exp[-2\pi i(n_1+n_2)]\}^{-1}\exp(-2\pi i n_1)$$
$$\times\sum_{\mu_1=0}^{l_1}\sum_{\mu_2=0}^{l_2}\sum_{\substack{N=0\\(2N+\lambda\geq\mu_1+\mu_2)}}^{\infty}R^{2N+\lambda}\frac{(l_1+\mu_1)!(l_2+\mu_2)!(-1)^{\mu_2}}{2^{\mu_1+\mu_2}(l_1-\mu_1)!(l_2-\mu_2)!\mu_1!\mu_2!\Gamma(\mu_1-n_1)\Gamma(\mu_2-n_2)}\frac{2^\lambda(\lambda+N)!}{N!(2N+2\lambda+1)!}$$
$$\times\int_{\Lambda_4} dx\,x^{2N+\lambda-\mu_1-\mu_2}(\zeta_1-x)^{\mu_1-n_1-1}(\zeta_2+x)^{\mu_2-n_2-1}. \tag{25}$$

The restriction $(2N+\lambda\geq\mu_1+\mu_2)$, which is clarified in the Appendix, makes it possible to integrate Eq. (25) in terms of simple functions. [There are *several* equivalent forms[5] for the integral of (25); we give only one.] Write

$$x^{2N+\lambda-\mu_1-\mu_2} = (\zeta_1+\zeta_2)^{\mu_1+\mu_2-2N-\lambda}[\zeta_1(\zeta_2+x)-\zeta_2(\zeta_1-x)]^{2N+\lambda-\mu_1-\mu_2} \tag{26}$$
$$= (\zeta_1+\zeta_2)^{\mu_1+\mu_2-2N-\lambda}(-\zeta_2)^{2N+\lambda-\mu_1-\mu_2}\sum_{M=0}^{2N+\lambda-\mu_1-\mu_2}\binom{2N+\lambda-\mu_1-\mu_2}{M}$$
$$\times(-\zeta_1)^M\zeta_2^{-M}(\zeta_1-x)^{2N+\lambda-\mu_1-\mu_2-M}(\zeta_2+x)^M, \tag{27}$$

[5] The author is not sure which of the many equivalent forms will be the most useful.

and use the integral representation[3c] of the beta function $[B(a,b)=\Gamma(a)\Gamma(b)/\Gamma(a+b)]$ to show that

$$-\tfrac{1}{2}i(\sin\pi n_1\sin\pi n_2)^{-1}\{1-\exp[-2\pi i(n_1+n_2)]\}^{-1}\exp(-2\pi i n_1)\int_{\Delta_4}dx(\zeta_1-x)^{2N+\lambda-n_1-\mu_2-M-1}(\zeta_2+x)^{\mu_2-n_2-1+M}$$
$$=[\sin\pi(n_1+n_2)]^{-1}(\zeta_1+\zeta_2)^{2N+\lambda-n_1-n_2-1}\Gamma(2N+\lambda-n_1-\mu_2-M)[\Gamma(\mu_2-n_2+M)/\Gamma(2N+\lambda-n_1-n_2)]. \quad (28)$$

The result for Eq. (24) is then

$$\mathcal{S}^\lambda\{\Delta_4 \text{ and } \Delta_6 \text{ contributions}\}$$
$$=-\pi[\sin\pi(n_1+n_2)]^{-1}\sum_{\substack{\mu_1=0\\(2N+\lambda\geq\mu_1+\mu_2)}}^{l_1}\sum_{\mu_2=0}^{l_2}\sum_{N=0}^{\infty}R^{2N+\lambda}\frac{(l_1+\mu_1)!(l_2+\mu_2)!}{2^{\mu_1+\mu_2}(l_1-\mu_1)!(l_2-\mu_2)!\mu_1!\mu_2!}$$
$$\times\frac{(-1)^{\mu_1}}{\Gamma(\mu_1-n_1)\Gamma(\mu_2-n_2)}\frac{2^\lambda(\lambda+N)!}{N!(2N+2\lambda+1)!}(\zeta_1+\zeta_2)^{\mu_1+\mu_2-n_1-n_2-1}\zeta_2^{2N+\lambda-\mu_1-\mu_2}$$
$$\times\sum_{M=0}^{2N+\lambda-\mu_1-\mu_2}\binom{2N+\lambda-\mu_1-\mu_2}{M}(-\zeta_1)^M\zeta_2^{-M}\Gamma(2N+\lambda-n_1-\mu_1-M)\frac{\Gamma(\mu_2-n_2+M)}{\Gamma(2N+\lambda-n_1-n_2)}. \quad (29)$$

$\oint dx$ TERMS

The remaining terms are from Eqs. (13) and (21):

$$\mathcal{S}^\lambda\{\text{the rest}\}=-\oint^{(0^+)}dx\,i(4\pi)^{-1}(-1)^{l_1}\Gamma(n_1-l_1+1)\Gamma(n_2-l_2+1)R^\lambda\left(R^{-1}\frac{d}{dR}\right)^\lambda R^{-1}e^{-xR}x^{1-\lambda+l_1+l_2}$$
$$\times\left[\left(x^{-1}\frac{d}{dx}\right)^{l_1}x^{-1}[(\zeta_1-x)^{l_1-n_1-1}-(\zeta_1+x)^{l_1-n_1-1}]\right]\left[\left(x^{-1}\frac{d}{dx}\right)^{l_2}x^{-1}(\zeta_2-x)^{l_2-n_2-1}\right]. \quad (30)$$

Equation (30)$\neq$0 only if the residue (the coefficient of x^{-1} in a Laurent series[4]) of the integrand at the origin does not vanish. The first odd power in the Laurent expansion of the integrand is $x^{l_1-l_2+\lambda+1}$. Since $l_1-l_2+\lambda+1\geq1$, there is no term $\sim x^{-1}$, and

$$\mathcal{S}^\lambda\{\text{the rest}\}=0. \quad (31)$$

OVERLAP SERIES. $n_1+n_2\neq$INTEGER

The complete series for $\mathcal{S}^\lambda(R)$ is obtained from Eqs. (9), (22), (29), (31), and (17):

$$\mathcal{S}^\lambda_{n_1l_1\zeta_1;n_2l_2\zeta_2}(R)=-\tfrac{1}{2}(-1)^{l_2}R^{n_1+n_2+1}$$
$$\times\sum_{\mu_1=0}^{l_1}\sum_{\mu_2=0}^{l_2}\sum_{N=0}^{\infty}(-R)^N\frac{(l_1+\mu_1)!(l_2+\mu_2)!}{2^{\mu_1+\mu_2}(l_1-\mu_1)!(l_2-\mu_2)!\mu_1!\mu_2!}\frac{2^\lambda\Gamma[\frac{1}{2}(n_1+n_2+1+N+\lambda)+1]}{\Gamma[\frac{1}{2}(n_1+n_2+1+N-\lambda)+1]\Gamma(n_1+n_2+3+N+\lambda)}$$
$$\times\sum_{M=0}^{N}\left(1+(-1)^{l_2+N-M}\frac{\sin\pi n_1}{\sin\pi(n_1+n_2)}+(-1)^{l_1+M}\frac{\sin\pi n_2}{\sin\pi(n_1+n_2)}\right)$$
$$\times\zeta_1^M\zeta_2^{N-M}[M!(N-M)!]^{-1}\Gamma(n_1-\mu_1+1+M)\Gamma(n_2-\mu_2+1+N-M)$$
$$+\sum_{\substack{\mu_1=0\\(2N+\lambda\geq\mu_1+\mu_2)}}^{l_1}\sum_{\mu_2=0}^{l_2}\sum_{N=0}^{\infty}R^{2N+\lambda}\frac{(l_1+\mu_1)!(l_2+\mu_2)!(-1)^{\mu_2}}{2^{\mu_1+\mu_2}(l_1-\mu_1)!(l_2-\mu_2)!\mu_1!\mu_2!}\frac{\Gamma(n_1-\mu_1+1)}{\Gamma(\mu_2-n_2)}$$
$$\times\frac{2^\lambda(\lambda+N)!}{N!(2N+2\lambda+1)!}\Gamma(n_1+n_2+1-2N-\lambda)(\zeta_1+\zeta_2)^{\mu_1+\mu_2-n_1-n_2-1}\zeta_2^{2N+\lambda-\mu_1-\mu_2}$$
$$\times\sum_{M=0}^{2N+\lambda-\mu_1-\mu_2}\binom{2N+\lambda-\mu_1-\mu_2}{M}\zeta_1^M\zeta_2^{-M}\frac{\Gamma(\mu_2-n_2+M)}{\Gamma(n_1+\mu_2+1-2N-\lambda+M)}. \quad (32)$$

CONVERGENCE

The discussion of convergence of Eq. (32) is simplified by rewriting $\mathcal{S}^{\lambda}(R)$ in terms of the hypergeometric function[3d]:

$$\mathcal{S}^{\lambda}(R)=-\tfrac{1}{2}(-1)^{l_2}R^{n_1+n_2+1}$$

$$\times\sum_{\mu_1=0}^{l_1}\sum_{\mu_2=0}^{l_2}\sum_{N=0}^{\infty}(-\zeta_2R)^N\frac{(l_1+\mu_1)!(l_2+\mu_2)!}{2^{\mu_1+\mu_2}(l_1-\mu_1)!(l_2-\mu_2)!\mu_1!\mu_2!}\frac{2^{\lambda}\Gamma[\frac{1}{2}(n_1+n_2+1+N+\lambda)+1]\Gamma(n_1-\mu_1+1)\Gamma(n_2-\mu_2+1+N)}{\Gamma[\frac{1}{2}(n_1+n_2+1+N-\lambda)+1]\Gamma(n_1+n_2+3+N+\lambda)N!}$$

$$\times\{F(-N,n_1-\mu_1+1;\mu_2-n_2-N;\zeta_1/\zeta_2)+[(-1)^{l_2+N}\sin\pi n_1+(-1)^{l_1}\sin\pi n_2]$$

$$\times[\sin\pi(n_1+n_2)]^{-1}F(-N,n_1-\mu_1+1;\mu_2-n_2-N;-\zeta_1/\zeta_2)\}$$

$$+\sum_{\substack{\mu_1=0\\(2N+\lambda\geq\mu_1+\mu_2)}}^{l_1}\sum_{\mu_2=0}^{l_2}\sum_{N=0}^{\infty}R^{2N+\lambda}\frac{(l_1+\mu_1)!(l_2+\mu_2)!(-1)^{\mu_2}}{2^{\mu_1+\mu_2}(l_1-\mu_1)!(l_2-\mu_2)!\mu_1!\mu_2!}\frac{2^{\lambda}(\lambda+N)!\Gamma(n_1-\mu_1+1)\Gamma(n_1+n_2+1-2N-\lambda)}{N!(2N+2\lambda+1)!\Gamma(n_1+\mu_2+1-2N-\lambda)}$$

$$\times(\zeta_1+\zeta_2)^{\mu_1+\mu_2-n_1-n_2-1}\zeta_2^{2N+\lambda-\mu_1-\mu_2}F(\mu_1+\mu_2-2N-\lambda,\mu_2-n_2;n_1+\mu_2+1-2N-\lambda;-\zeta_1/\zeta_2).\tag{33}$$

Consider the $R^{2N+\lambda}$ series. Fix μ_1 and μ_2, and assume that $\zeta_1<\zeta_2$. Denote the ratio of the $(N+1)$th-to-Nth term by $\rho_{N+1,N}$:

$$\rho_{N+1,N}=(\zeta_2R)^2\frac{(N+\lambda+1)(n_1+\mu_2-2N-\lambda)(n_1+\mu_2-2N-\lambda-1)}{(N+1)(2N+2\lambda+3)(2N+2\lambda+2)(n_1+n_2-2N-\lambda)(n_1+n_2-2N-\lambda-1)}$$

$$\times\frac{F(\mu_1+\mu_2-2N-\lambda-2,\mu_2-n_2;n_1+\mu_2+1-2N-\lambda-2;-\zeta_1/\zeta_2)}{F(\mu_1+\mu_2-2N-\lambda,\mu_2-n_2;n_1+\mu_2+1-2N-\lambda;-\zeta_1/\zeta_2)}.\tag{34}$$

When $|z|<1$,

$$\lim_{N\to\infty}F(a-2N,b;c-2N;z)=(1-z)^{-b}.\tag{35}$$

Thus,

$$\rho_{N+1,N}\underset{N\to\infty}{\sim}\tfrac{1}{4}(\zeta_2R)^2N^{-2},\tag{36}$$

which shows that the $R^{2N+\lambda}$ series converges absolutely for all $R<\infty$. [When $\zeta_2<\zeta_1$, a similar argument leads to Eq. (36) with ζ_2 replaced by ζ_1.] Similar conclusions apply to the $R^{n_1+n_2+1+N}$ series, and consequently the series for $\mathcal{S}^{\lambda}(R)$ [Eqs. (32) and (33)] are absolutely convergent for all finite R.

INTEGER n_1 AND n_2

When either n_1 or n_2 is an integer, the arguments of some of the gamma functions in the $R^{2N+\lambda}$ terms of Eq. (32) are nonpositive integers, and the expressions are indeterminate. Consideration of the limit of Eq. (32) as $n_1\to$ integer, however, leads to the modification

$$\sum_{M=0}^{2N+\lambda-\mu_1-\mu_2}\to\sum_{M=\max\{0,2N+\lambda-n_1-\mu_2\}}^{2N+\lambda-\mu_1-\mu_2},$$

while $n_2\to$ integer leads to

$$\sum_{M=0}^{2N+\lambda-\mu_1-\mu_2}\to\sum_{M=0}^{\min\{2N+\lambda-\mu_1-\mu_2,n_2-\mu_2\}}.$$

With the modified summations the Γ functions remain finite.

When both n_1 and n_2 are integers, it is easily seen that the limits of the $R^{n_1+n_2+1+N}$ and $R^{2N+\lambda}$ series depend upon the order that n_1 and n_2 become integers. Nevertheless, their sum, the whole series, does not depend on the order. We obtain (by first setting n_1, then n_2, equal to integers), after a minimum of manipulation,

$$\mathcal{S}^{\lambda}{}_{n_1l_1\zeta_1;n_2l_2\zeta_2}(R)\ \{n_1\text{ and }n_2\text{ both integers}\}$$

$$=\sum_{\substack{\mu_1=0\\(\mu_1+\mu_2\leq2N+\lambda\leq n_1+n_2)}}^{l_1}\sum_{\mu_2=0}^{l_2}\sum_{N\geq0}R^{2N+\lambda}\frac{(l_1+\mu_1)!(l_2+\mu_2)!(-1)^{\mu_2}(n_1-\mu_1)!(n_2-\mu_2)!2^{\lambda}(\lambda+N)!(n_1+n_2-2N-\lambda)!}{2^{\mu_1+\mu_2}(l_1-\mu_1)!(l_2-\mu_2)!\mu_1!\mu_2!N!(2N+2\lambda+1)!}$$

$$\times(\zeta_1+\zeta_2)^{\mu_1+\mu_2-n_1-n_2-1}\zeta_2^{2N+\lambda-\mu_1-\mu_2}\sum_{M=\max\{0,2N+\lambda-n_1-\mu_2\}}^{\min\{2N+\lambda-\mu_1-\mu_2,n_2-\mu_2\}}\binom{2N+\lambda-\mu_1-\mu_2}{M}$$

$$\times(-\zeta_1)^M\zeta_2^{-M}[(n_1+\mu_2-2N-\lambda+M)!(n_2-\mu_2-M)!]^{-1}-\tfrac{1}{2}(-1)^{l_2}R^{n_1+n_2+1}$$

$$\times\sum_{\mu_1=0}^{l_1}\sum_{\mu_2=0}^{l_2}\sum_{N=0}^{\infty}(-R)^N\frac{(l_1+\mu_1)!(l_2+\mu_2)!}{2^{\mu_1+\mu_2}(l_1-\mu_1)!(l_2-\mu_2)!\mu_1!\mu_2!}\frac{2^\lambda\Gamma[\frac{1}{2}(n_1+n_2+1+N+\lambda)+1]}{\Gamma[\frac{1}{2}(n_1+n_2+1+N-\lambda)+1](n_1+n_2+2+N+\lambda)!}$$

$$\times\sum_{M=0}^{N}[1+(-1)^{l_1+n_1+M}]\zeta_1^M\zeta_2^{N-M}[M!(N-M)!]^{-1}(n_1-\mu_1+M)!(n_2-\mu_2+N-M)!+(-1)^{n_1+l_1+l_2}$$

$$\times\sum_{\mu_1=0}^{l_1}\sum_{\mu_2=0}^{l_2}\sum_{\substack{N\\(2N+\lambda\geq n_1+n_2+1)}}R^{2N+\lambda}\frac{(l_1+\mu_1)!(l_2+\mu_2)!(n_2-\mu_2)!}{2^{\mu_1+\mu_2}(l_1-\mu_1)!(l_2-\mu_2)!\mu_1!\mu_2!}\frac{2^\lambda(\lambda+N)!}{N!(2N+2\lambda+1)}\frac{(2N+\lambda-\mu_1-\mu_2)!}{(2N+\lambda-n_1-n_2-1)!}$$

$$\times(\zeta_1+\zeta_2)^{\mu_1+\mu_2-n_1-n_2-1}\zeta_1^{2N+\lambda-n_1-\mu_2}\zeta_2^{n_1-\mu_1}\sum_{M=0}^{n_1-\mu_1}\binom{n_1-\mu_1}{M}\zeta_1^M\zeta_2^{-M}\frac{(2N+\lambda-n_1-n_2-1+M)!}{(2N+\lambda-n_1-\mu_2+M)!}. \qquad (37)$$

LOGARITHMIC CASE: n_1+n_2=INTEGER; n_1, $n_2\neq$INTEGER

When n_1+n_2 is an integer, while n_1 and n_2 are not, the series (32) fails catastrophically because of the vanishing of $\sin\pi(n_1+n_2)$ in the denominator and the infinity of $\Gamma(n_1+n_2+1-2N-\lambda)$ in the numerator. Examination of Eq. (20) reveals what has gone wrong. On Λ_3, the branch cut emanating from $-\zeta_2$ terminates at ζ_1, the infinite parts of Λ_3 cancel (see Λ'_3, Fig. 6) and the two terms in the numerator of Eq. (20) cancel:

$$[1-\exp(-2\pi in_1)]\int_{\Lambda_3'}dx+\exp(-2\pi in_1)\int_{\Lambda_4}dx=0. \qquad (38)$$

That is,

$$\lim_{n_1+n_2\to\text{integer}}\sin\pi(n_1+n_2)\,S^\lambda(R)=0. \qquad (39)$$

Consequently, the appropriate series expansion may be recovered from Eq. (32) by L'Hospital's rule:

$$S^\lambda(R)\{n_1+n_2=\text{ integer}\}=(-1)^{n_1+n_2}\pi^{-1}\lim_{n_2\to-n_1+\text{integer}}\frac{d}{dn_2}\sin\pi(n_1+n_2)\,S^\lambda(R)\{\text{Eq. (32)}\}. \qquad (40)$$

A logarithmic term is introduced by $(d/dn_2)R^{n_1+n_2+1+N}=R^{n_1+n_2+1+N}\log R$. The $\psi(n)$ denotes the derivative of the logarithm of the Γ function $[\psi(n)=(d/dn)\log\Gamma(n)]$:

$S^\lambda_{n_1l_1\zeta_1;n_2l_2\zeta_2}(R)$ {logarithmic case}

$$=\sum_{\substack{\mu_1=0\\(\mu_1+\mu_2\leq 2N+\lambda\leq n_1+n_2)}}^{l_1}\sum_{\mu_2=0}^{l_2}\sum_{N\geq0}R^{2N+\lambda}\frac{(l_1+\mu_1)!(l_2+\mu_2)!(-1)^{\mu_2}\Gamma(n_1-\mu_1+1)}{2^{\mu_1+\mu_1}(l_1-\mu_1)!(l_2-\mu_2)!\mu_1!\mu_2!\Gamma(\mu_2-n_2)}\frac{2^\lambda(\lambda+N)!}{N!(2N+2\lambda+1)!}$$

$$\times(n_1+n_2-2N-\lambda)!(\zeta_1+\zeta_2)^{\mu_1+\mu_2-n_1-n_2-1}\zeta_2^{2N+\lambda-\mu_1-\mu_2}$$

$$\times\sum_{M=0}^{2N+\lambda-\mu_1-\mu_2}\binom{2N+\lambda-\mu_1-\mu_2}{M}\zeta_1^M\zeta_2^{-M}\frac{\Gamma(\mu_2-n_2+M)}{\Gamma(n_1+\mu_2+1-2N-\lambda+M)}-\tfrac{1}{2}(-1)^{l_2}R^{n_1+n_2+1}$$

$$\times\sum_{\mu_1=0}^{l_1}\sum_{\mu_2=0}^{l_2}\sum_{N=0}^{\infty}(-R)^N\frac{(l_1+\mu_1)!(l_2+\mu_2)!}{2^{\mu_1+\mu_2}(l_1-\mu_1)!(l_2-\mu_2)!\mu_1!\mu_2!}\frac{2^\lambda\Gamma[\frac{1}{2}(n_1+n_2+1+N+\lambda)+1]}{\Gamma[\frac{1}{2}(n_1+n_2+1+N-\lambda)+1](n_1+n_2+2+N+\lambda)!}$$

$$\times\sum_{M=0}^{N}\zeta_1^M\zeta_2^{-M}[M!(N-M)!]^{-1}\Gamma(n_1-\mu_1+1+M)\Gamma(n_2-\mu_2+1+N-M)\{1+(-1)^{l_1+M}\cos\pi n_1$$

$$+\pi^{-1}(-1)^M\sin\pi n_1[(-1)^{l_2+n_1+n_2+N}-(-1)^{l_1}][\log R+\tfrac{1}{2}\psi(\tfrac{1}{2}(n_1+n_2+1+N+\lambda)+1)$$

$$-\tfrac{1}{2}\psi(\tfrac{1}{2}(n_1+n_2+1+N-\lambda)+1)-\psi(n_1+n_2+3+N+\lambda)+\psi(n_2-\mu_2+1+N-M)]\}-(-1)^{l_1+l_2}$$

$$\times\sum_{\mu_1=0}^{l_1}\sum_{\mu_2=0}^{l_2}\sum_{\substack{N\\(2N+\lambda\geq n_1+n_2+1)}}R^{2N+\lambda}\frac{(l_1+\mu_1)!(l_2+\mu_2)!\Gamma(n_1-\mu_1+1)\Gamma(n_2-\mu_2+1)}{2^{\mu_1+\mu_2}(l_1-\mu_1)!(l_2-\mu_2)!\mu_1!\mu_2!}\frac{2^\lambda(\lambda+N)!}{N!(2N+2\lambda+1)!}$$

$$\times[(2N+\lambda-n_1-n_2-1)!]^{-1}(\zeta_1+\zeta_2)^{\mu_1+\mu_2-n_1-n_2-1}\zeta_2^{2N+\lambda-\mu_1-\mu_2}$$

$$\times\sum_{M=0}^{2N+\lambda-\mu_1-\mu_2}\binom{2N+\lambda-\mu_1-\mu_2}{M}\zeta_1^M\zeta_2^{-M}\Gamma(\mu_2-n_2+M)[\Gamma(n_1+\mu_2+1-2N-\lambda+M)]^{-1}\pi^{-1}\sin\pi n_1$$

$$\times[-\log(\zeta_1+\zeta_2)+\psi(\mu_2-n_2)+\psi(2N+\lambda-n_1-n_2)-\psi(\mu_2-n_2+M)]. \quad (41)$$

REMARKS

By using "linear transformation formulas" and "contiguous relations" among hypergeometric functions,[3] (a) many alternative forms[5] for Eqs. (32), (33), (37), and (41) can be found, and (b) recurrence relations among the various coefficients of powers of R can be derived.

The important practical question,[6] "Which is the most efficient route for computations?" is as yet unanswered. A crude computer program based on Eq. (33) seems to be an order of magnitude faster than an equally crude program based on Eqs. (16) and (18) of I. The pitfall in using Eqs. (16) and (18) of I is the wiggly nature of the spherical Bessel functions, which requires many points for the numerical integration. The series expansion, moreover, has an advantage when more than one internuclear distance is involved, because the coefficients of the various powers of R need be computed just once. Finally, another numerical-integration route, as yet unexplored, could be based on Eqs. (8)–(11) for which the integrands die off exponentially, rather than oscillate interminably.

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APPENDIX

In Eq. (25), the $\sum_{\mu_1}\sum_{\mu_2}\sum_N$ was restricted by

$$2N+\lambda\geq\mu_1+\mu_2. \quad (A1)$$

An alternative statement of (A1) is that, in the expansion of (in Dirac notation) the integrand of

$$\langle[x^{-1}(d/dx)]^{l_1}x^{-1}\psi_1 \mid x^{2+\lambda+l_1+l_2+2N} \mid [x^{-1}(d/dx)]^{l_2}x^{-1}\psi_2\rangle \quad (A2)$$

in terms of derivatives of $\psi_1\times$ derivatives of $\psi_2\times$ powers of x, no negative powers of x occur.

If $2N+\lambda\geq l_1+l_2$, the assertion is trivial, so assume $2N+\lambda\leq l_1+l_2$. Also, assume $l_2\geq l_1$ (this is no loss of generality). Recall that $2N+\lambda+l_1+l_2$ is even, and $0\leq l_2-l_1\leq 2N+\lambda\leq l_1+l_2$. The restriction is proved by rewriting (A2) as

$$(-1)^{l_1}\left\langle\psi_1\left|\left(x^{-1}\frac{d}{dx}\right)^{l_1}x^{\lambda+l_1+l_2+2N}\left(\frac{d}{dx}x^{-1}\right)^{l_2}\right|\psi_2\right\rangle \quad (A3)$$

$$=(-1)^{l_1}\left\langle\psi_1\left|x^{2N+\lambda-l_1+l_2}\left(\frac{d}{dx}x^{-1}\right)^{1/2(2N+\lambda-l_1+l_2)}\left(\frac{d}{dx}\right)^{l_1+l_2-2N-\lambda}\left(x^{-1}\frac{d}{dx}\right)^{1/2(2N+\lambda+l_1-l_2)}x^{2N+\lambda+l_1-l_2}\right|\psi_2\right\rangle. \quad (A4)$$

When the operator part of (A4) is expanded in $x^\mu(d/dx)^{l_1+l_2-2N-\lambda+\mu}$, by inspection, no negative values of μ occur.

[6] It has been suggested that some remarks be included on the relative merits of the various possible computational routes so "that some new investigator can try the scheme out numerically and modify it, if necessary." The remarks of this paragraph are based on the author s meager experience in computations and are meant to be a preliminary guide for other investigators.