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On the Evaluation of Two-Center Overlap and Coulomb Integrals with Noninteger-n Slater-Type Orbitals*

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Some formulas are developed which facilitate computation of two-center overlap and Coulomb integrals with noninteger principal-quantum-number (n) Slater-type orbitals by the Fourier-transform convolution technique. A conceptually simple, closed-form analytical expression for the overlap and Coulomb integrals with integer-n Slater-type orbitals is also given.

INTRODUCTION

NONINTEGER principal-quantum-number (n) Slater-type orbitals (STO) provide a simple but more flexible basis for molecular quantum-mechanical calculations than integer-n STO's. But the large body of formulas[1–8] developed for the evaluation of two-center integrals for integer-n STO's does not generally apply to noninteger-n STO's: n is invariably used as an integer, e.g., as in a polynomial of degree n or in an n-step recursion formula. The purpose of this article is to point out that the Fourier-transform convolution-theorem method, employed recently by Prosser and Blanchard[9] and by Geller,[10–14] provides a convenient method for evaluating two-center noninteger-n integrals of the Coulomb and overlap type, and explicit formulas for the necessary Fourier transforms are developed. As a bonus, some interesting expressions for the integer-n integrals are also obtained.

SOME DEFINITIONS

The Fourier-transform convolution theorem[15] replaces a one-electron two-center overlap integral by an integral over the Fourier transforms:

$$\int dV\phi^*(\mathbf{r})\chi(\mathbf{r}-\mathbf{R})=(2\pi)^{-3}\int d^3\mathbf{k}\bar{\phi}^*(\mathbf{k})\bar{\chi}(\mathbf{k})\ \exp(i\mathbf{k}\cdot\mathbf{R}). \tag{1}$$

The vector between the two centers is denoted by $\mathbf{R}$, the asterisk denotes the complex conjugate, and $\bar{\phi}$ and $\bar{\chi}$ denote the Fourier transforms of ϕ and χ:

$$\bar{\phi}(\mathbf{k})=\int dV\ \exp(i\mathbf{k}\cdot\mathbf{r})\phi(\mathbf{r}),$$

$$\bar{\chi}(\mathbf{k})=\int dV\ \exp(i\mathbf{k}\cdot\mathbf{r})\chi(\mathbf{r}). \tag{2}$$

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

The matrix element of a two-electron operator between two one-center charge distributions is reduced from a six-dimensional to a three-dimensional integral:

$$\int dV_1 \int dV_2 \phi^*(\mathbf{r}_1) h(\mathbf{r}_{12}) \chi(\mathbf{r}_2-\mathbf{R}) = (2\pi)^{-3} \int d^3\mathbf{k} \bar{\phi}^*(\mathbf{k}) \bar{h}(\mathbf{k}) \bar{\chi}(\mathbf{k}) \exp(i\mathbf{k}\cdot\mathbf{R}). \quad (3)$$

In the case of the STO's, the nuclear attraction, kinetic energy, and matrix elements of powers of coordinates are essentially equivalent to overlap integrals. The most important two-electron integral is of the Coulomb type, for which $h(\mathbf{r}_{12}) = r_{12}^{-1}$ and $\bar{h}(\mathbf{k}) = 4\pi k^{-2}$.

A normalized STO is given by

$$\psi_{nlm\zeta}(\mathbf{r}) = N_{n\zeta} r^{n-1} \exp(-\zeta r) Y_l^m(\theta, \varphi), \quad (4)$$

where $Y_l^m(\theta, \varphi)$ is a (complex) spherical harmonic and $N_{n\zeta}$ a normalization constant:

$$N_{n\zeta} = (2\zeta)^{n+\frac{1}{2}} [\Gamma(2n+1)]^{-\frac{1}{2}}. \quad (5)$$

$\Gamma(x)$ denotes the gamma function. A Slater-type charge distribution is given by

$$\rho_{nlm\zeta}(\mathbf{r}) = M_{nl\zeta} r^{n-1} \exp(-\zeta r) Y_l^m(\theta, \varphi), \quad (6)$$

where three possible conventions for $M_{nl\zeta}$ are

$$M_{nl\zeta}(\text{Roothaan}^2) = [(2l+1)/4\pi]^{\frac{1}{2}} 2^l \zeta^{n+2} / \Gamma(n+l+2), \quad (7)$$

$$M_{nl\zeta}(\text{Ruedenberg}^8) = [(2l+1)/4\pi]^{\frac{1}{2}} [2^{n+1}\Gamma(n+2)]^{-1} \zeta^{n+2}, \quad (8)$$

$$M_{nl\zeta}(\text{unit multipole}) = \zeta^{n+l+2} / \Gamma(n+l+2). \quad (9)$$

The definition of Eq. (9) makes $\rho_{nlm\zeta}(\mathbf{r})$ correspond to a charge distribution with a unit multipole moment[16] of order l, m.

BASIC FOURIER TRANSFORM

To use Eqs. (1) and (3) to calculate overlap and Coulomb integrals we need the Fourier transform of $r^{n-1} \exp(-\zeta r) Y_l^m(\theta, \varphi)$:

$$F_{nlm\zeta}(\mathbf{k}) \equiv \int dV \exp(i\mathbf{k}\cdot\mathbf{r}) r^{n-1} \exp(-\zeta r) Y_l^m(\theta, \varphi). \quad (10)$$

The integral for $F_{nlm\zeta}(\mathbf{k})$ is easily evaluated. Using the expansion[17a] of $\exp(i\mathbf{k}\cdot\mathbf{r})$ in spherical Bessel functions and Rayleigh's formula[17b]

$$j_l(x) = (-x)^l [x^{-1}(d/dx)]^l (\sin x/x), \quad (11)$$

we obtain (θ_k and φ_k denote spherical polar coordinates in $\mathbf{k}$ space) explicitly

$$F_{nlm\zeta}(\mathbf{k}) = f_{nl\zeta}(k) Y_l^m(\theta_k, \varphi_k), \quad (12)$$

$$f_{nl\zeta}(k) = 4\pi i^l \int_0^\infty dr r^{n+1} \exp(-\zeta r) j_l(kr) dr$$

$$= 4\pi i^l \Gamma(n-l+1)(-k)^l [k^{-1}(d/dk)]^l (1/2ik) [(\zeta-ik)^{l-n-1} - (\zeta+ik)^{l-n-1}]. \quad (13)$$

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[16] J. D. Jackson, *Classical Electrodynamics* (John Wiley & Sons, Inc., New York, 1962), p. 99.

[17] *Handbook of Mathematical Functions*, M. Abramowitz and I. A. Stegun, Eds. (National Bureau of Standards, Appl. Math. Ser. No. 55, 1964): (a) p. 440, Eq. (10.1.47); (b) p. 439, Eq. (10.1.25); (c) p. 439, Eq. (10.1.19); (d) p. 439, Eq. (10.1.22); (e) p. 437–438, Eqs. (10.1.8)–(10.1.10).

Equations (1)–(13) yield the following expressions for the overlap and Coulomb integrals:

$$S_{n_1l_1m_1\zeta_1;n_2l_2m_2\zeta_2}(\mathbf{R})\equiv\int dV\psi^*_{n_1l_1m_1\zeta_1}(\mathbf{r})\psi_{n_2l_2m_2\zeta_2}(\mathbf{r}-\mathbf{R}) \tag{14}$$

$$=N_{n_1\zeta_1}N_{n_2\zeta_2}(2\pi)^{-3}\int d^3\mathbf{k}F^*_{n_1l_1m_1\zeta_1}(\mathbf{k})F_{n_2l_2m_2\zeta_2}(\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{R}) \tag{15}$$

$$=N_{n_1\zeta_1}N_{n_2\zeta_2}(2\pi^2)^{-1}\sum_{\lambda=|l_1-l_2|}^{l_1+l_2}c^\lambda(l_2,m_2;l_1,m_1)$$

$$\times(2\lambda+1)^{\frac{1}{2}}(4\pi)^{-\frac{1}{2}}Y_\lambda^{m_2-m_1}(\theta_R,\varphi_R)i^\lambda\int_0^\infty dkk^2f^*_{n_1l_1\zeta_1}(k)f_{n_2l_2\zeta_2}(k)j_\lambda(kR), \tag{16}$$

$$C_{n_1l_1m_1\zeta_1;n_2l_2m_2\zeta_2}(\mathbf{R})\equiv\int dV_1\int dV_2\rho^*_{n_1l_1m_1\zeta_1}(\mathbf{r}_1)r_{12}^{-1}\rho_{n_2l_2m_2\zeta_2}(\mathbf{r}_2-\mathbf{R}) \tag{17}$$

$$=M_{n_1l_1\zeta_1}M_{n_2l_2\zeta_2}2\pi^{-1}\sum_{\lambda=|l_1-l_2|}^{l_1+l_2}c^\lambda(l_2,m_2;l_1,m_1)$$

$$\times(2\lambda+1)^{\frac{1}{2}}(4\pi)^{-\frac{1}{2}}Y_\lambda^{m_2-m_1}(\theta_R,\varphi_R)i^\lambda\int_0^\infty dk\,f^*_{n_1l_1\zeta_1}(k)f_{n_2l_2\zeta_2}(k)j_\lambda(kR), \tag{18}$$

where θ_R and ϕ_R define the direction of $\mathbf{R}$, and (following Condon and Shortley[18]) the $c^\lambda(l_2,m_2;l_1,m_1)$ are

$$(2\lambda+1)^{\frac{1}{2}}(4\pi)^{-\frac{1}{2}}c^\lambda(l_2,m_2;l_1,m_1)=\int d\Omega(Y_{l_1}^{m_1}Y_\lambda^{m_2-m_1})^*Y_{l_2}^{m_2}. \tag{19}$$

Equations (16) and (18) give the overlap and Coulomb integrals in terms of one-dimensional integrals whose integrands are the product of two Fourier-transform radical functions and a spherical Bessel function. The S integrand differs from the C integrand only by a factor $(4\pi/k^2)^{-1}$.

There are some recurrence formulas that can simplify the calculation of $f_{nl\zeta}(k)$. From Eq. (13) it is seen that

$$f_{n,l,\zeta}(k)=-i\{(d/dk)-[(l-1)/k]\}f_{n-1,l-1,\zeta}(k). \tag{20}$$

By substituting certain recurrence formulas[17c,d] for the $j_l(kr)$ in Eq. (13) and integrating by parts, one also finds

$$f_{n,l,\zeta}(k)=i[(2l-1)/k]f_{n-1,l-1,\zeta}(k)+f_{n,l-2,\zeta}(k), \tag{21}$$

$$f_{n,l,\zeta}(k)=i[(2l-1)/(n-l+1)](\zeta/k)f_{n,l-1,\zeta}(k)+[(n+l)/(n-l+1)]f_{n,l-2,\zeta}(k). \tag{22}$$

A few $f_{n,l,\zeta}$ are given below. We have also defined $f_{n,-1,l}$, because of its inherent simplicity, from $f_{n,0,\zeta}$ and $f_{n,1,\zeta}$ with Eq. (22). Any $f_{n,l,\zeta}$ can be expressed in terms of $f_{n,-1,\zeta}$ and $f_{n,0,\zeta}$ by repeated application of Eq. (22):

$$f_{n,-1,\zeta}=-2\pi i\Gamma(n+1)k^{-1}[(\zeta-ik)^{-n-1}+(\zeta+ik)^{-n-1}], \tag{23}$$

$$f_{n,0,\zeta}=-2\pi i\Gamma(n+1)k^{-1}[(\zeta-ik)^{-n-1}-(\zeta+ik)^{-n-1}], \tag{24}$$

$$f_{n,1,\zeta}=2\pi\Gamma(n)k^{-2}[(\zeta-ik)^{-n}-(\zeta+ik)^{-n}]-2\pi i\Gamma(n+1)k^{-1}[(\zeta-ik)^{-n-1}+(\zeta+ik)^{-n-1}]. \tag{25}$$

Since there are very simple formulas[17e] for calculating $j_\lambda(kr)$, and by virtue of Eqs. (24), (23), (22), (18), and (16), it should not be difficult to program for a computer the overlap and Coulomb integrals for arbitrary $(n_1, l_1, \zeta_1, n_2, l_2, \zeta_2)$ for which the original integrals converge.

Note that $(-i)^lf_{nl\zeta}$ is real and is an even (odd) function of k when l is even (odd) and that in S and C [Eqs. (16) and (18)] the coefficients of the $Y_2^{m_2-m_1}$ are real. At the origin

$$f_{nl\zeta}(k)\xrightarrow[k\to0]{}k^l[2^{l+2}\pi i^l\zeta^{-l-n-2}\Gamma(l+1)\Gamma(n+l+2)/\Gamma(2l+2)]. \tag{26}$$

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[18] E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, London, 1935), p. 175, Eq. (6).

When n is an integer, the only singularities of $f_{nl\zeta}(k)$ are poles of order $n+1$ at $k=\pm i\zeta$. When n is not an integer, $k=\pm i\zeta$ are branch points.

ASYMPTOTIC BEHAVIOR OF THE COULOMB INTEGRAL: $R\rightarrow\infty$

Since the asymptotic behavior of a function is governed by the singularity of its Fourier transform nearest the origin, we recast Eq. (18) for the Coulomb integral as a Fourier transform. We use the information that $c^{\lambda}(l_2, m_2; l_1, m_1)=0$ when $\lambda+l_1+l_2$ is odd, that all the integrands in Eq. (18) are even functions of k, that a singularity at the origin can be "forced" only for the $\lambda=l_1+l_2$ term, and that $j_{\lambda}(kR)$ is given by Eq. (11). The behavior of $C(\mathbf{R})$ as $\mathbf{R}$ goes to infinity is given by

$$C_{n_1l_1m_1\zeta_1;n_2l_2m_2\zeta_2}(\mathbf{R})\underset{R\to\infty}{\longrightarrow}M_{n_1l_1\zeta_1}M_{n_2l_2\zeta_2}\pi^{-\frac{1}{2}}Y_{l_1+l_2}{}^{m_2-m_1}(\theta_R,\varphi_R)$$

$$\times(2l_1+2l_2+1)^{\frac{1}{2}}c^{l_1+l_2}(l_2,m_2;l_1,m_1)\,i^{l_1+l_2}\int_0^{\infty}dkf^*_{n_1l_1\zeta_1}(k)f_{n_2l_2\zeta_2}(k)j_{l_1+l_2}(kR) \tag{27}$$

$$=M_{n_1l_1\zeta_1}M_{n_2l_2\zeta_2}\pi^{-\frac{1}{2}}Y_{l_1+l_2}{}^{m_2-m_1}(\theta_R,\varphi_R)\,(2l_1+2l_2+1)^{\frac{1}{2}}c^{l_1+l_2}(l_2,m_2;l_1,m_1)$$

$$\times i^{l_1+l_2}(-R)^{l_1+l_2}\left(\frac{1}{R}\frac{d}{dR}\right)^{l_1+l_2}R^{-1}(4i)^{-1}\int_{-\infty}^{\infty}dkf^*_{n_1l_1\zeta_1}f_{n_2l_2\zeta_2}k^{-1-l_1-l_2}[\exp(ikR)-\exp(-ikR)]. \tag{28}$$

The nonexponential part of the integrand has a simple pole at $k=0$, so that the long-range behavior of $C(\mathbf{R})$ is just $(2\pi i)$ times the value of $k^{-l_1-l_2}f^*_{n_1l_1\zeta_1}f_{n_2l_2\zeta_2}$ at $k=0$:

$$C(\mathbf{R})\rightarrow R^{-l_1-l_2-1}\zeta_1^{-l_1-n_1-2}\zeta_2^{-l_2-n_2-2}Y_{l_1+l_2}{}^{m_2-m_1}(\theta_R,\varphi_R)M_{n_1l_1\zeta_1}M_{n_2l_2\zeta_2}8\pi^{\frac{1}{2}}(2l_1+2l_2+1)^{\frac{1}{2}}c^{l_1+l_2}(l_2,m_2;l_1,m_1)$$

$$\times\frac{(-1)^{l_2}(2l_1+2l_2)!l_1!l_2!\Gamma(l_1+n_1+2)\Gamma(l_2+n_2+2)}{(l_1+l_2)!(2l_1+1)!(2l_2+1)!} \tag{29}$$

$$=R^{-l_1-l_2-1}Y_{l_1+l_2}{}^{m_2-m_1}(\theta_R,\varphi_R)8\pi^{\frac{1}{2}}(-1)^{l_2+m_1}$$

$$\times[\zeta_1^{-l_1-n_1-2}M_{n_1l_1\zeta_1}(2l_1+1)^{-\frac{1}{2}}\Gamma(l_1+n_1+2)][\zeta_2^{-l_2-n_2-2}M_{n_2l_2\zeta_2}(2l_2+1)^{-\frac{1}{2}}\Gamma(l_2+n_2+2)]$$

$$\times(2l_1+2l_2+1)^{-\frac{1}{2}}[(l_1+l_2-m_1+m_2)!(l_1+l_2+m_1-m_2)!]^{\frac{1}{2}}[(l_1+m_1)!(l_1-m_1)!(l_2+m_2)!(l_2-m_2)!]^{-\frac{1}{2}}, \tag{30}$$

where in Eq. (30) we have evaluated $c^{l_1+l_2}(l_2, m_2; l_1, m_1)$. One can recover O-Ohata and Ruedenberg's[8] result by setting $\theta_R=\varphi_R=0$, $m_1=m_2=m$, and multiplying by $(-1)^{l_2+m_2}$.

WHEN n_1 AND n_2 ARE NOT INTEGERS

When n_1 and n_2 are *not* integers, the integrands in Eqs. (16) and (18) have branch points at $k=\pm i\zeta_1$, $\pm i\zeta_2$. A typical integral [cf. Eqs. (13) and (28)] involves

$$\int_{-\infty+i\epsilon}^{\infty+i\epsilon}dk\,\exp(ikR)\,(\zeta_1+ik)^{-\nu_1}(\zeta_2-ik)^{-\nu_2}k^{-N}, \tag{31}$$

where ν_1, ν_2 and N are nonnegative, ν_1 and ν_2 are *not* integers, and N *is* an integer. This integral (31) can be expressed as an infinite sum of confluent hypergeometric functions, but we have not found a closed analytical expression for the general case.[19] When $R=0$ (one-center case) or when for $C(\mathbf{R})\,n_1=l_1=m_1=\zeta_1=0$ (Coulomb attraction to off-center nucleus) both Eqs. (16) and (18) can be integrated analytically to give expressions already in the literature.[20]

WHEN n_1 AND n_2 ARE INTEGERS

When n_1 and n_2 are both integers, the only singularities in the integrands of Eqs. (16) and (18) are poles of order n_1+1 and n_2+1 at $k=\pm i\zeta_1$ and $\pm i\zeta_2$ (if $\zeta_1\neq\zeta_2$) or poles of order n_1+n_2+2 at $k=\pm i\zeta$ (if $\zeta_1=\zeta_2=\zeta$). Since there are no branch cuts, the integrations can be carried out immediately by contour integration and the residue

[19] One special case has been given, however, by M. Geller, Ref. 10, Eq. (21).
[20] H. W. Joy and R. G. Parr, J. Chem. Phys. **28**, 448 (1958).

theorem.[15] After a little algebraic manipulation one can obtain some master formulas giving all the integer-n overlap and Coulomb integrals in terms of derivatives of an algebraic expression and an exponential. These elegantly horrible results are:

for $\zeta_1 \neq \zeta_2$,

$$S_{n_1l_1m_1\zeta_1;n_2l_2m_2\zeta_2}(\mathbf{R})=N_{n_1\zeta_1}N_{n_2\zeta_2}(-1)^{l_1}\pi^{\frac{1}{2}}(n_1-l_1)!(n_2-l_2)!$$
$$\times\sum_{\lambda=|l_1-l_2|}^{l_1+l_2}(2\lambda+1)^{\frac{1}{2}}c^\lambda(l_2,m_2;l_1,m_1)Y_\lambda^{m_2-m_1}(\theta_R,\phi_R)R^\lambda[R^{-1}(d/dR)]^\lambda R^{-1}$$
$$\times((1/n_1!)(d/dx)^{n_1}|_{x=\zeta_1}(x-\zeta_1)^{n_1+1}x^{l_1+l_2-\lambda+1}\exp(-xR)\{[x^{-1}(d/dx)]^{l_1}x^{-1}(\zeta_1-x)^{l_1-n_1-1}\}$$
$$\times\{[x^{-1}(d/dx)]^{l_2}x^{-1}[(\zeta_2+x)^{l_2-n_2-1}-(\zeta_2-x)^{l_2-n_2-1}]\}$$
$$+(1/n_2!)(d/dx)^{n_2}|_{x=\zeta_2}(x-\zeta_2)^{n_2+1}x^{l_1+l_2-\lambda+1}\exp(-xR)\{[x^{-1}(d/dx)]^{l_2}x^{-1}(\zeta_2-x)^{l_2-n_2-1}\}$$
$$\times\{[x^{-1}(d/dx)]^{l_1}x^{-1}[(\zeta_1+x)^{l_1-n_1-1}-(\zeta_1-x)^{l_1-n_1-1}]\}), \tag{32}$$

$$C_{n_1l_1m_1\zeta_1;n_2l_2m_2\zeta_2}(\mathbf{R})=\{R^{-l_1-l_2-1}\text{ term}[\text{Eq. }(30)]\}-M_{n_1l_1\zeta_1}M_{n_2l_2\zeta_2}(-1)^{l_1}4\pi^{\frac{3}{2}}(n_1-l_1)!(n_2-l_2)!$$
$$\times\sum_{\lambda=|l_1-l_2|}^{l_1+l_2}(2\lambda+1)^{\frac{1}{2}}c^\lambda(l_2,m_2;l_1,m_1)Y_\lambda^{m_2-m_1}(\theta_R,\phi_R)R^\lambda[R^{-1}(d/dR)]^\lambda R^{-1}$$
$$\times((1/n_1!)(d/dx)^{n_1}|_{x=\zeta_1}(x-\zeta_1)^{n_1+1}x^{l_1+l_2-\lambda-1}\exp(-xR)\{[x^{-1}(d/dx)]^{l_1}x^{-1}(\zeta_1-x)^{l_1-n_1-1}\}$$
$$\times\{[x^{-1}(d/dx)]^{l_2}x^{-1}[(\zeta_2+x)^{l_2-n_2-1}-(\zeta_2-x)^{l_2-n_2-1}]\}$$
$$+(1/n_2!)(d/dx)^{n_2}|_{x=\zeta_2}(x-\zeta_2)^{n_2+1}x^{l_1+l_2-\lambda-1}\exp(-xR)\{[x^{-1}(d/dx)]^{l_2}x^{-1}(\zeta_2-x)^{l_2-n_2-1}\}$$
$$\times\{[x^{-1}(d/dx)^{l_1}x^{-1}[(\zeta_1+x)^{l_1-n_1-1}-(\zeta_1-x)^{l_1-n_1-1}]\}); \tag{33}$$

and for $\zeta_1=\zeta_2=\zeta$,

$$S_{n_1l_1m_1\zeta;n_2l_2m_2\zeta}(\mathbf{R})=-N_{n_1\zeta}N_{n_2\zeta}(-1)^{l_1}\pi^{\frac{1}{2}}(n_1-l_1)!(n_2-l_2)!$$
$$\times\sum_{\lambda=|l_1-l_2|}^{l_1+l_2}(2\lambda+1)^{\frac{1}{2}}c^\lambda(l_2,m_2;l_1,m_1)Y_\lambda^{m_2-m_1}(\theta_R,\phi_R)R^\lambda[R^{-1}(d/dR)]^\lambda R^{-1}$$
$$\times[(n_1+n_2+1)!]^{-1}(d/dx)^{n_1+n_2+1}|_{x=\zeta}(x-\zeta)^{n_1+n_2+2}x^{l_1+l_2-\lambda+1}\exp(-xR)$$
$$\times\{[x^{-1}(d/dx)]^{l_1}x^{-1}[(\zeta+x)^{l_1-n_1-1}-(\zeta-x)^{l_1-n_1-1}]\}$$
$$\times\{[x^{-1}(d/dx)]^{l_2}x^{-1}[(\zeta+x)^{l_2-n_2-1}-(\zeta-x)^{l_2-n_2-1}]\}, \tag{34}$$

$$C_{n_1l_1m_1\zeta;n_2l_2m_2\zeta}(\mathbf{R})=\{R^{-l_1-l_2-1}\text{ term}[\text{Eq. }(30)]\}+M_{n_1l_1\zeta}M_{n_2l_2\zeta}(-1)^{l_1}4\pi^{\frac{3}{2}}(n_1-l_1)!(n_2-l_2)!$$
$$\times\sum_{\lambda=|l_1-l_2|}^{l_1+l_2}(2\lambda+1)^{\frac{1}{2}}c^\lambda(l_2,m_2;l_1,m_1)Y_\lambda^{m_2-m_1}(\theta_R,\phi_R)R^\lambda[R^{-1}(d/dR)]^\lambda R^{-1}[(n_1+n_2+1)!]^{-1}$$
$$\times(d/dx)^{n_1+n_2+1}|_{x=\zeta}(x-\zeta)^{n_1+n_2+2}x^{l_1+l_2-\lambda-1}\exp(-xR)$$
$$\times\{[x^{-1}(d/dx)]^{l_1}x^{-1}[(\zeta+x)^{l_1-n_1-1}-(\zeta-x)^{l_1-n_1-1}]\}$$
$$\times\{[x^{-1}(d/dx)]^{l_2}x^{-1}[(\zeta+x)^{l_2-n_2-1}-(\zeta-x)^{l_2-n_2-1}]\}. \tag{35}$$

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