(Riemann-Lebesgue lemma). Such a procedure then assumes that we are discussing a system of independent two-level atoms with a given distribution of level separations.

However, despite the existence of a definite infinite time limit, it must still be noted that the final state depends on the initial condition, a rigorously demonstrated result in the *XY* model.

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Two-Center Integrals Involving Correlated Orbitals. I. Inclusion of James-Coolidge or Hylleraas r_{ij}^n Terms*

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All integrals needed to evaluate the wave function of the form

$$\Psi_{\rm tot}=\tilde{\mathfrak{a}}\left\{\left[\prod_j \sum_s a_{s_j}\Phi_s(j)\right]\left[1+\sum_{j<i}\sum w_{ij}\, r_{ij}^n\right]\right\} \qquad \text{for } n=1$$

and the Hamiltonian given are contained herein. For this form of the wave function, the integrals needed can be expressed as a product of integrals (involving at most four electrons). An indication of how to increase or decrease exponents of r_{ij}^n in steps of one or two is given. Some indication of how to proceed if the Hamiltonian contains $1/r_{ij}^3$ terms or if the wave function is of the form

$$\Psi_{\rm tot}=\tilde{\mathfrak{a}}\left\{\left[\prod_j \sum_s a_{sj}\,\Phi_s(j)\right]\left[1+\sum_{j<l<k}\sum\sum w_{jlk}\, r_{jl}^n\, r_{lk}^\nu\right]\right\}$$

is given. Consideration of all possible types of integrals (using picture-writing graph theory) involving $r_{ij}^a\, r_{kl}^b\, r_{mn}^c$ with $a<0$, $b>0$, $c>0$; $|a|=|b|=|c|=1$, is given. Integrals corresponding to the graphs (numbers next to the individual diagrams indicate the number of the equation) are given in analytical form. These can be evaluated by numerical-integration routines.

INTRODUCTION

Much success in *ab initio* calculations has been achieved with the use of correlated wave functions (wave functions that included the distance between two electrons explicitly). For the He atom,[1] the Li atom,[2] and the H_2 molecule,[3] these wave functions have yielded the most accurate energy levels and molecular properties.

Constructing the total wave function as a Slater determinant or antisymmetrized product is tantamount to using the Pauli principle, which excludes two electrons with identical quantum numbers and spin from occupying the same volume element at the same time. It does not tell us anything about two electrons with opposite spin, which we would expect to repel each other electrostatically. By including terms dependent upon the interelectronic separation, we cause the probability, calculated from this wave function, of finding two electrons at specified regions of space to decrease when the two electrons approach one another.

A correlated wave function can be an eigenfunction of spin and angular momentum. If $\mathfrak{a}(F)$ is an eigenfunction of the total and z component of spin and angular momentum, then Ψ is an eigenfunction of the same.[4] Using the Nth-order permutation group,[5] all spin states[6] for the N electron system can be included:

$$\Psi = \tilde{a}(FR),$$

$$F = F(1, 2, 3, \ldots, N) = (N!)^{-1/2}\Phi_1(1)\Phi_2(2)\cdots\Phi_N(N),$$

$$R = 1 + \sum_{j<l}\sum (w_{jl} r_{jl} + x_{jl} r_{jl}^2 + y_{jl} r_{jl}^3 + \cdots),$$

and $\tilde{a}$ is the antisymmetrization operator.

H is the Hamiltonian (in the Born-Oppenheimer approximation) in atomic units, Z_a and Z_b are the nuclear charges, R is the distance between nuclei a and b, $r_{i\lambda}$ is the distance between electron i and nucleus λ, r_{ij} is the distance between electron i and electron j:

$$\mathrm{H} = -\tfrac{1}{2}\sum_i \nabla_i^2 - \sum_i\left(\frac{Z_a}{r_{ia}} + \frac{Z_b}{r_{ib}}\right) + \sum_{i<j}\sum \frac{1}{r_{ij}} + \frac{Z_a Z_b}{R}.$$

The coordinate system[7] used is confocal elliptical. ϕ_i is the out-of-plane angle and R is the distance between nuclei a and b. $d\tau_i$ is the volume element and r_{12} the interelectronic distance. We have also

$$\xi_i = (r_{ai} + r_{bi})/R, \quad \eta_i = (r_{ai} - r_{bi})/R,$$

$$1 \le \xi_i < \infty, \quad -1 \le \eta_i \le 1, \quad 0 \le \phi_i < 2\pi,$$

$$d\tau_i = \tfrac{1}{8}R^3(\xi_i^2 - \eta_i^2)\,d\xi_i\,d\eta_i\,d\phi_i,$$

$$r_{12}^2 = \tfrac{1}{4}R^2\{\xi_1^2 + \xi_2^2 + \eta_1^2 + \eta_2^2 - 2 - 2\xi_1\xi_2\eta_1\eta_2 - 2[(\xi_1^2 - 1)(\xi_2^2 - 1)(1 - \eta_1^2)(1 - \eta_2^2)]^{1/2} \times \cos(\phi_1 - \phi_2)\}. \quad (1)$$

The basis functions $\Phi_s(j)$ and the total wave function are represented in Eqs. (2) and (3):

$$\Phi_s(j) = \xi_j^{p_s}\eta_j^{q_s}(\xi_j^2 - 1)^{\gamma_s/2}(1 - \eta_j^2)^{\nu_s/2}e^{-\alpha_s\xi_j}e^{\beta_s\eta_j}e^{im_s\phi_j},$$

$$s = (p_s, q_s, \gamma_s, \nu_s, \alpha_s, \beta_s, m_s), \quad i = \sqrt{(-1)} \quad (2)$$

$$\Psi_{\text{tot}} = \tilde{a}\{[\prod_j \sum_s a_{sj}\Phi_s(j)]\,[1 + \sum_{j<l}\sum \omega_{jl} r_{jl}^n]\}. \quad (3)$$

For molecules with more than two nuclei, the spherical coordinate system and Gaussian transforms[8] or ζ-function expansions[9] can be used for integral evaluation.

CLASSIFICATION OF INTEGRALS

The classification of types of integrals involving $r_{ij}^a r_{kl}^b r_{mn}^c$ can be considered in the notation of "picture-writing"[10] graph theory.[11] Figure 1 depicts the ten distinct integral types, for the case $a = b = 1$, $c = -1$. The small circles are electrons and the line segments connecting electrons i and j corresponds to the distance r_{ij}. The dashed line represents r_{ij}^{-1}. The numbers in parentheses next to each graph, in Fig. 1, correspond to the integral equation for that graph. If a line segment has no electron in common with any other line, it can be factored out of the integral. For the form of the wave function given in (3), the integrals needed can be expressed as a product of primitive integrals (involving at most four electrons). All the integrals needed to evaluate this wave function involving r_{ij} to the first power are given.

TWO-ELECTRON INTEGRALS

We have

$$\langle r_{12}^2\rangle = \langle\Phi_s(2)\,r_{12}^2\,\Phi_t(1)\rangle = \int d\tau\,\Phi_s(2)\,r_{12}^2\,\Phi_t(1)$$

$$= \tfrac{1}{64}R^8\pi^2\,\delta(m_s;0)\,\delta(m_t;0) \times \int_1^\infty\int_1^\infty\int_{-1}^1\int_{-1}^1 (\xi_1^2 - \eta_1^2)(\xi_2^2 - \eta_2^2)\,d\xi_1\,d\xi_2\,d\eta_1\,d\eta_2 \times \Phi_s(2)\,\Phi_t(1)\{\xi_1^2 + \xi_2^2 + \eta_1^2 + \eta_2^2 - 2 - 2\xi_1\xi_2\eta_1\eta_2 - [(\xi_1^2 - 1)(\xi_2^2 - 1)(1 - \eta_1^2)(1 - \eta_2^2)]^{1/2}\}. \quad (4)$$

The Neumann[12] expansion for $1/r_{12}$ in prolate elliptical coordinates is

$$\frac{1}{r_{12}} = \frac{4}{R}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}(-1)^m\,\frac{2l+1}{2}\left[\frac{(l-|m|)!}{(l+|m|)!}\right]^2 P_l^{|m|}(\xi_{1<2}) \times Q_l^{|m|}(\xi_{2>1})\,P_l^{|m|}(\eta_1)\,P_l^{|m|}(\eta_2)\,e^{im(\phi_1-\phi_2)}. \quad (5)$$

$P_l^m(\xi)$ and $Q_l^m(\xi)$ are associated Legendre polynomials of the first and second kind in the complex plane.[13] $\xi_{1<2}$ and $\xi_{2>1}$ mean the smaller and the larger, respectively, of ξ_1 and ξ_2. The $P_l^m(\xi)$ and $Q_l^m(\xi)$ have the range $[1, \infty]$. The $P_l^m(\eta)$ have the range $[-1, 1]$. For further details, see Refs. 13–23. We have

$$P_l^m(\xi) = \frac{(\xi^2 - 1)^{m/2}}{2^l\,l!}\,\frac{d^{l+m}}{d\xi^{l+m}}(\xi^2 - 1)^l,$$

$$P_l^m(\eta) = \frac{(1 - \eta^2)^{m/2}}{2^l\,l!}\,\frac{d^{l+m}}{d\eta^{l+m}}(\eta^2 - 1)^l,$$

$$Q_l^m(\xi) = (\xi^2 - 1)^{m/2}\,\frac{d^m}{d\xi^m}\,Q_l(\xi), \quad (6)$$

$$Q_l(\xi) = \tfrac{1}{2}P_l(\xi)\ln\left(\frac{\xi+1}{\xi-1}\right) - \sum_{j=1}^{\le(l+1)/2}\frac{2l - 4j + 3}{(2j-1)(l-j+1)}\,P_{l-2j+1}(\xi).$$

The $\langle 1/r_{12}\rangle$ [Eq. (10)] can be expressed more concisely, using the definitions of Eqs. (6)–(9),

$$a = (p_a, q_a, \gamma_a, \nu_a, \alpha_a, \beta_a, m_a),$$

$$b = (p_b, q_b, \gamma_b, \nu_b, \alpha_b, \beta_b, m_b),$$

$$K_{\mu,\mu',\alpha}^{\sigma}(z) = \int_1^z\int_{-1}^1 d\xi\,d\eta\,(\xi^2 - \eta^2)\,\xi^{p_a}\eta^{q_a}(\xi^2 - 1)^{\gamma_a/2} \times (1 - \eta^2)^{\nu_a/2}e^{-\alpha_a\xi}e^{+\beta_a\eta}P_\mu^\sigma(\xi)\,P_{\mu'}^\sigma(\eta), \quad (7)$$

$$F^\sigma_\mu(z)=\frac{-d}{dz}\left(\frac{Q^m_l(z)}{P^m_l(z)}\right)=\frac{(-1)^\sigma(\mu+\sigma)!/(\mu-\sigma)!}{[P^\sigma_\mu(z)]^2(z^2-1)}\,, \tag{8}$$

$$Z^\sigma_\mu=(-)^\sigma\left[\frac{(\mu-|\sigma|)!}{(\mu+|\sigma|)!}\right]^2\,, \tag{9}$$

$$\langle 1/r_{12}\rangle=\langle\Phi_a(1)\,(1/r_{12})\,\Phi_b(2)\rangle=\tfrac{1}{8}\pi^2R^5\,\delta(m_a+m_b;\,0)$$
$$\times\sum_{\mu=\sigma=|m_a|}^{\infty}(2\mu+1)Z^\sigma_\mu\int_1^\infty F^\sigma_\mu(z)K^\sigma_{\mu,\mu,a}(z)K^\sigma_{\mu,\mu,b}(z)\,dz\,. \tag{10}$$

For $\frac{1}{2}(\gamma_a+\sigma)$ and $\frac{1}{2}(\nu_a+\sigma)$ integers, the one-dimensional integral $K^\sigma_{\mu,\mu',a}(z)$ can be evaluated analytically for each z and inserted in the numerical integration at the appropriate mesh points:

$$K^\sigma_{\mu,\mu',a}(z)=\sum_{j=0}^{[(\mu-\sigma)/2]}\sum_{r=0}^{(\gamma_a+\sigma)/2}\sum_{k=0}^{[(\mu'-\sigma)/2]}\sum_{t=0}^{(\nu_a+\sigma)/2}\frac{(2\mu-2j)!\,(2\mu'-2k)!}{2^\mu j!\,(\mu-j)!\,(\mu-\sigma-2j)!\,2^{\mu'}k!\,(\mu'-k)!\,(\mu'-\sigma-2k)!}$$
$$\times\frac{(-1)^{(\nu_a+\sigma/2)-r}[\frac{1}{2}(\gamma_a+\sigma)]!\,(-1)^t[\frac{1}{2}(\nu_a+\sigma)]!}{r!\,[\frac{1}{2}(\gamma_a+\sigma)-r]!\,t!\,[\frac{1}{2}(\nu_a+\sigma)-t]!}\left\{S_2!\,V_0!\sum_{s=0}^{S_2}\sum_{v=0}^{V_0}\frac{[e^{-\alpha_a}-e^{-\alpha_a z}z^{S_2-s}]}{\alpha_a^{s+1}(S_2-s)!}\,\frac{[e^{\beta_a}(-1)^v-e^{-\beta_a}(-1)^{V_0}]}{\beta^{v+1}(V_0-v)!}\right.$$
$$\left.-S_0!\,V_2!\sum_{s=0}^{S_0}\sum_{v=0}^{V_2}\frac{[e^{-\alpha_a}-e^{-\alpha_a z}z^{S_0-s}]}{\alpha_a^{s+1}(S_0-s)!}\,\frac{[e^{\beta_a}(-1)^v-e^{-\beta_a}(-1)^{V_2}]}{\beta_a^{v+1}(V_2-v)!}\right\},\qquad S_0=\mu-\sigma+p_a-2j+2r,$$
$$S_2=S_0+2,\qquad V_0=\mu'-\sigma+q_a-2k+2t,\qquad V_2=V_0+2. \tag{11}$$

The upper limit of j is $\frac{1}{2}(\mu-\sigma)$ or $\frac{1}{2}(\mu-\sigma-1)$, whichever is an integral. The upper limit of k is $\frac{1}{2}(\mu'-\sigma)$ or $\frac{1}{2}(\mu'-\sigma-1)$, whichever is an integral. The upper limit of t is $\frac{1}{2}(\nu_a+\sigma)$ and the upper limit of r is $\frac{1}{2}(\gamma_a+\sigma)$; if these are not integrals, the summations are infinite ones. In practice, the $K^\sigma_{\mu,\mu',a}(z)$ are evaluated recursively and numerically.[24,25] If the $\Phi_a(j)$ of Eq. (10) are Slater-type orbitals, the integrals can be reexpressed[26] as a sum of "charge distributions." The r_{12} expansion is needed for the evaluation of r_{12} and for raising the value of n in r_{12}^n. This expansion [Eq. (12)] has been derived by Harris.[27] The partial integration of Eq. (14) is used in the evaluation of the corresponding integral [Eq. (15)]. In Eq. (14), for $z\to\infty$ and $\mu\neq0$, the first term approaches 0. For $\mu=0$, $X^\sigma_\mu=0$;

$$O_{\rm per}\binom{a}{b}$$

denotes interchange of a and b charge distributions. We have

$$r_{12}=\frac{R}{2}\sum_{\mu=0}^{\infty}\sum_{\sigma=-\mu}^{\mu}\left[(U^\sigma_\mu g^\sigma_\mu+V^\sigma_\mu h^\sigma_\mu+2W^\sigma_\mu)Q^{|\sigma|}_\mu(\xi_{2>1})+\frac{X^\sigma_\mu\,\xi_{2>1}}{P^{|\sigma|}_\mu(\xi_{2>1})}\right]P^{|\sigma|}_\mu(\xi_{1<2})P^{|\sigma|}_\mu(\eta_1)P^{|\sigma|}_\mu(\eta_2)\,e^{i\sigma(\phi_1-\phi_2)}\,,$$
$$g^\sigma_\mu=\frac{P^{|\sigma|}_{\mu+2}(\xi_1)}{P^{|\sigma|}_\mu(\xi_1)}+\frac{P^{|\sigma|}_{\mu+2}(\xi_2)}{P^{|\sigma|}_\mu(\xi_2)}+\frac{P^{|\sigma|}_{\mu+2}(\eta_1)}{P^{|\sigma|}_\mu(\eta_1)}+\frac{P^{|\sigma|}_{\mu+2}(\eta_2)}{P^{|\sigma|}_\mu(\eta_2)},\qquad h^\sigma_\mu=\frac{P^{|\sigma|}_{\mu-2}(\xi_1)}{P^{|\sigma|}_\mu(\xi_1)}+\frac{P^{|\sigma|}_{\mu-2}(\xi_2)}{P^{|\sigma|}_\mu(\xi_2)}+\frac{P^{|\sigma|}_{\mu-2}(\eta_1)}{P^{|\sigma|}_\mu(\eta_1)}+\frac{P^{|\sigma|}_{\mu-2}(\eta_2)}{P^{|\sigma|}_\mu(\eta_2)}\,,$$
$$U^\sigma_\mu=Z^\sigma_\mu\frac{(\mu-|\sigma|+1)(\mu-|\sigma|+2)}{(2\mu+3)^2}\,,\qquad V^\sigma_\mu=-Z^\sigma_\mu\frac{(\mu+|\sigma|-1)(\mu+|\sigma|)}{(2\mu-1)^2}\,, \tag{12}$$
$$W^\sigma_\mu=Z^\sigma_\mu\frac{2(2\mu+1)(4\sigma^2-1)}{(2\mu-1)^2(2\mu+3)^2}\,,\qquad X^\sigma_\mu=-\frac{(\mu-|\sigma|)!\,2(2\mu+1)}{(\mu+|\sigma|)!\,(2\mu-1)(2\mu+3)}\,,$$

$$G^\sigma_\mu(z)=\frac{-d}{dz}\left\{\frac{z}{[P^\sigma_\mu(z)]^2}\right\}=\frac{-l^\sigma_\mu}{[P^\sigma_\mu(z)]^2(z^2-1)}\,,\qquad l^\sigma_\mu(z)=(2\mu+3)z^2-2(\mu-\sigma+1)z\frac{P^\sigma_{\mu+1}(z)}{P^\sigma_\mu(z)}-1, \tag{13}$$

$$X^\sigma_\mu\int_1^z\frac{x}{P^\sigma_\mu(x)}w(x)\,dx=\frac{X^\sigma_\mu z}{[P^\sigma_\mu(z)]^2}\int_1^z P^\sigma_\mu(x)w(x)\,dx-X^\sigma_\mu\int_1^z\frac{l^\sigma_\mu(x)\,dx}{[P^\sigma_\mu(x)]^2(x^2-1)}\int_1^x P^\sigma_\mu(\xi)w(\xi)\,d\xi\,, \tag{14}$$

$$\langle r_{12}\rangle=\langle\Phi_a(1)\Phi_b(2)\,r_{12}\rangle=\tfrac{1}{32}R^7\pi^2\,\delta(m_a+m_b;\,0)$$
$$\times\left[1+O_{\rm per}\binom{a}{b}\right]\sum_{\mu=\sigma=|m_a|}^{\infty}\int_1^\infty dz\,K^\sigma_{\mu,\mu,a}(z)\,[F^\sigma_\mu(z)\tilde K^\sigma_{\mu,\mu,b}(z)+\tfrac{1}{2}X^\sigma_\mu G^\sigma_\mu(z)K^\sigma_{\mu,\mu,b}(z)], \tag{15}$$

$$\tilde{K}^{\sigma}_{\mu,\mu,a}(z) = U^{\sigma}_{\mu}[K^{\sigma}_{\mu+2,\mu,a}(z) + K^{\sigma}_{\mu,\mu+2,a}(z)] + V^{\sigma}_{\mu}[K^{\sigma}_{\mu-2,\mu,a}(z) + K^{\sigma}_{\mu,\mu-2,a}(z)] + W^{\sigma}_{\mu}K^{\sigma}_{\mu,\mu,a}(z). \quad (16)$$

THREE-ELECTRON INTEGRALS

The three- and four-electron integrals have been formulated in a straightforward manner, using partial integration. Equation (17) illustrates a technique of partial integration useful in the derivations. Whenever the product of two or more associated Legendre polynomials occurs, these can be replaced by a sum over a single associated Legendre polynomial. The coefficients involve products of Clebsch-Gordan coefficients. Equation (22) is a Clebsch-Gordan series. For further information see Refs. 23 and 28–35. We have

$$\int_1^\infty f(y)\,dy \int_{t=y}^\infty g(t)\,dt = \int_1^\infty g(y)\,dy \int_{t=1}^y f(t)\,dt, \qquad u(y) = \int_1^y f(t)\,dt, \quad v(y) = \int_1^y g(s)\,ds, \quad (17)$$

$$\langle r_{12} r_{13}\rangle = \langle \Phi_a(1)\Phi_b(2)\Phi_c(3) r_{12} r_{13}\rangle$$
$$= \tfrac{1}{128} R^{11}\pi^3 \delta(m_a + m_b + m_c; 0)\left[1 + O_{\text{per}}\binom{b}{c}\right] \sum_{\mu=\sigma=|m_b|}^{\infty} \sum_{\mu'=\sigma'=|m_c|}^{\infty}$$
$$\times \Bigg\{ \int_1^\infty dz\, [\tilde{\mathfrak{K}}^{\sigma'}_{\mu',\mu',c}(z) + X^{\sigma'}_{\mu'} \bar{\mathfrak{K}}^{\sigma'}_{\mu',\mu',c}(z)][F^{\sigma}_{\mu}(z)\tilde{N}^{(\sigma,\sigma')}_{(\mu,\mu'),a}(z) K^{\sigma}_{\mu,\mu,b}(z) + F^{\sigma}_{\mu}(z) N^{\sigma,\sigma'}_{\mu,\mu',a}(z)\tilde{K}^{\sigma}_{\mu,\mu,b}(z)$$
$$+ X^{\sigma}_{\mu} G^{\sigma}_{\mu}(z) N^{\sigma,\sigma'}_{\mu,\mu',a}(z) K^{\sigma}_{\mu,\mu,b}(z)]$$
$$+ \int_1^\infty dz\, \mathfrak{K}^{\sigma'}_{\mu',\mu',c}(z)[F^{\sigma}_{\mu}(z)\tilde{\tilde{N}}^{\sigma,\sigma'}_{\mu,\mu',a}(z) K^{\sigma}_{\mu,\mu,b}(z) + F^{\sigma}_{\mu}(z)\tilde{N}^{(\sigma',\sigma)}_{(\mu',\mu),a}(z)\tilde{K}^{\sigma}_{\mu,\mu,b}(z)$$
$$+ X^{\sigma}_{\mu} G^{\sigma}_{\mu}(z)\tilde{N}^{(\sigma',\sigma)}_{(\mu',\mu),a}(z) K^{\sigma}_{\mu,\mu,b}(z)]\Bigg\}, \quad (18)$$

$$\mathfrak{K}^{\sigma}_{\mu,\mu,b}(z) = \int_z^\infty F^{\sigma}_{\mu}(z) K^{\sigma}_{\mu,\mu,b}(z)\,dz, \quad (19)$$

$$\bar{\mathfrak{K}}^{\sigma}_{\mu,\mu,b}(z) = \int_z^\infty G^{\sigma}_{\mu}(z) K^{\sigma}_{\mu,\mu,b}(z)\,dz, \quad (20)$$

$$\tilde{\mathfrak{K}}^{\sigma}_{\mu,\mu,b}(z) = \int_z^\infty F^{\sigma}_{\mu}(z)\tilde{K}^{\sigma}_{\mu,\mu,b}(z)\,dz, \quad (21)$$

$$P^{m}_{l}(z) P^{m'}_{l'}(z) = \sum_j \begin{bmatrix} l & l' & l \\ m & m' & (m+m') \end{bmatrix} P^{(m+m')}_{j}(z), \quad (22)$$

$$\begin{bmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{bmatrix} = \begin{bmatrix} j_2 & j_1 & j \\ m_2 & m_1 & m \end{bmatrix} = \delta(m; m_1+m_2)\left[\frac{(j-m)!\,(j_1+m_1)!\,(j_2+m_2)!}{(j+m)!\,(j_1-m_1)!\,(j_2-m_2)!}\right]^{1/2}$$
$$\times C(j_1, j_2, j; m_1, m_2, m)\, C(j_1, j_2, j; 0, 0, 0)\, C(j_1, j_2, j; m_1, m_2, m)$$
$$= \delta(m; m_1+m_2)(2j+1)^{1/2}\, \Delta(j_1, j_2, j)$$
$$\times \sum_p \frac{(-1)^p[(j+m)!\,(j-m)!\,(j_1+m_1)!\,(j_1-m_1)!\,(j_2+m_2)!\,(j_2-m_2)!]^{1/2}}{p!\,(j_1+j_2-j-p)!\,(j_1-m_1-p)!\,(j-j_2+m_1+p)!\,(j_2+m_2-p)!\,(j-j_2-m_2+p)!},$$

$$\Delta(a,b,c) = \left[\frac{(a+b-c)!\,(b+c-a)!\,(c+a-b)!}{(a+b+c+1)!}\right]^{1/2},$$

$$N^{\sigma,\sigma'}_{\mu,\mu',a}(z) = N^{\sigma',\sigma}_{\mu',\mu,a}(z) = \int_1^z\int_{-1}^1 (\xi^2-\eta^2)\,d\xi\,d\eta\; P^{\sigma}_{\mu}(\xi) P^{\sigma'}_{\mu'}(\xi) P^{\sigma}_{\mu}(\eta) P^{\sigma'}_{\mu'}(\eta)\,\xi^{p_a}\eta^{q_a}(\xi^2-1)^{r_a/2}$$
$$\times (1-\eta^2)^{\nu_a/2} e^{-\alpha_a\xi} e^{\beta_a\eta} = \tfrac{1}{2}\delta(m;\sigma+\sigma')\sum_J\sum_{J'}\begin{bmatrix} \mu & \mu' & J \\ \sigma & \sigma' & m \end{bmatrix}\begin{bmatrix} \mu & \mu' & J' \\ \sigma & \sigma' & m \end{bmatrix}\{K^{m}_{J,J',a}(z) + K^{m}_{J',J,a}(z)\}, \quad (23)$$

$$\tilde{N}^{(\sigma,\sigma')}_{(\mu,\mu'),a}(z) = \delta(m;\sigma+\sigma')\sum_J \sum_{J'} \left\{ U^\sigma_\mu \begin{bmatrix} \mu+2 & \mu' & J \\ \sigma & \sigma' & m \end{bmatrix} + V^\sigma_\mu \begin{bmatrix} \mu-2 & \mu' & J \\ \sigma & \sigma' & m \end{bmatrix} \right\}$$

$$\times \begin{bmatrix} \mu & \mu' & J' \\ \sigma & \sigma' & m \end{bmatrix} \{K^m_{J,J',a}(z) + K^m_{J',J,a}(z)\} + W^\sigma_\mu N^{\sigma,\sigma'}_{\mu,\mu',a}(z), \tag{24}$$

$$\tilde{\tilde{N}}^{\sigma,\sigma'}_{\mu,\mu',a}(z) = \tilde{\tilde{N}}^{\sigma',\sigma}_{\mu',\mu,a}(z) = \delta(m;\sigma+\sigma')\sum_J \sum_{J'} \left\{ \left(U^\sigma_\mu U^{\sigma'}_{\mu'} \begin{bmatrix} \mu+2 & \mu'+2 & J \\ \sigma & \sigma' & m \end{bmatrix} + V^\sigma_\mu V^{\sigma'}_{\mu'} \right.\right.$$

$$\left. \times \begin{bmatrix} \mu-2 & \mu'-2 & J \\ \sigma & \sigma' & m \end{bmatrix} + U^\sigma_\mu V^{\sigma'}_{\mu'} \begin{bmatrix} \mu+2 & \mu'-2 & J \\ \sigma & \sigma' & m \end{bmatrix} + U^{\sigma'}_{\mu'} V^\sigma_\mu \begin{bmatrix} \mu-2 & \mu'+2 & J \\ \sigma & \sigma' & m \end{bmatrix} \right) \begin{bmatrix} \mu & \mu' & J' \\ \sigma & \sigma' & m \end{bmatrix}$$

$$\left. + \left(U^\sigma_\mu \begin{bmatrix} \mu+2 & \mu' & J \\ \sigma & \sigma' & m \end{bmatrix} + V^\sigma_\mu \begin{bmatrix} \mu-2 & \mu' & J \\ \sigma & \sigma' & m \end{bmatrix} \right) \left(U^{\sigma'}_{\mu'} \begin{bmatrix} \mu & \mu'+2 & J' \\ \sigma & \sigma' & m \end{bmatrix} + V^{\sigma'}_{\mu'} \begin{bmatrix} \mu & \mu'-2 & J' \\ \sigma & \sigma' & m \end{bmatrix} \right) \right\}$$

$$\times \{K^m_{J,J',a}(z) + K^m_{J',J,a}(z)\} + W^{\sigma'}_{\mu'} \tilde{N}^{(\sigma,\sigma')}_{(\mu,\mu'),a}(z) + W^\sigma_\mu \tilde{N}^{(\sigma',\sigma)}_{(\mu',\mu),a}(z) - W^{\sigma'}_{\mu'} W^\sigma_\mu N^{\sigma,\sigma'}_{\mu,\mu',a}(z) \quad , \tag{25}$$

$$\langle r_{12}/r_{13}\rangle = \langle \Phi_a(1)\Phi_b(2)\Phi_c(3) r_{12}/r_{13}\rangle = \tfrac{1}{64} R^9 \pi^3 \delta(m_a+m_b+m_c;0) \sum_{\mu=\sigma=|m_b|}^{\infty} \sum_{\mu'=\sigma'=|m_c|}^{\infty} (2\mu'+1) Z^{\sigma'}_{\mu'} \Big\{ \int_1^\infty dz\, F^\sigma_\mu(z)$$

$$\times \mathfrak{K}^{\sigma'}_{\mu',\mu',c}(z) [\tilde{N}^{(\sigma,\sigma')}_{(\mu,\mu'),a}(z) K^\sigma_{\mu,\mu,b}(z) + N^{\sigma,\sigma'}_{\mu,\mu',a}(z)\tilde{K}^\sigma_{\mu,\mu,b}(z)] + \int_1^\infty dz\, F^{\sigma'}_{\mu'}(z) K^{\sigma'}_{\mu',\mu',c}(z)$$

$$\times [\tilde{N}^{(\sigma,\sigma')}_{(\mu,\mu'),a}(z)\mathfrak{K}^\sigma_{\mu,\mu,b}(z) + N^{\sigma,\sigma'}_{\mu,\mu',a}(z)\tilde{\mathfrak{K}}^\sigma_{\mu,\mu,b}(z)] + X^\sigma_\mu \int_1^\infty dz\, N^{\sigma,\sigma'}_{\mu,\mu',a}(z) [K^\sigma_{\mu,\mu,b}(z)\, \mathfrak{K}^{\sigma'}_{\mu',\mu',c}(z) G^\sigma_\mu(z)$$

$$+ \overline{\mathfrak{K}}^\sigma_{\mu,\mu,b}(z) K^{\sigma'}_{\mu',\mu',c}(z) F^{\sigma'}_{\mu'}(z)]\Big\}, \tag{26}$$

$$\langle r_{12}r_{13}/r_{23}\rangle = \langle \Phi_a(1)\Phi_b(2)\Phi_c(3) r_{12}r_{13}/r_{23}\rangle = \tfrac{1}{128} R^{10}\pi^3 \delta(m_a+m_b+m_c;0)\left[1+O_{\mathrm{per}}\binom{b}{c}\right]$$

$$\times \sum_{\mu''=0}^{\infty} \sum_{w''=-\mu''}^{\mu''} \sum_{\mu'=\sigma'}^{\infty} \sum_{\mu=\sigma}^{\infty} \delta(w';m_c-w'')\,\delta(|w'|;\sigma')\,\delta(w;m_b+w'')\,\delta(|w|;\sigma)\,\delta(|w''|;\sigma'')$$

$$\times (2\mu''+1) Z^{\sigma''}_{\mu''} \Big\{ \int_1^\infty dz\; \mathfrak{N}^{\sigma',\sigma''}_{\mu',\mu'',c}(z) [N^{\sigma,\sigma''}_{\mu,\mu'',b}(z)\tilde{N}^{(\sigma',\sigma)}_{(\mu',\mu),a}(z) G^\sigma_\mu(z) X^\sigma_\mu + \tilde{N}^{(\sigma,\sigma'')}_{(\mu,\mu''),b}(z)\tilde{N}^{(\sigma',\sigma)}_{(\mu',\mu),a}(z) F^\sigma_\mu(z)$$

$$+ N^{\sigma,\sigma''}_{\mu,\mu'',b}(z)\tilde{\tilde{N}}^{\sigma,\sigma'}_{\mu,\mu',a}(z) F^\sigma_\mu(z)] + \int_1^\infty dz [X^\sigma_\mu\, \overline{\mathfrak{N}}^{(\sigma,\sigma'')}_{(\mu,\mu''),b}(z) + \tilde{\mathfrak{N}}^{(\sigma,\sigma'')}_{(\mu,\mu''),b}(z)] [N^{\sigma,\sigma'}_{\mu,\mu',a}(z) N^{\sigma',\sigma''}_{\mu',\mu'',c}(z)$$

$$\times G^{\sigma'}_{\mu'}(z) X^{\sigma'}_{\mu'} + \tilde{N}^{(\sigma',\sigma)}_{(\mu',\mu),a}(z) N^{\sigma',\sigma''}_{\mu',\mu'',c}(z) F^{\sigma'}_{\mu'}(z) + N^{\sigma,\sigma'}_{\mu,\mu',a}(z)\tilde{N}^{(\sigma',\sigma'')}_{(\mu',\mu''),c}(z) F^{\sigma'}_{\mu'}(z)]$$

$$+ \int_1^\infty dz\, F^{\sigma''}_{\mu''}(z) N^{\sigma,\sigma''}_{\mu,\mu'',b}(z) N^{\sigma',\sigma''}_{\mu',\mu'',c}(z) [X^{\sigma'}_{\mu'}\overline{\overline{\mathfrak{N}}}^{(\sigma,\sigma')}_{(\mu,\mu'),a}(z) + \tfrac{1}{2}\tilde{\tilde{\mathfrak{N}}}^{(\sigma,\sigma')}_{(\mu,\mu'),a}(z) + \tfrac{1}{2} X^\sigma_\mu X^{\sigma'}_{\mu'} \hat{\mathfrak{N}}^{\sigma,\sigma'}_{\mu,\mu',a}(z)]$$

$$+ \int_1^\infty dz\, F^{\sigma''}_{\mu''}(z) N^{\sigma,\sigma''}_{\mu,\mu'',b}(z)\tilde{N}^{(\sigma',\sigma'')}_{(\mu',\mu''),c}(z) [\tilde{\mathfrak{N}}^{(\sigma,\sigma')}_{(\mu,\mu'),a}(z) + X^\sigma_\mu \overline{\mathfrak{N}}^{(\sigma,\sigma')}_{(\mu,\mu'),a}(z)]$$

$$+ \frac{1}{2}\int_1^\infty dz\; F^{\sigma''}_{\mu''}(z)\tilde{N}^{(\sigma,\sigma'')}_{(\mu,\mu''),b}(z)\tilde{N}^{(\sigma',\sigma'')}_{(\mu',\mu''),c}(z)\mathfrak{N}^{\sigma,\sigma'}_{\mu,\mu',a}(z)\Big\}, \tag{27}$$

$$\mathfrak{N}^{\sigma,\sigma'}_{\mu,\mu',a}(z) = \mathfrak{N}^{\sigma',\sigma}_{\mu',\mu,a}(z) = \int_z^\infty F^{\sigma,\sigma'}_{\mu,\mu'}(x) N^{\sigma,\sigma'}_{\mu,\mu',a}(x)\,dx \quad , \tag{28}$$

$$F^{\sigma,\sigma'}_{\mu,\mu'}(x) = \frac{-d}{dx}\left[\frac{Q^\sigma_\mu(x)}{P^\sigma_\mu(x)}\frac{Q^{\sigma'}_{\mu'}(x)}{P^{\sigma'}_{\mu'}(x)}\right], \quad E^{(\sigma,\sigma')}_{(\mu,\mu')}(x) = \frac{-d}{dx}\left\{\frac{x}{[P^\sigma_\mu(x)]^2}\frac{Q^{\sigma'}_{\mu'}(x)}{P^{\sigma'}_{\mu'}(x)}\right\}, \quad G^{\sigma,\sigma'}_{\mu,\mu'}(x) = \frac{-d}{dx}\left\{\frac{x}{[P^\sigma_\mu(x)]^2}\frac{x}{[P^{\sigma'}_{\mu'}(x)]^2}\right\}, \tag{29}$$

$$\hat{\mathfrak{N}}^{\sigma,\sigma'}_{\mu,\mu',a}(z) = \hat{\mathfrak{N}}^{\sigma',\sigma}_{\mu',\mu,a}(z) = \int_z^\infty G^{\sigma,\sigma'}_{\mu,\mu'}(x) N^{\sigma,\sigma'}_{\mu,\mu',a}(x)\,dx, \tag{30}$$

$$\overline{\mathfrak{N}}^{(\sigma,\sigma')}_{(\mu,\mu'),a}(z) = \int_z^\infty E^{(\sigma,\sigma')}_{(\mu,\mu')}(x) N^{\sigma,\sigma'}_{\mu,\mu',a}(x)\,dx, \tag{31}$$

$$\tilde{\mathfrak{N}}^{(\sigma,\sigma')}_{(\mu,\mu'),a}(z)=\int_z^\infty F^{\sigma,\sigma'}_{\mu,\mu'}(x)\,\tilde{N}^{(\sigma,\sigma')}_{(\mu,\mu'),a}(x)\,dx\,, \tag{32}$$

$$\bar{\tilde{\mathfrak{N}}}^{(\sigma,\sigma')}_{(\mu,\mu'),a}(z)=\bar{\tilde{\mathfrak{N}}}^{(\sigma,\sigma')}_{(\mu,\mu'),a}(z)=\int_z^\infty E^{(\sigma',\sigma)}_{(\mu',\mu)}(x)\,\tilde{N}^{(\sigma,\sigma')}_{(\mu,\mu'),a}(x)\,dx, \tag{33}$$

$$\tilde{\tilde{\mathfrak{N}}}^{\sigma,\sigma'}_{\mu,\mu',a}(z)=\tilde{\tilde{\mathfrak{N}}}^{\sigma',\sigma}_{\mu',\mu,a}(z)=\int_z^\infty F^{\sigma,\sigma'}_{\mu,\mu'}(x)\,\tilde{\tilde{N}}^{\sigma,\sigma'}_{\mu,\mu',a}(x)\,dx\,. \tag{34}$$

FOUR-ELECTRON INTEGRALS

We have

$$\begin{aligned}
\langle r_{12}r_{13}/r_{14}\rangle &= \langle \Phi_a(1)\,\Phi_b(2)\,\Phi_c(3)\,\Phi_d(4)\,r_{12}r_{13}/r_{14}\rangle = \tfrac{1}{512}R^{13}\pi^4\,\delta(m_a+m_b+m_c+m_d;0)\left[1+O_{\rm per}\begin{pmatrix}b\\c\end{pmatrix}\right]\\
&\times\sum_{\mu=\sigma=|m_b|}^{\infty}\;\sum_{\mu'=\sigma'=|m_c|}^{\infty}\;\sum_{\mu''=\sigma''=|m_d|}^{\infty}(2\mu''+1)\,Z^{\sigma''}_{\mu''}\left\{\int_1^\infty dz\,\tilde{\tilde{M}}^{(\sigma,\sigma',\sigma'')}_{(\mu,\mu',\mu''),a}(z)\right.\\
&\times\mathfrak{K}^{\sigma'}_{\mu',\mu',c}(z)\,[F^{\sigma}_{\mu}(z)\,K^{\sigma}_{\mu,\mu,b}(z)\,\mathfrak{K}^{\sigma''}_{\mu'',\mu'',d}(z)+\tfrac{1}{2}F^{\sigma''}_{\mu''}(z)\,K^{\sigma''}_{\mu'',\mu'',d}(z)\,\mathfrak{K}^{\sigma}_{\mu,\mu,b}(z)]\\
&+\int_1^\infty dz\,M^{\sigma,\sigma',\sigma''}_{\mu,\mu',\mu'',a}(z)\,\mathfrak{K}^{\sigma''}_{\mu'',\mu'',d}(z)\,[F^{\sigma}_{\mu}(z)\,\tilde{K}^{\sigma}_{\mu,\mu,b}(z)+X^{\sigma}_{\mu}G^{\sigma}_{\mu}(z)\,K^{\sigma}_{\mu,\mu,b}(z)]\;[X^{\sigma'}_{\mu'}\bar{\mathfrak{K}}^{\sigma'}_{\mu',\mu',c}(z)\\
&+\tilde{\mathfrak{K}}^{\sigma'}_{\mu',\mu',c}(z)]+\frac{1}{2}\int_1^\infty dz\,F^{\sigma''}_{\mu''}(z)\,M^{\sigma,\sigma',\sigma''}_{\mu,\mu',\mu'',a}(z)\,K^{\sigma''}_{\mu'',\mu'',d}(z)\,[\tilde{\mathfrak{K}}^{\sigma}_{\mu,\mu,b}(z)+X^{\sigma}_{\mu}\,\bar{\mathfrak{K}}^{\sigma}_{\mu,\mu,b}(z)]\\
&\times[\tilde{\mathfrak{K}}^{\sigma'}_{\mu',\mu',c}(z)+X^{\sigma'}_{\mu'}\,\bar{\mathfrak{K}}^{\sigma'}_{\mu',\mu',c}(z)]+\int_1^\infty \tilde{M}^{(\sigma',\sigma,\sigma'')}_{(\mu',\mu,\mu''),a}(z)\,\mathfrak{K}^{\sigma'}_{\mu',\mu',c}(z)\,\mathfrak{K}^{\sigma''}_{\mu'',\mu'',d}(z)\\
&\times[F^{\sigma}_{\mu}(z)\,\tilde{K}^{\sigma}_{\mu,\mu,b}(z)+X^{\sigma}_{\mu}G^{\sigma}_{\mu}(z)\,K^{\sigma}_{\mu,\mu,b}(z)]+\int_1^\infty dz\,\tilde{M}^{(\sigma,\sigma',\sigma'')}_{(\mu,\mu',\mu''),a}(z)\,[\tilde{\mathfrak{K}}^{\sigma'}_{\mu',\mu',c}(z)+X^{\sigma'}_{\mu'}\,\bar{\mathfrak{K}}^{\sigma'}_{\mu',\mu',c}(z)]\\
&\left.\times[K^{\sigma}_{\mu,\mu,b}(z)\,\mathfrak{K}^{\sigma''}_{\mu'',\mu'',d}(z)\,F^{\sigma}_{\mu}(z)+K^{\sigma''}_{\mu'',\mu'',d}(z)\,\mathfrak{K}^{\sigma''}_{\mu'',\mu'',b}(z)\,F^{\sigma''}_{\mu''}(z)]\right\}\,,
\end{aligned}\tag{35}$$

$$\begin{aligned}
M^{\sigma,\sigma',\sigma''}_{\mu,\mu',\mu'',a}(z)&=\tfrac{1}{2}\,\delta(m;\sigma+\sigma'+\sigma'')\sum_{L'}\sum_{L}\sum_{J'}\sum_{J}\begin{bmatrix}\mu&\mu'&J\\\sigma&\sigma'&(\sigma+\sigma')\end{bmatrix}\begin{bmatrix}\mu&\mu'&J'\\\sigma&\sigma'&(\sigma+\sigma')\end{bmatrix}\begin{bmatrix}J&\mu''&L\\(\sigma+\sigma')&\sigma''&m\end{bmatrix}\\
&\times\begin{bmatrix}J'&\mu''&L'\\(\sigma+\sigma')&\sigma''&m\end{bmatrix}\{K^{m}_{L,L',a}(z)+K^{m}_{L',L,a}(z)\}\,,
\end{aligned}\tag{36}$$

$$\begin{aligned}
\tilde{M}^{(\sigma,\sigma',\sigma'')}_{(\mu,\mu',\mu''),a}(z)&=\tilde{M}^{(\sigma,\sigma'',\sigma')}_{(\mu,\mu'',\mu'),a}(z)=\delta(m;\sigma+\sigma'+\sigma'')\sum_{L}\sum_{L'}\sum_{J}\sum_{J'}\\
&\times\left\{U^{\sigma}_{\mu}\begin{bmatrix}\mu+2&\mu'&J\\\sigma&\sigma'&(\sigma+\sigma')\end{bmatrix}+V^{\sigma}_{\mu}\begin{bmatrix}\mu-2&\mu'&J\\\sigma&\sigma'&(\sigma+\sigma')\end{bmatrix}\right\}\begin{bmatrix}\mu&\mu'&J'\\\sigma&\sigma'&(\sigma+\sigma')\end{bmatrix}\begin{bmatrix}J&\mu''&L\\(\sigma+\sigma')&\sigma''&m\end{bmatrix}\\
&\times\begin{bmatrix}J'&\mu''&L'\\(\sigma+\sigma')&\sigma''&m\end{bmatrix}\{K^{m}_{L,L',a}(z)+K^{m}_{L',L,a}(z)\}\;+W^{\sigma}_{\mu}M^{\sigma,\sigma',\sigma''}_{\mu,\mu',\mu'',a}(z)\,,
\end{aligned}\tag{37}$$

$$\begin{aligned}
\tilde{\tilde{M}}^{(\sigma,\sigma',\sigma'')}_{(\mu,\mu',\mu''),a}(z)&=\tilde{\tilde{M}}^{(\sigma',\sigma,\sigma'')}_{(\mu',\mu,\mu''),a}(z)=\delta(m;\sigma+\sigma'+\sigma'')\sum_{J}\sum_{J'}\sum_{L}\sum_{L'}\left\{\left(U^{\sigma}_{\mu}U^{\sigma'}_{\mu'}\begin{bmatrix}\mu+2&\mu'+2&J\\\sigma&\sigma'&(\sigma+\sigma')\end{bmatrix}\right.\right.\\
&+V^{\sigma}_{\mu}V^{\sigma'}_{\mu'}\begin{bmatrix}\mu-2&\mu'-2&J\\\sigma&\sigma'&(\sigma+\sigma')\end{bmatrix}+U^{\sigma}_{\mu}V^{\sigma'}_{\mu'}\begin{bmatrix}\mu+2&\mu'-2&J\\\sigma&\sigma'&(\sigma+\sigma')\end{bmatrix}\\
&\left.+U^{\sigma'}_{\mu'}V^{\sigma}_{\mu}\begin{bmatrix}\mu-2&\mu'+2&J\\\sigma&\sigma'&(\sigma+\sigma')\end{bmatrix}\right)\begin{bmatrix}\mu&\mu'&J'\\\sigma&\sigma'&(\sigma+\sigma')\end{bmatrix}+\left(U^{\sigma}_{\mu}\begin{bmatrix}\mu+2&\mu'&J\\\sigma&\sigma'&(\sigma+\sigma')\end{bmatrix}+V^{\sigma}_{\mu}\begin{bmatrix}\mu-2&\mu'&J\\\sigma&\sigma'&(\sigma+\sigma')\end{bmatrix}\right)\\
&\left.\times\left(U^{\sigma'}_{\mu'}\begin{bmatrix}\mu&\mu'+2&J'\\\sigma&\sigma'&(\sigma+\sigma')\end{bmatrix}+V^{\sigma'}_{\mu'}\begin{bmatrix}\mu&\mu'-2&J\\\sigma&\sigma'&(\sigma+\sigma')\end{bmatrix}\right)\right\}\begin{bmatrix}J&\mu''&L\\(\sigma+\sigma')&\sigma''&m\end{bmatrix}\begin{bmatrix}J'&\mu''&L'\\(\sigma+\sigma')&\sigma''&m\end{bmatrix}\\
&\times\{K^{m}_{L,L',a}(z)+K^{m}_{L',L,a}(z)\}\;+W^{\sigma'}_{\mu'}\tilde{M}^{(\sigma,\sigma',\sigma'')}_{(\mu,\mu',\mu''),a}(z)+W^{\sigma}_{\mu}\tilde{M}^{(\sigma',\sigma,\sigma'')}_{(\mu',\mu,\mu''),a}(z)-W^{\sigma'}_{\mu'}W^{\sigma}_{\mu}M^{\sigma,\sigma',\sigma''}_{\mu,\mu',\mu'',a}(z)\,,
\end{aligned}\tag{38}$$

$$\langle r_{23}r_{14}/r_{12}\rangle = \langle \Phi_a(1)\Phi_b(2)\Phi_c(3)\Phi_d(4)\, r_{23}r_{14}/r_{12}\rangle = \tfrac{1}{512}R^{13}\pi^4\delta(\sigma^1;|m_c|)\delta(\sigma^{11};|m_d|)\,\delta(\sigma;|m_b+m_c|)$$

$$\times\delta(m_a+m_b+m_c+m_d;0)\sum_{\mu=\sigma}^{\infty}\sum_{\mu'=\sigma'}^{\infty}\sum_{\mu''=\sigma''}^{\infty}(2\mu+1)Z_\mu^\sigma\int_1^\infty dz\,F_\mu^\sigma(z)[N_{\mu',\mu,b}^{\sigma',\sigma}(z)\,\bar{\mathfrak{K}}_{\mu',\mu',c}^{\sigma'}(z)X_{\mu'}^{\sigma'}+\tilde{N}_{(\mu',\mu'),b}^{(\sigma',\sigma)}(z)\mathfrak{K}_{\mu',\mu',c}^{\sigma'}(z)$$

$$+N_{\mu',\mu,b}^{\sigma',\sigma}(z)\tilde{\mathfrak{K}}_{\mu',\mu',c}^{\sigma'}(z)+X_{\mu'}^{\sigma'}\bar{\mathfrak{J}}_{(\mu',\mu),c,b}^{(\sigma',\sigma)}(z)\;+\tilde{\mathfrak{S}}_{(\mu',\mu),c,b}^{(\sigma',\sigma)}(z)][N_{\mu'',\mu,a}^{\sigma'',\sigma}(z)\bar{\mathfrak{K}}_{\mu'',\mu'',d}^{\sigma''}(z)$$

$$\times X_{\mu''}^{\sigma''}+\tilde{N}_{(\mu'',\mu),a}^{(\sigma'',\sigma)}(z)\mathfrak{K}_{\mu'',\mu'',d}^{\sigma''}(z)\;+N_{\mu'',\mu,a}^{\sigma'',\sigma}(z)\tilde{\mathfrak{K}}_{\mu'',\mu'',d}^{\sigma''}(z)+X_{\mu''}^{\sigma''}\bar{\mathfrak{J}}_{(\mu'',\mu),d,a}^{(\sigma'',\sigma)}(z)+\tilde{\mathfrak{S}}_{(\mu'',\mu),d,a}^{(\sigma'',\sigma)}(z)], \tag{39}$$

$$\tilde{\mathfrak{S}}_{(\mu'',\mu),d,a}^{(\sigma'',\sigma)}(z)=\int_1^z dx F_{\mu''}^{\sigma''}(x)\,[K_{\mu'',\mu'',d}^{\sigma''}(x)\tilde{N}_{(\mu'',\mu),a}^{(\sigma'',\sigma)}(x)+\tilde{K}_{\mu'',\mu'',d}^{\sigma''}(x)N_{\mu'',\mu,a}^{\sigma'',\sigma}(x)], \tag{40}$$

$$\bar{\mathfrak{J}}_{(\mu,\mu'),d,a}^{(\sigma,\sigma')}(z)=\int_1^z dx G_\mu^\sigma(x)K_{\mu,\mu,d}^\sigma(x)N_{\mu,\mu',a}^{\sigma,\sigma'}(x), \tag{41}$$

$$\langle r_{12}r_{23}/r_{14}\rangle=\langle\Phi_a(1)\Phi_b(2)\Phi_c(3)\Phi_d(4)r_{12}r_{23}/r_{14}\rangle=\tfrac{1}{512}\;R^{13}\pi^4\delta(\sigma';|m_c|)\,\delta(\sigma'';|m_d|)\delta(\sigma;|m_b+m_c|)$$

$$\times\delta(m_a+m_b+m_c+m_d;0)\sum_{\mu=\sigma}^{\infty}\sum_{\mu'=\sigma'}^{\infty}\sum_{\mu''=\sigma''}^{\infty}(2\mu''+1)Z_{\mu''}^{\sigma''}\Big(\int_1^\infty dz\,\{X_\mu^\sigma G_\mu^\sigma(z)[\mathfrak{J}_{(\mu'',\mu),d,a}^{(\sigma'',\sigma)}(z)$$

$$+N_{\mu,\mu'',a}^{\sigma,\sigma''}(z)\mathfrak{K}_{\mu'',\mu'',d}^{\sigma''}(z)]+F_\mu^\sigma(z)[\tilde{\mathfrak{J}}_{(\mu,\mu''),d,a}^{(\sigma,\sigma'')}(z)\;+\tilde{N}_{(\mu,\mu''),a}^{(\sigma,\sigma'')}(z)\,\mathfrak{K}_{\mu'',\mu'',d}^{\sigma''}(z)]\}\{N_{\mu',\mu,b}^{\sigma',\sigma}(z)$$

$$\times\tilde{\mathfrak{K}}_{\mu',\mu',c}^{\sigma'}(z)+\tilde{N}_{(\mu',\mu),b}^{(\sigma',\sigma)}(z)\,\mathfrak{K}_{\mu',\mu',c}^{\sigma'}(z)\;+X_{\mu'}^{\sigma'}N_{\mu,\mu',b}^{\sigma,\sigma'}(z)\bar{\mathfrak{K}}_{\mu',\mu',c}^{\sigma'}(z)+X_{\mu'}^{\sigma'}\;\bar{\mathfrak{J}}_{(\mu',\mu),c,b}^{(\sigma',\sigma)}(z)$$

$$+\tilde{\mathfrak{S}}_{(\mu',\mu),c,b}^{(\sigma',\sigma)}(z)\}+\int_1^\infty dz\,F_\mu^\sigma(z)\;[\mathfrak{J}_{(\mu'',\mu),d,a}^{(\sigma'',\sigma)}(z)+N_{\mu,\mu'',a}^{\sigma,\sigma''}(z)\mathfrak{K}_{\mu'',\mu'',d}^{\sigma''}(z)]\,[\tilde{N}_{(\mu,\mu'),b}^{(\sigma,\sigma')}(z)\,\tilde{\mathfrak{K}}_{\mu',\mu',c}^{\sigma'}(z)$$

$$+\tilde{\tilde{N}}_{\mu,\mu',b}^{\sigma,\sigma'}(z)\,\mathfrak{K}_{\mu',\mu',c}^{\sigma'}(z)\;+X_{\mu'}^{\sigma'}\tilde{N}_{(\mu,\mu'),b}^{(\sigma,\sigma')}(z)\bar{\mathfrak{K}}_{\mu',\mu',c}^{\sigma'}(z)+X_{\mu'}^{\sigma'}\bar{\tilde{\mathfrak{J}}}_{(\mu,\mu'),c,b}^{(\sigma,\sigma')}(z)\;+\tilde{\tilde{\mathfrak{S}}}_{(\mu,\mu'),c,b}^{(\sigma,\sigma')}(z)]\Big), \tag{42}$$

$$\tilde{\mathfrak{J}}_{(\mu'',\mu),d,a}^{(\sigma'',\sigma)}(z)=\int_1^z F_\mu^\sigma(x)K_{\mu,\mu,d}^\sigma(x)\tilde{N}_{(\mu'',\mu),a}^{(\sigma'',\sigma)}(x)dx, \tag{43}$$

$$\bar{\mathfrak{J}}_{(\mu'',\mu),d,a}^{(\sigma'',\sigma)}(z)=\int_1^z G_\mu^\sigma(x)K_{\mu,\mu,d}^\sigma(x)\tilde{N}_{(\mu'',\mu),a}^{(\sigma'',\sigma)}(x)dx, \tag{44}$$

$$\tilde{\tilde{\mathfrak{S}}}_{(\mu,\mu'),c,b}^{(\sigma,\sigma')}(z)=\int_1^z F_{\mu'}^{\sigma'}(x)\,[K_{\mu',\mu',c}^{\sigma'}(x)\tilde{\tilde{N}}_{\mu,\mu',b}^{\sigma,\sigma'}(x)$$

$$+\tilde{K}_{\mu',\mu',c}^{\sigma'}(x)\tilde{N}_{(\mu,\mu'),b}^{(\sigma,\sigma')}(x)]dx, \tag{45}$$

$$\mathfrak{J}_{(\mu'',\mu),d,a}^{(\sigma'',\sigma)}(z)=\int_1^z F_{\mu''}^{\sigma''}(x)K_{\mu'',\mu'',d}^{\sigma''}(x)N_{\mu'',\mu,a}^{\sigma'',\sigma}(x)dx. \tag{46}$$

KINETIC ENERGY INTEGRAL

Essentially no new basic integrals are involved in the evaluation of the kinetic energy, nuclear attraction, and overlap integrals. In some cases, a modified $K_{\mu,\mu',s}^\sigma(z)$ integral is used. The modified integral $H_{\mu,\mu',s}^\sigma(z)$ is defined in Eq. (47); it differs in that the $\xi^2-\eta^2$ term is not included:

$$H_{\mu,\mu',s}^\sigma(z)=\int_1^z\int_{-1}^1\xi^{p_s}\eta^{q_s}(\xi^2-1)^{\gamma_s/2}(1-\eta^2)^{\nu_s/2}\;e^{-\alpha_s\xi}e^{\beta_s\eta}P_\mu^\sigma(\xi)P_{\mu'}^\sigma(\eta)\,d\xi\,d\eta, \tag{47}$$

$$-\frac{1}{2}\int d\tau\,\Phi_s(1)\Phi_t(2)\Phi_w(3)r_{13}^{l'}\nabla_1^2\,[r_{12}^l\Phi_a(1)\Phi_x(2)\Phi_y(3)]=-\frac{1}{2}\,l(l+1)\int d\tau\,\Phi_e(1)\Phi_f(2)\Phi_g(3)$$

$$\times r_{13}^{l'}r_{12}^{l-2}-\frac{2}{R^2}\int d\tau\,\frac{D_a(1)\Phi_e(1)}{\xi_1^2-\eta_1^2}\;\Phi_f(2)\Phi_g(3)r_{13}^{l'}r_{12}^l-l\int d\tau\;\frac{V_a(1,2)\Phi_e(1)}{\xi_1^2-\eta_1^2}\;\Phi_f(2)\Phi_g(3)\,r_{13}^{l'}r_{12}^{l-2}\;, \tag{48}$$

$$\Phi_s(1)\Phi_a(1)=\Phi_e(1),\quad\Phi_t(2)\Phi_x(2)=\Phi_f(2),\quad\Phi_w(3)\Phi_y(3)=\Phi_g(3)$$

$$D_a(1)=p_a^2+p_a+2p_a\gamma_a+\gamma_a-\alpha_a^2-q_a^2-q_a-2q_a\nu_a-\nu_a+\beta_a^2-2\alpha_a\xi_1(p_a+\gamma_a+1)$$

$$-2\beta_a\eta_1(q_a+\nu_a+1)+\frac{p_a-p_a^2}{\xi_1^2}\;+\frac{q_a^2-q_a}{\eta_1^2}\;+\frac{2\alpha_a p_a}{\xi_1}\;+\frac{2\beta_a q_a}{\eta_1}\;+\;\alpha_a^2\xi_1^2+\frac{\gamma_a^2\xi_1^2}{\xi_1^2-1}-\;\beta_a^2\eta_1^2+\frac{\nu_a^2\eta_1^2}{1-\eta_1^2}+\frac{m_a^2(\eta_1^2-\xi_1^2)}{(\xi_1^2-1)(1-\eta_1^2)}\;,$$

$$V_a(1,2)=q_a(1-\eta_1^2)+p_a(\xi_1^2-1)+\alpha_a\xi_2\eta_2\eta_1(\xi_1^2-1)-\nu_a\eta_1^2+\beta_a\eta_1(1-\eta_1^2)-p_a\xi_2\eta_2\eta_1(\xi_2^2-1)/\xi_1-\gamma_a\xi_2\eta_2\xi_1\eta_1$$
$$-\alpha_a\xi_1(\xi_1^2-1)-q_a\xi_2\eta_2\xi_1(1-\eta_1^2)/\eta_1+\nu_a\xi_2\eta_2\xi_1\eta_1-\beta_a\xi_2\eta_2\xi_1(1-\eta_1^2)+\gamma_a\xi_1^2$$
$$+\left(\alpha_a\xi_1+\beta_a\eta_1+q_a-p_a-\frac{\eta_1^2\nu_a}{1-\eta_1^2}-\frac{\xi_1^2\gamma_a}{\xi_1^2-1}\right)\left[\frac{e^{i(\phi_1-\phi_2)}+e^{-i(\phi_1-\phi_2)}}{2}\right]$$
$$\times[(\xi^2-1)(1-\eta_2^2)(\xi_1^2-1)(1-\eta_1^2)]^{1/2}+m_a(\xi_1^2-\eta_1^2)\left[\frac{(\xi_2^2-1)(1-\eta_2^2)}{(\xi_1^2-1)(1-\eta_1^2)}\right]^{1/2}[e^{i(\phi_1-\phi_2)}-e^{-i(\phi_1-\phi_2)}]\,. \quad (49)$$

For $l=l'=0$, the kinetic energy integral [Eq. (48)] over electron 1 is the sum of $-\frac{1}{2}\pi RH^{\sigma}_{\mu,\mu,e}(\infty)$ terms. For $l=0$ and $l'=1$, the integral is a sum of $\langle r_{12}\rangle$ terms [Eq. (15)], evaluated using $H^{\sigma}_{\mu,\mu',e}(z)$ [Eq. (47)] for electron 1 and the usual $K^{\sigma}_{\mu,\mu',f}(z)$ [Eq. (7)] for electron 2. For $l=0$ and $l'=2$, use Eq. (4) for $\langle r_{12}^2\rangle$ with $H^{\sigma}_{\mu,\mu',e}(z)$ for electron 1. For $l=1$ and $l'=0$, use the usual $\langle 1/r_{12}\rangle$ [Eq. (10)] and $\langle r_{12}\rangle$ [Eq. (15)] with Eq. (47) instead of Eq. (7) for electron 1. For $l=l'=1$, use $\langle r_{13}/r_{12}\rangle$ [Eq. (26)] and $\langle r_{12}r_{13}\rangle$ [Eq. (18)] with Eq. (47) instead of Eq. (7) for electron 1. For $l=2$ and $l'=0$, Eq. (48) is a sum of

$$-\tfrac{3}{4}\pi R^3(\tfrac{1}{4}\pi R^3)^2K^{\sigma}_{\mu,\mu,e}(\infty)K^{\sigma'}_{\mu',\mu',f}(\infty)K^{\sigma''}_{\mu'',\mu'',g}(\infty)$$

terms,

$$-\tfrac{1}{2}\pi R\,K^{\sigma}_{\mu,\mu,g}(\infty)\langle r_{12}^2\rangle$$

terms, and

$$-\tfrac{1}{2}\pi R^3(\tfrac{1}{4}\pi R^3)^2H^{\sigma}_{\mu,\mu,e}(\infty)K^{\sigma'}_{\mu',\mu',f}(\infty)K^{\sigma''}_{\mu'',\mu'',g}(\infty)$$

terms. The $\langle r_{12}^2\rangle$ are evaluated using Eq. (47) instead of Eq. (7) for electron 1. The case of the kinetic energy integral in which the Laplacian operates on r_{12} and this is multiplied by r_{12} is represented in Eq. (50):

$$-\tfrac{1}{2}\int d\tau\Phi_s(1)\Phi_t(2)r_{12}^{l'}\nabla_1^2[r_{12}^l\Phi_a(1)\Phi_x(2)]\,. \quad (50)$$

For $l=l'=1$, (50) equals

$$(\tfrac{1}{4}\pi R^3)^2\delta(m_s+m_a;0)\delta(m_t+m_x;0)K^{0}_{0,0,e}(\infty)K^{0}_{0,0,f}(\infty)$$
$$-\frac{1}{2}\int d\tau\,\frac{\Phi_f(2)r_{12}^2[D_a(1)+D_s(1)]\Phi_e(1)}{(\frac{1}{2}R)^2(\xi_1^2-\eta_1^2)}\,.$$

NUCLEAR-ELECTRON ATTRACTION AND OVERLAP INTEGRALS

We have

$$-\frac{2}{R}\int d\tau\left[\frac{(Z_a+Z_b)\xi_1+(Z_a-Z_b)\eta_1}{(\xi_1^2-\eta_1^2)}\right]\Phi_e(1)\Phi_f(2)\Phi_g(3)r_{12}^l r_{13}^{l'}\,. \quad (51)$$

For $l=l'=0$, the integral over electron 1 is

$$-\tfrac{1}{2}\pi R\delta(m_e;0)[(Z_a+Z_b)H^{0}_{1,0,e}(\infty)+(Z_a-Z_b)H^{0}_{0,1,e}(\infty)]$$

For $l'=0$ and $l=1$, use $\langle r_{12}\rangle$ [Eq. (15)] and Eq. (47) instead of Eq. (7) for electron 1. For $l'=0$ and $l=2$, use $\langle r_{12}^2\rangle$ [Eq. (4)] without the $(\xi_1^2-\eta_1^2)$ term. For $l'=l=1$, use $\langle r_{12}r_{13}\rangle$ [Eq. (18)] with Eq. (47) instead of Eq. (7) for electron 1. The nuclear-nuclear repulsion integral is Z_aZ_b/R times the overlap integral:

$$\langle r_{12}^l r_{13}^{l'}\rangle=\int d\tau\Phi_e(1)\Phi_f(2)\Phi_g(3)r_{12}^l r_{13}^{l'}\,. \quad (52)$$

For $l'=l=0$, the integral over electron 1 is $\frac{1}{4}\pi R^3\delta(m_e;0)K^{0}_{0,0,e}(\infty)$. For $l'=0$ and $l=1$, the integral is $\langle r_{12}\rangle$ [Eq. (15)]. For $l'=0$ and $l=2$, the integral is $\langle r_{12}^2\rangle$ [Eq. (4)]. For $l'=l=1$, the overlap is $\langle r_{12}r_{13}\rangle$ [Eq. (18)].

ADDITIONAL INTEGRALS

Some integrals can be generated from previously given integrals by raising or lowering the r_{12} index in even or odd steps [Eqs. (53) and (54)], using Eqs. (1), (5), (12), and (59). If the Hamiltonian contains the term $1/r_{ij}^3$, for the evaluation of spin-spin magnetic coupling or the relativistic effects of an external electric field, then $\langle 1/r_{ij}^3\rangle$ [Eq. (55)] and $\langle 1/r_{ij}^2\rangle$ [Eq. (56)] are some of the integrals needed. These results are based on a generalization of the Neumann expansion [Eq. (59)].[23,31,36,37] The $C_n^l(x)$ [Eq. (58)] are Gegenbauer polynomials. For $l=\frac{1}{2}$, the Gegenbauer polynomials are the same as Legendre polynomials. If the wave function [Eq. (3)] is modified to be

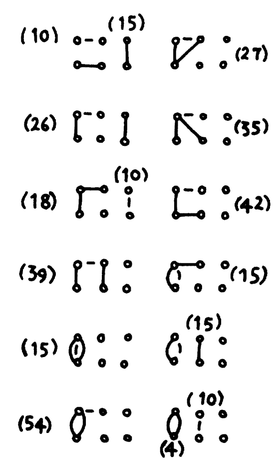

FIG. 1. Graphs for $r_{ij}r_{kl}^{-1}r_{mn}$. Numbers in parentheses correspond to the integral for that graph.

$$\Psi_{tot}=\tilde{\alpha}\left\{\left[\prod_j\sum_s a_{sj}\Phi_s(j)\right]\left[1+\sum_{j<l<k}\sum\sum w_{jlk}r_{jl}^{v}r_{lk}^{v}\right]\right\},$$

then terms $\langle 1/r_{12}r_{13}\rangle$ [Eq. (60)] will occur in the kinetic energy integrals:

$$\langle r_{12}^3\rangle=\int d\tau\,\Phi_e(1)\Phi_f(2)r_{12}^3=\tfrac{1}{4}R^2[\langle\Phi_{p_e+2,\ldots}(1)r_{12}\Phi_f(2)\rangle+\langle\Phi_{p_e,q_e+2,\ldots}(1)r_{12}\Phi_f(2)\rangle$$
$$-2\langle\Phi_e(1)r_{12}\Phi_f(2)\rangle+\langle\Phi_e(1)r_{12}\Phi_{p_f+2,\ldots}(2)\rangle+\langle\Phi_e(1)r_{12}\Phi_{p_f,q_f+2,\ldots}(2)\rangle$$
$$-2\langle\Phi_{p_e+1,q_e+1,\ldots}(1)r_{12}\Phi_{p_f+1,q_f+1,\ldots}(2)\rangle-\langle\Phi_{e_+}(1)r_{12}\Phi_{f_-}(2)\rangle-\langle\Phi_{e_-}(1)r_{12}\Phi_{f_+}(2)\rangle],$$

$$e_+=(p_e,q_e,\gamma_e+1,\nu_e+1,\alpha_e,\beta_e,m_e+1),\qquad e_-=(p_e,q_e,\gamma_e+1,\nu_e+1,\alpha_e,\beta_e,m_e-1)\tag{53}$$

$$\langle r_{13}^2/r_{12}\rangle=\int d\tau\,\Phi_a(1)\Phi_s(2)\Phi_t(3)r_{13}^2/r_{12}=\frac{R^2}{4}\{\langle\Phi_t(3)\rangle[\langle\Phi_{p_a+2,\ldots}(1)(1/r_{12})\Phi_s(2)\rangle$$
$$+\langle\Phi_{p_a,q_a+2,\ldots}(1)(1/r_{12})\Phi_s(2)\rangle-\langle\Phi_a(1)(1/r_{12})\Phi_s(2)\rangle]+\langle\Phi_a(1)(1/r_{12})\Phi_s(2)\rangle$$
$$\times[\langle\Phi_{p_t+2,\ldots}(3)\rangle+\langle\Phi_{p_t,q_t+2,\ldots}(3)\rangle-\langle\Phi_t(3)\rangle]-\langle\Phi_{t_-}(3)\rangle$$
$$\times\langle\Phi_{a_+}(1)(1/r_{12})\Phi_s(2)\rangle-\langle\Phi_{t_+}(3)\rangle\langle\Phi_{a_-}(1)(1/r_{12})\Phi_s(2)\rangle$$
$$-2\langle\Phi_{p_t+1,q_t+1,\ldots}(3)\rangle\langle\Phi_{p_a+1,q_a+1,\ldots}(1)(1/r_{12})\Phi_s(2)\rangle\},\tag{54}$$

$$\langle 1/r_{12}^3\rangle=\int d\tau\,\Phi_a(1)\Phi_b(2)1/r_{12}^3=\pi^2R^3\delta(m_a+m_b;0)$$
$$\times\sum_{l=0}^{\infty}\sum_{m=|m_a|+1}^{l}\tfrac{1}{2}\left|(-1)^{m_a+1}+(-1)^m\right|m(2l+1)$$
$$\times Z_l^m\int_1^\infty F_l^m(z)K_{l,1,a}^m(z)K_{l,1,b}^m(z)\,dz,\tag{55}$$

$$\langle 1/r_{12}^2\rangle=\int d\tau\,\Phi_a(1)\Phi_b(2)(1/r_{12}^2)=\tfrac{1}{2}\pi^2R^4$$
$$\times\sum_{n=0}^{\infty}\sum_{l=|m_a|}^{n}\delta(m_a+m_b;0)\left[\frac{1+(-1)^{l+m_a}}{2}\right]$$
$$\times\frac{(l!)^2(n-l)!(n+1)(2l+1)(l-m_a)!(l+m_a)!}{(n+l)!\{[\frac{1}{2}(l-m_a)]!\}^2\{[\frac{1}{2}(l+m_a)]!\}^2}$$
$$\times\int_1^\infty\frac{dz}{(z^2-1)^{l+3/2}[C_{n-l}^{l+1}(z)]^2}$$
$$\times L_{n-l,n-l,a(l)}^{l+1}(z)L_{n-l,n-l,b(l)}^{l+1}(z),$$

$$a(l)=(p_a,\ q_a,\ \gamma_a+l,\ \nu_a+l,\ \alpha_a,\ \beta_a,\ m_a),$$
$$b(l)=(p_b,\ q_b,\ \gamma_b+l,\ \nu_b+l,\ \alpha_b,\ \beta_b,\ m_b),\tag{56}$$

$$L_{n,n',s}^l(z)=\int_1^z\int_{-1}^1 d\xi\,d\eta\,\xi^{p_s}\eta^{q_s}(\xi^2-1)^{\gamma_s/2}$$
$$\times(1-\eta^2)^{\nu_s/2}e^{-\alpha_s\xi}e^{\beta_s\eta}C_n^l(\xi)C_{n'}^l(\eta),\tag{57}$$

$$C_n^l(x)=\sum_{j=0}^{[n/2]}\frac{2^{n-2j}(-1)^j(l+n-j-1)!}{j!(n-2j)!(l-1)!}x^{n-2j}.\tag{58}$$

The upper limit of the sum over j is $\frac{1}{2}n$ or $\frac{1}{2}(n-1)$, whichever is integral. We have[36,37]

$$\left(\frac{2r_{12}}{R}\right)^{-2p}=\sum_{n=0}^{\infty}\sum_{l=0}^{n}d_{nl}(p)[(1-\eta_1^2)$$
$$\times(1-\eta_2^2)(\xi_1^2-1)(\xi_2^2-1)]^{l/2}D_{n-l}^{l+p}(\xi_{1>2})$$
$$\times C_{n-l}^{p+l}(\xi_{2<1})C_{n-l}^{p+l}(\eta_1)C_{n-l}^{p+l}(\eta_2)$$
$$\times C_l^{p-1/2}[\cos(\phi_1-\phi_2)],\qquad p>0,\ p\neq\tfrac{1}{2}$$

$$d_{nl}(p)=\frac{-2^{2l+1}\Gamma(2p-1)[\Gamma(p+l)]^2}{[\Gamma(p)]^2\Gamma(2p+n+l)}$$
$$\times(n-l)!\,(n+p)(2p+2l-1),$$

$$D_m^u(\xi)=-C_m^u(\xi)\int_\xi^\infty\frac{(x^2-1)^{-u-1/2}dx}{[C_m^u(x)]^2},$$

$$\frac{d}{d\xi}\left[\frac{D_m^u(\xi)}{C_m^u(\xi)}\right]=\frac{(\xi^2-1)^{-u-1/2}}{[C_m^u(\xi)]^2},\tag{59}$$

$$\langle 1/r_{12}r_{13}\rangle=\int d\tau\,\Phi_a(1)\Phi_b(2)\Phi_c(3)1/r_{12}r_{13}$$
$$=\tfrac{1}{16}\pi^3R^7\delta(m_a+m_b+m_c;0)$$
$$\times\left[1+O_{per}\begin{pmatrix}b\\c\end{pmatrix}\right]\delta(\sigma;|m_b|)\delta(\sigma';|m_c|)$$
$$\times\sum_{l=\sigma}^{\infty}\sum_{j=\sigma'}^{\infty}(2l+1)(2j+1)Z_l^\sigma Z_j^{\sigma'}$$
$$\times\int_1^\infty dz\,N_{l,j,a}^{\sigma,\sigma'}(z)K_{l,1,b}^{\sigma}(z)\mathfrak{K}_{j,j,c}^{\sigma'}(z)F_l^\sigma(z).\tag{60}$$

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