Analytical evaluations of exponentially correlated unlinked one-center, three- and four-electron integrals

Cong Wang,[1] Peng Mei,[2] Yusaku Kurokawa,[1] Hiroyuki Nakashima,[1] and Hiroshi Nakatsuji[1,*]
[1]*Quantum Chemistry Research Institute, JST, CREST Kyodai Katsura Venture Plaza, North Building 106 1-36 Gory-Sahara, Nishikyo-ku, Kyoto, 615-8245 Japan*
[2]*Department of Mathematics and Statistics, P.O. Box 68, FI-00014, University of Helsinki, Finland*
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We discuss an extension of the Hylleraas configuration-interaction method by incorporation of an exponentially correlated term. The necessary unlinked one-center, three- and four-electron integrals are derived in a closed form. No three- or four-electron auxiliary integrals appear in the final expressions. The evaluation scheme is an extension of the recent development of Ruiz [J. Math. Chem. **46**, 1322 (2009)]. The prescription of combining diverged integrals to retrieve a finite value is avoided in the present approach.

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I. INTRODUCTION

In recent years, much attention has been focused on obtaining highly accurate solutions of the Schrödinger equation (SE) for few-electron systems [1–23]. Furthermore, a general method of solving the SE has been developed by one of the authors [24,25]. Then the need for accurate analytical Hamiltonian integrals over the wave functions including explicit r_{ij} terms has much increased. In the Hylleraas configuration-interaction (Hy-CI) ansatz [26,27], the wave function typically includes only linear r_{ij} terms. For such wave functions, all integrals are limited to four-electron integrals. For nonrelativistic atomic systems, analytical integrations are thus possible [28–33].

In this article, we propose a method to calculate analytically the atomic integrals over functions that includes correlation factors of the form $\exp(\omega_{ij}r_{ij})$, not only of the type r_{ij}^n. This makes it possible to study a wave function that has the form of an extension of the Hy-CI ansatz, which is

$$\Psi = \sum_K C_K \Phi_K, \tag{1}$$

$$\Phi_K = \mathcal{A}\left[r_{ij}^{n_{K_1}} \exp(\omega_{ij,K_2} r_{ij}) \phi_{K_3}(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N)\right]. \tag{2}$$

where K defines (K_1,K_2,K_3). We refer to this wave function ansatz as the extended Hy-CI (E-Hy-CI) ansatz. It includes the $r_{ij}^{n_{K_1}}$ term and the $\exp(\omega_{ij,K_2} r_{ij})$ term simultaneously, where the electron pairs are the same, i and j. In Eq. (2), $\mathcal{A}$ is the antisymmetrizer and $\phi_{K_3}(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N)$ is a general sum of the products of the spatial one-electron orbitals and the spin functions as appropriate for an eigenfunction of the spin operators. The terms of the form $r_i^{m_i}$ are included in ϕ_{K_3}. Note that in Eq. (2) some terms may have $n_{K_1} = 0$ and others may have $\omega_{ij,K_2} = 0$. So, in actual calculations, we use not only the present formulations of the integrals, but also the existing ones [28–33]. Some time ago, we examined the optimized values of ω_{ij} for the E-Hy-CI wave function of few-electron atoms [34]. However, there, we used the local Schrödinger equation (LSE) method [35] rather than the present method. In the LSE method, we do not use the analytical integrals but the sampling method.

In the following sections, we study the analytical evaluation of atomic integrals with up to four electrons based on the Slater-type orbitals appearing in correlated wave function theory including the E-Hy-CI ansatz expressed by Eq. (1). The integral includes both ordinary r_{ij}^n terms and the exponentially correlated term $\exp(\omega_{ij}r_{ij})$. The expressions for unlinked one-center, three- and four-electron integrals are derived by integrating over r_{ij} as a coordinate. The integration scheme is an extension of the recent articles due to Ruiz [32,33]. No three- or four-electron auxiliary integrals [29] appear in the final expressions. The calculation of such auxiliary integrals is computationally demanding [32]. As in linear geminal integration [33,36], the evaluation scheme involves individually diverged intermediate integrals. The prescription of combining singular integrals to finite values was discussed by Roberts [37] and Perkins [36] for low-order cases, and extended by Ruiz for the general situation [33]. In the present work, we manage to avoid such procedures. Nevertheless, in the original article [33], Ruiz wrote "In general, we have obtained the form of the combinations of A integrals and their value with the help of MAPLE." Although we tried to find a reference for the combined treatment of the diverged integrals A, we could not find the explicit derivations. We feel an explicit proof would still be helpful and in the Appendix, such a proof is given.

II. INTEGRALS APPEARING IN THE E-HY-CI ANSATZ

The correlated integrals arising from expansion (2) are

$$r_{12}^{\nu} e^{-\omega_{12}r_{12}}, \tag{3}$$

$$r_{12}^{\nu} r_{13}^{\mu} r_{23}^{\kappa} e^{-\omega_{12}r_{12}-\omega_{13}r_{13}}, \tag{4}$$

$$r_{12}^{\nu} r_{13}^{\mu} r_{14}^{\kappa} e^{-\omega_{12}r_{12}-\omega_{13}r_{13}}, \quad r_{12}^{\nu} r_{13}^{\mu} r_{34}^{\kappa} e^{-\omega_{12}r_{12}-\omega_{13}r_{13}}, \quad r_{12}^{\nu} r_{34}^{\mu} r_{23}^{\kappa} e^{-\omega_{12}r_{12}-\omega_{34}r_{34}}, \tag{5}$$

$$\nu,\mu,\kappa = -1,0,1,\ldots. \tag{6}$$

*h.nakatsuji@qcri.or.jp

Here we ignore the one-particle basis in the integration symbols. The exponent ω_{ij} can be zero by convention. Among these integrals, the exponentially correlated two-electron integrals (3) have been derived by Calais and Löwdin [28] for the regular case. The singular two-electron integrals were studied by Yan and Drake [38,39], Caro [40], Korobov [41], and Harris *et al*. [42]. Three-electron integrals were evaluated analytically by Fromm and Hill [30]. The original formulation was improved and extended by many authors [31,43–55]. The four-electron integrals were discussed by Frolov as an expansion of the exponentially correlated function into a power series [56,57].

In the next section, we integrate over r_{ij} directly to derive expressions for unlinked three- and four-electron integrals. The term "unlinked" means that no cyclic indices such as $r_{12}r_{13}r_{23}$ appear in the integral. The present evaluation scheme is based on the work of Calais and Löwdin [28] and Perkins [36], and especially on the recent development of Ruiz [32,33].

III. EXPRESSIONS FOR UNLINKED THREE- AND FOUR-ELECTRON INTEGRALS

A. Three-electron integral

Since the angular structure of the integral (4) is the same as that of the linear r_{12} ones [32], only the radial part is essential:

$$\begin{aligned}&\mathcal{J}(N_1,N_2,N_3;\omega_1,\omega_2,\omega_3;\omega_{12},\omega_{13};\nu,\mu;L_2,L_3)\\&:=\int_0^\infty r_1^{N_1+1}e^{-\omega_1 r_1}dr_1\int_0^\infty r_2^{N_2+1}e^{-\omega_2 r_2}dr_2\int_{|r_1-r_2|}^{r_1+r_2}\frac{1}{2}\frac{r_{12}^{\nu+1}}{r_1r_2}P_{L_2}(\cos\theta_{12})e^{-\omega_{12}r_{12}}dr_{12}\int_0^\infty r_3^{N_3+1}e^{-\omega_3 r_3}dr_3\\&\quad\times\int_{|r_1-r_3|}^{r_1+r_3}\frac{1}{2}\frac{r_{13}^{\mu+1}}{r_1r_3}P_{L_3}(\cos\theta_{13})e^{-\omega_{13}r_{13}}dr_{13},\end{aligned}\tag{7}$$

$$|L_2-L_3|\leqslant L_1\leqslant L_2+L_3.\tag{8}$$

The inequality (8) is the nonzero condition for the full integral (4) arising from evaluating the angular variables [32].

Using a similar treatment to the linear geminal integration method in Ruiz's work [32], we expand the Legendre polynomial $P_{L_2}(\cos\theta_{12})$ [32], Eq. (24)] as $r_{12}^2=r_1^2+r_2^2-2r_1r_2\cos\theta_{12}$, and the angular variable $\cos\theta_{12}$ is converted into power series of r_1,r_2, and r_{12}. We then integrate r_{12} and r_2 in domains D_1 and D_2 [36]:

$$\int_0^\infty dr_1\int_0^\infty dr_2\int_{|r_1-r_2|}^{r_1+r_2}dr_{12}=D_1-D_2,\tag{9}$$

$$D_1:=\int_0^\infty dr_1\int_0^\infty dr_2\int_{r_1-r_2}^{r_1+r_2}dr_{12},\tag{10}$$

$$D_2:=\int_0^\infty dr_1\int_{r_1}^\infty dr_2\int_{r_1-r_2}^{r_2-r_1}dr_{12}=\int_0^\infty dr_1\int_0^\infty dy\int_{-y}^{y}dr_{12},\ \ r_2\to r_1+y.\tag{11}$$

The exponential correlated function can be integrated [[58], Eq. (2.321.2)] by using

$$\int z^n e^{-az}dz=-\frac{n!}{a^{n+1}}e^{-az}\sum_{i=0}^{n}\frac{(az)^i}{i!}+\text{const.},\tag{12}$$

with $n\geqslant 0$. We then obtain

$$\begin{aligned}\mathcal{J}=&\sum_{k=0}^{\lfloor L_2/2\rfloor}\sum_{q=0}^{L_2-2k}\sum_{p=0}^{L_2-2k-q}\frac{(-1)^{k+q}}{2^{2L_2-2k+1}}\frac{(\nu+2q+1)!}{\omega_{12}^{\nu+2q+2}}\binom{L_2}{k}\binom{2L_2-2k}{L_2}\binom{L_2-2k}{q}\binom{L_2-2k-q}{p}\\&\times\sum_{i=0}^{\nu+2q+1}\frac{\omega_{12}^i}{i!}\Bigg\{\sum_{j=0}^{i}\binom{i}{j}[(-1)^jA(N_2-L_2+2k+2p+j,\omega_2-\omega_{12})-A(N_2-L_2+2k+2p+j,\omega_2+\omega_{12})]\\&\times\mathcal{I}(N_1+L_2-2k-2q-2p+i-j-1,N_3;\omega_1+\omega_{12},\omega_3,\omega_{13};\mu;L_3)\\&-\sum_{j=0}^{N_2-L_2+2k+2p}\binom{N_2-L_2+2k+2p}{j}[(-1)^iA(i+j,\omega_2-\omega_{12})-A(i+j,\omega_2+\omega_{12})]\\&\times\mathcal{I}(N_1+N_2-2q-j-1,N_3;\omega_1+\omega_2,\omega_3,\omega_{13};\mu;L_3)\Bigg\},\ \ N_2\geqslant L_2,\end{aligned}\tag{13}$$

$$
\begin{aligned}
&= \sum_{k=0}^{\lfloor L_3/2 \rfloor} \sum_{q=0}^{L_3-2k} \sum_{p=0}^{L_3-2k-q} \frac{(-1)^{k+q}}{2^{2L_3-2k+1}} \frac{(\mu+2q+1)!}{\omega_{13}^{\mu+2q+2}} \binom{L_3}{k}\binom{2L_3-2k}{L_3}\binom{L_3-2k}{q}\binom{L_3-2k-q}{p} \\
&\times \sum_{i=0}^{\mu+2q+1} \frac{\omega_{13}^i}{i!} \Bigg\{ \sum_{j=0}^{i} \binom{i}{j} [(-1)^j A(N_3-L_3+2k+2p+j,\omega_3-\omega_{13}) - A(N_3-L_3+2k+2p+j,\omega_3+\omega_{13})] \\
&\times \mathcal{I}(N_1+L_3-2k-2q-2p+i-j-1,N_2;\omega_1+\omega_{13},\omega_2,\omega_{12};\nu;L_2) \\
&- \sum_{j=0}^{N_3-L_3+2k+2p} \binom{N_3-L_3+2k+2p}{j} [(-1)^i A(i+j,\omega_3-\omega_{13}) - A(i+j,\omega_3+\omega_{13})] \\
&\times \mathcal{I}(N_1+N_3-2q-j-1,N_2;\omega_1+\omega_3,\omega_2,\omega_{12};\nu;L_2) \Bigg\}, \quad N_3 \geqslant L_3,
\end{aligned} \tag{14}
$$

where (::) is a binomial coefficient. $\lfloor\ \rfloor$ is a floor function, defined as the largest integral that is less than its argument. A and $\mathcal{I}$ are one- and two-electron integrals,

$$A(n,\alpha) := \int_0^\infty r^n e^{-\alpha r} dr, \tag{15}$$

$$\mathcal{I}(N_1,N_2;\omega_1,\omega_2,\omega_{12};\nu,L) := \int_0^\infty r_1^{N_1+1} e^{-\omega_1 r_1} dr_1 \int_0^\infty r_2^{N_2+1} e^{-\omega_2 r_2} dr_2 \int_{|r_1-r_2|}^{r_1+r_2} \frac{1}{2} \frac{r_{12}^{\nu+1}}{r_1 r_2} P_L(\cos\theta_{12}) e^{-\omega_{12} r_{12}} dr_{12}. \tag{16}$$

The expression (13) is derived by assuming $N_2 - L_2 \geqslant 0$; otherwise the closed-form binomial expansion of $(r_1 + y)^{N_2-L_2+2k+2p}$ as one of the intermediate steps is not possible. This condition can always be satisfied in the three- and four-electron integrals $\mathcal{L}$ and $\mathcal{K}_2$. For the four-electron integral $\mathcal{K}_1$ in the next section the indices obey $N_3 - L_3 \geqslant 0$. Such integrals are evaluated by exchanging the indices 2 and 3. The result is given in Eq. (14).

The two-electron integrals $\mathcal{I}$ in Eq. (13) will always converge, since the index range obeys $N_i \geqslant L_i$ in Eq. (7). This can be seen as follows: the exponentially correlated geminal and $\nu > -1$ will not increase the singularity of integral (13). Therefore the convergence condition of $\mathcal{I}$ is no weaker than in the $\omega_{12} = 0$ and $\nu = -1$ case. In this situation, it can be shown that the index ranges [33]

$$N_1 + L \geqslant -1, \tag{17}$$

$$N_2 + L \geqslant -1, \tag{18}$$

$$N_1 + N_2 \geqslant -2 \tag{19}$$

guarantee the convergence of $\mathcal{I}$. We shall check these conditions. The lower bounds of the first argument of both $\mathcal{I}$'s in Eq. (13) are $N_1 - L_2 - 1$. Thus we start from the left-hand side (LHS) of Eq. (17), $N_1 - L_2 - 1 + L_3 \geqslant L_1 - (L_2 - L_3) - 1 \geqslant L_1 - |L_2 - L_3| - 1 \geqslant -1$, fulfilling the right-hand side (RHS). Here the nonzero condition of the Clebsch-Gordan coefficient (8) has been used. Equation (18) is trivially satisfied. Equation (19) can be ensured by the condition $N_1 - L_2 - 1 + N_3 \geqslant L_1 - L_2 + L_3 - 1 \geqslant L_1 - |L_2 - L_3| - 1 \geqslant -1 > -2$.

The evaluation of the two-electron integral $\mathcal{I}$ has been discussed in the literature [28,41,42]. Our current approach is to integrate over r_{12} directly:

$$
\begin{aligned}
\mathcal{I} &= \sum_{k=0}^{\lfloor L/2 \rfloor} \sum_{q=0}^{L-2k} \sum_{p=0}^{L-2k-q} \frac{(-1)^{k+q}}{2^{2L-2k+1}} \frac{(\nu+2q+1)!}{\omega_{12}^{\nu+2q+2}} \binom{L}{k}\binom{2L-2k}{L}\binom{L-2k}{q}\binom{L-2k-q}{p} \\
&\times \sum_{i=0}^{\nu+2q+1} \frac{\omega_{12}^i}{i!} \Bigg\{ \sum_{j=0}^{i} \binom{i}{j} [(-1)^j A(N_2-L+2k+2p+j,\omega_2-\omega_{12}) - A(N_2-L+2k+2p+j,\omega_2+\omega_{12})] \\
&\times A(N_1+L-2k-2q-2p+i-j,\omega_1+\omega_{12}) \\
&- \sum_{j=0}^{N_2-L+2k+2p} \binom{N_2-L+2k+2p}{j} [(-1)^i A(i+j,\omega_2-\omega_{12}) - A(i+j,\omega_2+\omega_{12})] A(N_1+N_2-2q-j,\omega_1+\omega_2) \Bigg\}.
\end{aligned} \tag{20}
$$

In addition, when $\omega_{12} = 0$, Eq. (13) is not suitable for numerical evaluation.

We can integrate r_{12} by the nonexponentially correlated formalism; the result is similar to the linear geminal integration [33]:

$$\mathcal{J} = \sum_{k=0}^{\lfloor L_2/2\rfloor}\sum_{q=0}^{L_2-2k}\sum_{p=0}^{L_2-2k-q}\frac{(-1)^{k+q}}{2^{2L_2-2k}(\nu+2q+2)}\binom{L_2}{k}\binom{2L_2-2k}{L_2}\binom{L_2-2k}{q}\binom{L_2-2k-q}{p}$$
$$\times\Bigg[\sum_{i=1}^{\lfloor(\nu+2q+3)/2\rfloor}\binom{\nu+2q+2}{2i-1}A(N_2-L_2+2k+2p+2i-1,\omega_2)$$
$$\times\mathcal{I}(N_1+L_2-2k-2p-2i+\nu+2,N_3;\omega_1,\omega_3;\omega_{13};\mu;L_3)$$
$$-\delta_{\nu,2n+1}\sum_{j=1}^{N_2-L_2+2k+2p+1}\binom{N_2-L_2+2k+2p}{j-1}A(\nu+2q+j+1,\omega_2)$$
$$\times\mathcal{I}(N_1+N_2-2q-j,N_3;\omega_1+\omega_2,\omega_3;\omega_{13};\mu;L_3)\Bigg]\Bigg|_{\omega_{12}=0},\quad N_2\geqslant L_2. \tag{21}$$

For small but nonzero ω_{12}, it has been suggested that the integral be evaluated by expanding the exponentially correlated function into a Taylor series [56,57]. The same prescription also applies to the four-electron integrals in the next section.

B. Four-electron integrals

As in the linear case [33], the unlinked four-electron integrals can be classified into three types: $\mathcal{K}_1$, $\mathcal{K}_2$, and $\mathcal{L}$. Since the angular structures are the same as the linear case, we focus on only the radial parts:

$$\mathcal{K}_1(N_1,N_2,N_3,N_4;\omega_1,\omega_2,\omega_3,\omega_4;\omega_{12},\omega_{13};\nu,\mu,\kappa;L_2,L_3,L_4)$$
$$:=\int_0^\infty r_1^{N_1+1}e^{-\omega_1 r_1}dr_1\int_0^\infty r_2^{N_2+1}e^{-\omega_2 r_2}dr_2\int_{|r_1-r_2|}^{r_1+r_2}\frac{1}{2}\frac{r_{12}^{\nu+1}}{r_1r_2}P_{L_2}(\cos\theta_{12})e^{-\omega_{12}r_{12}}\,dr_{12}$$
$$\times\int_0^\infty r_3^{N_3+1}e^{-\omega_3 r_3}dr_3\int_{|r_1-r_3|}^{r_1+r_3}\frac{1}{2}\frac{r_{13}^{\mu+1}}{r_1r_3}P_{L_3}(\cos\theta_{13})e^{-\omega_{13}r_{13}}dr_{13}\int_0^\infty r_4^{N_4+1}e^{-\omega_4 r_4}dr_4\int_{|r_3-r_4|}^{r_3+r_4}\frac{1}{2}\frac{r_{34}^{\kappa+1}}{r_3r_4}P_{L_4}(\cos\theta_{34})dr_{34}, \tag{22}$$

$$\mathcal{K}_2(N_1,N_2,N_3,N_4;\omega_1,\omega_2,\omega_3,\omega_4;\omega_{12},\omega_{34};\nu,\mu,\kappa;L_2,L_3,L_4)$$
$$:=\int_0^\infty r_1^{N_1+1}e^{-\omega_1 r_1}dr_1\int_0^\infty r_2^{N_2+1}e^{-\omega_2 r_2}dr_2\int_{|r_1-r_2|}^{r_1+r_2}\frac{1}{2}\frac{r_{12}^{\nu+1}}{r_1r_2}P_{L_2}(\cos\theta_{12})\,e^{-\omega_{12}r_{12}}dr_{12}$$
$$\times\int_0^\infty r_3^{N_3+1}e^{-\omega_3 r_3}dr_3\int_{|r_2-r_3|}^{r_2+r_3}\frac{1}{2}\frac{r_{23}^{\kappa+1}}{r_2r_3}P_{L_3}(\cos\theta_{23})dr_{23}\int_0^\infty r_4^{N_4+1}e^{-\omega_4 r_4}dr_4\int_{|r_3-r_4|}^{r_3+r_4}\frac{1}{2}\frac{r_{34}^{\mu+1}}{r_3r_4}P_{L_4}(\cos\theta_{34})e^{-\omega_{34}r_{34}}dr_{34}, \tag{23}$$

$$\mathcal{L}(N_1,N_2,N_3,N_4;\omega_1,\omega_2,\omega_3,\omega_4;\omega_{12},\omega_{13};\nu,\mu,\kappa;L_2,L_3,L_4)$$
$$:=\int_0^\infty r_1^{N_1+1}e^{-\omega_1 r_1}dr_1\int_0^\infty r_2^{N_2+1}e^{-\omega_2 r_2}dr_2\int_{|r_1-r_2|}^{r_1+r_2}\frac{1}{2}\frac{r_{12}^{\nu+1}}{r_1r_2}P_{L_2}(\cos\theta_{12})e^{-\omega_{12}r_{12}}\,dr_{12}$$
$$\times\int_0^\infty r_3^{N_3+1}e^{-\omega_3 r_3}dr_3\int_{|r_1-r_3|}^{r_1+r_3}\frac{1}{2}\frac{r_{13}^{\mu+1}}{r_1r_3}P_{L_3}(\cos\theta_{13})e^{-\omega_{13}r_{13}}dr_{13}\int_0^\infty r_4^{N_4+1}e^{-\omega_4 r_4}dr_4\int_{|r_1-r_4|}^{r_1+r_4}\frac{1}{2}\frac{r_{14}^{\kappa+1}}{r_1r_4}P_{L_4}(\cos\theta_{14})dr_{14}. \tag{24}$$

The parameter $\kappa=-1$ covers all essential possibilities.

As in the linear geminal case, the four-electron integration formulas contain individually diverged one- and two-electron integrals. Our evaluation scheme is to integrate the exponential correlated functions first, leaving the diverged part as linear correlated two-electron integrals, except in certain cases of $\mathcal{K}_1$. As with the three-electron integration in the previous section, we start from the variable r_{12} for $\mathcal{K}_1$ and $\mathcal{L}$, and from r_{34} for $\mathcal{K}_2$. After a few manipulations, the results are

$$\mathcal{K}_1=\sum_{k=0}^{\lfloor L_2/2\rfloor}\sum_{q=0}^{L_2-2k}\sum_{p=0}^{L_2-2k-q}\frac{(-1)^{k+q}}{2^{2L_2-2k+1}}\frac{(\nu+2q+1)!}{\omega_{12}^{\nu+2q+2}}\binom{L_2}{k}\binom{2L_2-2k}{L_2}\binom{L_2-2k}{q}\binom{L_2-2k-q}{p}$$
$$\times\sum_{i=0}^{\nu+2q+1}\frac{\omega_{12}^i}{i!}\left\{\sum_{j=0}^{i}\binom{i}{j}[(-1)^jA(N_2-L_2+2k+2p+j,\omega_2-\omega_{12})-A(N_2-L_2+2k+2p+j,\omega_2+\omega_{12})]\right.$$
$$\times\mathcal{J}(N_3,N_1+L_2-2k-2q-2p+i-j-1,N_4;\omega_3,\omega_1+\omega_{12},\omega_4;\omega_{13},0;\mu,\kappa;L_3,L_4)$$

$$- \sum_{j=0}^{N_2-L_2+2k+2p} \binom{N_2-L_2+2k+2p}{j}[(-1)^i A(i+j,\omega_2-\omega_{12}) - A(i+j,\omega_2+\omega_{12})]$$

$$\times \mathcal{J}(N_3,N_1+N_2-2q-j-1,N_4;\omega_3,\omega_1+\omega_2,\omega_4;\omega_{13},0;\mu,\kappa;L_3,L_4)\Bigg\}, \quad (25)$$

$$\mathcal{K}_1 = \sum_{k=0}^{\lfloor L_2/2\rfloor}\sum_{q=0}^{L_2-2k}\sum_{p=0}^{L_2-2k-q} \frac{(-1)^{k+q}}{2^{2L_2-2k}(\nu+2q+2)}\binom{L_2}{k}\binom{2L_2-2k}{L_2}\binom{L_2-2k}{q}\binom{L_2-2k-q}{p}$$
$$\times \Bigg[\sum_{i=1}^{\lfloor(\nu+2q+3)/2\rfloor}\binom{\nu+2q+2}{2i-1}A(N_2-L_2+2k+2p+2i-1,\omega_2)$$
$$\times \mathcal{J}(N_3,N_1+L_2-2k-2p-2i+\nu+2,N_4;\omega_3,\omega_1,\omega_4;\omega_{13},0;\mu,\kappa;L_3,L_4)$$
$$-\delta_{\nu,2n+1}\sum_{j=1}^{N_2-L_2+2k+2p+1}\binom{N_2-L_2+2k+2p}{j-1}A(\nu+2q+j+1,\omega_2)$$
$$\times \mathcal{J}(N_3,N_1+N_2-2q-j,N_4;\omega_3,\omega_1+\omega_2,\omega_4;\omega_{13},0;\mu,\kappa;L_3,L_4)\Bigg]\Bigg|_{\omega_{12}=0}, \quad (26)$$

$$\mathcal{K}_2 = \sum_{k=0}^{\lfloor L_4/2\rfloor}\sum_{q=0}^{L_4-2k}\sum_{p=0}^{L_4-2k-q} \frac{(-1)^{k+q}}{2^{2L_4-2k+1}}\frac{(\mu+2q+1)!}{\omega_{34}^{\mu+2q+2}}\binom{L_4}{k}\binom{2L_4-2k}{L_4}\binom{L_4-2k}{q}\binom{L_4-2k-q}{p}$$
$$\times \sum_{i=0}^{\mu+2q+1}\frac{\omega_{34}^i}{i!}\Bigg\{\sum_{j=0}^{i}\binom{i}{j}[(-1)^j A(N_4-L_4+2k+2p+j,\omega_4-\omega_{34}) - A(N_4-L_4+2k+2p+j,\omega_4+\omega_{34})]$$
$$\times \mathcal{J}(N_2,N_1,N_3+L_4-2k-2q-2p+i-j-1;\omega_2,\omega_1,\omega_3+\omega_{34};\omega_{12},0;\nu,\kappa;L_2,L_3)$$
$$- \sum_{j=0}^{N_4-L_4+2k+2p}\binom{N_4-L_4+2k+2p}{j}[(-1)^i A(i+j,\omega_4-\omega_{34}) - A(i+j,\omega_4+\omega_{34})]$$
$$\times \mathcal{J}(N_2,N_1,N_3+N_4-2q-j-1;\omega_2,\omega_1,\omega_3+\omega_4;\omega_{12},0;\nu,\kappa;L_2,L_3)\Bigg\}, \quad (27)$$

$$\mathcal{K}_2 = \sum_{k=0}^{\lfloor L_4/2\rfloor}\sum_{q=0}^{L_4-2k}\sum_{p=0}^{L_4-2k-q} \frac{(-1)^{k+q}}{2^{2L_4-2k}(\mu+2q+2)}\binom{L_4}{k}\binom{2L_4-2k}{L_4}\binom{L_4-2k}{q}\binom{L_4-2k-q}{p}$$
$$\times \Bigg[\sum_{i=1}^{\lfloor(\mu+2q+3)/2\rfloor}\binom{\mu+2q+2}{2i-1}A(N_4-L_4+2k+2p+2i-1,\omega_4)$$
$$\times \mathcal{J}(N_2,N_1,N_3+L_4-2k-2p-2i+\mu+2;\omega_2,\omega_1,\omega_3;\omega_{12},0;\nu,\kappa;L_2,L_3)$$
$$-\delta_{\mu,2n+1}\sum_{j=1}^{N_4-L_4+2k+2p+1}\binom{N_4-L_4+2k+2p}{j-1}A(\mu+2q+j+1,\omega_4)$$
$$\times \mathcal{J}(N_2,N_1,N_3+N_4-2q-j,N_4;\omega_2,\omega_1,\omega_3+\omega_4;\omega_{12},0;\nu,\kappa;L_2,L_3)\Bigg]\Bigg|_{\omega_{34}=0}, \quad (28)$$

$$\mathcal{L} = \sum_{k=0}^{\lfloor L_2/2\rfloor}\sum_{q=0}^{L_2-2k}\sum_{p=0}^{L_2-2k-q} \frac{(-1)^{k+q}}{2^{2L_2-2k+1}}\frac{(\nu+2q+1)!}{\omega_{12}^{\nu+2q+2}}\binom{L_2}{k}\binom{2L_2-2k}{L_2}\binom{L_2-2k}{q}\binom{L_2-2k-q}{p}$$
$$\times \sum_{i=0}^{\nu+2q+1}\frac{\omega_{12}^i}{i!}\Bigg\{\sum_{j=0}^{i}\binom{i}{j}[(-1)^j A(N_2-L_2+2k+2p+j,\omega_2-\omega_{12}) - A(N_2-L_2+2k+2p+j,\omega_2+\omega_{12})]$$
$$\times \mathcal{J}(N_1+L_2-2k-2q-2p+i-j-1,N_3,N_4;\omega_1+\omega_{12},\omega_3,\omega_4;\omega_{13},0;\mu,\kappa;L_3,L_4)$$

$$- \sum_{j=0}^{N_2-L_2+2k+2p} \binom{N_2-L_2+2k+2p}{j}[(-1)^i A(i+j,\omega_2-\omega_{12}) - A(i+j,\omega_2+\omega_{12})]$$

$$\times \mathcal{J}(N_1+N_2-2q-j-1,N_3,N_4;\omega_1+\omega_2,\omega_3,\omega_4;\omega_{13},0;\mu,\kappa;L_3,L_4)\Bigg\}, \tag{29}$$

$$\mathcal{L} = \sum_{k=0}^{\lfloor L_2/2\rfloor}\sum_{q=0}^{L_2-2k}\sum_{p=0}^{L_2-2k-q} \frac{(-1)^{k+q}}{2^{2L_2-2k}(\nu+2q+2)}\binom{L_2}{k}\binom{2L_2-2k}{L_2}\binom{L_2-2k}{q}\binom{L_2-2k-q}{p}$$
$$\times \Bigg[\sum_{i=1}^{\lfloor(\nu+2q+3)/2\rfloor}\binom{\nu+2q+2}{2i-1}A(N_2-L_2+2k+2p+2i-1,\omega_2)$$
$$\times \mathcal{J}(N_1+L_2-2k-2p-2i+\nu+2,N_3,N_4;\omega_1,\omega_3,\omega_4;\omega_{13},0;\mu,\kappa;L_3,L_4)$$
$$- \delta_{\nu,2n+1}\sum_{j=1}^{N_2-L_2+2k+2p+1}\binom{N_2-L_2+2k+2p}{j-1}A(\nu+2q+j+1,\omega_2)$$
$$\times \mathcal{J}(N_1+N_2-2q-j,N_3,N_4;\omega_1+\omega_2,\omega_3,\omega_4;\omega_{13},0;\mu,\kappa;L_3,L_4)\Bigg]\Bigg|_{\omega_{12}=0}. \tag{30}$$

The terms $\delta_{\mu,2n+1}$ equal 0 and 1 for even and odd μ, respectively. The same convention holds for $\delta_{\nu,2n+1}$. Like the three-electron integral, when $\omega_{12}=0$ in Eqs. (25) and (29), and $\omega_{34}=0$ in Eq. (27), the expressions are not suitable for numerical evaluation. We can evaluate the integral as in the linear geminal case [33]. The results are given in Eqs. (26), (28), and (30). They have essentially identical structures as in Ruiz's original article [33].

Since the exponentially correlated function does not increase the singularity in the integrals, the divergence in the one- and two-electron integrals in Eqs. (25)–(30) originates from nonexponential geminals and such diverging terms must be eliminated from the expressions for the $\mathcal{L}$ and $\mathcal{K}_2$ integrals [33]. As we have seen, the possible divergence has been absorbed into the nonexponentially correlated two-electron integrals $\mathcal{I}|_{\omega_{12}=0}$. Therefore we can adopt the prescription of combining singular integrals as suggested by Ruiz [33]. In the Appendix, we give an explicit formulation using this prescription. This makes it possible to calculate the integrals without assuming the cancellation of infinite values. We can avoid such treatment in the evaluation of the integrals.

Notice that the diverged one-electron integral $A(-n,\alpha)$ ($n>0$) can be related to a scaled exponential integral $L_n(\alpha,\varepsilon)$, introduced by Harris *et al.* [42],

$$A(-n,\alpha) = \lim_{\varepsilon\to 0} L_n(\alpha,\varepsilon), \tag{31}$$

$$L_n(\alpha,\varepsilon) := \int_\varepsilon^\infty t^{-n}e^{-\alpha t}dt. \tag{32}$$

The function L_n has the following properties [[59], Eq. (8.19.8)] when $n>0$:

$$L_n(\alpha,\varepsilon) = (-\alpha)^{n-1}\left[\frac{\psi(n)-\ln\alpha-\ln\varepsilon}{(n-1)!} + \sum_{\substack{j=-\infty\\ j\neq 0}}^{n-1}\frac{(-\alpha\varepsilon)^{-j}}{j(n-j-1)!}\right]$$

$$= (-\alpha)^{n-1}\left[\frac{\psi(n)-\ln\alpha-\ln\varepsilon}{(n-1)!} + \sum_{j=1}^{n-1}\frac{(-\alpha\varepsilon)^{-j}}{j(n-j-1)!}\right] \text{ (when } \varepsilon\to 0); \tag{33}$$

here $\psi(n)$ is the digamma function, defined as $\psi(z) := d\,[\ln\gamma(z)]/dz$. For an integer argument, $\psi(n) = -\gamma_E + \sum_{m=1}^{n-1} m^{-1}$. γ_E is the Euler constant [[60], Eq. (6.3.2)]. Therefore we can write the diverged integral A as

$$A(-n,\alpha) = (-\alpha)^{n-1}\left[\frac{\psi(n)-\ln\alpha}{(n-1)!}\right] + \lim_{\varepsilon\to 0} O(\ln\varepsilon), \tag{34}$$

since the inverse power has a stronger singularity than the logarithm function. As the final four-electron integral converges, all diverged terms eventually have zero contribution. The reason for this can be seen as follows. In a four-electron integral, the ε in each diverged term is the same. It is not possible to obtain a nonzero value by addition and multiplication operations with $\ln\varepsilon$ and ε^{-j} terms. Therefore we can denote the finite part of Eq. (34) as an effective value of the integral $A(-n,\alpha)$. Furthermore, the diverged terms will cancel pairwise. This can also be seen in Eq. (A1) of the Appendix. The Euler constant will not appear in the final expressions. Then Eq. (34) can be replaced by

$$A(-n,\alpha) \to (-\alpha)^{n-1}\left[\frac{H(n-1)-\ln\alpha}{(n-1)!}\right], \tag{35}$$

with $H(n-1) := \sum_{m=1}^{n-1} m^{-1}$ as the harmonic number [[61], p. 75].

In the integral $\mathcal{K}_2$, one needs to handle the diverged two-electron auxiliary integral V. In this case, we can start from Eq. (B.10) in Ruiz's article [33]:

$$\begin{aligned} V(k,-l;\alpha,\gamma) &= \int_0^\infty\int_{r_1}^\infty r_1^k e^{-\alpha r_1} r_2^{-l} e^{-\gamma r_2} dr_1 dr_2 = \int_0^\infty\int_0^{r_2} r_1^k e^{-\alpha r_1} r_2^{-l} e^{-\gamma r_2} dr_1 dr_2 \\ &= \int_0^\infty\int_0^\infty r_1^k e^{-\alpha r_1} r_2^{-l} e^{-\gamma r_2} dr_1 dr_2 - \int_0^\infty\int_{r_2}^\infty r_1^k e^{-\alpha r_1} r_2^{-l} e^{-\gamma r_2} dr_1 dr_2 \ (k,l \geqslant 0). \end{aligned} \tag{36}$$

Integrating over r_1 for the last term in the second line of Eq. (36) yields

$$V(k,-l;\alpha,\gamma) = A(k,\alpha)A(-l,\gamma) - \frac{k!}{\alpha^{k+1}}\sum_{q=0}^{k}\frac{\alpha^q}{q!}A(q-l,\alpha+\gamma), \tag{37}$$

where k and $l \geqslant 0$. The singular integrals $A(-l,\gamma)$ and $A(q-l,\alpha+\gamma)$ are then evaluated according to Eq. (35). This method of skipping diverged terms was proposed by Yan and Drake [38], and by Korobov [41] in a different context.

In $\mathcal{K}_1$ each exponentially correlated two-electron integral is finite, since the indices are in the converged region, Eqs. (17)–(19). However, this condition is weaker than $N_1 \geqslant L$ or $N_2 \geqslant L$ which Eqs. (14)–(21) can apply. In practice, we do encounter an integral in which $L > N_1 \geqslant -L-1$ and $L > N_2 \geqslant -L-1$. Converting the Legendre polynomial into a power series of r_1, r_2, and r_{12} yields individually diverged exponentially correlated two-electron integrals. The low-order singular integrals were studied by Korobov [41] and by Harris *et al.* [42]. We generalize such results in the present work. Expanding the Legendre polynomial in $\mathcal{I}$, Eq. (16) becomes

$$\begin{aligned} \mathcal{I} = &\sum_{k=0}^{\lfloor L/2\rfloor}\sum_{q=0}^{L-2k}\sum_{p=0}^{L-2k-q}\frac{(-1)^{k+q}}{2^{2L-2k+1}}\binom{L}{k}\binom{2L-2k}{L}\binom{L-2k}{q}\binom{L-2k-q}{p} \\ &\times \Gamma_{N_1+L-2k-2q-2p,N_2-L+2k+2p,\nu+2q+1}(\omega_1,\omega_2,\omega_{12}). \end{aligned} \tag{38}$$

The two-electron integral $\mathcal{I}$ is transformed into a linear combination of polynomials of r_1, r_2, and r_{12} times the exponential functions. The integral $\Gamma_{l,m,n}(\alpha,\beta,\gamma)$ follows the convention of Harris *et al.* [42]:

$$\Gamma_{l,m,n}(\alpha,\beta,\gamma) := \int_0^\infty r_1^l e^{-\alpha r_1} dr_1 \int_0^\infty r_2^m e^{-\beta r_2} dr_2 \int_{|r_1-r_2|}^{r_1+r_2} r_{12}^n e^{-\gamma r_{12}} dr_{12}. \tag{39}$$

Starting from $\Gamma_{-p,-q,0}$ ($p > 0, q > 0$), Eq. (D1) in the paper of Harris *et al.* [42] becomes

$$\begin{aligned} \Gamma_{-p,-q,0} = &\frac{1}{\gamma}\int_0^\infty \frac{dr_1}{r_1^p} e^{-(\alpha+\gamma)r_1}\int_0^\infty \frac{dr_2}{r_2^q}[e^{-(\beta-\gamma)r_2} - e^{-(\beta+\gamma)r_2}] \\ &-\frac{1}{\gamma}\int_0^\infty \frac{dr_1}{r_1^p} e^{-(\alpha+\gamma)r_1}\int_{r_1}^\infty \frac{dr_2}{r_2^q} e^{-(\beta-\gamma)r_2} + \frac{1}{\gamma}\int_0^\infty \frac{dr_1}{r_1^p} e^{-(\alpha-\gamma)r_1}\int_{r_1}^\infty \frac{dr_2}{r_2^q} e^{-(\beta+\gamma)r_2} \\ = &\frac{1}{\gamma}L_p(\alpha+\gamma)[L_q(\beta-\gamma) - L_q(\beta+\gamma)] \\ &-\frac{1}{\gamma}\int_0^\infty \frac{dr_1}{r_1^{p+q-1}} e^{-(\alpha+\gamma)r_1} E_q[(\beta-\gamma)r_1] + \frac{1}{\gamma}\int_0^\infty \frac{dr_1}{r_1^{p+q-1}} e^{-(\alpha-\gamma)r_1} E_q[(\beta+\gamma)r_1]; \end{aligned} \tag{40}$$

here the function $L_n(\alpha,\varepsilon)$, Eq. (32), is taken at the $\varepsilon \to 0$ limit. For $q > 1$ we can use the recurrence relation of the generalized exponential integral [[60], Eq. (5.1.14)]

$$E_{q+1}(z) = \frac{1}{q}[e^{-z} - zE_q(z)]q = 1,2,3,\cdots \tag{41}$$

to reduce $E_q[(\beta-\gamma)r_1]$ and $E_q[(\beta+\gamma)r_1]$ to $q = 1$, which has been solved in earlier literature [41,42]. The general expression is

$$\begin{aligned}\Gamma_{-p,-q,0} &= \frac{1}{\gamma}L_p(\alpha+\gamma)[L_q(\beta-\gamma) - L_q(\beta+\gamma)]\\ &\quad - \frac{1}{\gamma}\sum_{i=1}^{q-2}\frac{(-1)^i}{(q-1)\cdots(q-i-1)}[(\beta-\gamma)^i - (\beta+\gamma)^i]L_{p+q-i-1}(\alpha+\beta)\\ &\quad - \frac{1}{\gamma}\frac{(-1)^{q-1}}{(q-1)!}(\beta-\gamma)^{q-1}I_p(\alpha+\gamma,\beta-\gamma) + \frac{1}{\gamma}\frac{(-1)^{q-1}}{(q-1)!}(\beta+\gamma)^{q-1}I_p(\alpha-\gamma,\beta+\gamma).\end{aligned} \tag{42}$$

Equation (42) is valid for $p > 0$ and $q > 0$. For $q = 2,3,4$ the expressions are

$$\Gamma_{-p,-2,0} = \frac{1}{\gamma}L_p(\alpha+\gamma)\,[L_2(\beta-\gamma) - L_2(\beta+\gamma)] + \frac{\beta-\gamma}{\gamma}I_p(\alpha+\gamma,\beta-\gamma) - \frac{\beta+\gamma}{\gamma}I_p(\alpha-\gamma,\beta+\gamma), \tag{43}$$

$$\begin{aligned}\Gamma_{-p,-3,0} &= \frac{1}{\gamma}L_p(\alpha+\gamma)\,[L_3(\beta-\gamma) - L_3(\beta+\gamma)] - L_{p+1}(\alpha+\beta)\\ &\quad - \frac{(\beta-\gamma)^2}{2\gamma}I_p(\alpha+\gamma,\beta-\gamma) + \frac{(\beta+\gamma)^2}{2\gamma}I_p(\alpha-\gamma,\beta+\gamma),\end{aligned} \tag{44}$$

$$\begin{aligned}\Gamma_{-p,-4,0} &= \frac{1}{\gamma}L_p(\alpha+\gamma)\,[L_4(\beta-\gamma) - L_4(\beta+\gamma)] - \frac{1}{3}L_{p+2}(\alpha+\beta) + \frac{2\beta}{3}L_{p+1}(\alpha+\beta)\\ &\quad + \frac{(\beta-\gamma)^3}{6\gamma}I_p(\alpha+\gamma,\beta-\gamma) - \frac{(\beta+\gamma)^3}{6\gamma}I_p(\alpha-\gamma,\beta+\gamma).\end{aligned} \tag{45}$$

Notice that in Eq. (D2) of the original article by Harris *et al.* [42], $E_1(\beta-\gamma)$ and $E_1(\beta+\gamma)$ should be $E_1[(\beta-\gamma)r_1]$ and $E_1[(\beta+\gamma)r_1]$, respectively.

The higher power of the r_{12} term can be generated by taking the derivative

$$\Gamma_{-p,-q,n}(\alpha,\beta,\gamma) = (-1)^n\Gamma^{(0,0,n)}_{-p,-q,0}(\alpha,\beta,\gamma), \tag{46}$$

where the superscript in parentheses is the partial derivative:

$$f^{(l,m,n)}(x,y,z) := \frac{\partial^{l+m+n}}{\partial x^l\partial y^m\partial z^n}f(x,y,z). \tag{47}$$

With the help of the generalized Leibniz rule [62,63]

$$\left[\prod_{i=1}^{r} f_i(x)\right]^{(n)} = \sum_{n_1+\cdots+n_r=n}\binom{n}{n_1,\ldots,n_r}\prod_{i=1}^{r} f_i^{(n_i)}(x), \tag{48}$$

where $\binom{n}{n_1,\ldots,n_r}$ is a multinomial coefficient defined as

$$\binom{n}{n_1,\ldots,n_r} := \frac{n!}{n_1!\cdots n_r!}, \tag{49}$$

$\Gamma_{-p,-q,n}$ can be obtained from Eqs. (42), (46), and (48):

$$\begin{aligned}\Gamma_{-p,-q,n} &= (-1)^n\sum_{n_1+n_2+n_3=n}\binom{n}{n_1,n_2,n_3}\left(\frac{1}{\gamma}\right)^{(n_1)}L_p^{(n_2)}(\alpha+\gamma)[L_q(\beta-\gamma) - L_q(\beta+\gamma)]^{(n_3)}\\ &\quad - (-1)^n\sum_{n_1+n_2=n}\binom{n}{n_1,n_2}\left(\frac{1}{\gamma}\right)^{(n_1)}\sum_{i=1}^{q-2}\frac{(-1)^i}{(q-1)\cdots(q-i-1)}[(\beta-\gamma)^i - (\beta+\gamma)^i]^{(n_2)}L_{p+q-i-1}(\alpha+\beta)\end{aligned}$$

$$-(-1)^n \sum_{n_1+n_2+n_3+n_4=n} (-1)^{n_4} \binom{n}{n_1,n_2,n_3,n_4} \left(\frac{1}{\gamma}\right)^{(n_1)} \frac{(-1)^{q-1}}{(q-1)!} [(\beta-\gamma)^{q-1}]^{(n_2)} I_p^{(n_3,n_4)}(\alpha+\gamma,\beta-\gamma)$$
$$+(-1)^n \sum_{n_1+n_2+n_3+n_4=n} (-1)^{n_3} \binom{n}{n_1,n_2,n_3,n_4} \left(\frac{1}{\gamma}\right)^{(n_1)} \frac{(-1)^{q-1}}{(q-1)!} [(\beta+\gamma)^{q-1}]^{(n_2)} I_p^{(n_3,n_4)}(\alpha-\gamma,\beta+\gamma). \quad (50)$$

Notice that Eq. (48) is valid for a single-variable function. In evaluating the derivative of $I_p(x,y)$ we have performed these steps:

$$\frac{\partial^n}{\partial \gamma^n} I_p(\alpha-\gamma,\beta+\gamma) = \sum_{n_1+n_2=n} \binom{n}{n_1,n_2} (-1)^{n_1} I_p^{(n_1,n_2)}(\alpha-\gamma,\beta+\gamma), \quad (51)$$

$$\frac{\partial^n}{\partial \gamma^n} I_p(\alpha+\gamma,\beta-\gamma) = \sum_{n_1+n_2=n} \binom{n}{n_1,n_2} (-1)^{n_2} I_p^{(n_1,n_2)}(\alpha+\gamma,\beta-\gamma). \quad (52)$$

By inserting the explicit expressions of the derivatives into Eq. (50), we obtain

$$\Gamma_{-p,-q,n} = (-1)^n \sum_{n_1+n_2+n_3=n} \binom{n}{n_1,n_2,n_3} \frac{(-1)^{n_1+n_2} n_1!}{\gamma^{n_1+1}} L_{p-n_2}(\alpha+\gamma)[L_{q-n_3}(\beta-\gamma) - (-1)^{n_3} L_{q-n_3}(\beta+\gamma)]$$
$$-(-1)^n \sum_{n_1+n_2=n} \binom{n}{n_1,n_2} \frac{(-1)^{n_1} n_1!}{\gamma^{n_1+1}} \sum_{i=1}^{q-2} \frac{(-1)^i\ i\cdots(i-n_2+1)}{(q-1)\cdots(q-i-1)} [(-1)^{n_2}(\beta-\gamma)^{i-n_2} - (\beta+\gamma)^{i-n_2}]\theta(i-n_2)$$
$$\times\ L_{p+q-i-1}(\alpha+\beta) - (-1)^{n+q-1} \sum_{n_1+n_2+n_3+n_4=n} \binom{n}{n_1,n_2,n_3,n_4} \frac{(-1)^{n_1+n_2+n_4} n_1!}{\gamma^{n_1+1}} \frac{(\beta-\gamma)^{q-n_2-1}}{(q-n_2-1)!} \theta(q-n_2-1)$$
$$\times \begin{cases} (-1)^{n_3} I_{p-n_3}(\alpha+\gamma,\beta-\gamma), & n_4=0, \\ \sum_{n_5+n_6=n_4-1} \binom{n_4-1}{n_5,n_6} (-1)^{n_3+n_5+n_6-1} \frac{n_5!}{(\beta-\gamma)^{n_5+1}} L_{p-n_3-n_6}(\alpha+\beta), & n_4>0 \end{cases}$$
$$+(-1)^{n+q-1} \sum_{n_1+n_2+n_3+n_4=n} \binom{n}{n_1,n_2,n_3,n_4} \frac{(-1)^{n_1+n_3} n_1!}{\gamma^{n_1+1}} \frac{(\beta+\gamma)^{q-n_2-1}}{(q-n_2-1)!} \theta(q-n_2-1)$$
$$\times \begin{cases} (-1)^{n_3} I_{p-n_3}(\alpha-\gamma,\beta+\gamma), & n_4=0, \\ \sum_{n_5+n_6=n_4-1} \binom{n_4-1}{n_5,n_6} (-1)^{n_3+n_5+n_6-1} \frac{n_5!}{(\beta+\gamma)^{n_5+1}} L_{p-n_3-n_6}(\alpha+\beta), & n_4>0. \end{cases} \quad (53)$$

Here θ is a step function, defined as

$$\theta(n) = \begin{cases} 0, & n<0, \\ 1, & n \geqslant 0. \end{cases} \quad (54)$$

In Eq. (53) if $p-n_3 \leqslant 0$, I_{p-n_3} is finite. The value is [[58], Eq. (6.228.2)]

$$I_p(x,y) = \frac{p!}{(p+1)(x+y)^{p+1}}\ {}_2F_1\left(1,p+1;p+2;\frac{x}{x+y}\right), \quad (55)$$

where ${}_2F_1$ is the hypergeometric function [[60], p. 556].

In practical calculations it is more efficient to set up a recursive scheme rather than a direct evaluation of Eq. (53). As a special case of the Sack *et al*. method [64], if a function can be written as

$$F_n(\alpha,\beta,\gamma) = \left(-\frac{\partial}{\partial\gamma}\right)^n \frac{f(\alpha,\beta,\gamma)}{\gamma}, \quad (56)$$

the following relation holds for $n \geqslant 1$:

$$F_n(\alpha,\beta,\gamma) = \frac{1}{\gamma}\left[F_{n-1}(\alpha,\beta,\gamma) + \left(-\frac{\partial}{\partial\gamma}\right)^n f(\alpha,\beta,\gamma)\right]. \tag{57}$$

Applying Eq. (57) to Eq. (46), we can establish

$$\Gamma_{-p,-q,n} = \frac{1}{\gamma}(n\Gamma_{-p,-q,n-1} + G_{-p,-q,n}), \tag{58}$$

where

$$\begin{aligned}
G_{-p,-q,n} :=& \left(-\frac{\partial}{\partial\gamma}\right)^n \Bigg\{L_p(\alpha+\gamma)[L_q(\beta-\gamma) - L_q(\beta+\gamma)] \\
& - \sum_{i=1}^{q-2} \frac{(-1)^i}{(q-1)\cdots(q-i-1)}\left[(\beta-\gamma)^i - (\beta+\gamma)^i\right] L_{p+q-i-1}(\alpha+\beta) \\
& - \frac{(-1)^{q-1}}{(q-1)!}(\beta-\gamma)^{q-1} I_p(\alpha+\gamma,\beta-\gamma) + \frac{(-1)^{q-1}}{(q-1)!}(\beta+\gamma)^{q-1} I_p(\alpha-\gamma,\beta+\gamma)\Bigg\} \\
=& (-1)^n \sum_{n_1+n_2=n} \binom{n}{n_1,n_2} (-1)^{n_1} L_{p-n_1}(\alpha+\gamma)[L_{q-n_2}(\beta-\gamma) - (-1)^{n_2} L_{q-n_2}(\beta+\gamma)] \\
& - (-1)^n \sum_{i=1}^{q-2} \frac{(-1)^i\ i\cdots(i-n+1)}{(q-1)\cdots(q-i-1)}[(-1)^n(\beta-\gamma)^{i-n} - (\beta+\gamma)^{i-n}]\theta(i-n) \\
& \times L_{p+q-i-1}(\alpha+\beta) - (-1)^{n+q-1} \sum_{n_1+n_2+n_3=n} \binom{n}{n_1,n_2,n_3} (-1)^{n_1+n_3} \frac{(\beta-\gamma)^{q-n_1-1}}{(q-n_2-1)!}\theta(q-n_1-1) \\
& \times \begin{cases} (-1)^{n_2} I_{p-n_2}(\alpha+\gamma,\beta-\gamma), & n_3 = 0, \\ \sum_{n_4+n_5=n_3-1} \binom{n_3-1}{n_4,n_5} (-1)^{n_2+n_4+n_5-1} \frac{n_4!}{(\beta-\gamma)^{n_4+1}} L_{p-n_2-n_5}(\alpha+\beta), & n_3 > 0, \end{cases} \\
& + (-1)^{n+q-1} \sum_{n_1+n_2+n_3=n} \binom{n}{n_1,n_2,n_3} (-1)^{n_2} \frac{(\beta+\gamma)^{q-n_1-1}}{(q-n_1-1)!}\theta(q-n_1-1) \\
& \times \begin{cases} (-1)^{n_2} I_{p-n_2}(\alpha-\gamma,\beta+\gamma), & n_3 = 0, \\ \sum_{n_4+n_5=n_3-1} \binom{n_3-1}{n_4,n_5} (-1)^{n_2+n_4+n_5-1} \frac{n_4!}{(\beta+\gamma)^{n_4+1}} L_{p-n_2-n_5}(\alpha+\beta), & n_3 > 0. \end{cases}
\end{aligned} \tag{59}$$

Equation (59) has onefold summation fewer than Eq. (53).

TABLE I. Values of two-electron integral $\mathcal{I}$, Eq. (16).

N_1	N_2	ω_1	ω_2	ω_{12}	ν	L	$\mathcal{I}$
−1	0	4.0	2.0	−0.5	−1	0	**1.437 324 001 953 832 013 664 951 297 055 19**7 × 10^{-1}
−1	0	4.0	2.0	−0.5	0	0	**1.145 191 162 425 783 775 072 558 441 119 48**6 × 10^{-1}
−1	0	4.0	2.0	−0.5	1	0	**1.595 028 495 832 393 726 782 454 173 284 9**80 × 10^{-1}
0	0	4.0	2.0	−0.5	−1	0	**3.174 603 174 603 174 603 174 603 174 603 174** × 10^{-2}
0	0	4.0	2.0	−0.5	0	0	**3.023 431 594 860 166 288 737 717 309 145 87**2 × 10^{-2}
0	0	4.0	2.0	−0.5	1	0	**4.549 544 685 599 107 367 814 850 808 048** 120 × 10^{-2}
1	0	4.0	2.0	−0.5	1	0	**2.699 835 288 108 692 708 627 920 808 030 94**4 × 10^{-2}
1	1	4.0	2.0	−0.5	1	0	**4.673 407 113 748 329 599 749 532 802 118 91**2 × 10^{-2}
1	1	4.0	2.0	−0.5	1	1	**−9.867 859 128 198 184 455 608 059 970 4**48 2 × 10^{-3}
2	2	4.0	2.0	−0.5	1	1	**−2.431 564 634 556 186 430 148 411 010 294 65** × 10^{-2}

TABLE II. Values of three-electron integral $\mathcal{J}$, Eq. (7).

N_1	N_2	N_3	ω_1	ω_2	ω_3	ω_{12}	ω_{13}	ν	μ	L_2	L_3	$\mathcal{J}$
0	1	1	6.0	4.0	2.0	−0.5	0.0	−1	0	0	0	5.009 276 437 847 866 419 294 990 723 562 145 × 10^{-4}
0	1	1	6.0	4.0	2.0	−0.5	0.0	0	0	0	0	3.402 163 699 009 710 141 435 558 875 262 040 × 10^{-4}
0	1	1	6.0	4.0	2.0	−0.5	0.0	1	0	0	0	3.266 607 859 046 959 834 854 685 829 314 128 × 10^{-4}
1	1	1	6.0	4.0	2.0	−0.5	0.0	−1	0	0	0	1.541 575 307 809 074 042 840 276 606 510 372 × 10^{-4}
1	1	1	6.0	4.0	2.0	−0.5	0.0	0	0	0	0	1.185 106 005 480 436 244 477 398 128 941 392 × 10^{-4}
1	1	1	6.0	4.0	2.0	−0.5	0.0	1	0	0	0	1.249 025 368 815 175 904 696 267 955 878 976 × 10^{-4}
2	2	2	6.0	4.0	2.0	−0.5	0.0	−1	0	1	0	7.561 424 913 423 564 123 513 524 761 627 8 × 10^{-6}
2	2	2	6.0	4.0	2.0	−0.5	0.0	0	0	1	0	−6.982 228 365 392 342 585 667 055 092 049 6 × 10^{-6}
2	2	2	6.0	4.0	2.0	−0.5	0.0	1	0	1	0	−2.417 662 538 431 947 826 713 986 489 464 68 × 10^{-5}
2	2	2	6.0	4.0	2.0	−0.5	0.0	1	−1	1	1	−2.615 759 285 094 083 555 892 702 111 012 18 × 10^{-6}
0	1	1	6.0	4.0	2.0	−0.5	−0.5	−1	0	0	0	1.215 166 719 484 094 376 352 887 862 332 437 × 10^{-3}
0	1	1	6.0	4.0	2.0	−0.5	−0.5	0	0	0	0	8.307 575 028 794 119 806 230 161 609 520 50 × 10^{-4}
0	1	1	6.0	4.0	2.0	−0.5	−0.5	1	0	0	0	8.026 762 164 322 698 855 868 381 913 747 400 × 10^{-4}
1	1	1	6.0	4.0	2.0	−0.5	−0.5	−1	0	0	0	3.825 773 050 336 459 474 879 547 838 183 266 × 10^{-4}
1	1	1	6.0	4.0	2.0	−0.5	−0.5	0	0	0	0	2.980 753 462 738 371 954 794 858 483 016 718 × 10^{-4}
1	1	1	6.0	4.0	2.0	−0.5	−0.5	1	0	0	0	3.183 245 452 149 235 698 199 669 529 408 872 × 10^{-4}
2	2	2	6.0	4.0	2.0	−0.5	−0.5	−1	0	1	0	2.525 717 461 258 712 398 749 836 685 360 63 × 10^{-5}
2	2	2	6.0	4.0	2.0	−0.5	−0.5	0	0	1	0	−2.432 450 005 271 229 916 526 278 743 090 41 × 10^{-5}
2	2	2	6.0	4.0	2.0	−0.5	−0.5	1	0	1	0	−8.475 881 930 997 630 463 595 145 867 367 48 × 10^{-5}
2	2	2	6.0	4.0	2.0	−0.5	−0.5	1	−1	1	1	−8.120 788 621 430 925 892 524 954 668 746 80 × 10^{-5}

TABLE III. Values of four-electron integral $\mathcal{K}_1$, Eq. (22).

N_1	N_2	N_3	N_4	ω_1	ω_2	ω_3	ω_4	ω_{12}	ω_{13}	ν	μ	κ	L_2	L_3	L_4	$\mathcal{K}_1$
1	1	1	1	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	0	0	0	4.932 012 038 777 262 926 861 676 603 092 256 × 10^{-7}
2	2	2	2	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	0	0	0	9.723 625 354 173 994 947 050 888 948 241 52 × 10^{-8}
2	2	2	2	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	1	0	0	−6.314 113 122 206 599 835 153 824 108 674 4 × 10^{-9}
2	2	2	2	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	1	1	0	5.183 696 218 741 692 075 780 581 590 202 92 × 10^{-10}
2	2	2	2	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	1	1	1	1.041 001 980 702 750 962 914 776 868 380 95 × 10^{-10}
3	3	3	3	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	0	0	0	6.573 955 325 992 439 005 351 895 740 006 212 × 10^{-8}
3	3	3	3	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	2	0	0	−2.639 184 813 383 406 534 009 563 729 142 6 × 10^{-10}
3	3	3	3	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	2	2	0	7.618 693 019 575 205 369 196 829 629 516 × 10^{-13}
3	3	3	3	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	2	2	2	4.838 627 101 675 689 383 370 301 951 764 × 10^{-14}
3	3	3	3	8.0	6.0	4.0	2.0	−0.5	−0.5	1	1	−1	2	2	2	1.161 557 445 600 211 830 743 332 255 003 0 × 10^{-13}

TABLE IV. Values of four-electron integral $\mathcal{K}_2$, Eq. (23).

N_1	N_2	N_3	N_4	ω_1	ω_2	ω_3	ω_4	ω_{12}	ω_{34}	ν	μ	κ	L_2	L_3	L_4	$\mathcal{K}_2$
1	1	1	1	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	0	0	0	1.465 423 281 172 008 340 718 675 056 269 763 × 10^{-6}
2	2	2	2	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	0	0	0	3.455 948 258 119 907 308 258 045 381 210 140 × 10^{-7}
2	2	2	2	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	1	0	0	−2.131 868 102 234 955 748 873 926 631 509 776 × 10^{-8}
2	2	2	2	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	1	1	0	−4.479 303 653 926 613 814 855 805 199 716 874 × 10^{-9}
2	2	2	2	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	1	1	1	5.623 732 368 534 378 098 402 718 867 978 85 × 10^{-10}
3	3	3	3	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	0	0	0	2.799 519 792 819 307 124 798 406 613 728 066 × 10^{-7}
3	3	3	3	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	2	0	0	−1.161 863 685 712 510 582 515 311 687 013 099 × 10^{-9}
3	3	3	3	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	2	2	0	−1.036 582 942 644 425 513 882 521 709 129 422 × 10^{-10}
3	3	3	3	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	2	2	2	−5.381 773 582 248 076 958 003 411 278 978 8 × 10^{-13}
3	3	3	3	8.0	6.0	4.0	2.0	−0.5	−0.5	1	1	−1	2	2	2	−1.438 964 823 159 370 296 803 316 838 538 9 × 10^{-12}

TABLE V. Values of four-electron integral $\mathcal{L}$, Eq. (24).

N_1	N_2	N_3	N_4	ω_1	ω_2	ω_3	ω_4	ω_{12}	ω_{13}	ν	μ	κ	L_2	L_3	L_4	$\mathcal{L}$
1	1	1	1	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	0	0	0	**5.757 249 082 801 392 218 172 468 820 882 18** × 10^{-7}
2	2	2	2	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	0	0	0	**1.095 599 985 633 336 705 357 419 158 111 10**2 × 10^{-7}
2	2	2	2	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	1	0	0	**−7.029 957 673 654 003 660 063 080 964 0**30 3 × 10^{-9}
2	2	2	2	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	1	1	0	**5.787 345 803 218 052 342 632 091 056** 243 9 × 10^{-10}
2	2	2	2	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	1	1	1	**9.574 389 125 220 778 379 545 715 227** 653 4 × 10^{-11}
3	3	3	3	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	0	0	0	**7.220 579 580 660 073 929 030 826 772 816 4**60 × 10^{-8}
3	3	3	3	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	2	0	0	**−2.899 424 717 488 939 534 340 207 8**88 064 6 × 10^{-10}
3	3	3	3	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	2	2	0	**7.585 365 260 760 225 169 170** 964 001 884 × 10^{-13}
3	3	3	3	8.0	6.0	4.0	2.0	−0.5	−0.5	0	0	−1	2	2	2	**3.643 122 172 782 238 928 668** 814 032 947 8 × 10^{-14}
3	3	3	3	8.0	6.0	4.0	2.0	−0.5	−0.5	1	1	−1	2	2	2	**1.684 904 654 636 257 728 954** 787 087 091 6 × 10^{-13}

IV. INTEGRAL VALUES

To test the numerical abilities of the present formulas, we have calculated the numerical values of some typical two-, three-, and four-electron integrals and they are summarized in Tables I–V. The calculations were performed with the MAPLE [65] program package with 34-digit accuracy which corresponds to quadruple arithmetic precision. At the same time, to examine the accuracy of the calculated integrals, we performed the calculations with 100-digit precision. In Tables I–V, the boldface characters indicate the correct numbers by comparison with the results of the calculations with 100-digit precision. Even in the least accurate case, namely, certain $\mathcal{K}_1$-type integrals, precision of about 18 significant figures could be obtained.

V. SUMMARY

When we adopt the wave function ansatz as given by the E-Hy-CI method that includes single r_{ij}^n and $\exp(-\omega_{ij} r_{ij})$ at the same time, Eq. (2), to formulate up to four-electron integrals; their analytical expressions for atoms are given in this paper. This integration scheme is an extension of the works of Calais and Löwdin [28], Perkins [36], and especially Ruiz [33]. No three- or four-electron auxiliary integral appears in the final expressions. These formulas cover a wider class of correlation factors. Together with the Fromm-Hill formula [30] for the linked three-electron case, all necessary nonrelativistic atomic integrals in this approach can be evaluated in a closed form. The prescription of combining diverged integrals to obtain finite values in the previous schemes [33,36,37] is avoided in the present work.

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APPENDIX

In the article of Ruiz [33] an identity for eliminating divergence, Eq. (B.5), was obtained with the help of a symbolic computation program package, MAPLE [65]. The derivation details are unknown to the best of the present authors' knowledge. We think an explicit proof will be helpful. In this Appendix, we present such a proof.

After slightly rearranging the original expression, we obtain

$$A(-n,\alpha) - A(-n,\alpha+\gamma) - \sum_{l=1}^{n-1} \frac{\gamma^l}{l!} A(-n+l,\alpha+\gamma) = \frac{1}{(n-1)!}\left[(-\alpha)^{n-1} \ln\left(\frac{\alpha+\gamma}{\alpha}\right) + \sum_{k=1}^{n-1} \frac{\gamma^k(-\alpha)^{n-k-1}}{k}\right], \tag{A1}$$

where $n > 0$. By Eqs. (31)–(33), after binomial expansion and rearrangement of the summation indices, the LHS of Eq. (A1) becomes

$$\frac{(-\alpha)^{n-1}}{(n-1)!} \ln\left(\frac{\alpha+\gamma}{\alpha}\right) + \sum_{k=1}^{n-1} \frac{(-1)^{k-1}}{k!(n-k-1)!} \gamma^k (-\alpha)^{n-k-1} \left[\psi(n) + \sum_{l=1}^{k} \frac{(-1)^l k!}{l!(k-l)!} \psi(n-l)\right]$$
$$+ \lim_{\varepsilon\to 0} \sum_{k=1}^{n-1} \frac{(-1)^k}{k!(n-k-1)!} \gamma^k (-\alpha)^{n-k-1} \ln[(\alpha+\gamma)\varepsilon]$$
$$+ \lim_{\varepsilon\to 0} \sum_{k=1}^{n-1} \sum_{l=1}^{k} \frac{(-1)^{k-l}}{l!(k-l)!(n-k-1)!} \gamma^k (-\alpha)^{n-k-1} \ln[(\alpha+\gamma)\varepsilon]$$

$$+\lim_{\varepsilon\to 0}\sum_{j=1}^{n-1}\sum_{k=1}^{n-j-1}\frac{(-1)^{k-1}}{j\,k!\,(n-j-k-1)!}\,\gamma^k(-\alpha)^{n-j-k-1}\varepsilon^{-j}$$
$$+\lim_{\varepsilon\to 0}\sum_{j=1}^{n-1}\sum_{k=1}^{n-j-1}\sum_{l=1}^{k}\frac{(-1)^{k-l-1}}{j\,l!\,(k-l)!\,(n-j-k-1)!}\,\gamma^k(-\alpha)^{n-j-k-1}\varepsilon^{-j}. \quad (A2)$$

Inside a four-electron integral, all ε's are the same. Therefore, the logarithms and polynomial divergence terms have zero contributions:

$$\lim_{\varepsilon\to 0}\sum_{k=1}^{n-1}\frac{(-1)^k}{k!(n-k-1)!}\left[1+\sum_{l=1}^{k}\frac{(-1)^l k!}{l!(k-l)!}\right]\gamma^k(-\alpha)^{n-k-1}\ln[(\alpha+\gamma)\varepsilon]=0, \quad (A3)$$

$$\lim_{\varepsilon\to 0}\sum_{j=1}^{n-1}\sum_{k=1}^{n-j-1}\frac{(-1)^{k-1}}{j\,k!\,(n-j-k-1)!}\left[1+\sum_{l=1}^{k}\frac{(-1)^l k!}{l!(k-l)!}\right]\gamma^k(-\alpha)^{n-j-k-1}\varepsilon^{-j}=0. \quad (A4)$$

The remaining terms can be written as

$$\frac{(-\alpha)^{n-1}}{(n-1)!}\ln\left(\frac{\alpha+\gamma}{\alpha}\right)+\sum_{k=1}^{n-1}\frac{(-1)^{k-1}}{k!(n-k-1)!}\left[\psi(n)+\sum_{l=1}^{k}\frac{(-1)^l k!}{l!(k-l)!}\psi(n-l)\right]\gamma^k\,(-\alpha)^{n-k-1}$$
$$=\frac{(-\alpha)^{n-1}}{(n-1)!}\ln\left(\frac{\alpha+\gamma}{\alpha}\right)+\sum_{k=1}^{n-1}\frac{(-1)^k}{k!(n-k-1)!}\left[\sum_{l=0}^{k}\frac{(-1)^l k!}{l!(k-l)!}\sum_{m=1}^{l}\frac{1}{n-m}\right]\gamma^k\,(-\alpha)^{n-k-1}$$
$$=\frac{(-\alpha)^{n-1}}{(n-1)!}\ln\left(\frac{\alpha+\gamma}{\alpha}\right)+\sum_{k=1}^{n-1}\frac{(-1)^k}{k!(n-k-1)!}\left[\sum_{l=0}^{k}\frac{(-1)^l k!}{l!(k-l)!}\sum_{m=1}^{l}\int_0^1 x^{n-m-1}dx\right]\gamma^k\,(-\alpha)^{n-k-1}$$
$$=\frac{(-\alpha)^{n-1}}{(n-1)!}\ln\left(\frac{\alpha+\gamma}{\alpha}\right)+\sum_{k=1}^{n-1}\frac{(-1)^k}{k!(n-k-1)!}\left[\sum_{l=0}^{k}\frac{(-1)^l k!}{l!(k-l)!}\int_0^1\frac{x^{n-l-1}}{1-x}dx\right]\gamma^k\,(-\alpha)^{n-k-1}$$
$$=\frac{(-\alpha)^{n-1}}{(n-1)!}\ln\left(\frac{\alpha+\gamma}{\alpha}\right)+\sum_{k=1}^{n-1}\frac{1}{k!(n-k-1)!}\left[\int_0^1(1-x)^k\frac{x^{n-k-1}}{1-x}dx\right]\gamma^k\,(-\alpha)^{n-k-1}$$
$$=\frac{(-\alpha)^{n-1}}{(n-1)!}\ln\left(\frac{\alpha+\gamma}{\alpha}\right)+\sum_{k=1}^{n-1}\frac{1}{k!(n-k-1)!}\mathrm{B}(k,n-k)\gamma^k\,(-\alpha)^{n-k-1}$$
$$=\frac{1}{(n-1)!}\left[(-\alpha)^{n-1}\ln\left(\frac{\alpha+\gamma}{\alpha}\right)+\sum_{k=1}^{n-1}\frac{\gamma^k\,(-\alpha)^{n-k-1}}{k}\right]; \quad (A5)$$

here $\mathrm{B}(x,y)$ is the beta function) [[60], Eq. (6.2.2)]. Thus we obtain the RHS of Eq. (A1).

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