Extended Hylleraas three-electron integral

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A closed-form expression for the three-electron Hylleraas integral involving the inverse quadratic power of one interparticle coordinate is obtained, and recursion relations are derived for positive powers of other coordinates. This result is suited for high-precision calculations of relativistic effects in lithium and light lithiumlike ions.

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I. INTRODUCTION

The subject of this work is the extended three-electron Hylleraas integrals involving $1/r_{ij}^2$ and $1/r_i^2$ terms, which appear in matrix elements of relativistic operators in the Breit-Pauli Hamiltonian. These integrals are defined as

$$f(n_1,n_2,n_3,n_4,n_5,n_6) = \int \frac{d^3r_1}{4\pi} \int \frac{d^3r_2}{4\pi} \int \frac{d^3r_3}{4\pi} e^{-w_1 r_1 - w_2 r_2 - w_3 r_3} \times r_{23}^{n_1-1} r_{31}^{n_2-1} r_{12}^{n_3-1} r_1^{n_4-1} r_2^{n_5-1} r_3^{n_6-1}, \tag{1}$$

with one of n_i equal to −1 and all other n_i nonnegative integers. They have been studied in detail in a series of papers by King and co-workers [1–3] and by Yan and Drake [4]. Their approach is based on the expansion of $1/r_{ij}^n$ in an infinite series of some orthogonal polynomials. The resulting multiple summation is performed with the help of convergence accelerators. In some special cases [1] this expansion can be avoided and Eq. (1) can be expressed in terms of the two-electron Hylleraas integral. Using these methods leading relativistic and QED corrections to energies [5,6], isotope shifts [7], and g factors [8] have been calculated to a high degree of accuracy. The analytic approach to the Hylleraas integral has been so far much less successful. Fromm and Hill in Ref. [9] were able to obtain an analytic expression for a more general integral with exponents in r_i, as well as in r_{ij}. However, their expression is quite complicated, involves multivalued dilogarithmic functions, and thus is of limited use. In parallel Remiddi in [10] obtained a simple analytic expression for the Hylleraas integral with $n_i=0$. Recently, together with Remiddi we derived recursion relations [11] for Hylleraas integrals for arbitrary large powers of r_i and r_{ij}. This result allows for a convenient calculation of the nonrelativistic wave function of the lithium atom and light lithium-like ions.

In this work we present an analytic approach which allows for a fast and high-precision calculation of extended three-electron Hylleraas integrals. This sets the ground for improving the precision of theoretical energy levels by including higher-order relativistic corrections [12]. We obtain here the closed-form expression for the master integral $f(-1,0,0,0,0,0)$ and derive recursion relations for increasing values of arguments n_i of $f(-1,n_2,n_3,n_4,n_5,n_6)$. The other integrals, such as $f(n_1,n_2,n_3,-1,n_5,n_6)$, can be obtained by using already derived recursion relations for $f(n_1,n_2,n_3,n_4,n_5,n_6)$ with nonnegative n_i followed by a one-dimensional numerical integration with respect to the corresponding parameter w_i.

II. RECURSION RELATIONS FOR r_{23}^{-2} INTEGRAL

Our derivation is based on integration by parts identities which are commonly used for the calculations of multiloop Feynman diagrams [13]. We follow here the former work [11] and first consider the integral G,

$$G(m_1,m_2,m_3;m_4,m_5,m_6) = \frac{1}{8\pi^6} \int d^3k_1 \int d^3k_2 \int d^3k_3\, (k_1^2+u_1^2)^{-m_1}(k_2^2+u_2^2)^{-m_2} \times (k_3^2+u_3^2)^{-m_3}(k_{32}^2+w_1^2)^{-m_4}(k_{13}^2+w_2^2)^{-m_5}(k_{21}^2+w_3^2)^{-m_6}, \tag{2}$$

which is related to f by $f(0,0,0,0,0,0,0) = G(1,1,1,1,1,1)|_{u_1=u_2=u_3=0}$. The following nine integration by parts identities are valid because the integral of the derivative of a function vanishing at infinity vanishes,

$$0 \equiv \mathrm{id}(i,j) = \int d^3k_1 \int d^3k_2 \int d^3k_3 \frac{\partial}{\partial \vec{k}_i}[\vec{k}_j (k_1^2+u_1^2)^{-1}(k_2^2+u_2^2)^{-1} \times (k_3^2+u_3^2)^{-1}(k_{32}^2+w_1^2)^{-1}(k_{13}^2+w_2^2)^{-1}(k_{21}^2+w_3^2)^{-1}], \tag{3}$$

where $i,j=1,2,3$. The reduction of the scalar products from the numerator leads to the identities for the linear combination of the G function. If any of the arguments is equal to 0, then G becomes a known two-electron Hylleraas-type integral, Eq. (B6). The explicit form of all nine identities is presented in Eq. (A1) and the whole derivation presented below is performed with the help of the MATHEMATICA program for symbolic computation.

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In the first step of deriving recursion relations we take the difference $\mathrm{id}(3,2)-\mathrm{id}(2,2)$ and use it as an equation for $G(1,2,1,1,1,1)$,

$$\begin{aligned}G(1,2,1,1,1,1)(u_2^2-u_3^2+w_1^2) &= G(1,1,1,0,1,2)-G(1,1,1,1,0,2)+G(1,1,1,1,1,1)\\ &\quad -G(1,2,0,1,1,1)+G(1,2,1,0,1,1)\\ &\quad -2G(1,1,1,2,1,1)w_1^2\\ &\quad +G(1,1,1,1,1,2)(w_2^2-w_1^2-w_3^2).\end{aligned} \tag{4}$$

Similarly, the difference $\mathrm{id}(2,3)-\mathrm{id}(3,3)$ is used to obtain $G(1,1,2,1,1,1)$,

$$\begin{aligned}G(1,1,2,1,1,1)(u_2^2-u_3^2-w_1^2) &= G(1,0,2,1,1,1)-G(1,1,1,0,2,1)-G(1,1,1,1,1,1)\\ &\quad +G(1,1,1,1,2,0)-G(1,1,2,0,1,1)\\ &\quad +2G(1,1,1,2,1,1)w_1^2\\ &\quad +G(1,1,1,1,2,1)(w_1^2+w_2^2-w_3^2).\end{aligned} \tag{5}$$

These two equations are used now to derive recursions in n_2 and n_3. With the help of the trivial formula

$$\int_0^\infty du \frac{e^{-ur}}{r} = \frac{1}{r^2}, \tag{6}$$

one integrates with respect to u_1, which lowers the first argument n_1 to -1. Next, one differentiates with respect to u_2, u_3, w_1, w_2, w_3 at $u_2=u_3=0$ to generate arbitrary powers of $r_{13}, r_{12}, r_1, r_2, r_3$ and obtains quite long recursion relations for n_2 and n_3,

$$\begin{aligned}f(-1,n_2+2,n_3,n_4,n_5,n_6) = \frac{1}{w_1^2w_3}\big[& n_4(n_4-1)(n_2+1)f(-1,n_2,n_3,n_4-2,n_5,n_6+1)-n_5(n_5-1)(n_2+1)f(-1,n_2,n_3,n_4,n_5-2,n_6\\ &+1)+n_6(1+n_2+2n_4+n_6)(n_2+1)f(-1,n_2,n_3,n_4,n_5,n_6-1)-n_3(n_3-1)n_6f(-1,n_2+2,n_3\\ &-2,n_4,n_5,n_6-1)+n_4(n_4-1)n_6f(-1,n_2+2,n_3,n_4-2,n_5,n_6-1)-2n_4(n_2+1)w_1f(-1,n_2,n_3,n_4\\ &-1,n_5,n_6+1)-2n_6(n_2+1)w_1f(-1,n_2,n_3,n_4+1,n_5,n_6-1)-2n_4n_6w_1f(-1,n_2+2,n_3,n_4-1,n_5,n_6\\ &-1)+n_6w_1^2f(-1,n_2+2,n_3,n_4,n_5,n_6-1)+2n_5(n_2+1)w_2f(-1,n_2,n_3,n_4,n_5-1,n_6+1)-(2+n_2\\ &+2n_4+2n_6)(n_2+1)w_3f(-1,n_2,n_3,n_4,n_5,n_6)+(n_3-1)n_3w_3f(-1,n_2+2,n_3-2,n_4,n_5,n_6)-n_4(n_4\\ &-1)w_3f(-1,2+n_2,n_3,-2+n_4,n_5,n_6)+2(n_2+1)w_1w_3f(-1,n_2,n_3,n_4+1,n_5,n_6)w_1w_3\\ &+2n_4w_1w_3f(-1,n_2+2,n_3,n_4-1,n_5,n_6)+(n_2+1)(w_1^2-w_2^2+w_3^2)f(-1,n_2,n_3,n_4,n_5,n_6+1)\\ &+\delta_{n_4}w_3\Gamma(n_3+n_5-1,n_2+n_6+1,-1;w_2,w_3,0)-\delta_{n_3}w_3\Gamma(-1+n_4+n_5,n_6,n_2;w_1+w_2,w_3,0)\\ &-(n_2+n_6+1)\,\delta_{n_4}\Gamma(n_3+n_5-1,n_2+n_6,-1;w_2,w_3,0)+n_6\delta_{n_3}\Gamma(n_4+n_5-1,n_6-1,n_2;w_1+w_2,w_3,0)\\ &+(n_2+1)\,\delta_{n_5}\Gamma(n_6-1,n_3+n_4-1,n_2;w_3,w_1,0)\big],\end{aligned} \tag{7}$$

$$\begin{aligned}f(-1,n_2,n_3+2,n_4,n_5,n_6) = \frac{1}{w_1^2w_2}\big[&-n_2(n_2-1)n_5f(-1,-n_2-2,n_3+2,n_4,n_5-1,n_6)+(n_3+1)n_4(n_4-1)f(-1,n_2,n_3,n_4\\ &-2,n_5+1,n_6)+(n_3+1)n_5(1+n_3+2n_4+n_5)f(-1,n_2,n_3,n_4,n_5-1,n_6)-(n_3+1)n_6(n_6\\ &-1)f(-1,n_2,n_3,n_4,n_5+1,n_6-2)+n_4(n_4-1)n_5f(-1,n_2,n_3+2,n_4-2,n_5-1,n_6)-2(n_3\\ &+1)n_4w_1f(-1,n_2,n_3,n_4-1,n_5+1,n_6)-2(n_3+1)n_5w_1f(-1,n_2,n_3,n_4+1,n_5-1,n_6)\\ &-2n_4n_5w_1f(-1,n_2,2+n_3,n_4-1,n_5-1,n_6)+(n_3+1)(w_1^2+w_2^2-w_3^2)f(-1,n_2,n_3,n_4,n_5+1,n_6)\\ &+n_5w_1^2f(-1,n_2,n_3+2,n_4,n_5-1,n_6)+n_2(n_2-1)w_2f(-1,n_2-2,n_3+2,n_4,n_5,n_6)-(n_3+1)(n_3+2n_4\\ &+2n_5+2)w_2f(-1,n_2,n_3,n_4,n_5,n_6)-n_4(n_4-1)w_2f(-1,n_2,2+n_3,n_4-2,n_5,n_6)+2(n_3+1)\\ &\times w_1w_2f(-1,n_2,n_3,n_4+1,n_5,n_6)+2n_4w_1w_2f(-1,n_2,n_3+2,n_4-1,n_5,n_6)+2(n_3\\ &+1)n_6w_3f(-1,n_2,n_3,n_4,n_5+1,n_6-1)+\delta_{n_4}w_2\Gamma(n_3+n_5+1,n_2+n_6-1,-1;w_2,w_3,0)\\ &-\delta_{n_2}w_2\Gamma(n_4+n_6-1,n_5,n_3;w_1+w_3,w_2,0)+(n_3+1)\,\delta_{n_6}\Gamma(n_2+n_4-1,n_5-1,n_3;w_1,w_2,0)-(1+n_3\\ &+n_5)\,\delta_{n_4}\Gamma(n_3+n_5,n_2+n_6-1,-1;w_2,w_3,0)+n_5\delta_{n_2}\Gamma(n_4+n_6-1,n_5,n_3-1;w_1+w_3,w_2,0)\big],\end{aligned} \tag{8}$$

where δ_n denotes the Kronecker delta $\delta_{n,0}$ and Γ is a two-electron Hylleraas integral, which is defined in Eq. (B1). These recursions assume that the values of $f(-1,0,0,n_4,n_5,n_6)$, $f(-1,1,0,n_4,n_5,n_6)$, $f(-1,0,1,n_4,n_5,n_6)$, and $f(-1,1,1,n_4,n_5,n_6)$ are known. We calculate master integrals for the last three cases explicitly and express them in terms of two-electron Hylleraas integrals as in [1],

$$f(-1,1,1,0,0,0) = \int \frac{d^3r_1}{4\pi}\int \frac{d^3r_2}{4\pi}\int \frac{d^3r_3}{4\pi}\frac{e^{-w_1r_1-w_2r_2-w_3r_3}}{r_{23}^2 r_1 r_2 r_3} = \frac{1}{w_1^2(w_2^2-w_3^2)}\ln\frac{w_2}{w_3} = \frac{1}{w_1^2}\Gamma(0,0,-1;w_2,w_3,0), \tag{9}$$

$$\begin{aligned}f(-1,0,1,0,0,0) &= \int \frac{d^3r_1}{4\pi}\int \frac{d^3r_2}{4\pi}\int \frac{d^3r_3}{4\pi}\frac{e^{-w_1r_1-w_2r_2-w_3r_3}}{r_{23}^2 r_{13} r_1 r_2 r_3}\\ &= \frac{1}{4w_1^2 w_2}\bigg[\ln^2\left(\frac{w_2}{w_2+w_3}\right) - \ln^2\left(\frac{w_2}{w_1+w_2+w_3}\right) + 2\mathrm{Li}_2\left(\frac{w_2}{w_2+w_3}\right)\\ &\quad - 2\mathrm{Li}_2\left(\frac{w_2}{w_1+w_2+w_3}\right) + 2\mathrm{Li}_2\left(1-\frac{w_3}{w_2}\right) - 2\mathrm{Li}_2\left(1-\frac{w_1+w_3}{w_2}\right)\bigg]\\ &= \frac{1}{w_1^2}[\Gamma(-1,0,-1;w_3,w_2,0) - \Gamma(-1,0,-1;w_1+w_3,w_2,0)],\end{aligned} \tag{10}$$

$$\begin{aligned}f(-1,1,0,0,0,0) &= \int \frac{d^3r_1}{4\pi}\int \frac{d^3r_2}{4\pi}\int \frac{d^3r_3}{4\pi}\frac{e^{-w_1r_1-w_2r_2-w_3r_3}}{r_{23}^2 r_{12} r_1 r_2 r_3}\\ &= \frac{1}{w_1^2}[\Gamma(-1,0,-1;w_2,w_3,0) - \Gamma(-1,0,-1;w_1+w_2,w_3,0)],\end{aligned} \tag{11}$$

where Li_2 is a dilogarithmic function, Eq. (C13). The recursion relations in n_4,n_5,n_6 are obtained by differentiation with respect to w_1, w_2, and w_3,

$$\begin{aligned}f(-1,n_2,n_3,n_4,n_5,n_6) &= \frac{1}{w_1^2}[-n_4(n_4-1)f(-1,n_2,n_3,n_4-2,n_5,n_6)\\ &\quad + 2n_4 w_1 f(-1,n_2,n_3,n_4-1,n_5,n_6)\\ &\quad + \delta_{n_4}\Gamma(n_5+n_3-1,n_6+n_2-1,-1;w_2,w_3,0)\\ &\quad - \delta_{n_3}\Gamma(n_4+n_5-1,n_6,-1;w_1+w_2,w_3,0)\\ &\quad - \delta_{n_2}\Gamma(n_4+n_6-1,n_5,-1;w_1+w_3,w_2,0)],\end{aligned} \tag{12}$$

for $(n_2,n_3)\in\{(1,1),(1,0),(0,1)\}$.

The calculation of the integral $f(-1,0,0,n_4,n_5,n_6)$ is much more elaborate and we have to return to integration by parts identities; see Appendix A. These are nine equations, which we solve against the following $X_{i=1,9}$ unknowns at $u_2=u_3=0$,

$$\begin{aligned}X_1 &= G(1,2,1,1,1,1)u_1,\\ X_2 &= G(1,1,2,1,1,1)u_1,\\ X_3 &= G(1,1,1,1,2,1)u_1,\\ X_4 &= G(1,1,1,1,1,2)u_1,\\ X_5 &= G(1,2,1,1,1,1),\\ X_6 &= G(1,1,2,1,1,1),\\ X_7 &= G(1,1,1,1,2,1),\\ X_8 &= G(1,1,1,1,1,2),\\ X_9 &= G(2,1,1,1,1,1).\end{aligned} \tag{13}$$

The solution for X_7 and X_8 is

$$\begin{aligned}G(1,1,1,1,2,1) &= -G(2,1,1,1,1,1)\frac{u_1^2}{2w_2^2} - G(1,1,1,2,1,1)\frac{w_1^2+w_2^2-w_3^2}{2w_2^2}\\ &\quad + G(1,1,1,1,1,1)\frac{3w_1^2+w_2^2-w_3^2}{4w_1^2w_2^2} + \frac{F(u_1)}{4w_1^2w_2^2},\end{aligned} \tag{14}$$

$$\begin{aligned}G(1,1,1,1,1,2) &= -G(2,1,1,1,1,1)\frac{u_1^2}{2w_3^2} - G(1,1,1,2,1,1)\frac{w_1^2-w_2^2+w_3^2}{2w_3^2}\\ &\quad + G(1,1,1,1,1,1)\frac{3w_1^2-w_2^2+w_3^2}{4w_1^2w_3^2} - \frac{F(u_1)}{4w_1^2w_3^2},\end{aligned} \tag{15}$$

where

$$\begin{aligned}F(u_1) &= 2[G(1,1,1,0,2,1)w_2^2 - G(1,1,1,1,2,0)w_2^2\\ &\quad + G(2,0,1,1,1,1)w_2^2 - G(2,1,1,1,1,0)w_2^2\\ &\quad - G(1,1,1,0,1,2)w_3^2 + G(1,1,1,1,0,2)w_3^2\\ &\quad - G(2,1,0,1,1,1)w_3^2 + G(2,1,1,1,0,1)w_3^2].\end{aligned} \tag{16}$$

We now use the explicit form of two-electron integrals in Eq. (B6) and integrate both equations with respect to u_1,

$$\begin{aligned}f(-1,0,0,0,1,0) &= \frac{1}{2w_1^2w_2}[F + (2w_1^2+w_2^2-w_3^2)\\ &\quad \times f(-1,0,0,0,0,0) - w_1(w_1^2+w_2^2-w_3^2)\\ &\quad \times f(-1,0,0,1,0,0)],\end{aligned} \tag{17}$$

$$f(-1,0,0,0,0,1) = \frac{1}{2w_1^2 w_3}[-F + (2w_1^2 - w_2^2 + w_3^2) f(-1,0,0,0,0,0) - w_1(w_1^2 - w_2^2 + w_3^2) f(-1,0,0,1,0,0)], \tag{18}$$

where

$$\begin{aligned} F &= \int_0^\infty du_1 F(u_1) = \frac{1}{2}\Bigg[2\mathrm{Li}_2\left(-\frac{w_2}{w_1}\right) - \mathrm{Li}_2\left(1 - \frac{w_2}{w_3}\right) + \mathrm{Li}_2\left(1 - \frac{w_1 + w_2}{w_3}\right) - 2\mathrm{Li}_2\left(-\frac{w_3}{w_1}\right) + \mathrm{Li}_2\left(\frac{w_2}{w_2 + w_3}\right) - \mathrm{Li}_2\left(\frac{w_3}{w_2 + w_3}\right) \\ &\quad + \mathrm{Li}_2\left(\frac{w_2}{w_1 + w_2 + w_3}\right) - \mathrm{Li}_2\left(\frac{w_3}{w_1 + w_2 + w_3}\right) + \mathrm{Li}_2\left(1 - \frac{w_3}{w_2}\right) - \mathrm{Li}_2\left(1 - \frac{w_1 + w_3}{w_2}\right) + \ln\left(\frac{w_2}{w_3}\right)\ln\left(\frac{w_1 + w_2 + w_3}{w_2 + w_3}\right)\Bigg] \\ &= \Gamma(0,-1,-2;w_2,w_1 + w_3,0) - \Gamma(0,-1,-2;w_3,w_1 + w_2,0) + \Gamma(0,-1,-2,0;w_1,w_2) - \Gamma(0,-1,-2,0;w_1,w_3) \\ &\quad + w_2\Gamma(-1,0,-1;w_1,0,w_2) - w_3\Gamma(-1,0,-1;w_1,0,w_3) + w_2\Gamma(-1,0,-1;0,w_2,w_3) - w_3\Gamma(-1,0,-1;0,w_3,w_2). \end{aligned} \tag{19}$$

Next, we multiply both equations by powers of w_i to eliminate any w_i from the denominator and differentiate with respect to w_1, w_2, and w_3. This leads to the following recursion relations in n_5 and n_6 of the f function:

$$\begin{aligned} f(-1,0,0,n_4,n_5+1,n_6) &= \frac{1}{2w_1^2 w_2}\{n_4(n_4-1)(n_4+2n_5) f(-1,0,0,n_4-2,n_5,n_6) - 2n_4(n_4-1)w_2 f(-1,0,0,n_4-2,n_5+1,n_6) \\ &\quad - n_4(3n_4+4n_5+1)w_1 f(-1,0,0,n_4-1,n_5,n_6) + 4n_4 w_1 w_2 f(-1,0,0,n_4-1,n_5+1,n_6) + (n_4+1)(n_5-1)n_5 f(-1,0,0,n_4,n_5 \\ &\quad -2,n_6) - 2(n_4+1)n_5 w_2 f(-1,0,0,n_4,n_5-1,n_6) - (n_4+1)(n_6-1)n_6 f(-1,0,0,n_4,n_5,n_6-2) + 2(n_4+1)n_6 w_3 f(-1,0,0, \\ &\quad n_4,n_5,n_6-1) + [(3n_4+2n_5+2)w_1^2 + (n_4+1)w_2^2 - (n_4+1)w_3^2] f(-1,0,0,n_4,n_5,n_6) - (n_5-1)n_5 w_1 f(-1,0,0,n_4+1,n_5-2,n_6) \\ &\quad + 2n_5 w_1 w_2 f(-1,0,0,n_4+1,n_5-1,n_6) + (n_6-1)n_6 w_1 f(-1,0,0,n_4+1,n_5,n_6-2) - 2n_6 w_1 w_3 f(-1,0,0,n_4+1,n_5,n_6-1) \\ &\quad - w_1(w_1^2 + w_2^2 - w_3^2) f(-1,0,0,n_4+1,n_5,n_6) + F(n_4,n_5,n_6)\}, \end{aligned} \tag{20}$$

$$\begin{aligned} f(-1,0,0,n_4,n_5,n_6+1) &= \frac{1}{2w_1^2 w_3}\{n_4(n_4-1)(n_4+2n_6) f(-1,0,0,n_4-2,n_5,n_6) - 2(n_4-1)n_4 w_3 f(-1,0,0,n_4-2,n_5,n_6+1) \\ &\quad - n_4(3n_4+4n_6+1)w_1 f(-1,0,0,n_4-1,n_5,n_6) + 4n_4 w_1 w_3 f(-1,0,0,n_4-1,n_5,n_6+1) - (n_4+1)(n_5-1)n_5 f(-1,0,0,n_4,n_5 \\ &\quad -2,n_6) + 2(n_4+1)n_5 w_2 f(-1,0,0,n_4,n_5-1,n_6) + (n_4+1)(n_6-1)n_6 f(-1,0,0,n_4,n_5,n_6-2) - 2(n_4+1)n_6 w_3 f(-1,0,0, \\ &\quad n_4,n_5,n_6-1) + [(3n_4+2n_6+2)w_1^2 - (n_4+1)w_2^2 + (n_4+1)w_3^2] f(-1,0,0,n_4,n_5,n_6) + (n_5-1)n_5 w_1 f(-1,0,0,n_4+1,n_5-2,n_6) \\ &\quad - 2n_5 w_1 w_2 f(-1,0,0,n_4+1,n_5-1,n_6) - (n_6-1)n_6 w_1 f(-1,0,0,n_4+1,n_5,n_6-2) + 2n_6 w_1 w_3 f(-1,0,0,n_4+1,n_5,n_6-1) \\ &\quad - w_1(w_1^2 - w_2^2 + w_3^2) f(-1,0,0,n_4+1,n_5,n_6) - F(n_4,n_5,n_6)\}, \end{aligned} \tag{21}$$

where

$$\begin{aligned} F(n_4,n_5,n_6) &= (-\partial_{w_1})^{n_4}(-\partial_{w_2})^{n_5}(-\partial_{w_3})^{n_6} F = (n_6 - n_5)\,\delta_{n_4}\Gamma(-1,n_5-1,n_6-1;0,w_2,w_3) + w_2\delta_{n_4}\Gamma(-1,n_5,n_6-1;0,w_2,w_3) \\ &\quad - w_3\delta_{n_4}\Gamma(-1,n_6,n_5-1;0,w_3,w_2) - (n_5-1)\,\delta_{n_6}\Gamma(n_4-1,0,n_5-2;w_1,0,w_2) + w_2\delta_{n_6}\Gamma(n_4-1,0,n_5-1;w_1,0,w_2) \\ &\quad + (n_6-1)\,\delta_{n_5}\Gamma(n_4-1,0,n_6-2;w_1,0,w_3) - w_3\delta_{n_5}\Gamma(-1+n_4,0,n_6-1;w_1,0,w_3) + \Gamma(n_5,n_4+n_6-1,-2;w_2,w_1+w_3,0) \\ &\quad - \Gamma(n_6,n_4+n_5-1,-2;w_3,w_1+w_2,0). \end{aligned} \tag{22}$$

What remains is the calculation of $f(-1,0,0,n_4,0,0)$. In the following we derive a differential equation for $h(w_1) \equiv f(-1,0,0,0,0,0)$, from which we obtain $f(-1,0,0,n_4,0,0)$. The solutions for

$$G(2,1,1,1,1,1) = X_9 \tag{23}$$

and for the difference

$$X_1 u_1^{-2} - X_5 = 0 \tag{24}$$

form two algebraic equations, which, however, are too long to be written here. They involve the terms $G(2,1,1,1,1,1)$, $G(2,1,1,1,1,1)u_1^2$, $G(1,1,1,1,1,1)$, $G(1,1,1,1,1,1)u_1^{-2}$, $G(1,1,1,2,1,1)$, $G(1,1,1,2,1,1)u_1^{-2}$, and the known two-electron terms, where one of the arguments of the G function is equal to 0. We integrate both equations in u_1 from ϵ to ∞, approach the limit $\epsilon \to 0$, and drop $\ln \epsilon$,

$$\int_\epsilon^\infty du_1 G(2,1,1,1,1,1) = -\frac{g(w_1)}{2},$$

$$\int_\epsilon^\infty du_1 u_1^2 G(2,1,1,1,1,1) = \frac{h(w_1)}{2},$$

$$\int_\epsilon^\infty du_1 G(1,1,1,1,1,1) = h(w_1),$$

$$\int_\epsilon^\infty du_1 u_1^{-2} G(1,1,1,1,1,1) = g(w_1) - f(1,0,0,0,0,0),$$

$$\int_\epsilon^\infty du_1 G(1,1,1,2,1,1) = -\frac{h'(w_1)}{2},$$

$$\int_\epsilon^\infty du_1 u_1^{-2} G(1,1,1,2,1,1) = -\frac{g'(w_1)}{2} + \frac{1}{2}\frac{\partial f(1,0,0,0,0,0)}{\partial w_1}, \tag{25}$$

where

$$h(w_1) = f(-1,0,0,0,0,0),$$

$$g(w_1) = \int \frac{d^3r_1}{4\pi}\int \frac{d^3r_2}{4\pi}\int \frac{d^3r_3}{4\pi} \times e^{-w_1r_1-w_2r_2-w_3r_3}(\ln r_{23}+\gamma) r_{31}^{-1}r_{12}^{-1}r_1^{-1}r_2^{-1}r_3^{-1}, \tag{26}$$

and

$$f(1,0,0,0,0,0) = -\frac{1}{w_2^2w_3^2}\ln\left[\frac{w_1(w_1+w_2+w_3)}{(w_1+w_2)(w_1+w_3)}\right]. \tag{27}$$

The set of both equations forms first-order differential equations for $h(w_1)$ and $g(w_1)$. We eliminate $g(w_1)$ to obtain the following second-order differential equation for $h(w_1)$:

$$ww_1^2h''(w_1) + w_1[4w_1^2(w_1^2-w_2^2-w_3^2)+w]h'(w_1) + [w_1^4 + 4w_1^2(w_1^2-w_2^2-w_3^2) - w]h(w_1) = R(w_1), \tag{28}$$

where

$$R(w_1) = w_1w_2\ln\left(1+\frac{w_1}{w_2}\right) + w_1w_3\ln\left(1+\frac{w_1}{w_3}\right) + (w_2^2-w_3^2)\ln\left(\frac{w_1+w_3}{w_1+w_2}\right) + 2w_1^2\ln\left(\frac{w_1(w_1+w_2+w_3)}{(w_1+w_2)(w_1+w_3)}\right) + (w_2^2-w_3^2)F \tag{29}$$

and

$$w = w_1^4+w_2^4+w_3^4-2w_1^2w_2^2-2w_2^2w_3^2-2w_1^2w_3^2 = -(-w_1+w_2+w_3)(w_1-w_2+w_3)(w_1+w_2-w_3)(w_1+w_2+w_3). \tag{30}$$

Two linearly independent solutions of the homogeneous equation are

$$h_1(w_1) = \frac{1}{w_1\sqrt{w_2w_3}}K\left[\frac{(w_1+w_2-w_3)(w_1-w_2+w_3)}{4w_2w_3}\right],$$

$$h_2(w_1) = \frac{1}{w_1\sqrt{w_2w_3}}K\left[\frac{(-w_1+w_2+w_3)(w_1+w_2+w_3)}{4w_2w_3}\right], \tag{31}$$

where K is a complete elliptic integral of the first kind as defined in Eq. (C1), and the Wronskian W is

$$W = h_1(w_1)h_2'(w_1) - h_1'(w_1)h_2(w_1) = \frac{2\pi}{ww_1}, \tag{32}$$

where w is defined in Eq. (30). The solution in Eq. (31) is valid for w_1 in the range $|w_2-w_3|<w_1<w_2+w_3$, because the elliptic integral K has a branch cut for arguments exceeding 1. We use the identity in Eq. (C8), to obtain the solution h_1 of the homogeneous equation for $w_1>w_2+w_3$,

$$h_1(w_1) = \frac{2}{w_1\sqrt{(w_1+w_2-w_3)(w_1-w_2+w_3)}} \times K\left[\frac{4w_2w_3}{(w_1+w_2-w_3)(w_1-w_2+w_3)}\right], \tag{33}$$

and h_2 for $w_1<|w_2-w_3|$,

$$h_2(w_1) = \frac{2}{w_1\sqrt{(-w_1+w_2+w_3)(w_1+w_2+w_3)}} \times K\left[\frac{4w_2w_3}{(-w_1+w_2+w_3)(w_1+w_2+w_3)}\right]. \tag{34}$$

The solution of the inhomogeneous equation is obtained by Euler's method of variation of the constant,

$$h(w_1) = \frac{h_1(w_1)}{2\pi}\int_{w_1}^{w_2+w_3} dw' \frac{R(w')h_2(w')}{w'} + \frac{h_2(w_1)}{2\pi}\int_{|w_2-w_3|}^{w_1} dw' \frac{R(w')h_1(w')}{w'}. \tag{35}$$

There is no additional term that is a solution of the homogeneous equation, because $h(w_1)$ is finite for all values of w_1, but not $h_1(w_1)$ and $h_2(w_1)$. Therefore this is the right solution. Having obtained $f(-1,0,0,0,0,0)\equiv h(w_1)$ and $f(-1,0,0,1,0,0)=-h'(w_1)$ we calculate $f(-1,0,0,n_4,0,0) = h(w_1,n_4) = (-\partial_{w_1})^{n_4}h(w_1)$ recursively. The inhomogeneous differential equation (28) is differentiated n times with respect to w_1, to obtain

$$h(w_1,n+2) = \frac{1}{ww_1^2}\{-(n-3)(n-2)^3(n-1)nh(w_1,n-4) + (n-2)(n-1)n(13-17n+6n^2)w_1h(w_1,n-3) - (n-1)n[(14-25n+15n^2)w_1^2 - 2(n-1)^2w_s]h(w_1,n-2) + 2nw_1[(3-5n+10n^2)w_1^2 + (-1+3n-4n^2)w_s]h(w_1,n-1) + [-(4+10n+15n^2)w_1^4 + (1-n^2)w_p^2 + 2(1+3n+6n^2)w_1^2w_s]h(w_1,n) + w_1[(5+6n)w_1^4 + (1+2n)w_p^2 - 2(3+4n)w_1^2w_s]h(w_1,n+1) + R(w_1,n)\}, \tag{36}$$

where $w_s = w_2^2 + w_3^2$, $w_p = w_2^2 - w_3^2$, and

$$R(w_1,n) = (-\partial_{w_1})^n R(w_1) = -\frac{4(n-3)!}{w_1^{n-2}} + \frac{5w_2(n-2)!}{(w_1+w_2)^{n-1}} + \frac{4(n-3)!}{(w_1+w_2)^{n-2}} + \frac{5w_3(n-2)!}{(w_1+w_3)^{n-1}} + \frac{4(n-3)!}{(w_1+w_3)^{n-2}} - \frac{2(w_2+w_3)^2(n-1)!}{(w_1+w_2+w_3)^n} - \frac{4(w_2+w_3)(n-2)!}{(w_1+w_2+w_3)^{n-1}} - \frac{4(n-3)!}{(w_1+w_2+w_3)^{n-2}} + \frac{(4w_2^2-w_3^2)(n-1)!}{(w_1+w_2)^n} + \frac{(4w_3^2-w_2^2)(n-1)!}{(w_1+w_3)^n} + (w_2^2-w_3^2)F(n,0,0)$$

for $n > 2$,

$$R(w_1,0) = R(w_1),$$

$$R(w_1,1) = -(w_2+w_3) + \frac{4w_2^2-w_3^2}{w_1+w_2} - 2\frac{(w_2+w_3)^2)}{w_1+w_2+w_3} + \frac{4w_3^2-w_2^2}{w_1+w_3} - w_2\ln\left(1+\frac{w_1}{w_2}\right) - w_3\ln\left(1+\frac{w_1}{w_3}\right) - 4w_1\ln\left[\frac{w_1(w_1+w_2+w_3)}{(w_1+w_2)(w_1+w_3)}\right] + (w_2^2-w_3^2)F(1,0,0),$$

$$R(w_1,2) = \frac{5w_2}{w_1+w_2} + \frac{5w_3}{w_1+w_3} - \frac{2(w_2+w_3)^2}{(w_1+w_2+w_3)^2} - \frac{4(w_2+w_3)}{w_1+w_2+w_3} + \frac{4w_2^2-w_3^2}{(w_1+w_2)^2} + \frac{4w_3^2-w_2^2}{(w_1+w_3)^2} + 4\ln\left[\frac{w_1(w_1+w_2+w_3)}{(w_1+w_2)(w_1+w_3)}\right] + (w_2^2-w_3^2)F(2,0,0). \tag{37}$$

In the case $w_1 \approx w_{\text{sing}} = w_2+w_3$ or $|w_2-w_3|$, the recursion in Eq. (36) is not numerically stable. Therefore, instead of this recursion, one calculates the recursion exactly at $w_1 = w_{\text{sing}}$, which corresponds to setting $w=0$ in Eq. (36),

$$h(w_1,n+1) = \frac{-1}{w_1[(5+6n)w_1^4 + (1+2n)w_p^2 - 2(3+4n)w_1^2w_s]} \times\{-(n-3)(n-2)^3(n-1)nh(w_1,n-4) + (n-2)(n-1)n(13-17n+6n^2)w_1h(w_1,n-3) - (n-1)n[(14-25n+15n^2)w_1^2 - 2(n-1)^2w_s]h(w_1,n-2) + 2nw_1[(3-5n+10n^2)w_1^2 + (-1+3n-4n^2)w_s]h(w_1,n-1) + [-(4+10n+15n^2)w_1^4 + (1-n^2)w_p^2 + 2(1+3n+6n^2)w_1^2w_s]h(w_1,n) + R(w_1,n)\}, \tag{38}$$

where $w_1 = w_{\text{sing}}$. This completes the recursion relations for the extended Hylleraas integral with r_{23}^{-2}.

III. NUMERICAL EVALUATION

We pass now to numerical implementation of recursions and integration of the master integral in Eq. (35). All the computation is performed with extended precision arithmetic, namely, quadruple and sextuple precision. Even higher precision, the octuple one, is used for checking numerical accuracy. The starting point is the master integral. One needs to calculate it with the highest possible accuracy, because the recursions depend most significantly on the value of initial terms. The integrand in Eq. (35) is a product of the function R and the complete elliptic integral K. The function R defined in Eq. (29) has singularities only at $w_i = 0$ and ∞, and the complete elliptic integral has logarithmic singularities at $w_1 = w_{\text{sing}} \equiv |w_2-w_3|$ or w_2+w_3 which correspond to zeros of w in Eq. (30). In the following we assume that $w_2 - w_3 \neq 0$. When $|w_2-w_3| + \epsilon_1 < w_1 < w_2+w_3-\epsilon_2$, the integral in Eq. (35) can be performed by the Gauss-Legendre quadrature [14]. We have verified that for $\epsilon_i \approx 0.2$ the integration with 100 points gives an accuracy of at least 32 digits if not more. For the cases $w_1 > w_2+w_3+\epsilon_2$ and $w_1 < |w_2$

TABLE I. Values of the master integral for selected w_1, w_2, and w_3. The number in brackets represent power of ten.

w_1	w_2	w_3	$f(-1,0,0,0,0,0)$
4.0	1.0	0.5	1.243 735 828 073 620 173 310 981 564 244[−1]
4.0	1.0	1.0	9.855 133 136 060 504 470 218 647 797 889[−2]
4.0	1.0	1.5	8.181 412 007 841 597 436 460 514 476 518[−2]
4.0	1.0	2.0	6.983 588 391 604 680 181 982 031 823 035[−2]
4.0	1.0	2.5	6.077 218 287 692 100 226 048 417 176 715[−2]
4.0	1.0	3.0	5.365 400 720 042 544 709 716 176 264 176[−2]
4.0	1.0	3.5	4.791 010 346 652 078 406 517 300 908 585[−2]
4.0	1.0	4.0	4.317 729 831 064 450 749 511 048 756 748[−2]
4.0	1.0	4.5	3.921 185 585 221 614 693 378 573 393 156[−2]
4.0	1.0	5.0	3.584 332 630 993 527 980 351 431 968 712[−2]
4.0	1.0	5.5	3.294 856 745 699 432 037 984 459 599 008[−2]

TABLE II. Three-electron Hylleraas integral involving $1/r_{12}^2$. n_i and w_i are from Table II of Ref. [3]. Function I from this reference should be divided by $(4\pi)^3$ for comparison with our function f. The numbers in brackets represent power of ten.

	w_1	w_2	w_3	
$f(-1,2,2,2,2,2)$	2.700	2.700	2.700	3.622 072 193 238 069 065 841 911 460 566[−3]
$f(-1,2,4,1,1,1)$	2.700	2.900	0.650	2.044 941 897 990 188 175 637 070 889 313[−1]
$f(-1,0,2,1,1,1)$	2.700	2.900	0.650	8.560 152 684 198 427 372 519 849 562 718[−3]
$f(-1,0,0,1,1,1)$	2.700	2.900	0.650	7.695 548 443 927 856 456 193 296 733 495[−3]
$f(-1,4,4,3,2,2)$	7.384	4.338	4.338	2.516 457 130 304 929 175 434 829 560 592[−6]
$f(-1,0,0,2,2,2)$	3.000	2.000	1.000	7.759 319 533 814 226 728 190 558 692 235[−3]
$f(-1,0,0,1,3,2)$	3.000	1.000	2.000	1.528 428 874 506 937 507 531 543 743 291[−2]
$f(-1,0,4,2,4,3)$	2.000	3.000	4.000	6.208 037 315 282 433 323 108 011 184 899[−3]
$f(-1,2,2,1,1,1)$	2.700	2.900	0.650	4.036 629 272 285 446 411 970 138 933 470[−2]
$f(-1,2,2,1,1,1)$	2.500	2.500	0.600	1.025 702 855 657 754 018 359 340 659 240[−1]
$f(-1,2,2,0,0,0)$	2.700	2.900	0.650	3.674 068 373 009 625 515 617 159 197 784[−2]
$f(-1,2,2,1,2,3)$	1.000	1.000	1.000	4.576 295 463 451 984 514 935 097 879 411[2]
$f(-1,2,2,2,2,2)$	1.000	1.000	1.000	5.436 536 048 634 697 021 325 813 246 683[2]
$f(-1,2,4,4,3,1)$	3.000	2.000	1.000	6.126 463 692 215 932 446 059 888 955 061[0]
$f(-1,2,4,1,0,0)$	1.000	1.000	1.000	4.219 398 540 932 754 336 898 663 066 822[2]
$f(-1,4,4,1,1,1)$	2.700	2.900	0.650	3.826 213 635 276 544 192 395 399 453 200[0]
$f(-1,4,6,1,1,1)$	2.700	2.900	0.650	4.206 326 264 336 604 338 380 540 655 410[1]
$f(-1,6,6,1,1,1)$	2.700	2.900	0.650	1.886 948 258 407 236 970 462 772 961 418[3]

$-w_3| - \epsilon_1$, the integration contour is deformed on the complex plane to avoid the singularity. So this contour consists of two lines on a real axis, joined by a half circle with origin at the singular point, and integration is performed independently on each part using the Gauss-Legendre quadrature. When w_1 is close to the singular point, we first obtain $h(w_{\rm sing} \pm \epsilon)$; next we calculate $h(w_{\rm sing})$ by matching the Taylor expansion from recursion in Eq. (38) with $h(w_{\rm sing} \pm \epsilon)$; and in the last step we again use recursion in Eq. (38) to obtain $h(w_1)$. For $w_2 - w_3 = 0$ we separate R in Eq. (29) into the part that is free of $\ln w_1$ and the part that is proportional to $\ln w_1$. The first part is integrated using the Gauss-Legendre quadrature and the second one is integrated using the Gauss quadrature adapted for the logarithmic weight function. Several numerical results for some selected w_i are presented in Table I.

Considering recursions, all but one involve denominators limited from below. Only that in Eq. (36) for increasing n_4 has a denominator that can be arbitrarily close to zero. Therefore, if $w_1 \approx w_{\rm sing}$, instead of recursion in Eq. (36), one uses the recursion in Eq. (38) and calculates $h(w_1, n)$ from Taylor expansion at $w_1 = w_{\rm sing}$. All other recursions are calculated directly as in Eqs. (7), (8), (12), (20), and (21). They involve two-electron integrals Γ. The calculation of Γ including singular cases has recently been described in detail in Refs. [16,17], and it does not pose any problem. Finally, several numerical results for three-electron integral involving powers of r_i and r_{ij} are presented in Table II. For comparison with the former results obtained in Ref. [3], we have taken the same n_i and w_i as in Table II of this reference. Our results agree up to the precision achieved in Ref. [3] with the one correction. In the fifth position instead of $I(2,1,1,3,3,-2,4.338,4.338,7.384)$, it should be $I(1,1,2,3,3,-2,4.338,4.338,7.384)$.

Considering the extended Hylleraas integral with r_1^{-2}, we calculate it by numerical integration with respect to w_1,

$$f(n_1,n_2,n_3,-1,n_5,n_6) = \int_{w_1}^{\infty} dw_1 f(n_1,n_2,n_3,0,n_5,n_6). \tag{39}$$

The recursion relations for $f(n_1,n_2,n_3,n_4,n_5,n_6)$ with non-negative n_i have been derived previously [11], and they seem to be stable enough to perform this integration numerically. Since we have not found in the literature a method of integration that is adapted to two weight functions, the constant and the logarithmic one, we use the standard Gauss-Legendre quadrature. In Table III we present several numerical results. A significant loss of precision is observed due to

TABLE III. Three-electron Hylleraas integral involving $1/r_1^2$ at $w_1=2$, $w_2=3$, $w_3=4$.

$f(0,0,0,-1,0,0)$	5.112 034 507 187 907 543[−2]
$f(0,1,0,-1,0,0)$	1.376 985 263 507 039 164[−2]
$f(0,2,0,-1,0,0)$	6.942 269 369 095 712 105[−3]
$f(0,3,0,-1,0,0)$	5.403 223 451 815 895 118[−3]
$f(0,4,0,-1,0,0)$	5.907 661 306 554 417 555[−3]
$f(0,5,0,-1,0,0)$	8.587 459 945 883 427 557[−3]
$f(0,6,0,-1,0,0)$	1.598 496 287 482 975 980[−2]
$f(0,7,0,-1,0,0)$	3.698 745 219 132 481 190[−2]
$f(0,8,0,-1,0,0)$	1.036 442 843 454 920 448[−1]
$f(0,9,0,-1,0,0)$	3.434 721 508 609 856 189[−1]

the presence of $(\ln w_1/w_1^n)$ at the large w_1 asymptotic. Therefore, precise integration requires in some cases the subtraction of these terms.

IV. SUMMARY

An analytic approach is presented for the calculation of three-electron Hylleraas integrals involving one inverse quadratic power of the interparticle coordinate. This approach is based on exact recursion relations in powers of coordinates. These recursions involve initial terms and two-electron integrals. For the initial term $f(-1,0,0,0,0,0)$ as a function of w_1, one constructs a linear second-order differential equation. Its solution is expressed as a one-dimensional integral over dilogarithmic and elliptic function K, which can be obtained numerically with arbitrarily high precision. The two-electron Hylleraas integrals have already been derived in the literature and they also can be obtained with arbitrarily high precision.

These extended Hylleraas integrals are necessary for the calculation of relativistic effects in lithium and light lithium-like ions [5–8]. One interesting goal is the high-precision calculation of the lithium hyperfine splitting [18], which can serve as a benchmark result for other less accurate methods. Moreover, it has recently become possible to derive nuclear parameters such as the charge radius from the measurement of the isotope shift [7]. The hyperfine splitting (hfs) is sensitive to the distribution of magnetic moment. Therefore the measurement of hfs in various odd isotopes of Li or light lithiumlike ions may lead to the determination of the so-called magnetic radius, which is very difficult to access experimentally. Even more interesting is the possible extension of this analytic method to beryllium and berylliumlike ions, the four-electron systems. The use of the Hylleraas basis set will allow for a high-precision calculation of the wave function and, for example, various transition rates which are of astrophysical relevance.

Note added in proof. Authors after submission of this work, became aware of a paper by J. Ma *et al.* [19], where a method of numerical integration adapted to two weight functions is presented. This method allows one to perform the integral in Eq. (39) with precision of 32 digits using about 40 nodes only.

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APPENDIX A: INTEGRATION BY PARTS IDENTITIES

The complete set of recursion relations as obtained from integration by parts identities is presented below. Function G is defined in Eq. (2) and $\mathrm{id}(i,j)=0$ for $i,j=1,2,3$.

$$\begin{aligned}\mathrm{id}(1,1) = &-G(0,1,1,1,1,2)-G(0,1,1,1,2,1)\\ &+G(1,0,1,1,1,2)+G(1,1,0,1,2,1)\\ &-G(1,1,1,1,1,1)+2G(2,1,1,1,1,1)u_1^2\\ &+G(1,1,1,1,2,1)(u_1^2-u_3^2+w_2^2)+G(1,1,1,1,1,2)\\ &\times(u_1^2-u_2^2+w_3^2),\end{aligned}$$

$$\begin{aligned}\mathrm{id}(2,1) = &-G(0,1,1,1,1,2)-G(0,1,1,1,2,1)\\ &+G(1,0,1,1,1,2)+G(1,1,0,1,2,1)\\ &-G(1,1,1,0,2,1)+G(1,1,1,1,2,0)\\ &-G(2,0,1,1,1,1)+G(2,1,1,1,1,0)\\ &+G(1,1,1,1,1,2)(u_1^2-u_2^2-w_3^2)+G(2,1,1,1,1,1)\\ &\times(u_1^2+u_2^2-w_3^2)+G(1,1,1,1,2,1)\\ &\times(u_1^2-u_3^2+w_1^2-w_3^2),\end{aligned}$$

$$\begin{aligned}\mathrm{id}(3,1) = &-G(0,1,1,1,1,2)-G(0,1,1,1,2,1)\\ &+G(1,0,1,1,1,2)+G(1,1,0,1,2,1)\\ &-G(1,1,1,0,1,2)+G(1,1,1,1,0,2)\\ &-G(2,1,0,1,1,1)+G(2,1,1,1,0,1)\\ &+G(1,1,1,1,2,1)(u_1^2-u_3^2-w_2^2)+G(2,1,1,1,1,1)\\ &\times(u_1^2+u_3^2-w_2^2)+G(1,1,1,1,1,2)\\ &\times(u_1^2-u_2^2+w_1^2-w_2^2),\end{aligned}$$

$$\begin{aligned}\mathrm{id}(2,2) = &\,G(0,1,1,1,1,2)-G(1,0,1,1,1,2)\\ &-G(1,0,1,2,1,1)+G(1,1,0,2,1,1)\\ &-G(1,1,1,1,1,1)+2G(1,2,1,1,1,1)u_2^2\\ &+G(1,1,1,2,1,1)(u_2^2-u_3^2+w_1^2)+G(1,1,1,1,1,2)\\ &\times(-u_1^2+u_2^2+w_3^2),\end{aligned}$$

$$\begin{aligned}\mathrm{id}(1,2) = &\,G(0,1,1,1,1,2)-G(0,2,1,1,1,1)\\ &-G(1,0,1,1,1,2)-G(1,0,1,2,1,1)\\ &+G(1,1,0,2,1,1)-G(1,1,1,2,0,1)\\ &+G(1,1,1,2,1,0)+G(1,2,1,1,1,0)\\ &+G(1,1,1,1,1,2)(-u_1^2+u_2^2-w_3^2)+G(1,2,1,1,1,1)\\ &\times(u_1^2+u_2^2-w_3^2)+G(1,1,1,2,1,1)\\ &\times(u_2^2-u_3^2+w_2^2-w_3^2),\end{aligned}$$

$$\begin{aligned}\mathrm{id}(3,2) = &\,G(0,1,1,1,1,2)-G(1,0,1,1,1,2)\\ &-G(1,0,1,2,1,1)+G(1,1,0,2,1,1)\\ &+G(1,1,1,0,1,2)-G(1,1,1,1,0,2)\\ &-G(1,2,0,1,1,1)+G(1,2,1,0,1,1)\\ &+G(1,1,1,2,1,1)(u_2^2-u_3^2-w_1^2)+G(1,2,1,1,1,1)\\ &\times(u_2^2+u_3^2-w_1^2)+G(1,1,1,1,1,2)\end{aligned}$$

$$\times(-u_1^2+u_2^2-w_1^2+w_2^2),$$

$$\begin{aligned}\mathrm{id}(3,3) = {} & G(0,1,1,1,2,1)+G(1,0,1,2,1,1)\\ & -G(1,1,0,1,2,1)-G(1,1,0,2,1,1)\\ & -G(1,1,1,1,1,1)+2G(1,1,2,1,1,1)u_3^2\\ & +G(1,1,1,2,1,1)(-u_2^2+u_3^2+w_1^2)\\ & +G(1,1,1,1,2,1)(-u_1^2+u_3^2+w_2^2),\end{aligned}$$

$$\begin{aligned}\mathrm{id}(2,3) = {} & G(0,1,1,1,2,1)+G(1,0,1,2,1,1)\\ & -G(1,0,2,1,1,1)-G(1,1,0,1,2,1)\\ & -G(1,1,0,2,1,1)+G(1,1,1,0,2,1)\\ & -G(1,1,1,1,2,0)+G(1,1,2,0,1,1)\\ & +G(1,1,1,2,1,1)(-u_2^2+u_3^2-w_1^2)+G(1,1,2,1,1,1)\\ & \times(u_2^2+u_3^2-w_1^2)+G(1,1,1,1,2,1)\\ & \times(-u_1^2+u_3^2-w_1^2+w_3^2),\end{aligned}$$

$$\begin{aligned}\mathrm{id}(1,3) = {} & G(0,1,1,1,2,1)-G(0,1,2,1,1,1)\\ & +G(1,0,1,2,1,1)-G(1,1,0,1,2,1)\\ & -G(1,1,0,2,1,1)+G(1,1,1,2,0,1)\\ & -G(1,1,1,2,1,0)+G(1,1,2,1,0,1)\\ & +G(1,1,1,1,2,1)(-u_1^2+u_3^2-w_2^2)+G(1,1,2,1,1,1)\\ & \times(u_1^2+u_3^2-w_2^2)+G(1,1,1,2,1,1)\\ & \times(-u_2^2+u_3^2-w_2^2+w_3^2). \qquad \text{(A1)}\end{aligned}$$

APPENDIX B: TWO-ELECTRON INTEGRALS

The two-electron integral Γ is defined by

$$\Gamma(n_1,n_2,n_3;\alpha_1,\alpha_2,\alpha_3) = \int\frac{d^3r_1}{4\pi}\int\frac{d^3r_2}{4\pi}e^{-\alpha_1 r_1-\alpha_2 r_2-\alpha_3 r_{12}}r_1^{n_1-1}r_2^{n_2-1}r_{12}^{n_3-1}. \qquad \text{(B1)}$$

In the simplest case of $n_1=n_2=n_3=0$ it is

$$\Gamma(0,0,0,;\alpha_1,\alpha_2,\alpha_3)=\frac{1}{(\alpha_1+\alpha_2)(\alpha_2+\alpha_3)(\alpha_3+\alpha_1)}. \qquad \text{(B2)}$$

In the general case of $n_i \geqslant 0$

$$\Gamma(n_1,n_2,n_3;\alpha_1,\alpha_2,\alpha_3)=\left(-\frac{d}{d\alpha_1}\right)^{n_1}\left(-\frac{d}{d\alpha_2}\right)^{n_2}\left(-\frac{d}{d\alpha_3}\right)^{n_3}\times\frac{1}{(\alpha_1+\alpha_2)(\alpha_2+\alpha_3)(\alpha_3+\alpha_1)}, \qquad \text{(B3)}$$

and recursions relations for its evaluation have been derived in Ref. [15]. The two-electron integral Γ for $n_i<0$ can be obtained by integration over α_i. Typical examples are

$$\Gamma(-1,n_2,n_3;\alpha_1,\alpha_2,\alpha_3)=\left(-\frac{d}{d\alpha_2}\right)^{n_2}\left(-\frac{d}{d\alpha_3}\right)^{n_3}\times\frac{\ln(\alpha_1+\alpha_2)-\ln(\alpha_1+\alpha_3)}{(\alpha_2-\alpha_3)(\alpha_2+\alpha_3)}, \qquad \text{(B4)}$$

$$\begin{aligned}\Gamma(-1,n_2,-1;\alpha_1,\alpha_2,\alpha_3) &= \left(-\frac{d}{d\alpha_2}\right)^{n_2}\frac{1}{2\alpha_2}\left[\frac{\pi^2}{6}+\frac{1}{2}\ln^2\left(\frac{\alpha_1+\alpha_2}{\alpha_2+\alpha_3}\right)\right.\\ &\quad\left.+\mathrm{Li}_2\left(1-\frac{\alpha_1+\alpha_3}{\alpha_1+\alpha_2}\right)+\mathrm{Li}_2\left(1-\frac{\alpha_1+\alpha_3}{\alpha_2+\alpha_3}\right)\right]. \qquad \text{(B5)}\end{aligned}$$

Other examples together with recursion relations to calculate derivatives may be found in Refs. [16,17]. Some three-electron integrals G can be expressed in terms of Γ. This is when any of the arguments is equal to zero. The complete list of all cases is

$$\begin{aligned}G(0,1,1,1,1,1) &= \Gamma(-1,0,-1;w_2+w_3,w_1,u_2+u_3),\\ G(1,0,1,1,1,1) &= \Gamma(-1,0,-1;w_1+w_3,w_2,u_1+u_3),\\ G(1,1,0,1,1,1) &= \Gamma(-1,0,-1;w_1+w_2,w_3,u_1+u_2),\\ G(1,1,1,0,1,1) &= \Gamma(-1,0,-1;w_2+u_3,u_1,w_3+u_2),\\ G(1,1,1,1,0,1) &= \Gamma(-1,0,-1;w_1+u_3,u_2;w_3+u_1),\\ G(1,1,1,1,1,0) &= \Gamma(-1,0,-1;w_1+u_2,u_3,w_2+u_1). \qquad \text{(B6)}\end{aligned}$$

APPENDIX C: SPECIAL FUNCTIONS

The complete elliptic integrals of the first and second kinds, K and E, respectively, are defined according to [20] as

$$K(m)=\int_0^1 dt(1-t^2)^{-1/2}(1-mt^2)^{-1/2}, \qquad \text{(C1)}$$

$$E(m)=\int_0^1 dt(1-t^2)^{-1/2}(1-mt^2)^{1/2}. \qquad \text{(C2)}$$

They are related to hypergeometric functions

$$K(m)=\frac{\pi}{2}{}_2F_1(1/2,1/2;1;m), \qquad \text{(C3)}$$

$$E(m)=\frac{\pi}{2}{}_2F_1(-1/2,1/2;1;m), \qquad \text{(C4)}$$

and satisfy the Legendre relation

$$E(m)K(1-m)+E(1-m)K(m)-K(m)K(1-m)=\frac{\pi}{2}. \tag{C5}$$

Their first derivatives are

$$K'(m)=\frac{E(m)}{2m(1-m)}-\frac{K(m)}{2m}, \tag{C6}$$

$$E'(m)=\frac{E(m)-K(m)}{2m}. \tag{C7}$$

Elliptic functions for $|m|\leqslant 1$ can be conveniently calculated numerically as described in [14]. For $m>1$ one uses the identities [19]

$$K(m\pm i\epsilon)=\frac{1}{\sqrt{m}}K\left(\frac{1}{m}\right)\pm iK(1-m), \tag{C8}$$

$$E(m\pm i\epsilon)=\sqrt{m}E\left(\frac{1}{m}\right)+\frac{1-m}{\sqrt{m}}K\left(\frac{1}{m}\right) \pm i[K(1-m)-E(1-m)], \tag{C9}$$

and for $m<-1$

$$K(m)=\frac{1}{\sqrt{1-m}}K\left(\frac{m}{m-1}\right), \tag{C10}$$

$$E(m)=\sqrt{1-m}E\left(\frac{m}{m-1}\right). \tag{C11}$$

The Laurent expansion near the singularity $m=1$ is

$$K(m)=\sum_{n=0}^{\infty}\left[\frac{1}{n!}\left(\frac{1}{2}\right)_n\right]^2\left[\psi(n+1)-\psi(n+1/2) -\frac{1}{2}\ln(1-m)\right](1-m)^n, \tag{C12}$$

where ψ is a logarithmic derivative of the Euler Gamma function.

The dilogarithmic function Li_2 is defined by

$$\mathrm{Li}_2(z)=-\int_0^z\frac{\ln(1-z)}{z}. \tag{C13}$$

The Taylor expansion around the origin,

$$\mathrm{Li}_2(z)=\sum_{i=1}^{\infty}\frac{z^i}{i^2}, \tag{C14}$$

is convergent for $|z|\leqslant 1$. Two useful relations

$$\mathrm{Li}_2(-x)+\mathrm{Li}_2\left(-\frac{1}{x}\right)=-\frac{\pi^2}{6}-\frac{\ln^2 x}{2}, \tag{C15}$$

$$\mathrm{Li}_2(x)+\mathrm{Li}_2(1-x)=\frac{\pi^2}{6}-\ln x\ln(1-x) \tag{C16}$$

are used for simplification of the result of integrations in Eqs. (10) and (19). Further formulas may be found in Ref. [20] and an efficient numerical evaluation is described among others in Ref. [16].

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