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Singular Hylleraas three-electron integrals

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Abstract

Calculations of the leading quantum electrodynamics effects in few electron systems involve singular matrix elements of the inter-electronic distances of the form $1/r_i^3$ and $1/r_{ij}^3$. Integrals that result when the nonrelativistic wave function is represented with a Hylleraas basis representation are studied. Recursion relations for various powers of the electron coordinates and the master integrals are derived in a form suited for high precision numerical evaluations.

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I. INTRODUCTION

A challenging task in high precision calculations of energy levels of few electron atoms or ions is the accurate solution ψ of the nonrelativistic Schrödinger equation. This wave function ψ is next used to obtain relativistic and quantum electrodynamics (QED) effects including finite nuclear mass corrections. The most accurate representation of the three-electron wave function ψ achieved so far [1, 2] uses the Hylleraas basis set [3], namely

$$\begin{aligned} \psi &= \sum_i c_i\,\phi_i \\ \phi &= e^{-w_1\,r_1-w_2\,r_2-w_3\,r_3}\,r_{23}^{n_1}\,r_{31}^{n_2}\,r_{12}^{n_3}\,r_1^{n_4}\,r_2^{n_5}\,r_3^{n_6}, \end{aligned} \tag{1}$$

with n_i being nonnegative integers. This basis set allows the Kato cusp condition to be satisfied to a high degree, thus ensuring good convergence for matrix elements of relativistic and QED operators. All these matrix elements can be expressed in terms of the Hylleraas integrals f, see Eq. (2). The calculation of the nonrelativistic energy involves integrals with nonnegative n_i. Such integrals have been worked out by King *et al.* in the series of works [4], and more recently by Yan and Drake [1, 5], Sims and Hegstrom [6], and by us in Ref. [7]. Our approach relies on analytic recursion relations, which are highly efficient and sufficiently stable to achieve accurate numerical results.

Matrix elements of relativistic operators involve the so called extended Hylleraas integral, where one of $n_i = -1$ (see Eq. (2)). These integrals have been worked out first by King *et al.* in [8], and later by Yan and Drake in Refs. [9] and by us in [2, 10]. The use of recursion relations allows for a significant increase in the size of the basis set and the accuracy of the obtained results [2]. Finally, matrix elements of QED operators involve integrals with $n_i = -2$. Such integrals have been worked out by Yan in [11], but no numerical results for any particular integral have been published, which would serve as a test of achieved accuracy. In this work we develop recursion relations for three-electron Hylleraas integrals either with $1/r_{ij}^3$ or with $1/r_i^3$, and obtain a one dimensional integral representation for the master integral which is suitable for precise numerical evaluation.

In Section II we recall known results for the regular Hylleraas integrals, in Section III we treat integrals involving $1/r_i^2$, and in Section IV we treat integrals involving $1/r_{ij}^2$. Apart from known results, we present also a new form of the master integral with the hope that it can be used in the future to obtain a fully analytic result. In Section V we develop recursion relations for integrals involving $1/r_i^3$ which are very similar to those involving $1/r_i^2$. In Section VI, which is the most difficult one, we obtain a full set of recursions for Hylleraas integrals with $1/r_{ij}^3$, and in Section VII we present numerical results together with a short summary.

II. REGULAR THREE-ELECTRON HYLLERAAS INTEGRAL

The regular three-electron Hylleraas integral is

$$f(n_1, n_2, n_3; n_4, n_5, n_6) = \int \frac{d^3 r_1}{4\pi} \int \frac{d^3 r_2}{4\pi} \int \frac{d^3 r_3}{4\pi} e^{-w_1 r_1 - w_2 r_2 - w_3 r_3} r_{23}^{n_1-1} r_{31}^{n_2-1} r_{12}^{n_3-1} r_1^{n_4-1} r_2^{n_5-1} r_3^{n_6-1}, \tag{2}$$

with all $n_i \geq 0$. The most convenient way to perform this integral is by using recursion relations. The initial values with $n_i = 0, 1$ are known explicitly [7, 12].

$$f(0,0,0;0,0,0) = \frac{-1}{2\, w_1\, w_2\, w_3} \left[\mathrm{Lg}\left(\frac{w_3}{w_1 + w_2}\right) + \mathrm{Lg}\left(\frac{w_2}{w_3 + w_1}\right) + \mathrm{Lg}\left(\frac{w_1}{w_2 + w_3}\right)\right], \tag{3}$$

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

$$f(0,1,0;0,0,0) = -\frac{1}{w_1^2\, w_3^2} \ln\left[\frac{w_2\,(w_1 + w_2 + w_3)}{(w_2 + w_3)(w_2 + w_1)}\right], \tag{5}$$

$$f(0,0,1;0,0,0) = -\frac{1}{w_1^2\, w_2^2} \ln\left[\frac{w_3\,(w_1 + w_2 + w_3)}{(w_3 + w_1)(w_3 + w_2)}\right], \tag{6}$$

$$f(1,1,0;0,0,0) = \frac{1}{w_1\, w_2\,(w_1 + w_2)\, w_3^2}, \tag{7}$$

$$f(1,0,1;0,0,0) = \frac{1}{w_1\, w_3\,(w_1 + w_3)\, w_2^2}, \tag{8}$$

$$f(0,1,1;0,0,0) = \frac{1}{w_2\, w_3\,(w_2 + w_3)\, w_1^2}, \tag{9}$$

$$f(1,1,1;0,0,0) = \frac{1}{w_1^2\, w_2^2\, w_3^2}, \tag{10}$$

where

$$\mathrm{Lg}(x) = \mathrm{Li}_2(1-x) + \mathrm{Li}_2(-x) + \ln(x)\,\ln(1+x), \tag{11}$$

and $\mathrm{Li}_2(x)$ is the dilogarithmic function. All other Hylleraas integrals for arbitrary but nonnegative n_i can be obtained by 6 independent recursion relations for each n_i, see Ref. [7]. The numerical stability of these recursions is an issue. For the maximal number $\Omega = \sum_i n_i = 30$ we used sextuple precision arithmetic and verified against octuple precision that results for nonrelativistic energies are numerically significant for at least 16 digits.

III. EXTENDED HYLERAAS INTEGRAL WITH $1/r_i^2$

More difficult to evaluate are extended Hylleraas three-electron integrals involving additional single powers of r_i or r_{ij} in the denominator. The first kind of integral with $1/r_i^2$ can be obtained by integration with respect to a corresponding parameter w_i, namely

$$f(0,0,0;-1,n_5,n_6) = \int_{w_1}^{\infty} dw_1\, f(0,0,0;0,n_5,n_6), \tag{12}$$

where $f(0,0,0;0,n_5,n_6)$ is obtained by recursions which are numerically stable at high values of w_1. The integration in Eq. (12) is performed using the adapted quadrature [13] for the class of functions involving logarithms [13], which allows one to achieve high precision at low evaluation cost. The function $f(n_1,n_2,n_3;-1,n_5,n_6)$ for arbitrary integer values of n_1,n_2 and n_3 can be obtained [2] by recursion relations starting from $f(0,0,0;-1,n_5,n_6)$.

IV. EXTENDED HYLERAAS INTEGRAL WITH $1/r_{ij}^2$

The second kind of extended Hylleraas integral involves $1/r_{ij}^2$, and we will investigate it here in more detail. Recursion relations start from the master integral

$$\begin{aligned} h(w_1,w_2,w_3) &\equiv f(-1,0,0;0,0,0) \\ &= \int \frac{d^3 r_1}{4\pi} \int \frac{d^3 r_2}{4\pi} \int \frac{d^3 r_3}{4\pi}\, e^{-w_1 r_1 - w_2 r_2 - w_3 r_3}\, r_{23}^{-2}\, r_{31}^{-1}\, r_{12}^{-1}\, r_1^{-1}\, r_2^{-1}\, r_3^{-1}\,. \end{aligned} \tag{13}$$

and some other simpler two electron-like integrals. By using integration by parts identities [14], the following differential equations for the h function have been obtained in Ref. [10]

$$\frac{\partial h}{\partial w_2} = \frac{-1}{2\,w_1^2\,w_2}\Big[F + (2\,w_1^2 + w_2^2 - w_3^2)\,h + w_1\,(w_1^2 + w_2^2 - w_3^2)\,\frac{\partial h}{\partial w_1}\Big], \tag{14}$$

$$\frac{\partial h}{\partial w_3} = \frac{-1}{2\,w_1^2\,w_3}\Big[-F + (2\,w_1^2 - w_2^2 + w_3^2)\,h + w_1\,(w_1^2 - w_2^2 + w_3^2)\,\frac{\partial h}{\partial w_1}\Big], \tag{15}$$

and

$$w\,w_1^2\,\frac{\partial^2 h}{\partial w_1^2} + w_1\,[4\,w_1^2\,(w_1^2 - w_2^2 - w_3^2) + w]\,\frac{\partial h}{\partial w_1} + [w_1^4 + 4\,w_1^2\,(w_1^2 - w_2^2 - w_3^2) - w]\,h(w_1) = R, \tag{16}$$

where

$$\begin{aligned} R = {} & w_1\,w_2\,\ln\Big(1 + \frac{w_1}{w_2}\Big) + w_1\,w_3\,\ln\Big(1 + \frac{w_1}{w_3}\Big) + (w_2^2 - w_3^2)\,\ln\Big(\frac{w_1 + w_3}{w_1 + w_2}\Big) \\ & + 2\,w_1^2\,\ln\Big(\frac{w_1\,(w_1 + w_2 + w_3)}{(w_1 + w_2)\,(w_1 + w_3)}\Big) + (w_2^2 - w_3^2)\,F, \end{aligned} \tag{17}$$

$$
\begin{aligned}
F &= \frac{1}{2}\Big[2\,\mathrm{Li}_2\Big(-\frac{w_2}{w_1}\Big) - \mathrm{Li}_2\Big(1-\frac{w_2}{w_3}\Big) + \mathrm{Li}_2\Big(1-\frac{w_1+w_2}{w_3}\Big) - 2\,\mathrm{Li}_2\Big(-\frac{w_3}{w_1}\Big) \\
&\quad + \mathrm{Li}_2\Big(\frac{w_2}{w_2+w_3}\Big) - \mathrm{Li}_2\Big(\frac{w_3}{w_2+w_3}\Big) + \mathrm{Li}_2\Big(\frac{w_2}{w_1+w_2+w_3}\Big) - \mathrm{Li}_2\Big(\frac{w_3}{w_1+w_2+w_3}\Big) \\
&\quad + \mathrm{Li}_2\Big(1-\frac{w_3}{w_2}\Big) - \mathrm{Li}_2\Big(1-\frac{w_1+w_3}{w_2}\Big) + \ln\Big(\frac{w_2}{w_3}\Big)\,\ln\Big(\frac{w_1+w_2+w_3}{w_2+w_3}\Big)\Big], \qquad (18) \\
w &= (w_1-w_2-w_3)(w_1-w_2+w_3)(w_1+w_2-w_3)(w_1+w_2+w_3). \qquad (19)
\end{aligned}
$$

It is convenient to express the function h

$$
h(w_1,w_2,w_3) = \frac{1}{w_1\,\sqrt{w_2\,w_3}}\,H\Big(\frac{w_1^2-w_2^2-w_3^2}{4\,w_2\,w_3},\frac{w_2}{w_3}\Big), \qquad (20)
$$

in terms of a dimensionless function $H(x,y)$ of two variables x and y. Then the first two differential equations become apparently equivalent and take the form

$$
\frac{\partial H}{\partial y} = -\frac{1}{2\,y}\left(4\,x+y+\frac{1}{y}\right)^{-1/2} F, \qquad (21)
$$

where

$$
F = F(w_1,w_2,w_3) = F\Big(\sqrt{4\,x+y+\frac{1}{y}},\sqrt{y},\frac{1}{\sqrt{y}}\Big), \qquad (22)
$$

and the third differential equation, with respect to w_1 becomes

$$
(4\,x^2-1)\,\frac{\partial^2 H}{\partial x^2} + 8\,x\,\frac{\partial H}{\partial x} + H = R'(x,y), \qquad (23)
$$

where

$$
\begin{aligned}
R'(x,y) &= \frac{\sqrt{w_2\,w_3}}{w_1^3}\,R(w_1,w_2,w_3) \\
&= \left(4\,x+y+\frac{1}{y}\right)^{-3/2} R\Big(\sqrt{4\,x+y+\frac{1}{y}},\sqrt{y},\frac{1}{\sqrt{y}}\Big). \qquad (24)
\end{aligned}
$$

The homogenous differential equation in (23) is satisfied by complete elliptic integrals $K(1/2\pm x)$, and the solution of the inhomogeneous equation is obtained by Euler's method of variation of constants [10]

$$
\begin{aligned}
H(x,y) &= \frac{1}{\pi}\left[K\Big(\frac{1}{2}+x\Big)\int_x^{1/2} dz\,R'(z,y)\,K\Big(\frac{1}{2}-z\Big)\right. \\
&\quad \left. + K\Big(\frac{1}{2}-x\Big)\int_{-1/2}^{x} dz\,R'(z,y)\,K\Big(\frac{1}{2}+z\Big)\right]. \qquad (25)
\end{aligned}
$$

This integral form is convenient for the numerical calculation of the master integral $h(w_1,w_2,w_3)$ and its derivatives. However, a different and apparently simpler form can be obtained from Eq. (21)

$$H\Big(x,\frac{w_2}{w_3}\Big) = \int_0^{w_2/w_3} dy\,\Big(-\frac{1}{2\,y}\Big)\,\Big(4\,x+y+\frac{1}{y}\Big)^{-1/2}\,F$$
$$= \int_0^{\sqrt{w_2/w_3}} \frac{du}{u}\,\frac{1}{\sqrt{4\,x'+(u-1/u)^2}}\,F(\sqrt{4\,x'+(u-1/u)^2},1/u,u), \qquad (26)$$

where $x' = x+1/2$. This integral can be further transformed to a form involving Jacobi elliptic functions, but we have not been able to perform it analytically. In particular cases, where $x=\pm 1/2$, this integral becomes ($w_2 < w_3$)

$$H\Big(\frac{1}{2},\frac{w_2}{w_3}\Big) = \int_0^{\sqrt{w_2/w_3}} du\,\frac{1}{1+u^2}\,F(1+u^2,1,u^2), \qquad (27)$$
$$H\Big(-\frac{1}{2},\frac{w_2}{w_3}\Big) = \int_0^{\sqrt{w_2/w_3}} du\,\frac{1}{1-u^2}\,F(1-u^2,1,u^2), \qquad (28)$$

and this can be expressed in terms of Li_3, Li_2, and logarithmic functions. We use Eqs. (27,28) in cases $w_1 > w_2+w_3$ and $w_1 < |w_2-w_3|$, and for its numerical calculations we employ adapted quadrature [13] with 120 points, to achieve about 64 significant digits accuracy.

Recursion relations for $f(-1,n_2,n_3,n_4,n_5,n_6)$ have been derived in [10]. Among them, the most numerically unstable is the one which increases the parameter n_4, see Eq. (36) of Ref. [10]. Namely, close to singularity points, $x=\pm 1/2$ and for small ω_1, we use Taylor expansion to avoid numerical instabilities.

V. SINGULAR HYLLERAAS INTEGRAL WITH $1/r_i^3$

The singular Hylleraas integrals which involve $1/r_i^3$ and $1/r_{ij}^3$ are needed for the computation of QED effects [11]. Let us first define a distribution $P(1/r^3)$

$$\langle\phi|P\left(\frac{1}{r^3}\right)|\psi\rangle = \lim_{\epsilon\to 0}\int d^3r\,\phi^*(\vec r)\left[\frac{1}{r^3}\,\Theta(r-\epsilon)+4\,\pi\,\delta^3(r)\,(\gamma+\ln\epsilon)\right]\,\psi(\vec r)\,. \qquad (29)$$

Any factor $1/r^3$ in the following will be understood to be defined in the above sense, and we will drop the symbol $P()$. It follows from this definition that

$$\left\langle\frac{e^{-w\,r}}{r^3}\right\rangle = C\,\ln(w)+O(1/\omega) \qquad (30)$$

for large ω. Moreover, we will use in the derivation below the following integral representations

$$\frac{1}{r^3} = \lim_{\Lambda\to\infty}\Big\{\int_0^\Lambda dt\,t\,\frac{e^{-t\,r}}{r}+4\,\pi\,\delta^3(r)\,(1-\ln\Lambda)\Big\}$$
$$= \frac{1}{2}\lim_{\Lambda\to\infty}\Big\{\int_0^\Lambda dt\,t^2\,e^{-t\,r}+4\,\pi\,\delta^3(r)\,[2\,(1-\ln\Lambda)+1]\Big\}. \qquad (31)$$

To obtain recursion relations for the singular three-electron Hylleraas integral one first considers the integral G

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

which is related to f by $f(0,0,0,0,0,0) = G(1,1,1,1,1,1)|_{u_1=u_2=u_3=0}$. The following 9 integration by parts (IBP) identities are valid because the integral of the derivative of a function vanishing at infinity vanishes,

$$0 \equiv \mathrm{id}(i,j) = \int d^3k_1\int d^3k_2\int d^3k_3\,\frac{\partial}{\partial\,\vec{k}_i}\Big[\vec{k}_j\,(k_1^2+u_1^2)^{-1}\\ (k_2^2+u_2^2)^{-1}\,(k_3^2+u_3^2)^{-1}(k_{32}^2+w_1^2)^{-1}\,(k_{13}^2+w_2^2)^{-1}\,(k_{21}^2+w_3^2)^{-1}\Big], \quad (33)$$

where $i,j=1,2,3$. The reduction of the scalar products from the numerator leads to identities for linear combination of the G functions. If any of the arguments is equal to 0, then G becomes a known two-electron Hylleraas type integral. These identities can be used to derive various recursion relations. Here we derive a set of recursions for $f(n_1,n_2,n_3,-2,n_5,n_6)$. This is achieved in a few steps. In the first step we use integration by parts identities in momentum representation Eq. (33), to form the following linear combination

$$\begin{aligned}\mathrm{id}(2,2)+\mathrm{id}(3,3)-\mathrm{id}(1,1) &= 2\,[G(0,1,1,1,1,2)+G(0,1,1,1,2,1)-G(1,0,1,1,1,2)\\ &\quad -G(1,1,0,1,2,1)-G(1,1,1,1,1,1)/2-G(2,1,1,1,1,1)\,u_1^2\\ &\quad -G(1,1,1,1,1,2)\,(u_1^2-u_2^2)+G(1,2,1,1,1,1)\,u_2^2\\ &\quad -G(1,1,1,1,2,1)\,(u_1^2-u_3^2)+G(1,1,2,1,1,1)\,u_3^2\\ &\quad +G(1,1,1,2,1,1)\,w_1^2]=0\,. \qquad (34)\end{aligned}$$

We use Eq. (31) to integrate with respect to w_1 and differentiate over u_1, u_2, u_3, w_2, and w_3 to obtain the main formula

$$\begin{aligned}f(n_1,n_2,n_3,-2,n_5,n_6) &= \frac{1}{(n_2+n_3-n_1-1)\,w_2\,w_3}\Big[\\ &\quad (n_1-1)\,n_1\,n_5\,f(n_1-2,n_2,n_3,-2,n_5-1,n_6+1)\\ &\quad +(n_1-1)\,n_1\,n_6\,f(n_1-2,n_2,n_3,-2,n_5+1,n_6-1)\\ &\quad -(n_2-1)\,n_2\,n_5\,f(n_1,n_2-2,n_3,-2,n_5-1,n_6+1)\\ &\quad -(n_3-1)\,n_3\,n_6\,f(n_1,n_2,n_3-2,-2,n_5+1,n_6-1)\end{aligned}$$

$$
\begin{aligned}
&+(n_1-n_2-n_3+1)\,n_5\,n_6\,f(n_1,n_2,n_3,-2,n_5-1,n_6-1)\\
&+n_5\,n_6\,f(n_1,n_2,n_3,-1,n_5-1,n_6-1)\,w_1\\
&-(n_1-1)\,n_1\,f(n_1-2,n_2,n_3,-2,n_5,n_6+1)\,w_2\\
&+(n_2-1)\,n_2\,f(n_1,n_2-2,n_3,-2,n_5,n_6+1)\,w_2\\
&-(n_1-n_2-n_3+1)\,n_6\,f(n_1,n_2,n_3,-2,n_5,n_6-1)\,w_2\\
&-n_6\,f(n_1,n_2,n_3,-1,n_5,n_6-1)\,w_1\,w_2\\
&-(n_1-1)\,n_1\,f(n_1-2,n_2,n_3,-2,n_5+1,n_6)\,w_3\\
&+(n_3-1)\,n_3\,f(n_1,n_2,n_3-2,-2,n_5+1,n_6)\,w_3\\
&-(n_1-n_2-n_3+1)\,n_5\,f(n_1,n_2,n_3,-2,n_5-1,n_6)\,w_3\\
&-n_5\,f(n_1,n_2,n_3,-1,n_5-1,n_6)\,w_1\,w_3\\
&+f(n_1,n_2,n_3,-1,n_5,n_6)\,w_1\,w_2\,w_3\\
&-n_5\,\delta(n_1)\,\Gamma(n_5+n_6-1,-2,n_2+n_3-1,w_2+w_3,w_1,0)\\
&-n_6\,\delta(n_1)\,\Gamma(n_5+n_6-1,-2,n_2+n_3-1,w_2+w_3,w_1,0)\\
&+\delta(n_1)\,\Gamma(n_5+n_6,-2,n_2+n_3-1,w_2+w_3,w_1,0)\,w_2\\
&+\delta(n_1)\,\Gamma(n_5+n_6,-2,n_2+n_3-1,w_2+w_3,w_1,0)\,w_3\\
&+n_5\,\delta(n_2)\,\Gamma(n_6-2,n_5-1,n_1+n_3-1,w_1+w_3,w_2,0)\\
&-\delta(n_2)\,\Gamma(n_6-2,n_5,n_1+n_3-1,w_1+w_3,w_2,0)\,w_2\\
&+n_6\,\delta(n_3)\,\Gamma(n_5-2,n_6-1,n_1+n_2-1,w_1+w_2,w_3,0)\\
&-\delta(n_3)\,\Gamma(n_5-2,n_6,n_1+n_2-1,w_1+w_2,w_3,0)\,w_3\\
&-n_5\,n_6\,\Gamma(n_3+n_5-2,n_2+n_6-2,n_1,w_2,w_3,0)\\
&+n_6\,\Gamma(n_3+n_5-1,n_2+n_6-2,n_1,w_2,w_3,0)\,w_2\\
&+n_5\,\Gamma(n_3+n_5-2,n_2+n_6-1,n_1,w_2,w_3,0)\,w_3\\
&-\Gamma(n_3+n_5-1,n_2+n_6-1,n_1,w_2,w_3,0)\,w_2\,w_3\Big]\,. \qquad (35)
\end{aligned}
$$

It takes a particularly simple form when all n_i are equal to 0:

$$
\begin{aligned}
f(0,0,0,-2,0,0) \;=\; & \frac{1}{w_2\,w_3}\Big[-w_1\,w_2\,w_3\,f(0,0,0,-1,0,0)+w_3\,\Gamma(-2,0,-1,w_1+w_2,w_3,0)\\
&+w_2\,\Gamma(-2,0,-1,w_1+w_3,w_2,0)+w_2\,w_3\,\Gamma(-1,-1,0,w_2,w_3,0)\\
&-(w_2+w_3)\,\Gamma(0,-2,-1,w_2+w_3,w_1,0)\Big]\\
=\; & -w_1\,f(0,0,0,-1,0,0)-w_1\,(w_1+w_2+w_3)\,f(0,0,0,0,0,0) \qquad (36)
\end{aligned}
$$

$$+\frac{1}{w_2}\bigg[(2-\ln(w_1))\,\ln\Big(1+\frac{w_2}{w_3}\Big)+\frac{1}{2}\,\ln^2\Big(\frac{w_3}{w_1}\Big)+\mathrm{Li}_2\Big(1-\frac{w_1+w_2}{w_3}\Big)+\mathrm{Li}_2\Big(1-\frac{w_2+w_3}{w_1}\Big)\bigg]$$
$$+\frac{1}{w_3}\bigg[(2-\ln(w_1))\,\ln\Big(1+\frac{w_3}{w_2}\Big)+\frac{1}{2}\,\ln^2\Big(\frac{w_2}{w_1}\Big)+\mathrm{Li}_2\Big(1-\frac{w_1+w_3}{w_2}\Big)+\mathrm{Li}_2\Big(1-\frac{w_2+w_3}{w_1}\Big)\bigg],$$

where Γ is the two electron Hylleraas integral, defined in the appendix. The general formula in Eq. (35) does not work in the case $1+n_1=n_2+n_3$. In this special case we use IBP identities in coordinate space and limit ourselves only to identities of the form

$$0\equiv \mathrm{id}(i)=\int d^3r_1\int d^3r_2\int d^3r_3\,(g\,\nabla_i^2 h-h\,\nabla_i^2 g)\,, \tag{37}$$

where

$$g = e^{-w_1\,r_1-w_2\,r_2-w_3\,r_3}\,r_1^{n_4-1}\,r_2^{n_5-1}\,r_3^{n_6-1}\,, \tag{38}$$
$$h = r_{23}^{n_1-1}\,r_{31}^{n_2-1}\,r_{12}^{n_3-1}\,. \tag{39}$$

The identities id(2) and id(3)

$$\begin{aligned}
f(n_1,n_2,n_3,-2,n_5,n_6) &= \frac{1}{w_2^2}\Big[(n_1-1)\,(n_1+n_3-1)\,f(n_1-2,n_2,n_3,-2,n_5,n_6)\\
&\quad -(n_1-1)\,(n_3-1)\,f(n_1-2,2+n_2,n_3-2,-2,n_5,n_6)\\
&\quad +(n_3-1)\,(n_1+n_3-1)\,f(n_1,n_2,n_3-2,-2,n_5,n_6)\\
&\quad -(n_5-1)\,n_5\,f(n_1,n_2,n_3,-2,n_5-2,n_6)\\
&\quad +2\,n_5\,f(n_1,n_2,n_3,-2,n_5-1,n_6)\,w_2\\
&\quad +\delta(n_5)\,\Gamma(n_1+n_6-1,n_3-3,n_2,w_3,w_1,0)\Big], \qquad (40)\\
f(n_1,n_2,n_3,-2,n_5,n_6) &= \frac{1}{w_3^2}\Big[-(n_1-1)\,(n_2-1)\,f(n_1-2,n_2-2,n_3+2,-2,n_5,n_6)\\
&\quad +(n_1-1)\,(n_1+n_2-1)\,f(n_1-2,n_2,n_3,-2,n_5,n_6)\\
&\quad +(n_2-1)\,(n_1+n_2-1)\,f(n_1,n_2-2,n_3,-2,n_5,n_6)\\
&\quad -(n_6-1)\,n_6\,f(n_1,n_2,n_3,-2,n_5,n_6-2)\\
&\quad +2\,n_6\,f(n_1,n_2,n_3,-2,n_5,n_6-1)\,w_3\\
&\quad +\delta(n_6)\,\Gamma(n_2-3,n_1+n_5-1,n_3,w_1,w_2,0)\Big], \qquad (41)
\end{aligned}$$

replace the main recursion in Eq. (35) for the case $1+n_1=n_2+n_3$, and can be used also for all other n_i under the conditions that $n_1>0$, $n_3>0$ or $n_1>0$, $n_2>0$, respectively. The case of $n_1=0,n_2=0,n_3=1$ or $n_1=0,n_2=1,n_3=0$, which is not covered by above recursions, remains to be treated. Therefore, in the third step one obtains the necessary recursions from the following combination of IBP identities in the momentum space: id$(1,1)$ + id$(2,1)$ + id$(3,1) \equiv 0$

$$
\begin{aligned}
f(0,1,0,-2,n_5,n_6) \;=\; & -\frac{1}{w_3^2}\Big[(n_6-1)\,n_6\,f(0,1,0,-2,n_5,n_6-2) \\
& -2\,n_6\,f(0,1,0,-2,n_5,n_6-1)\,w_3 \\
& +\Gamma(n_5+n_6-1,-2,0,w_2+w_3,w_1,0) \\
& -\delta(n_6)\,\Gamma(-2,n_5-1,0,w_1,w_2,0)\Big], \qquad (42)\\
f(0,0,1,-2,n_5,n_6) \;=\; & -\frac{1}{w_2^2}\Big[(n_5-1)\,n_5\,f(0,0,1,-2,n_5-2,n_6) \\
& -2\,n_5\,f(0,0,1,-2,n_5-1,n_6)\,w_2 \\
& +\Gamma(n_5+n_6-1,-2,0,w_2+w_3,w_1,0) \\
& -\delta(n_5)\,\Gamma(n_6-1,-2,0,w_3,w_1,0)\Big]. \qquad (43)
\end{aligned}
$$

This completes the evaluation of singular Hylleraas integrals involving $1/r_i^3$.

VI. SINGULAR HYLLERAAS INTEGRAL WITH $1/r_{ij}^3$

The derivation of recursion relations and the master integral is similar to the one for Hylleraas integral with $1/r_{ij}^2$, see Ref. [10]. In the first step of deriving recursion relations we take the difference id$(3,2)$ − id$(2,2)$ and use it as an equation for $G(1,2,1,1,1,1)$,

$$
\begin{aligned}
G(1,2,1,1,1,1)\,(u_2^2-u_3^2+w_1^2) \;=\; & G(1,1,1,0,1,2)-G(1,1,1,1,0,2) \\
& +G(1,1,1,1,1,1)-G(1,2,0,1,1,1) \\
& +G(1,2,1,0,1,1)-2\,G(1,1,1,2,1,1)\,w_1^2 \\
& +G(1,1,1,1,1,2)\,(w_2^2-w_1^2-w_3^2). \qquad (44)
\end{aligned}
$$

Similarly, the difference id$(2,3)$ − id$(3,3)$ is used to obtain $G(1,1,2,1,1,1)$. These two equations are used now to derive recursions in n_2 and n_3. With the help of Eq. (31) one integrates Eq. (44) with respect to u_1, which lowers the first argument n_1 to -2. 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 the recursion relation in n_2

$$
\begin{aligned}
f(-2,n_2+1,n_3,n_4,n_5,n_6) \;=\; & \frac{1}{w_1^2\,w_3}\Big[n_2\,(n_4-1)\,n_4\,f(-2,n_2-1,n_3,n_4-2,n_5,n_6+1) \\
& -2\,n_2\,n_4\,w_1\,f(-2,n_2-1,n_3,n_4-1,n_5,n_6+1)
\end{aligned}
$$

$$
\begin{aligned}
&-n_2\,(n_5-1)\,n_5\,f(-2,n_2-1,n_3,n_4,n_5-2,n_6+1)\\
&+2\,n_2\,n_5\,w_2\,f(-2,n_2-1,n_3,n_4,n_5-1,n_6+1)\\
&+n_2\,n_6\,(n_2+2\,n_4+n_6)\,f(-2,n_2-1,n_3,n_4,n_5,n_6-1)\\
&-n_2\,(n_2+2\,n_4+2\,n_6+1)\,w_3\,f(-2,n_2-1,n_3,n_4,n_5,n_6)\\
&+n_2\,(w_1^2-w_2^2+w_3^2)\,f(-2,n_2-1,n_3,n_4,n_5,n_6+1)\\
&-2\,n_2\,n_6\,w_1\,f(-2,n_2-1,n_3,n_4+1,n_5,n_6-1)\\
&+2\,n_2\,w_1\,w_3\,f(-2,n_2-1,n_3,n_4+1,n_5,n_6)\\
&-(n_3-1)\,n_3\,n_6\,f(-2,n_2+1,n_3-2,n_4,n_5,n_6-1)\\
&+(n_3-1)\,n_3\,w_3\,f(-2,n_2+1,n_3-2,n_4,n_5,n_6)\\
&+(n_4-1)\,n_4\,n_6\,f(-2,n_2+1,n_3,n_4-2,n_5,n_6-1)\\
&-(n_4-1)\,n_4\,w_3\,f(-2,n_2+1,n_3,n_4-2,n_5,n_6)\\
&-2\,n_4\,n_6\,w_1\,f(-2,n_2+1,n_3,n_4-1,n_5,n_6-1)\\
&+2\,n_4\,w_1\,w_3\,f(-2,n_2+1,n_3,n_4-1,n_5,n_6)\\
&+n_6\,w_1^2\,f(-2,n_2+1,n_3,n_4,n_5,n_6-1)\\
&-(n_2+n_6)\,\delta(n_4)\,\Gamma(n_3+n_5-1,n_2+n_6-1,-2,w_2,w_3,0)\\
&+w_3\,\delta(n_4)\,\Gamma(n_3+n_5-1,n_2+n_6,-2,w_2,w_3,0)\\
&+n_6\,\delta(n_3)\,\Gamma(n_4+n_5-1,n_6-1,n_2-2,w_1+w_2,w_3,0)\\
&-w_3\,\delta(n_3)\,\Gamma(n_4+n_5-1,n_6,n_2-2,w_1+w_2,w_3,0)\\
&+n_2\,\delta(n_5)\,\Gamma(n_6-2,n_3+n_4-1,n_2-1,w_3,w_1,0)\Big], \qquad (45)
\end{aligned}
$$

where $n_i \geq 0$, and the formula for $f(-2,n_2,1+n_3,n_4,n_5,n_6)$ can be obtained from the above one using symmetries of the function f. These recursions assumes that values of $f(-2,0,0;n_4,n_5,n_6)$ are known. We again obtain them using IBP identities. These are 9 equations, which we solve against the following $X_{i=1,9}$ unknowns at $u_2=u_3=0$

$$
\begin{aligned}
X_1 &= G(1,2,1,1,1,1)\,u_1^2\,,\\
X_2 &= G(1,1,2,1,1,1)\,u_1^2\,,\\
X_3 &= G(1,1,1,1,2,1)\,u_1^2\,,\\
X_4 &= G(1,2,1,1,1,2)\,u_1^2\,,\\
X_5 &= G(1,2,1,1,1,1)\,,
\end{aligned}
$$

$$
\begin{aligned}
X_6 &= G(1,1,2,1,1,1)\,,\\
X_7 &= G(1,1,1,2,1,1)\,,\\
X_8 &= G(1,1,1,1,2,1)\,,\\
X_9 &= G(1,1,1,1,1,2). \qquad (46)
\end{aligned}
$$

Equations for X_7, X_8, and X_9 are

$$
\begin{aligned}
0 &= (3\,w_1^2+w_2^2-w_3^2)\,G(1,1,1,1,1,1)-2\,u_1^2\,w_1^2\,G(2,1,1,1,1,1)\\
&\quad -4\,w_1^2\,w_2^2\,G(1,1,1,1,2,1)-2\,w_1^2\,(w_1^2+w_2^2-w_3^2)\,G(1,1,1,2,1,1)\\
&\quad +F_1(u_1)\,w_2-F_2(u_1)\,w_3\,, \qquad (47)\\
0 &= (3\,w_1^2-w_2^2+w_3^2)\,G(1,1,1,1,1,1)-2\,u_1^2\,w_1^2\,G(2,1,1,1,1,1)\\
&\quad -4\,w_1^2\,w_3^2\,G(1,1,1,1,1,2)-2\,w_1^2\,(w_1^2-w_2^2+w_3^2)\,G(1,1,1,2,1,1)\\
&\quad -F_1(u_1)\,w_2+F_2(u_1)\,w_3\,, \qquad (48)\\
0 &= (3\,w_1^4-4\,w_1^2\,w_2^2+w_2^4-4\,w_1^2\,w_3^2-2\,w_2^2\,w_3^2+w_3^4)\,G(1,1,1,1,1,1)\\
&\quad -2\,w_1^2\,(w_1^4-2\,w_1^2\,w_2^2+w_2^4-2\,w_1^2\,w_3^2-2\,w_2^2\,w_3^2+w_3^4)\,G(1,1,1,2,1,1)\\
&\quad -2\,w_1^2\,(u_1^2\,(w_1^2-\,w_2^2-\,w_3^2)+2\,w_2^2\,w_3^2)\,G(2,1,1,1,1,1)\\
&\quad -F_1(u_1)\,w_2\,(w_1^2-w_2^2+w_3^2)-F_2(u_1)\,w_3\,(w_1^2+w_2^2-w_3^2)\,, \qquad (49)
\end{aligned}
$$

where

$$
\begin{aligned}
F_1(u_1) &= 2\,w_2\,[G(1,1,1,0,2,1)-G(1,1,1,1,2,0)+G(2,0,1,1,1,1)-G(2,1,1,1,1,0)]\,, \qquad (50)\\
F_2(u_1) &= 2\,w_3\,[G(1,1,1,0,1,2)-G(1,1,1,1,0,2)+G(2,1,0,1,1,1)-G(2,1,1,1,0,1)]\,. \qquad (51)
\end{aligned}
$$

One performs the u_1 integration and obtains

$$
\begin{aligned}
0 &= F_1\,w_2-F_2\,w_3+(w_1^2+w_2^2-w_3^2)\,f(-2,0,0,0,0,0)\\
&\quad -2\,w_1^2\,w_2\,f(-2,0,0,0,1,0)-w_1\,(w_1^2+w_2^2-w_3^2)\,f(-2,0,0,1,0,0)\\
&\quad +w_1^2\,\Gamma(0,-1,-1,w_1,w_2+w_3,0)\,, \qquad (52)\\
0 &= -F_1\,w_2+F_2\,w_3+(w_1^2-w_2^2+w_3^2)\,f(-2,0,0,0,0,0)\\
&\quad -2\,w_1^2\,w_3\,f(-2,0,0,0,0,1)-w_1\,(w_1^2-w_2^2+w_3^2)\,f(-2,0,0,1,0,0)
\end{aligned}
$$

$$
\begin{aligned}
&\quad +w_1^2\,\Gamma(0,-1,-1,w_1,w_2+w_3,0)\,, && (53)\\
0 &= -F_2\,w_3\,(w_1^2+w_2^2-w_3^2)-F_1\,w_2\,(w_1^2-w_2^2+w_3^2)+w\,f(-2,0,0,0,0,0)\\
&\quad -w\,w_1\,f(-2,0,0,1,0,0)-2\,w_1^2\,w_2^2\,w_3^2\,f(0,0,0,0,0,0)\\
&\quad +w_1^2\,(w_1^2-w_2^2-w_3^2)\,\Gamma(0,-1,-1,w_1,w_2+w_3,0)\,, && (54)
\end{aligned}
$$

where w is defined in Eq. (19) and

$$
F_i=\int_0^\infty du_1\,u_1\,F_i(u_1) \qquad (55)
$$

in the sense of the integral defined in Eq. (31), with the result

$$
\begin{aligned}
F_1 &= \frac{1}{2}\Bigg[\ln\Big(1+\frac{w_2}{w_3}\Big)\,\ln\Big(\frac{w_2}{w_3}\Big)-\ln^2\Big(\frac{w_3}{w_1}\Big)+2\,\ln\Big(\frac{w_1}{w_2+w_3}\Big)-2\,\ln(w_3)\,\ln\Big(\frac{w_1}{w_2+w_3}\Big)\\
&\quad -\ln\Big(\frac{w_2}{w_1+w_3}\Big)\,\ln\Big(1+\frac{w_2}{w_1+w_3}\Big)-2\,\mathrm{Li}_2\Big(-\frac{w_2}{w_1}\Big)+\mathrm{Li}_2\Big(1-\frac{w_2}{w_3}\Big)-\mathrm{Li}_2\Big(-\frac{w_2}{w_3}\Big)\\
&\quad -\mathrm{Li}_2\Big(-\frac{w_2}{w_1+w_3}\Big)-\mathrm{Li}_2\Big(1-\frac{w_2}{w_1+w_3}\Big)\Bigg] && (56)\\
&= \Gamma(0,-1,-2,w_2,w_3,0)-\Gamma(0,-1,-2,0,w_1,w_2)\\
&\quad -w_2\,\Gamma(0,-1,-1,0,w_1,w_2)+w_2\,\Gamma(0,-1,-1,w_2,w_1+w_3,0)\,, && (57)
\end{aligned}
$$

$$
\begin{aligned}
F_2 &= \frac{1}{2}\Bigg[\ln\Big(1+\frac{w_3}{w_2}\Big)\,\ln\Big(\frac{w_3}{w_2}\Big)-\ln^2\Big(\frac{w_2}{w_1}\Big)+2\,\ln\Big(\frac{w_1}{w_2+w_3}\Big)-2\,\ln(w_2)\,\ln\Big(\frac{w_1}{w_2+w_3}\Big)\\
&\quad -\ln\Big(\frac{w_3}{w_1+w_2}\Big)\,\ln\Big(1+\frac{w_3}{w_1+w_2}\Big)-2\,\mathrm{Li}_2\Big(-\frac{w_3}{w_1}\Big)+\mathrm{Li}_2\Big(1-\frac{w_3}{w_2}\Big)-\mathrm{Li}_2\Big(-\frac{w_3}{w_2}\Big)\\
&\quad -\mathrm{Li}_2\Big(-\frac{w_3}{w_1+w_2}\Big)-\mathrm{Li}_2\Big(1-\frac{w_3}{w_1+w_2}\Big)\Bigg] && (58)\\
&= \Gamma(0,-1,-2,w_3,w_2,0)-\Gamma(0,-1,-2,0,w_1,w_3)\\
&\quad -w_3\,\Gamma(0,-1,-1,0,w_1,w_3)+w_3\,\Gamma(0,-1,-1,w_3,w_1+w_2,0)\,. && (59)
\end{aligned}
$$

Under the replacement $f(-2,0,0,0,0,0)=h/w_1\equiv h(0,0,0)/w_1$ one obtains simplified differential equations

$$
\begin{aligned}
0 &= 2\,w_1\,w_2\,\frac{\partial h}{\partial w_2}+(w_1^2+w_2^2-w_3^2)\,\frac{\partial h}{\partial w_1}+F_1\,w_2-F_2\,w_3+w_1^2\,\Gamma(0,-1,-1,w_1,w_2+w_3,0)\,, && (60)\\
0 &= 2\,w_1\,w_3\,\frac{\partial h}{\partial w_3}+(w_1^2-w_2^2+w_3^2)\,\frac{\partial h}{\partial w_1}-F_1\,w_2+F_2\,w_3+w_1^2\,\Gamma(0,-1,-1,w_1,w_2+w_3,0)\,, && (61)\\
0 &= w\,\frac{\partial h}{\partial w_1}-F_2\,w_3\,(w_1^2+w_2^2-w_3^2)-F_1\,w_2\,(w_1^2-w_2^2+w_3^2)-2\,w_1^2\,w_2^2\,w_3^2\,f(0,0,0,0,0,0)\\
&\quad +w_1^2\,(w_1^2-w_2^2-w_3^2)\,\Gamma(0,-1,-1,w_1,w_2+w_3,0)\,. && (62)
\end{aligned}
$$

One differentiates Eq. (60) with respect to w_1, w_2, and w_3, and obtains in this way recursions for h in n_5

$$\begin{aligned}
h(n_4, n_5+1, n_6) \;=\; & \frac{1}{2\,w_1\,w_2}\Big[-n_5\,F_1(n_4, n_5-1, n_6) + w_2\,F_1(n_4, n_5, n_6) \\
& +n_6\,F_2(n_4, n_5, n_6-1) - w_3\,F_2(n_4, n_5, n_6) \\
& +(n_4-1)\,n_4\,\Gamma(-1, n_4-2, n_5+n_6-1, 0, w_1, w_2+w_3) \\
& -2\,n_4\,w_1\,\Gamma(-1, n_4-1, n_5+n_6-1, 0, w_1, w_2+w_3) \\
& +w_1^2\,\Gamma(-1, n_4, n_5+n_6-1, 0, w_1, w_2+w_3) \\
& -n_4\,(n_4+2\,n_5-1)\,h(n_4-1, n_5, n_6) \\
& +2\,n_4\,w_2\,h(n_4-1, n_5+1, n_6) \\
& +2\,(n_4+n_5)\,w_1\,h(n_4, n_5, n_6) \\
& -(n_5-1)\,n_5\,h(n_4+1, n_5-2, n_6) \\
& +2\,n_5\,w_2\,h(n_4+1, n_5-1, n_6) \\
& +(n_6-1)\,n_6\,h(n_4+1, n_5, n_6-2) \\
& -2\,n_6\,w_3\,h(n_4+1, n_5, n_6-1) \\
& -(w_1^2+w_2^2-w_3^2)\,h(n_4+1, n_5, n_6)\Big]\,, \qquad (63)
\end{aligned}$$

where

$$\begin{aligned}
F_1(n_4, n_5, n_6) \;=\; & \delta(n_4)\,\Gamma(-2, n_5, n_6-1, 0, w_2, w_3) \\
& -n_5\,\Gamma(-1, n_5-1, n_4+n_6-1, 0, w_2, w_1+w_3) \\
& +w_2\,\Gamma(-1, n_5, n_4+n_6-1, 0, w_2, w_1+w_3) \\
& +(n_5-1)\,\delta(n_6)\,\Gamma(0, n_4-1, n_5-2, 0, w_1, w_2)\,, \\
& -w_2\,\delta(n_6)\,\Gamma(0, n_4-1, n_5-1, 0, w_1, w_2), \qquad (64) \\
F_2(n_4, n_5, n_6) \;=\; & \delta(n_4)\,\Gamma(-2, n_5-1, n_6, 0, w_2, w_3) \\
& -n_6\,\Gamma(-1, n_6-1, n_4+n_5-1, 0, w_3, w_1+w_2) \\
& +w_3\,\Gamma(-1, n_6, n_4+n_5-1, 0, w_3, w_1+w_2) \\
& +(n_6-1)\,\delta(n_5)\,\Gamma(0, n_4-1, n_6-2, 0, w_1, w_3) \\
& -w_3\,\delta(n_5)\,\Gamma(0, n_4-1, n_6-1, 0, w_1, w_3)\,, \qquad (65)
\end{aligned}$$

and the formula for $h(n_4, n_5, 1+n_6)$ is analogous. Eq. (62) is transformed now to the more explicit form

$$\frac{\partial h}{\partial w_1} = \frac{g_1}{w_1+w_2+w_3} + \frac{g_2}{w_1-w_2-w_3} + \frac{g_3}{w_1-w_2+w_3} + \frac{g_4}{w_1+w_2-w_3}\,, \tag{66}$$

$$\begin{aligned} g_1 &= \frac{1}{4}\biggl[-\frac{\pi^2}{6} + \ln\Bigl(\frac{w_1}{w_2}\Bigr)\ln\Bigl(\frac{w_1}{w_3}\Bigr) + [\ln(w_2\,w_3)-2]\ln\Bigl(\frac{w_1}{w_2+w_3}\Bigr) \\ &\quad + \mathrm{Li}_2\Bigl(-\frac{w_2}{w_1}\Bigr) + \mathrm{Li}_2\Bigl(-\frac{w_3}{w_1}\Bigr)\biggr]\,, \end{aligned} \tag{67}$$

$$\begin{aligned} g_2 &= \frac{1}{4}\biggl[-\ln\Bigl(\frac{w_1}{w_2}\Bigr)\ln\Bigl(\frac{w_1}{w_3}\Bigr) + [2-\ln(w_2\,w_3)]\ln\Bigl(\frac{w_1}{w_2+w_3}\Bigr) \\ &\quad - \mathrm{Li}_2\Bigl(-\frac{w_2}{w_1}\Bigr) - \mathrm{Li}_2\Bigl(-\frac{w_3}{w_1}\Bigr) - \mathrm{Lg}\Bigl(\frac{w_3}{w_1+w_2}\Bigr) - \mathrm{Lg}\Bigl(\frac{w_2}{w_1+w_3}\Bigr)\biggr]\,, \end{aligned} \tag{68}$$

$$\begin{aligned} g_3 &= \frac{1}{8}\biggl[-\frac{\pi^2}{6} + 2\,\mathrm{Lg}\Bigl(\frac{w_3}{w_1+w_2}\Bigr) + 2\,\mathrm{Lg}\Bigl(\frac{w_1}{w_2+w_3}\Bigr) - 2\,\mathrm{Li}_2\Bigl(-\frac{w_2}{w_1}\Bigr) + \mathrm{Li}_2\Bigl(1-\frac{w_2}{w_3}\Bigr) \\ &\quad - \mathrm{Li}_2\Bigl(-\frac{w_2}{w_3}\Bigr) + 2\,\mathrm{Li}_2\Bigl(-\frac{w_3}{w_1}\Bigr) + \mathrm{Li}_2\Bigl(-\frac{w_3}{w_2}\Bigr) - \mathrm{Li}_2\Bigl(1-\frac{w_3}{w_2}\Bigr)\biggr]\,, \end{aligned} \tag{69}$$

$$\begin{aligned} g_4 &= \frac{1}{8}\biggl[-\frac{\pi^2}{6} + 2\,\mathrm{Lg}\Bigl(\frac{w_2}{w_1+w_3}\Bigr) + 2\,\mathrm{Lg}\Bigl(\frac{w_1}{w_2+w_3}\Bigr) + 2\,\mathrm{Li}_2\Bigl(-\frac{w_2}{w_1}\Bigr) - \mathrm{Li}_2\Bigl(1-\frac{w_2}{w_3}\Bigr) \\ &\quad + \mathrm{Li}_2\Bigl(-\frac{w_2}{w_3}\Bigr) - 2\,\mathrm{Li}_2\Bigl(-\frac{w_3}{w_1}\Bigr) - \mathrm{Li}_2\Bigl(-\frac{w_3}{w_2}\Bigr) + \mathrm{Li}_2\Bigl(1-\frac{w_3}{w_2}\Bigr)\biggr]\,, \end{aligned} \tag{70}$$

These formulae are used to obtain forward recursions for $h(n_4,0,0)$ similar to those used in two-electron Hylleraas integrals [15]. Namely, if we denote by $h_i = g_i/(w_1+\ldots)$ the corresponding term in Eq. (66), then the recursion for example for $h_2(n)$ defined by

$$h_2(n) = \Bigl(-\frac{\partial}{\partial w_1}\Bigr)^n h_2\,, \tag{71}$$

in the general case is the following

$$h_2(n) = \frac{g_2(n) + n\,h_2(n-1)}{w_1-w_2-w_3}\,. \tag{72}$$

In the special case of $w_1 \approx w_2+w_3$ one calculates at first recursions exactly at $w_1 = w_2+w_3$

$$h_2(n) = -\frac{g_2(n+1)}{n+1}\,, \tag{73}$$

and obtains $h_2(n)$ for $w_1 \neq w_2+w_3$ using the Taylor formula. For this one notes that first derivatives of g_i are quite simple,

$$\frac{\partial g_1}{\partial w_1} = \frac{1}{4\,w_1}\,[\ln(w_1+w_2)+\ln(w_1+w_3)-2], \tag{74}$$

$$\frac{\partial g_2}{\partial w_1} = -\frac{1}{4\,w_1}\,[\ln(w_1+w_2)+\ln(w_1+w_3)-2] + \frac{1}{4\,(w_1+w_2-w_3)}\,\ln\Bigl(\frac{w_3}{w_1+w_2}\Bigr) + \frac{1}{4\,(w_1-w_2+w_3)}\,\ln\Bigl(\frac{w_2}{w_1+w_3}\Bigr) - \frac{1}{4\,(w_1+w_2+w_3)}\,\Bigl[\ln\Bigl(\frac{w_3}{w_1+w_2}\Bigr)+\ln\Bigl(\frac{w_2}{w_1+w_3}\Bigr)\Bigr], \tag{75}$$

$$\frac{\partial g_3}{\partial w_1} = \frac{1}{4\,w_1}\,\ln\Bigl(\frac{w_1+w_3}{w_1+w_2}\Bigr) - \frac{1}{4\,(w_1+w_2-w_3)}\,\ln\Bigl(\frac{w_3}{w_1+w_2}\Bigr) - \frac{1}{4\,(w_1-w_2-w_3)}\,\ln\Bigl(\frac{w_1}{w_2+w_3}\Bigr) + \frac{1}{4\,(w_1+w_2+w_3)}\,\Bigl[\ln\Bigl(\frac{w_3}{w_1+w_2}\Bigr)+\ln\Bigl(\frac{w_1}{w_2+w_3}\Bigr)\Bigr], \tag{76}$$

$$\frac{\partial g_4}{\partial w_1} = \frac{1}{4\,w_1}\,\ln\Bigl(\frac{w_1+w_2}{w_1+w_3}\Bigr) - \frac{1}{4\,(w_1-w_2+w_3)}\,\ln\Bigl(\frac{w_2}{w_1+w_3}\Bigr) - \frac{1}{4\,(w_1-w_2-w_3)}\,\ln\Bigl(\frac{w_1}{w_2+w_3}\Bigr) + \frac{1}{4\,(w_1+w_2+w_3)}\,\Bigl[\ln\Bigl(\frac{w_2}{w_1+w_3}\Bigr)+\ln\Bigl(\frac{w_1}{w_2+w_3}\Bigr)\Bigr]. \tag{77}$$

Independly of recursions one needs the function h. It is obtained from Eq. (66)

$$h = \int_0^{w_1} dw_1\,\frac{\partial h}{\partial w_1}, \tag{78}$$

and this integral can be explicitly performed in terms of Li_3, Li_2 and logarithmic functions, but the result is quite complicated. For numerical calculations, the integral representation of Eq. (78) with the adapted quadrature [13] is used to achieve about 64 digits accuracy.

Having $h(n_4, n_5, n_6)$, the function $f(-2,0,0,n_4,n_5,n_6)$ is obtained by

$$f(-2,0,0,n_4,n_5,n_6) = \frac{1}{w_1}[h(n_4,n_5,n_6) + n_4\,f(-2,0,0,n_4-1,n_5,n_6)], \tag{79}$$

which completes the evaluation of singular Hylleraas integrals.

VII. SUMMARY

We have obtained recursion relations for three-electron Hylleraas integrals involving $1/r_i^3$ and $1/r_{ij}^3$. The initial multi dimensional master integral is expressed in the form of a one dimensional integral, which is suitable for high precision numerical evaluation. A set of numerical examples for $f(-2,0,0,0,0,0)$ is presented in Table I and for $f(0,0,0,-2,0,0)$ in Table II. Together with regular and extended Hylleraas integrals they allow for the calculation of leading QED effects in three electron atoms or ions. Accurate results for the lithium atom have already been obtained by Yan and Drake in [19] and several precise measuements have been performed in [16, 17]. While we intend to verify their result, we aim also to calculate QED effects in the Be^+ ion for the determination of the nuclear charge radii from planned isotope shift measurements. Moreover, we aim to calculate higher order QED effects for energy levels along with fine and hyperfine splittings [18] to verify certain discrepancies, for example the difference between experimental values and theoretical predictions for the 2S-3S transition frequency in Li [17, 19].

TABLE I: Values of the master integral $f(-2,0,0,0,0,0)$ for selected w_1, w_2, and w_3

w_1	w_2	w_3	$f(-2,0,0,0,0,0)$
4.0	1.0	0.5	-0.712 305 106 830 898 240 034 381 269 753 396
4.0	1.0	1.0	-0.699 249 073 328 162 683 321 507 663 896 763
4.0	1.0	1.5	-0.691 399 920 204 079 424 318 079 206 069 445
4.0	1.0	2.0	-0.680 940 098 270 060 661 183 207 296 253 486
4.0	1.0	2.5	-0.667 068 654 115 517 811 166 904 215 261 918
4.0	1.0	3.0	-0.651 691 691 901 107 499 331 195 660 199 574
4.0	1.0	3.5	-0.640 014 560 205 730 366 159 157 581 017 121
4.0	1.0	4.0	-0.627 151 433 983 103 414 178 318 921 819 093
4.0	1.0	4.5	-0.614 807 615 676 494 534 607 896 770 432 226
4.0	1.0	5.0	-0.602 911 457 174 426 959 108 113 476 921 161
4.0	1.0	5.5	-0.591 697 977 384 241 861 061 839 402 802 568

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[1] Z.-C. Yan and G. W. F. Drake, Phys. Rev. A **52**, 3711 (1995).

[2] M. Puchalski and K. Pachucki, Phys. Rev. A **73**, 022503 (2006).

[3] E.A. Hylleraas, Z. Phys. **54**, 347 (1929).

[4] F. W. King and V. Shoup, Phys. Rev. A **33**, 2940 (1986); F. W. King and M. P. Bergsbaken, J. Chem. Phys. **93**, 2570 (1990); F. W. King, J. Chem. Phys. **99**, 3622 (1993); F. W. King,

TABLE II: Values of the master integral $f(0,0,0,-2,0,0)$ for selected w_1, w_2, and w_3

w_1	w_2	w_3	$f(0,0,0,-2,0,0)$
4.0	1.0	0.5	-3.457 452 854 159 239 112 750 191 117 485 829
4.0	1.0	1.0	-2.650 037 638 635 495 670 871 341 393 412 236
4.0	1.0	1.5	-2.234 238 493 311 187 793 632 537 945 604 453
4.0	1.0	2.0	-1.967 448 655 334 872 044 627 131 808 094 930
4.0	1.0	2.5	-1.777 079 267 715 778 085 428 017 041 995 909
4.0	1.0	3.0	-1.632 246 974 419 083 835 406 405 271 425 506
4.0	1.0	3.5	-1.517 186 855 826 194 722 590 295 936 030 308
4.0	1.0	4.0	-1.422 872 681 980 733 011 235 327 186 357 640
4.0	1.0	4.5	-1.343 706 445 824 538 744 395 243 994 507 941
4.0	1.0	5.0	-1.276 004 428 705 473 405 554 500 648 664 743
4.0	1.0	5.5	-1.217 228 914 605 386 522 608 906 840 145 094

THEOCHEM: J. Mol. Struct. **400**, 7 (1997); P.J. Pelzl and F.W. King, Phys. Rev. E **57**, 7268 (1998); F.W. King, Adv. At. Mol. Opt. Phys. **40**, 57 (1999).

[5] D. K. McKenzie and G. W. F. Drake, Phys. Rev. A **44**, R6973 (1991); G.W.F. Drake and Z.-C. Yan, Phys. Rev. A **46**, 2378 (1992).

[6] J. S. Sims and S. A. Hagstrom, J. Phys. B: At. Mol. Opt. Phys. **37**, 1519 (2004); *ibid.* **40**, 1575 (2007).

[7] K. Pachucki, M. Puchalski and E. Remiddi, Phys. Rev. A **70**, 032502 (2004).

[8] D.M. Feldman, P.J. Pelzl, and F. W. King, J. Math. Phys. **39**, 6262 (1998); F. W. King *et al.* Phys. Rev. A **58**, 3597 (1998); F. W. King, Int. J. Quant. Chem. **72**, 93 (1999); P.J. Pelzl, G.J. Smethells, and F.W. King, Phys. Rev. E **65**, 036707 (2002).

[9] G. W. F. Drake and Z.-C. Yan, Phys. Rev. A **52**, 3681 (1995); J. Phys. B: At. Mol. Opt. Phys. **30**, 4723 (1997); Z.-C. Yan and G. W. F. Drake, Phys. Rev. A **61**, 022504 (2000); Phys. Rev. A **66**, 042504 (2002); Phys. Rev. Lett. **91**, 113004 (2003).

[10] K. Pachucki and M. Puchalski, Phys. Rev. A **71**, 032514 (2005),

[11] Z.-C. Yan, J. Phys. B: At. Mol. Opt. Phys. **33**, 2437 (2000).

[12] E. Remiddi, Phys. Rev. A **44**, 5492 (1991).

[13] J. Ma, V. Rokhlin, and S. Wandzura, SIAM J. Numer. Anal. **33**, 971 (1996).

[14] F.V. Tkachov, Phys. Lett. B **100**, 65 (1981); K.G. Chetyrkin and F.V. Tkachov, Nucl. Phys. B **192**, 159 (1981).

[15] R.A. Sack, C.C.J Roothaan and W. Kołos, J. Math. Phys. **8**, 1093 (1967); V.I. Korobov, J. Phys. B **35**, 1959 (2002); F.E Harris, A.M. Frolov and V.S. Smith, Jr., J. Chem. Phys **121**, 6323 (2004).

[16] W. DeGraffenreid and C.J. Sansonetti, Phys. Rev. A **67**, 012509 (2003).

[17] B. A. Bushaw, W. Nörtershäuser, G. Ewald, A. Dax, and G. W. F. Drake, Phys. Rev. Lett. **91**, 043004 (2003).

[18] K. Pachucki, Phys. Rev. A **66**, 062501 (2002).

[19] Z.-C. Yan and G. W. F. Drake, Phys. Rev. A 66, 042504 (2002), Phys. Rev. Lett. **91**, 113004 (2003).

Appendix: Singular two electron integrals

The definition of the distribution $P(1/r^3)$ assumes that it is integrated with a smooth function of r. This is not always the case with Hylleraas integrals. One can not apply directly the definition of Eq. (29), because the integrand is logarithmic in r for certain negative powers of electron coordinates. Therefore, here we assume the following recursive definition

$$-\frac{\partial}{\partial\gamma}\,\Gamma(n_1,n_2,n_3,\alpha,\beta,\gamma) = \Gamma(n_1,n_2,n_3+1,\alpha,\beta,\gamma) \tag{80}$$

and set the boundary condition for large γ, by the requirement that only powers of $\ln\gamma$ are present, but no constant term. Using this definition, which is consistent with Eq. (29), one obtains

$$\Gamma(n_1,n_2,n_3,\alpha,\beta,\gamma) \equiv \int\frac{d^3r_1}{4\,\pi}\int\frac{d^3r_2}{4\,\pi}\,e^{-\alpha\,r_1-\beta\,r_2-\gamma\,r_{12}}\,r_1^{n_1-1}\,r_2^{n_2-1}\,r_{12}^{n_3-1} \tag{81}$$

$$\Gamma(0,0,0,\alpha,\beta,\gamma) = \frac{1}{(\alpha+\beta)\,(\alpha+\gamma)\,(\beta+\gamma)} \tag{82}$$

$$\Gamma(0,0,-1,\alpha,\beta,\gamma) = \frac{1}{(\alpha-\beta)\,(\alpha+\beta)}\ln\Bigl(\frac{\gamma+\alpha}{\gamma+\beta}\Bigr) \tag{83}$$

$$\Gamma(0,0,-2,\alpha,\beta,\gamma) \;=\; \frac{(\beta+\gamma)\,\ln(\beta+\gamma)-(\alpha+\gamma)\,\ln(\alpha+\gamma)}{(\alpha^2-\beta^2)}+\frac{1}{\alpha+\beta} \tag{84}$$

$$\Gamma(0,-1,-1,0,\beta,\gamma) \;=\; \frac{1}{\gamma}\,\ln\Bigl(1+\frac{\gamma}{\beta}\Bigr)+\frac{1}{\beta}\,\ln\Bigl(1+\frac{\beta}{\gamma}\Bigr) \tag{85}$$

$$\Gamma(0,-1,-1,\alpha,\beta,0) \;=\; \frac{1}{2\,\alpha}\left[\frac{\pi^2}{6}-\ln\Bigl(1+\frac{\alpha}{\beta}\Bigr)\,\ln\frac{\alpha}{\beta}-\mathrm{Li}_2\Bigl(1-\frac{\alpha}{\beta}\Bigr)-\mathrm{Li}_2\Bigl(-\frac{\alpha}{\beta}\Bigr)\right] \tag{86}$$

$$\Gamma(0,-1,-1,\alpha,\beta,\gamma) \;=\; \frac{1}{2\,\alpha}\left[\frac{\pi^2}{6}+\frac{1}{2}\,\ln^2\Bigl(\frac{\alpha+\beta}{\alpha+\gamma}\Bigr)+\mathrm{Li}_2\Bigl(1-\frac{\beta+\gamma}{\alpha+\beta}\Bigr)+\mathrm{Li}_2\Bigl(1-\frac{\beta+\gamma}{\alpha+\gamma}\Bigr)\right] \tag{87}$$

$$\Gamma(0,-1,-2,0,\beta,\gamma) \;=\; \mathrm{Li}_2\Bigl(-\frac{\gamma}{\beta}\Bigr)-\frac{\gamma}{\beta}\,\ln\Bigl(1+\frac{\beta}{\gamma}\Bigr)+\frac{1}{2}\,\ln^2\beta-\ln(\beta+\gamma)+\frac{\pi^2}{6}+1 \tag{88}$$

$$\begin{aligned}\Gamma(0,-1,-2,\alpha,\beta,0) \;=\;& \frac{1}{2}\,\mathrm{Li}_2\Bigl(1-\frac{\alpha}{\beta}\Bigr)-\frac{1}{2}\,\mathrm{Li}_2\Bigl(-\frac{\alpha}{\beta}\Bigr)+\frac{1}{2}\,\ln\alpha\,\ln\Bigl(1+\frac{\alpha}{\beta}\Bigr)\\ &+\Bigl(\frac{\ln\beta}{2}-1\Bigr)\,\ln(\alpha+\beta)+\frac{\pi^2}{12}+1\end{aligned} \tag{89}$$

$$\begin{aligned}\Gamma(0,-1,-2,\alpha,\beta,\gamma) \;=\;& \frac{1}{2}\Bigl(1-\frac{\gamma}{\alpha}\Bigr)\,\mathrm{Li}_2\Bigl(1-\frac{\beta+\gamma}{\alpha+\beta}\Bigr)-\frac{1}{2}\Bigl(1+\frac{\gamma}{\alpha}\Bigr)\,\mathrm{Li}_2\Bigl(1-\frac{\beta+\gamma}{\alpha+\gamma}\Bigr)\\ &-\frac{1}{4}\Bigl(1+\frac{\gamma}{\alpha}\Bigr)\,\ln^2\Bigl(\frac{\alpha+\gamma}{\alpha+\beta}\Bigr)+\frac{1}{2}\,\ln^2(\alpha+\beta)-\ln(\alpha+\beta)\\ &+\frac{\pi^2}{12}\Bigl(1-\frac{\gamma}{\alpha}\Bigr)+1\end{aligned} \tag{90}$$