Recursion relations for the generic Hylleraas three-electron integral

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Abstract

Recursion relations for the generic Hylleraas three-electron integral are obtained in a closed form by using integration by parts identities. Numerically fast algorithms suitable for high precision calculations of the integral with high powers of inter-electronic coordinates are presented.

PACS numbers: 31.25.-v, 31.15.Pf, 02.70.-c

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I. INTRODUCTION

The explicitely correlated Hylleraas basis set [1] is one of the most efficient representation of a few-electron wave function. It has been applied mostly to helium [2] and lithium atoms [3, 4]. While the general analytic formula for two-electron Hylleraas integrals is quite simple [5], the three-electron case is much more complicated. Fromm and Hill in [6] were able to derive a closed form formula for the generic integral

$$\int d^3r_1 \int d^3r_2 \int d^3r_3\, e^{-w_1\,r_1-w_2\,r_2-w_3\,r_3-u_1\,r_{23}-u_2\,r_{31}-u_3\,r_{12}}\, r_{23}^{-1}\, r_{31}^{-1}\, r_{12}^{-1}\, r_1^{-1}\, r_2^{-1}\, r_3^{-1}\,, \tag{1}$$

which consists of the sum of many multi-valued dilogarithmic functions. This formula was later simplified by Harris [7] to a more symmetric form, in which many spurious singularities have been eliminated. However, only few preliminary results have been reported so far with these functions, namely in Refs. [8, 9]. The more convenient basis set for applications to 3- or 4-electron atoms happen to consist of functions with all u_i equal to 0, and include polynomials in r_{ij} and additionally in r_i, namely the 3-electron Hylleraas functions

$$\phi = e^{-w_1\,r_1-w_2\,r_2-w_3\,r_3}\, r_{23}^{n_1-1}\, r_{31}^{n_2-1}\, r_{12}^{n_3-1}\, r_1^{n_4-1}\, r_2^{n_5-1}\, r_3^{n_6-1}\,. \tag{2}$$

A compact expression for the integral with all $n_i = 0$ and with $n_1 = 2, n_2 = 0, n_3 = 2, n_4 = n_5 = n_6 = 1$ was derived in [10]. Other integrals with small values of n_i have recently been derived in Ref. [11]. Integrals for arbitrary n_i can in principle be obtained from the general formula by Fromm and Hill in Ref. [6] by differentiation with respect to u_i and w_i. In practice that is quite complicated for large powers of r_{ij}. For testing results obtained in this work we have written a Mathematica code for derivation of Hylleraas type of integrals using the Fromm-Hill formula, and obtained results for all n_i such that $n_1+n_2+n_3+n_4+n_5+n_6 < 10$. Despite the existence of an analytical result for the generic integral (1), the most advanced results for lithium have been obtained so far in series of papers by King [3] and Yan, Drake [4], where Hylleraas integrals where calculated by series expansion in angular momenta.

For helium atom recursion relations [5] are available, which allow to express Hylleraas integrals with $n_1 + n_2 + n_3 = N$ [see Eq. (A5)] as a linear combination of integrals from the lower shell $N - 1$. In this work we derive a similar complete set of recursion relations for the three-electron Hylleraas integrals

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

These recursions eliminate the principal drawback of Hylleraas basis sets, namely the complexity of various integrals for nonrelativistic matrix elements for the lithium atom. Moreover they can be applied also to more than three-electron atoms as in [12], with the condition that the basis set contains at most one odd power of r_{ij}. In the next section we present our main result, a complete set of recursion relations for the three-electron Hylleraas integrals defined in Eq. (3). In Section III we analyze boundary terms and two-electron recursions, and in Section IV we sketch the derivation of the main result. Finally in Section V we analyze numerical stability and present numerical results for some selected integrals.

II. THREE-ELECTRON RECURSION RELATIONS

The recursion relations are conveniently divided into two sets. The first set of three recursions increases by 2 any of the first three indices n_1, n_2, n_3 at $n_4 = n_5 = n_6 = 0$, starting from the shell $n_1 + n_2 + n_3 = 0$ (as initial conditions, the values with $n_i = 0, 1, i = 1, 2, 3$ and $n_4 = n_5 = n_6 = 0$ are therefore needed). With the notation of Appendix A, (the symbol $\star$ means that $r^{n_i - 1}$ is replaced by $4\,\pi\,\delta(r)$ in the integral representation of function f), these recursions read

$$
\begin{aligned}
f(n_1, n_2, n_3+2; 0,0,0) \;=\; & \frac{1+n_3}{2}\Bigg\{ \\
& \frac{1}{w_1^2}\Bigg[\frac{n_2\,(n_2-1)}{n_3+1}\, f(n_1, n_2-2, n_3+2; 0,0,0) \\
& +(n_1+2\,n_2+n_3+2)\, f(n_1, n_2, n_3; 0,0,0) \\
& +\frac{1}{n_3+1}\, f(n_1, n_2, n_3+2; \star, 0, 0) \\
& +\frac{n_2\,(n_2-1)}{n_1+1}\, f(n_1+2, n_2-2, n_3; 0,0,0) \\
& +\frac{1}{n_1+1}\, f(n_1+2, n_2, n_3; 0,0,\star) \\
& -\frac{\delta_{n_2}}{n_3+1}\, f(n_1, \star, n_3+2; 0,0,0) \\
& -\frac{\delta_{n_2}}{n_1+1}\, f(n_1+2, \star, n_3; 0,0,0)\Bigg] \\
& +\frac{1}{w_2^2}\Bigg[\frac{n_1\,(n_1-1)}{n_3+1}\, f(n_1-2, n_2, n_3+2; 0,0,0) \\
& +(2\,n_1+n_2+n_3+2)\, f(n_1, n_2, n_3; 0,0,0) \\
& +\frac{1}{n_3+1}\, f(n_1, n_2, n_3+2; 0, \star, 0) +
\end{aligned}
$$

$$
\begin{aligned}
&\frac{n_1\,(n_1-1)}{n_2+1}\,f(n_1-2,n_2+2,n_3;0,0,0)+\\
&\frac{1}{n_2+1}\,f(n_1,n_2+2,n_3;0,0,\star)\\
&-\frac{\delta_{n_1}}{n_3+1}\,f(\star,n_2,n_3+2;0,0,0)\\
&-\frac{\delta_{n_1}}{n_2+1}\,f(\star,n_2+2,n_3;0,0,0)\Big]\\
-\frac{w_3^2}{w_1^2\,w_2^2}\Big[&\frac{n_3\,(n_3-1)}{n_2+1}\,f(n_1,n_2+2,n_3-2;0,0,0)\\
&+(n_1+n_2+2\,n_3+2)\,f(n_1,n_2,n_3;0,0,0)\\
&+\frac{1}{n_2+1}\,f(n_1,2+n_2,n_3;\star,0,0)\\
&+\frac{n_3\,(n_3-1)}{n_1+1}\,f(n_1+2,n_2,n_3-2;0,0,0)\\
&+\frac{1}{n_1+1}\,f(n_1+2,n_2,n_3;0,\star 0)\\
&-\frac{\delta_{n_3}}{n_2+1}\,f(n_1,n_2+2,\star;0,0,0)\\
&-\frac{\delta_{n_3}}{n_1+1}\,f(n_1+2,n_2,\star;0,0,0)\Big]\Big\}\,. \qquad (4)
\end{aligned}
$$

Formulas for $f(n_1,n_2+2,n_3,0,0,0)$ and $f(n_1+2,n_2,n_3,0,0,0)$ can be obtained from Eqs. (3) and (4) by interchanging (r_2,r_3) or (r_1,r_3) respectively.

The next three recursions increase by 1 any of n_4,n_5,n_6 of a given subshell $n_4+n_5+n_6$ for arbitrary n_1,n_2 and n_3

$$
\begin{aligned}
f(n_1,n_2,n_3;n_4,n_5,n_6+1) \;=\; &\frac{1}{w_1\,w_2\,w_3}\Big\{\\
&(n_1-1)\,n_1\,n_4\,f(n_1-2,n_2,n_3;n_4-1,n_5+1,n_6)\\
&+(n_2-1)\,n_2\,n_5\,f(n_1,n_2-2,n_3;n_4+1,n_5-1,n_6)\\
&-(n_3-1)\,n_3\,n_4\,f(n_1,n_2,n_3-2;n_4-1,n_5+1,n_6)\\
&-(n_3-1)\,n_3\,n_5\,f(n_1,n_2,n_3-2;n_4+1,n_5-1,n_6)\\
&+n_4\,n_5\,(n_1+n_2-n_3+n_6+1)\,f(n_1,n_2,n_3;n_4-1,n_5-1,n_6)\\
&-(n_1-1)\,n_1\;f(n_1-2,n_2,n_3;n_4,n_5+1,n_6)\,w_1\\
&+(n_3-1)\,n_3\;f(n_1,n_2,n_3-2;n_4,n_5+1,n_6)\,w_1\\
&-n_5\,(n_1+n_2-n_3+n_6+1)\,f(n_1,n_2,n_3;n_4,n_5-1,n_6)\,w_1\\
&-(n_2-1)\,n_2\,f(n_1,n_2-2,n_3;n_4+1,n_5,n_6)\,w_2\\
&+(n_3-1)\,n_3\,f(n_1,n_2,n_3-2;n_4+1,n_5,n_6)\,w_2
\end{aligned}
$$

$$
\begin{aligned}
&-n_4\,(n_1+n_2-n_3+n_6+1)\,f(n_1,n_2,n_3;n_4-1,n_5,n_6)\,w_2\\
&-n_4\,n_5\,f(n_1,n_2,n_3;n_4-1,n_5-1,n_6+1)\,w_3\\
&+(n_1+n_2-n_3+n_6+1)\,f(n_1,n_2,n_3;n_4,n_5,n_6)\,w_1\,w_2\\
&+n_4\,f(n_1,n_2,n_3;n_4-1,n_5,n_6+1)\,w_2\,w_3\\
&+n_5\,f(n_1,n_2,n_3;n_4,n_5-1,n_6+1)\,w_3\,w_1\\
&-\delta_{n_1}\,n_4\,f(\star,n_2,n_3;n_4-1,n_5+1,n_6)\\
&+\delta_{n_1}\,f(\star,n_2,n_3;n_4,n_5+1,n_6)\,w_1\\
&-\delta_{n_2}\,n_5\,f(n_1,\star,n_3;n_4+1,n_5-1,n_6)\\
&+\delta_{n_2}\,f(n_1,\star,n_3;n_4+1,n_5,n_6)\,w_2\\
&+\delta_{n_3}\,n_4\,f(n_1,n_2,\star;n_4-1,n_5+1,n_6)\\
&+\delta_{n_3}\,n_5\,f(n_1,n_2,\star;n_4+1,n_5-1,n_6)\\
&-\delta_{n_3}\,f(n_1,n_2,\star;n_4,n_5+1,n_6)\,w_1\\
&-\delta_{n_3}\,f(n_1,n_2,\star;n_4+1,n_5,n_6)\,w_2\}\,. \qquad (5)
\end{aligned}
$$

Two other recursions for $f(n_1,n_2,n_3,n_4,n_5+1,n_6)$ and $f(n_1,n_2,n_3,n_4+1,n_5,n_6)$ are obtained from Eqs. (3) and (5) by interchanging arguments of f-function, using the identities

$$
\begin{aligned}
&f(n_1,n_2,n_3;n_4,n_5,n_6;w_1,w_2,w_3) =\\
&f(n_2,n_1,n_3;n_5,n_4,n_6;w_2,w_1,w_3) =\\
&f(n_3,n_2,n_1;n_6,n_5,n_4;w_3,w_2,w_1) =\\
&f(n_1,n_3,n_2;n_4,n_6,n_5;w_1,w_3,w_2)\,, \qquad (6)
\end{aligned}
$$

where any of n_i can become a $\star$.

III. BOUNDARY TERMS

These recursion relations in Eqs. (4) and (5) involve boundary terms. They are initial terms to start recursions and the two-electron integrals, namely the terms which contain the symbol $\star$. The first initial term was derived in Ref. [10], (with correction of misprints; see Ref. [13]), the 7 remaining initial terms to start the first set of recursions are obtained from the generic Fromm-Hill formula [6] or by direct integration [11]

$$
f(0,0,0;0,0,0) \;=\; \frac{-1}{2\,w_1\,w_2\,w_3}\Big\{
$$

$$
\begin{aligned}
& \ln\Big(\frac{w_3}{w_1+w_2}\Big)\,\ln\Big(1+\frac{w_3}{w_1+w_2}\Big)+\mathrm{Li}_2\Big(-\frac{w_3}{w_1+w_2}\Big)+\mathrm{Li}_2\Big(1-\frac{w_3}{w_1+w_2}\Big) \\
& +\ln\Big(\frac{w_2}{w_3+w_1}\Big)\,\ln\Big(1+\frac{w_2}{w_1+w_3}\Big)+\mathrm{Li}_2\Big(-\frac{w_2}{w_1+w_3}\Big)+\mathrm{Li}_2\Big(1-\frac{w_2}{w_1+w_3}\Big) \\
& +\ln\Big(\frac{w_1}{w_2+w_3}\Big)\,\ln\Big(1+\frac{w_1}{w_1+w_2}\Big)+\mathrm{Li}_2\Big(-\frac{w_1}{w_2+w_3}\Big)+\mathrm{Li}_2\Big(1-\frac{w_1}{w_2+w_3}\Big)\Big\}
\end{aligned}
$$

$$
\begin{aligned}
f(1,0,0;0,0,0) &= -\frac{1}{w_2^2\,w_3^2}\,\ln\Big[\frac{w_1\,(w_1+w_2+w_3)}{(w_1+w_2)(w_1+w_3)}\Big]\,, \\
f(0,1,0;0,0,0) &= -\frac{1}{w_1^2\,w_3^2}\,\ln\Big[\frac{w_2\,(w_1+w_2+w_3)}{(w_2+w_3)(w_2+w_1)}\Big]\,, \\
f(0,0,1;0,0,0) &= -\frac{1}{w_1^2\,w_2^2}\,\ln\Big[\frac{w_3\,(w_1+w_2+w_3)}{(w_3+w_1)(w_3+w_2)}\Big]\,, \\
f(1,1,0;0,0,0) &= \frac{1}{w_1\,w_2\,(w_1+w_2)\,w_3^2}\,, \\
f(1,0,1;0,0,0) &= \frac{1}{w_1\,w_3\,(w_1+w_3)\,w_2^2}\,, \\
f(0,1,1;0,0,0) &= \frac{1}{w_2\,w_3\,(w_2+w_3)\,w_1^2}\,, \\
f(1,1,1;0,0,0) &= \frac{1}{w_1^2\,w_2^2\,w_3^2}\,, \qquad (7)
\end{aligned}
$$

where $\mathrm{Li}_2(x)$ is the dilogarithmic function. Besides the initial terms one needs also as boundary terms the following two-electron integrals

$$
\begin{aligned}
f(\star,n_2,n_3;n_4,n_5,n_6) &= \Gamma(n_5+n_6-1,n_4,n_3+n_2-1;w_2+w_3,w_1,0)\,, \\
f(n_1,\star,n_3;n_4,n_5,n_6) &= \Gamma(n_4+n_6-1,n_5,n_1+n_3-1;w_1+w_3,w_2,0)\,, \\
f(n_1,n_2,\star;n_4,n_5,n_6) &= \Gamma(n_4+n_5-1,n_6,n_1+n_2-1;w_1+w_2,w_3,0)\,, \\
f(n_1,n_2,n_3;\star,0,0) &= \Gamma(n_3-1,n_2-1,n_1;w_2,w_3,0)\,, \\
f(n_1,n_2,n_3;0,\star,0) &= \Gamma(n_1-1,n_3-1,n_2;w_3,w_1,0)\,, \\
f(n_1,n_2,n_3;0,0,\star) &= \Gamma(n_2-1,n_1-1,n_3;w_1,w_2,0)\,, \qquad (8)
\end{aligned}
$$

where Γ is defined in Eq. (A5). Recursion relations for Γ have already been worked out in the literature and can be found for example in [5, 14]. For completeness we include below generic formulas for two cases: nonnegative n_1,n_2,n_3,

$$
\Gamma(n_1,n_2,n_3;\alpha_1,\alpha_2,\alpha_3)=\Big(-\frac{\mathrm{d}}{\mathrm{d}\alpha_1}\Big)^{n_1}\Big(-\frac{\mathrm{d}}{\mathrm{d}\alpha_2}\Big)^{n_2}\Big(-\frac{\mathrm{d}}{\mathrm{d}\alpha_3}\Big)^{n_3}\frac{1}{(\alpha_1+\alpha_2)(\alpha_2+\alpha_3)(\alpha_3+\alpha_1)}, \qquad (9)
$$

and the second case: $n_1=-1$, and nonnegative n_2,n_3

$$
\Gamma(-1,n_2,n_3;\alpha_1,\alpha_2,\alpha_3)=\Big(-\frac{\mathrm{d}}{\mathrm{d}\alpha_2}\Big)^{n_2}\Big(-\frac{\mathrm{d}}{\mathrm{d}\alpha_3}\Big)^{n_3}\frac{\ln(\alpha_1+\alpha_2)-\ln(\alpha_1+\alpha_3)}{(\alpha_2-\alpha_3)(\alpha_2+\alpha_3)}\,. \qquad (10)
$$

The complete set of recursion relations have been checked by comparison with analytic expressions obtained by differentiation of Fromm and Hill's formula [6] with respect to the u_i and w_i parameters (in our notation).

IV. DERIVATION OF THREE-ELECTRON RECURSION FORMULAS

We use the method of the integration by parts identities [15], which is by now standard in the analytical calculation of Feynman diagrams. In our case, it amounts to considering the following 9 identities in the momentum representation of the integral G, [see Eq. (A6)]

$$0 \equiv \mathrm{id}(i,j) = \int d^3k_1 \int d^3k_2 \int d^3k_3 \, \frac{\partial}{\partial \vec{k}_i} \Big[\vec{k}_j \, (k_1^2+u_1^2)^{-m_1} \\ (k_2^2+u_2^2)^{-m_2} \, (k_3^2+u_3^2)^{-m_3} (k_{32}^2+w_1^2)^{-m_4} \, (k_{13}^2+w_2^2)^{-m_5} \, (k_{21}^2+w_3^2)^{-m_6} \Big], \qquad (11)$$

which are trivially valid (the integral of the derivative of a function vanishing at infinity vanishes).

These identities group naturally into three sets. The first set consists of $\mathrm{id}(1,1)$, $\mathrm{id}(2,1)$, and $\mathrm{id}(3,1)$. Other sets are obtained by changing the second argument from 1 into 2 or 3. The reduction of the scalar products from the numerator leads to the following identities of the first set

$$\begin{aligned}
\mathrm{id}(1,1) \;=\; & -m_6\, G(m_1-1, m_6+1) - m_5\, G(m_1-1, m_5+1) + m_6\, G(m_2-1, m_6+1) \\
& + m_5\, G(m_3-1, m_5+1) + (3 - 2\,m_1 - m_5 - m_6)\, G() + m_6\, G(m_6+1)\, u_1^2 \\
& + m_5\, G(m_5+1)\, u_1^2 + 2\,m_1\, G(m_1+1)\, u_1^2 - m_6\, G(m_6+1)\, u_2^2 - m_5\, G(m_5+1)\, u_3^2 \\
& + m_5\, G(m_5+1)\, w_2^2 + m_6\, G(m_6+1)\, w_3^2\,,
\end{aligned}$$

$$\begin{aligned}
\mathrm{id}(2,1) \;=\; & -m_6\, G(m_1-1, m_6+1) - m_5\, G(m_1-1, m_5+1) + m_6\, G(m_2-1, m_6+1) \\
& + m_5\, G(m_3-1, m_5+1) - m_5\, G(m_4-1, m_5+1) + (m_6 - m_1)\, G() \\
& + m_5\, G(m_5+1, m_6-1) - m_1\, G(m_1+1, m_2-1) + m_1\, G(m_1+1, m_6-1) \\
& + m_6\, G(m_6+1)\, u_1^2 + m_5\, G(m_5+1)\, u_1^2 + m_1\, G(m_1+1)\, u_1^2 - m_6\, G(m_6+1)\, u_2^2 \\
& + m_1\, G(m_1+1)\, u_2^2 - m_5\, G(m_5+1)\, u_3^2 + m_5\, G(m_5+1)\, w_1^2 - m_6\, G(m_6+1)\, w_3^2 \\
& - m_5\, G(m_5+1)\, w_3^2 - m_1\, G(m_1+1)\, w_3^2\,,
\end{aligned}$$

$$
\begin{aligned}
\mathrm{id}(3,1) \;=\; & -m_6\, G(m_1-1, m_6+1) - m_5\, G(m_1-1, m_5+1) + m_6\, G(m_2-1, m_6+1) \\
& + m_5\, G(m_3-1, m_5+1) - m_6\, G(m_4-1, m_6+1) + m_6\, G(-m_5+1, m_6+1) \\
& + (m_5-m_1)\, G() - m_1\, G(m_1+1, m_3-1) + m_1\, G(m_1+1, m_5-1) \\
& + m_6\, G(m_6+1)\, u_1^2 + m_5\, G(m_5+1)\, u_1^2 + m_1\, G(m_1+1)\, u_1^2 - m_6\, G(m_6+1)\, u_2^2 \\
& - m_5\, G(m_5+1)\, u_3^2 + m_1\, G(m_1+1)\, u_3^2 + m_6\, G(m_6+1)\, w_1^2 - m_6\, G(m_6+1)\, w_2^2 \\
& - m_5\, G(m_5+1)\, w_2^2 - m_1\, G(m_1+1)\, w_2^2\,. \qquad (12)
\end{aligned}
$$

The function G is defined as in Eq. (A6), but for ease of writing only the arguments which contain a ± 1 are shown explicitly [so that, for instance, $G(m_5+1)$ stands for $G(m_1, m_2, m_3; m_4, m_5+1, m_6)$ etc.]

The general solution of these recursions is of great interest, but we consider here only the case $u_1 = u_2 = u_3 = 0$ which corresponds to Hylleraas basis set. For this we put $m_1 = m_2 = m_3 = 1$ and differentiate these identities over u_1, u_2, u_3 at $u_1 = u_2 = u_3 = 0$. It leads to recursions for the h function of Eq. (A7). The first subset of identities forms 3 linear equations for $h(n_1+2), h(m_5+1), h(m_6+1)$ (same convention for the explicitly written indices as for the function G) which can easily be solved. Since there are 9 equations for 6 unknowns, two different solutions for $h(m_4+1), h(m_5+1), h(m_6+1)$ can be used to simplify recursion formulas. We achieve this by solving three equations

$$
\begin{aligned}
h_1(m_4+1) - h_2(m_4+1) &= 0\,, \\
h_1(m_5+1) - h_2(m_5+1) &= 0\,, \\
h_1(m_6+1) - h_2(m_6+1) &= 0\,, \qquad (13)
\end{aligned}
$$

against the following linear combinations

$$
\begin{aligned}
& h(m_5-1, m_6+1) - h(m_4-1, m_6+1)\,, \\
& h(m_5+1, m_6-1) - h(m_4-1, m_5+1)\,, \\
& h(m_4+1, m_5-1) - h(m_4+1, m_6-1)\,. \qquad (14)
\end{aligned}
$$

The solutions obtained are inserted back into recursion formulas for $h(n_i+2)$ and $h(m_i+1)$, and they take the form

$$
\frac{2\, w_2^2\, w_3^2}{n_1+1}\, h(n_1+2) \;=\; [w_3^2\,(2+n_1+n_2+2\,n_3) + w_2^2\,(2+n_1+2\,n_2+n_3) -
$$

$$
\begin{aligned}
& w_1^2\,(2+2\,n_1+n_2+n_3)]\,h()+w_3^2\,Q_3+w_2^2\,Q_2-w_1^2\,Q_1+\ldots \\
\frac{2\,w_1^2\,w_3^2}{n_2+1}\,h(n_2+2) \;=\; & [w_3^2\,(2+n_1+n_2+2\,n_3)-w_2^2\,(2+n_1+2\,n_2+n_3)+ \\
& w_1^2\,(2+2\,n_1+n_2+n_3)]\,h()+w_3^2\,Q_3-w_2^2\,Q_2+w_1^2\,Q_1+\ldots \\
\frac{2\,w_1^2\,w_2^2}{n_3+1}\,h(n_3+2) \;=\; & [-w_3^2\,(2+n_1+n_2+2\,n_3)+w_2^2\,(2+n_1+2\,n_2+n_3)+ \\
& w_1^2\,(2+2\,n_1+n_2+n_3)]\,h()-w_3^2\,Q_3+w_2^2\,Q_2+w_1^2\,Q_1+\ldots \qquad (15)
\end{aligned}
$$

$$
\begin{aligned}
w_1^2\,m_4\,h(m_4+1) &= (-n_1+n_2+n_3+2\,m_4-1)\,h()+2\,(X_3-X_2)+\ldots \\
w_2^2\,m_5\,h(m_5+1) &= (n_1-n_2+n_3+2\,m_5-1)\,h()+2\,(X_1-X_3)+\ldots \\
w_3^2\,m_6\,h(m_6+1) &= (n_1+n_2-n_3+2\,m_6-1)\,h()+2\,(X_2-X_1)+\ldots \qquad (16)
\end{aligned}
$$

where by $\ldots$ we denote the omitted boundary terms, which are proportional to δ_{n_i}, and

$$
\begin{aligned}
Q_1 &= \frac{n_1\,(n_1-1)}{n_3+1}\,h(n_1-2,n_3+2)+\frac{n_1\,(n_1-1)}{n_2+1}\,h(n_1-2,n_2+2)+ \\
&\quad \frac{1}{n_3+1}\,h(n_3+2,m_5-1)+\frac{1}{n_2+1}\,h(n_2+2,m_6-1)\,, \\
Q_2 &= \frac{n_2\,(n_2-1)}{n_3+1}\,h(n_2-2,n_3+2)+\frac{n_2\,(n_2-1)}{n_1+1}\,h(n_1+2,n_2-2)+ \\
&\quad \frac{1}{n_3+1}\,h(n_3+2,m_4-1)+\frac{1}{n_2+1}\,h(n_1+2,m_6-1)\,, \\
Q_3 &= \frac{n_3\,(n_3-1)}{n_2+1}\,h(n_2+2,n_3-2)+\frac{n_3\,(n_3-1)}{n_1+1}\,h(n_1+2,n_3-2)+ \\
&\quad \frac{1}{n_2+1}\,h(n_2+2,m_4-1)+\frac{1}{n_1+1}\,h(n_1+2,m_5-1)\,, \qquad (17)
\end{aligned}
$$

$$
\begin{aligned}
X_1 &= (n_2-1)\,n_2\,m_4\,h(n_2-2,m_4+1)-(n_3-1)\,n_3\,m_4\,h(n_3-2,m_4+1)\,, \\
X_2 &= (n_3-1)\,n_3\,m_5\,h(n_3-2,m_5+1)-(n_1-1)\,n_1\,m_5\,h(n_1-2,m_5+1)\,, \\
X_3 &= (n_1-1)\,n_1\,m_6\,h(n_1-2,m_6+1)-(n_2-1)\,n_2\,m_6\,h(n_2-2,m_6+1)\,. \qquad (18)
\end{aligned}
$$

There is obviously some freedom in using Eqs. (13) to simplify recursions, and our choice allows us to separate recursions into two subshells of $n_1+n_2+n_3$ and $m_4+m_5+m_6$. We put $m_4=m_5=m_6=1$ in Eq. (15) and immediately obtain the first subset of recursions, Eq. (4). The second subset Eq. (5) is obtained from Eq. (16) in three steps. The first step is setting $m_4=m_5=m_6=1$. The second step is multiplication of recursion formulas by $w_i\,w_j$ to remove any w_i from the denominator. The third step is differentiation with respect to w_1, w_2, and w_3, which converts the function $h()$ into the function $f()$. That completes the derivation of recursion relations for three-electron Hylleraas integrals.

V. SUMMARY

We have derived a complete set of recursion relations for the three-electron Hylleraas integral f. They are sufficiently stable for a precise numerical calculation [16]. Since all w_i are bounded from below by approximately $\sqrt{2\,E}$, where E is the ionization energy, the denominators of the three-electron recursions are also bounded from below. Therefore, by using extended precision arithmetic (octuple precision) we can safely devote 1 digit per iteration, and still preserve quad precision for about 30 iterations, which is the maximum we aim to use. Possible instabilities in two-electron integrals are avoided by applying inverse recursions [14]. Further analysis of numerical stability is postponed to a separate work. Numerical results for some specific n_i and w_i are shown in Table I.

TABLE I: Values of three-electron Hylleraas integral at $w_1 = w_2 = w_3 = 1$, [m] denotes 10^m

n	$f(n,0,0;0,0,0)$	$f(0,0,0;n,0,0)$
0	2.208 310 154 388 618 874 536 424[-1]	2.208 310 154 388 618 874 536 424[-1]
1	2.876 820 724 517 809 274 392 190[-1]	2.208 310 154 388 618 874 536 424[-1]
2	6.071 253 765 587 525 062 881 067[-1]	3.658 582 716 243 175 207 969 277[-1]
3	1.801 456 579 614 247 419 513 752[0]	8.803 723 087 040 150 596 505 449[-1]
4	6.949 688 537 201 117 333 162 822[0]	2.849 464 173 126 685 211 199 798[0]
5	3.316 893 553 498 521 645 367 878[1]	1.176 795 411 671 425 935 279 582[1]
6	1.892 427 697 247 010 803 401 964[2]	5.962 899 567 501 152 778 486 008[1]
7	1.258 719 915 821 483 876 136 660[3]	3.596 955 116 745 326 378 301 909[2]
8	9.575 385 319 725 442 534 735 866[3]	2.522 862 411 307 814 783 043 058[3]
9	8.206 804 555 680 135 296 239 238[4]	2.019 476 554 953 447 619 512 494[4]

The obtained recursion relations can be used for a high precision calculation of a lithium wave function with a small computational effort. We think that similar recursions can be derived also for beryllium, which involves four electrons, but the generic integral with all powers of r_{ij} equal to -1 has not yet been obtained. However, this generic integral can be represented as a multiple sum as recently indicated by Sims and Hagstrom [17] and Frolov [18] and thus obtained numerically. Coming back to lithium, our aim is the high precision calculation of higher order relativistic and QED effects like that for lithium hyperfine splitting [19]. It requires, however, also the calculation of Hylleraas integrals with various negative powers of r_i and r_{ij}. $1/r_i^n$ with $n > 1$ can be expressed in terms of harmonic polylogarithms, which were introduced recently in [20], and $1/r_{ij}^n$ can be obtained, we think, by generalization of the recursion relations obtained in this work.

In summary, we have presented a simple method to derive recursion relations and solved them for the three-electron Hylleraas integral.

VI. ACKNOWLEDGMENTS

We are grateful to Vladimir Korobov for his source code of the fast multiprecision arithmetics and of two-electron recursions in the singular case. This work was supported by EU grant HPRI-CT-2001-50034.

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APPENDIX A: DEFINITIONS OF FUNCTIONS AND RELATIONS

We use the symbol δ_n which denotes the Kronecker $\delta_{n,0}$. Definitions of all functions used in this work are presented below. r_{ij} denotes $|\vec{r}_i - \vec{r}_j|$ and $k_{ij} = |\vec{k}_i - \vec{k}_j|$. All the n_i and m_i are assumed to be nonnegative integer and w_i, u_i to be real and positive.

$$F(n_1, n_2, n_3; n_4, n_5, n_6) = \int \frac{d^3 r_1}{4\pi} \int \frac{d^3 r_2}{4\pi} \int \frac{d^3 r_3}{4\pi}\, e^{-w_1 r_1 - w_2 r_2 - w_3 r_3 - u_1 r_{23} - u_2 r_{31} - u_3 r_{12}}\, r_{23}^{n_1-1}\, r_{31}^{n_2-1}\, r_{12}^{n_3-1}\, r_1^{n_4-1}\, r_2^{n_5-1}\, r_3^{n_6-1} \tag{A1}$$

$$f(n_1, n_2, n_3; n_4, n_5, n_6) = \int \frac{d^3 r_1}{4\pi} \int \frac{d^3 r_2}{4\pi} \int \frac{d^3 r_3}{4\pi}\, e^{-w_1 r_1 - w_2 r_2 - w_3 r_3}\, r_{23}^{n_1-1}\, r_{31}^{n_2-1}\, r_{12}^{n_3-1}\, r_1^{n_4-1}\, r_2^{n_5-1}\, r_3^{n_6-1} \tag{A2}$$

$$f(\star, n_2, n_3; n_4, n_5, n_6) = \int \frac{d^3 r_1}{4\pi} \int \frac{d^3 r_2}{4\pi} \int \frac{d^3 r_3}{4\pi}\, e^{-w_1 r_1 - w_2 r_2 - w_3 r_3}\, 4\pi\, \delta^3(r_{23})\, r_{31}^{n_2-1}\, r_{12}^{n_3-1}\, r_1^{n_4-1}\, r_2^{n_5-1}\, r_3^{n_6-1} \tag{A3}$$

$$f(n_1, n_2, n_3; \star, n_5, n_6) = \int \frac{d^3 r_1}{4\pi} \int \frac{d^3 r_2}{4\pi} \int \frac{d^3 r_3}{4\pi}\, e^{-w_1 r_1 - w_2 r_2 - w_3 r_3}\, r_{23}^{n_1-1}\, r_{31}^{n_2-1}\, r_{12}^{n_3-1}\, 4\pi\, \delta^3(r_1)\, r_2^{n_5-1}\, r_3^{n_6-1} \tag{A4}$$

$$\Gamma(n_1, n_2, n_3; \alpha_1, \alpha_2, \alpha_3) = \int \frac{d^3 r_1}{4\pi} \int \frac{d^3 r_2}{4\pi}\, e^{-\alpha_1 r_1 - \alpha_2 r_2 - \alpha_3 r_{12}}\, r_1^{n_1-1}\, r_2^{n_2-1}\, r_{12}^{n_3-1} \tag{A5}$$

$$G(m_1,m_2,m_3;m_4,m_5,m_6) = \frac{1}{8\,\pi^6}\int d^3k_1\int d^3k_2\int d^3k_3\,(k_1^2+u_1^2)^{-m_1}\,(k_2^2+u_2^2)^{-m_2} \\ (k_3^2+u_3^2)^{-m_3}\,(k_{32}^2+w_1^2)^{-m_4}\,(k_{13}^2+w_2^2)^{-m_5}\,(k_{21}^2+w_3^2)^{-m_6} \tag{A6}$$

$$h(n_1,n_2,n_3;m_4,m_5,m_6) = (-1)^{n_1}\,\frac{\partial^{n_1}}{\partial u_1^{n_1}}\Big|_{u_1=0}(-1)^{n_2}\,\frac{\partial^{n_2}}{\partial u_2^{n_2}}\Big|_{u_2=0}(-1)^{n_3}\,\frac{\partial^{n_3}}{\partial u_3^{n_3}}\Big|_{u_3=0} \\ G(1,1,1,m_4,m_5,m_6) \tag{A7}$$

$$f(n_1,n_2,n_3;n_4,n_5,n_6) = (-1)^{n_4}\,\frac{\partial^{n_4}}{\partial w_1^{n_4}}\,(-1)^{n_5}\,\frac{\partial^{n_5}}{\partial w_2^{n_5}}\,(-1)^{n_6}\,\frac{\partial^{n_6}}{\partial w_3^{n_6}}\,h(n_1,n_2,n_3,1,1,1) \tag{A8}$$