Convergence Accelerator Approach for the Evaluation of Some Three-Electron Integrals Containing Explicit r_{ij} Factors

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ABSTRACT: A simplified analysis is presented for the evaluation of the three-electron one-center integrals of the form $\int r_1^i r_2^j r_3^k r_{23}^l r_{31}^m r_{12}^n e^{-\alpha r_1 - \beta r_2 - \gamma r_3} d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3$, for the cases $i, j, k, \geq -2, l = -2, m \geq -1, n \geq -1$. These integrals arise in the calculation of lower bounds for energy levels and certain relativistic corrections to the energy when Hylleraas-type basis sets are employed. Convergence accelerator techniques are employed to obtain a reasonable number of digits of precision, without excessive CPU requirements.
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Key words: convergence accelerator; three-electron integrals

Introduction

There has been considerable recent progress on high-precision calculations for atomic three-electron systems, and the lithium atom has been the focus of much of this effort (see [1] and [2] for reviews on recent progress). Two principal areas where progress has been significantly restricted are the evaluation of lower bounds [3, 4] for energy levels and the evaluation of high-precision estimates for some of the relativistic corrections [5]. The highest precision results for several properties of the ^2S states of three-electron systems have been obtained using the Hylleraas or CI–Hylleraas techniques [3, 4, 6–11]. Using Hylleraas-type functions, the integration problem reduces to the evaluation of the integrals

$$I(i, j, k, l, m, n, \alpha, \beta, \gamma)$$
$$= \int r_1^i r_2^j r_3^k r_{23}^l r_{31}^m r_{12}^n e^{-\alpha r_1 - \beta r_2 - \gamma r_3} d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3, \quad (1)$$

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where r_i denotes an electron–nuclear distance and r_{ij} is an electron–electron separation.

The integrals in Eq. (1) can be divided into two basic groups: those integrals having $l, m, n \geq -1$ and those integrals having one of the indices $l, m, n = -2$. To evaluate the energy and a large number of other properties, only the case l, m, n, each ≥ -1, arises. These integrals and some related generalizations have been extensively discussed in the literature [12–23]. Evaluating lower bounds to the energy, or some of the relativistic corrections to the energy levels, requires integrals where one of $l, m, n = -2$. This is a much more difficult case and is the underlying reason why success on the aforementioned two problems has been somewhat limited. The purpose of this work was to discuss the evaluation of Eq. (1) for cases where one of $l, m, n = -2$. These integrals and some related generalizations have received considerably less attention than has the other case mentioned above [24–29].

In what follows, we will set $l = -2$. Previous work [24–28] on the evaluation of Eq. (1) for $l = -2$ can be broken up into three distinct groups: (i) m and n *not* both odd and ≥ -1, (ii) m and n *both* odd, and (iii) one of m or $n = -2$. Fairly effective methods have been devised to treat integrals in case (i) [24]. The integrals in case (iii) [26, 27] arise when the most general Hylleraas-type expansion is employed, but these integrals can be circumvented by some minor restrictions on the basis set. The integrals in case (ii) *cannot* be avoided with any realistic restrictions imposed on the basis set. These integrals are a principal focus of this work. In previous efforts with the integrals in case (ii), the following approaches have been employed: The first involves a series expansion of some integrals involving logarithmic functions [25, 26]. Methods to solve these integrals via special logarithmic-function quadratures have been developed [25]. A scheme based on the series expansion of r_{ij}^{-2} in terms of Gegenbauer polynomials has been developed [27] and an alternative series approach has been discussed [28].

Theory

In the present work, r_{23}^{-2} is expanded as the product $(r_{23}^{-1})(r_{23}^{-1})$ and the standard expansion of r_{23}^{-1} in terms of Legendre polynomials is employed. At first sight, this approach would not appear to be useful, because the expansion of r_{23}^{-2} [24, 27, 30, 31] has the following form [24]:

$$
\begin{aligned}
\frac{1}{r_{23}^2} = \sum_{l=0}^{\infty}\left[\frac{2l+1}{2}\right]4^{-l}
&\times\Bigg[\ln\left|\frac{r_2+r_3}{r_2-r_3}\right|\sum_{\kappa=0}^{l} r_2^{2\kappa-l-1}r_3^{l-2\kappa-1}\\
&\times\sum_{\nu=0}^{\min[\kappa,l-\kappa]}(-4)^{\nu}\binom{l}{\nu}\binom{2l-2\nu}{l}\binom{l-2\nu}{\kappa-\nu}\\
&-2\sum_{\kappa=0}^{l-1} r_2^{-l+2\kappa}r_3^{l-2\kappa-2}\\
&\times\sum_{j=0}^{\min[\kappa,l-\kappa-1]}4^{j}\binom{l-2j-1}{\kappa-j}\\
&\times\sum_{\nu=0}^{j}\frac{(-1)^{\nu}\binom{l}{\nu}\binom{2l-2\nu}{l}}{2j-2\nu+1}\Bigg]P_l(\cos\theta_{23}).
\end{aligned}
\tag{2}
$$

Equation (2) can be written in a symmetric form in the variables r_2 and r_3, which is more suitable for examining the convergence behavior of the expansion in terms of r_2 and r_3. However, that form is less useful for the evaluation of integrals (see [24] for details). Dealing with the logarithmic terms in Eq. (2) leads to considerable additional complexities [24]. Employing the standard expansion of r_{23}^{-1} leads to much simpler integration problems, but at the cost, not surprisingly, of producing a much more slowly converging series. This latter problem can be addressed by resorting to convergence accelerator techniques to carry out the required summations. Some useful discussion on the expansion of r_{ij}^{-2} can be found in the work of Steinborn and Filter [32].

Inserting the standard expansion for r_{23}^{-1} and the Sack expansions [33] for r_{31}^{m} and r_{12}^{n} into Eq. (1) leads to the result

$$
\begin{aligned}
I &\equiv I(i,j,k,-2,m,n,\alpha,\beta,\gamma)\\
&= \sum_{l_1=0}^{\infty}\sum_{l_2=0}^{\infty}\sum_{p=0}^{\infty}\sum_{q=0}^{\infty}\int r_1^i r_2^j r_3^k e^{-\alpha r_1-\beta r_2-\gamma r_3}\\
&\quad\times\frac{r_{23<}^{l_1+l_2}}{r_{23>}^{l_1+l_2+2}}R_{mp}(r_3,r_1)R_{nq}(r_1,r_2)
\end{aligned}
$$

$$\times P_{l_1}(\cos\theta_{23})P_{l_2}(\cos\theta_{23})P_p(\cos\theta_{31}) \times P_q(\cos\theta_{12})d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3. \tag{3}$$

In Eq. (3), $R_{mp}(r_3, r_1)$ is a Sack radial function [33], $P_p(\cos\theta_{31})$ denotes a Legendre polynomial, $r_{23<}$ represents $\min(r_2, r_3)$, and $r_{23>}$ signifies $\max(r_2, r_3)$. The angular integral I_Ω in Eq. (3) is

$$I_\Omega = \int P_{l_1}(\cos\theta_{23})P_{l_2}(\cos\theta_{23})P_p(\cos\theta_{31}) \times P_q(\cos\theta_{12})\, d\Omega_1 d\Omega_2 d\Omega_3, \tag{4}$$

which can be evaluated by expanding the Legendre polynomials in terms of spherical harmonics, leading to

$$I_\Omega = \frac{256\pi^4}{(2l_1+1)(2l_2+1)(2p+1)(2q+1)} \times \sum_{m_1=-l_1}^{l_1}\sum_{m_2=-l_2}^{l_2}\sum_{P=-p}^{p}\sum_{Q=-q}^{q}\int Y^*_{qQ}(\theta_1,\phi_1) \times Y_{pP}(\theta_1,\phi_1)\, d\Omega_1 \times \int Y^*_{l_1m_1}(\theta_2,\phi_2)Y^*_{l_2m_2}(\theta_2,\phi_2)Y_{qQ}(\theta_2,\phi_2)\, d\Omega_2 \times \int Y_{l_1m_1}(\theta_3,\phi_3)Y_{l_2m_2}(\theta_3,\phi_3)Y_{pP}(\theta_3,\phi_3)\, d\Omega_3. \tag{5}$$

Using standard results for the integrals over spherical harmonics, Eq. (5) can be simplified to

$$I_\Omega = \frac{64\pi^3}{(2p+1)}\delta_{pq}\begin{pmatrix} l_1 & l_2 & p \\ 0 & 0 & 0 \end{pmatrix}^2, \tag{6}$$

where δ_{pq} is a Kronecker delta and $\left(\begin{smallmatrix} a & b & c \\ d & e & f\end{smallmatrix}\right)$ denotes a 3-j symbol. For large values of l_1, the 3-j symbols can be computed effectively using a recursive scheme [34, 35]. The optimal approach is to table them, thereby making the calculation of the 3-j symbols a rather minor part of the overall calculation.

The Sack radial functions can be written as [33]

$$R_{mp}(r_3, r_1) = r_{13>}^{m-p} r_{13<}^{p} \sum_{t=0}^{\infty} a_{pmt}\left(\frac{r_{13<}}{r_{13>}}\right)^{2t}, \tag{7}$$

where

$$a_{pmt} = \frac{\left(\frac{-m}{2}\right)_p \left(p - \frac{m}{2}\right)_t \left(-\frac{1}{2} - \frac{m}{2}\right)_t}{\left(\frac{1}{2}\right)_p t! \left(p + \frac{3}{2}\right)_t}, \tag{8}$$

and $(a)_b$ denotes a Pochhammer symbol.

If Eq. (7) and the analogous result for $R_{np}(r_1, r_2)$ and Eq. (6) are substituted into Eq. (3), then

$$I = 64\pi^3 \sum_{l_1=0}^{\infty}\sum_{l_2=0}^{\infty}\sum_{p=0}^{\infty}\frac{\begin{pmatrix} l_1 & l_2 & p \\ 0 & 0 & 0\end{pmatrix}^2}{(2p+1)} \times \sum_{t=0}^{\infty} a_{pmt}\sum_{u=0}^{\infty} a_{pnu}\int r_1^{i+2}r_2^{j+2}r_3^{k+2}r_{23<}^{l_1+l_2} \times r_{23>}^{-l_1-l_2-2} r_{13<}^{p+2t} r_{13>}^{m-p-2t} r_{12<}^{p+2u} r_{12>}^{n-p-2u} \times e^{-\alpha r_1 - \beta r_2 - \gamma r_3}\, dr_1\, dr_2\, dr_3. \tag{9}$$

On splitting the integration domain, the radial integral in Eq. (9) can be simplified into a sum of integrals of the form

$$W(I, J, K, \alpha, \beta, \gamma) = \int_0^\infty x^I e^{-\alpha x}\, dx \int_x^\infty y^J e^{-\beta y}\, dy \int_y^\infty z^K e^{-\gamma z}\, dz. \tag{10}$$

These W-integrals have been discussed extensively in the literature [12, 13, 17, 20, 21, 36–38]. Equation (9) simplifies to

$$I = 64\pi^3 \sum_{l_1=0}^{\infty}\sum_{l_2=0}^{\infty}\sum_{p=0}^{\infty}\frac{\begin{pmatrix} l_1 & l_2 & p \\ 0 & 0 & 0\end{pmatrix}^2}{2p+1} \times \sum_{t=0}^{\infty} a_{pmt}\sum_{u=0}^{\infty} a_{pnu} \times \{W(i+2+2p+2u+2t, j+2+n+l_{12} - p - 2u, k+m-p-2t-l_{12}, \alpha, \beta, \gamma) + W(i+2+2p+2u+2t, k+2+m+l_{12}-p-2t, j+n-p-2u-l_{12}, \alpha, \gamma, \beta) + W(j+2+p+2u+l_{12}, i+2+2t+n-2u, k+m-l_{12}-p-2t, \beta, \alpha, \gamma) + W(j+2+p+2u+l_{12}, k+p+2t-l_{12}, i+2, m+n-2p-2t-2u, \beta, \gamma, \alpha)$$

$$+W(k+2+p+2t+l_{12}, i+2+m+2u-2t, j+n-p-2u-l_{12}, \gamma, \alpha, \beta) + W(k+2+p+2t+l_{12}, j+p+2u-l_{12}, i+2+m+n-2p-2t-2u, \gamma, \beta, \alpha)\}, \tag{11}$$

where $l_{12} = l_1 + l_2$. Equation (11) is a key result of this work.

We now focus on some computational simplifications. The t-summation in Eq. (11) is finite:

$$t_{\max} = \left(\frac{m}{2} - p\right) \quad \text{for } m \text{ even} \tag{12}$$

$$t_{\max} = \frac{m+1}{2} \quad \text{for } m \text{ odd}, \tag{13}$$

which follows from the definition of the a_{pmt} coefficient in Eq. (8) and the properties of the Pochhammer symbol. In a similar fashion, the u-summation terminates at $u_{\max} = (n/2) - p$ for n even, or $u_{\max} = (n+1)/2$ for n odd. The p-summation terminates at

$$p_{\max} = \begin{cases} l_1 + l_2 & m \text{ and } n \text{ both odd} \\ \min\left[l_1 + l_2, \frac{m}{2}\right] & m \text{ even}, n \text{ odd} \\ \min\left[l_1 + l_2, \frac{n}{2}\right] & n \text{ even}, m \text{ odd} \\ \min\left[l_1 + l_2, \frac{m}{2}, \frac{n}{2}\right] & m \text{ and } n \text{ both even}. \end{cases} \tag{14}$$

In Eq. (14), the constraints depending on m and/or n arise from the term $(-m/2)_p(-n/2)_p$ in Eq. (11), which comes from the product $a_{pmt}a_{pnu}$. The constraint involving $l_1 + l_2$ follows from the triangle inequality condition for the 3-j symbol:

$$|l_1 - l_2| \le p \le l_1 + l_2. \tag{15}$$

The triple sum in Eq. (11) can be simplified by noting that the W-integrals depend on $l_1 + l_2$. Hence, the triple sum can be decomposed as

$$\sum_{l_1=0}^{\infty} \sum_{l_2=0}^{\infty} \sum_{p=0}^{\infty} \{\,\} = \sum_{\substack{l_1=0 \\ (l_2=l_1)}}^{\infty} \sum_{p=0}^{\infty} \{\,\} + 2 \sum_{l_1=1}^{\infty} \sum_{l_2=0}^{l_1-1} \sum_{p=0}^{\infty} \{\,\} \tag{16}$$

and

$$\sum_{\substack{l_1=0 \\ (l_2=l_1)}}^{\infty} \sum_{p=0}^{\infty} \{\,\} = \sum_{\substack{l_1=0 \\ (l_2=l_1)}}^{\infty} \sum_{\substack{p=0 \\ (p,\ even)}}^{p_{\max}} \{\,\}, \tag{17}$$

with $p_{\max}$ given in Eq. (14) (with $l_1 + l_2 \to 2l_1$). The even condition on p in Eq. (17) follows from the condition that the 3-j symbol

$$\begin{pmatrix} l_1 & l_1 & p \\ 0 & 0 & 0 \end{pmatrix} = 0 \quad \text{for } p \text{ odd}. \tag{18}$$

The triple summation in Eq. (16) can be written as

$$\sum_{l_1=1}^{\infty} \sum_{l_2=0}^{l_1-1} \sum_{p=0}^{\infty} \{\,\} = \sum_{l_1=1}^{\infty} \sum_{l_2=0}^{l_1-1} \left[\sum_{p=l_1-l_2}^{p_{\max}} \{\,\} \right]. \quad (l_1 + l_2 \text{ even} \Rightarrow p \text{ even}) \quad (l_1 + l_2 \text{ odd} \Rightarrow p \text{ odd}) \tag{19}$$

Computational Approach

In light of the remarks made in the last section, particularly those connected with the replacement of Eq. (2) by a double-infinite summation, a direct numerical evaluation of the I-integrals by series summation using Eq. (11) is not feasible. Instead, evaluation of Eq. (11) is facilitated by the use of convergence accelerator techniques. For a recent review of accelerator techniques, see Weniger [39–41] or the recent text on extrapolation methods [42]. The technique employed to sum the series in Eq. (11) is the Levin u transform [43]. The Levin u transform is a powerful general-purpose convergence accelerator technique. For the type of series behavior expected in this work, the Levin u transform is expected to be among the better choices to achieve reasonable convergence [44, 45].

A sequence of partial sums for a particular series are defined by

$$S_n = \sum_{w=0}^{n} A_w \tag{20}$$

and we suppose these converge to the limit S. Then, an improved set of approximations to the sum is given by

$$u_k = \frac{\sum_{j=0}^{k} c_j(k, A_j) S_j}{\sum_{j=0}^{k} c_j(k, A_j)}, \qquad (21)$$

with

$$c_j(k, A_j) = (-1)^j \binom{k}{j} (j+1)^{k-2} A_j^{-1} \qquad (22)$$

and $\binom{k}{j}$ denotes a binomial coefficient. Equation (21) is Levin's u transformation, which is well known to be particularly effective to numerically sum series with logarithmic convergence characteristics. Equation (21) can be evaluated in a recursive manner [46]. The Levin u transformation was applied to Eq. (11) with the triple infinite sum (*over* l_1, l_2, p) simplified as in Eqs. (16), (17), and (19). The l_1-summation is evaluated up to some maximum value, which becomes the termination point for u_k.

Table I illustrates the convergence behavior of a representative I-integral as a function of the index k in Eq. (21). The precision level employed for the calculation was 30 digits (which corresponds to approximately Fortran double precision with a 64-bit word or quadruple precision with a 32-bit word). Table II shows the results for a number of I-integrals. The first 15 results have been previously evaluated using alternative methods [24], and these represent the easier of the more difficult $l = -2$ cases. These 15 values were evaluated using higher-precision arithmetic, and the results can therefore serve as benchmarks for alternative evaluation schemes. In several cases, these results improve on the accuracy of values given elsewhere [24]. The second group of examples, those involving both m and n odd, provide a good test of the procedure. For these cases, the results presented in Table II agree with results from more complicated evaluations to the precision level that is apparent from the earlier work [25, 27,* 28].

TABLE I
Convergence of the integral $I(1, 1, 1, -2, 1, 1, 2.7, 2.7, 2.7)$ as a function of the index k in the Levin u transform.

Levin index k	I-integral[a]
0	5.096
1	6.483
2	7.078
3	7.177
4	7.18666
5	7.18799
6	7.187861
7	7.187624
8	7.1876386
9	7.1876467
10	7.18764638
11	7.187646258
12	7.187646242
13	7.1876462442
14	7.18764624507
15	7.187646245098
16	7.187646245088
17	7.187646245089
18	7.1876462450905
19	7.1876462450912
20	7.1876462450915
21	7.1876462450917
22	7.1876462450917
23	7.18764624509178
24	7.18764624509180
25	7.18764624509182
26	7.1876462450918
27	7.1876462450918
28	7.187646245092
29	7.187646245092
30	7.18764624509
31	7.18764624509
32	7.1876462451
33	7.1876462451
34	7.187646245
35	7.18764625
36	7.18764625

[a] Value of the integral computed using higher-precision arithmetic is 7.1876462450918377526396.

Discussion

The I-integrals for the more difficult odd m-odd n cases were evaluated to a precision level of around 12–15 digits (with one exception) in a rather straightforward approach. The convergence is relatively quick to reach this precision level. Typically, about 25 terms in the sum are required to reach the aforementioned level of precision. The most slowly converging cases in the present study have $l = -2$, $m = -1$, $n = -1$. For these cases, alternative methods give improved precision [28].

* A typographical error has been found in this work: There is a factor of $\tau!$ missing from the denominator of Eq. (14).

TABLE II
Some representative *I*-integrals computed using Eq. (11).

i	j	k	l	m	n	α	β	γ	I-integral
0	0	0	−2	0	0	2	2	2	$2.0670851120199880116984210044 7 \times 10^{1}$
2	2	2	−2	0	0	2.7	2.9	0.65	$3.0519140965850573055900245 75 \times 10^{2}$
−2	−2	−1	−2	0	0	2.7	2.9	0.65	$6.4043353229072602890633999842 3 \times 10^{2}$
0	0	0	−2	0	2	2.7	2.9	0.65	$5.8346389252505330054048206453 \times 10^{1}$
0	0	0	−2	0	4	2.7	2.9	0.65	$3.4340509393876867695194904738 \times 10^{2}$
3	3	2	−2	2	4	2.7	2.9	0.65	$8.3820939334531531196177093106 2 \times 10^{6}$
0	0	0	−2	6	4	0.5	0.5	1.0	$2.3581983027829121164584068815 7 \times 10^{16}$
3	3	2	−2	−1	0	2.7	2.9	0.65	$2.5733614215267942389457451615 6 \times 10^{2}$
1	1	1	−2	1	0	2.7	2.9	0.65	$1.6549150099585140789822711495 9 \times 10^{2}$
3	2	3	−2	3	0	2.7	2.9	0.65	$1.2620751004179325494963810220 5 \times 10^{6}$
−1	−1	3	−2	5	4	2.5	3.0	0.6	$1.1057391366407830629785132400 0 \times 10^{9}$
3	2	3	−2	−1	2	2.7	2.9	0.65	$4.5804291719808937134810767194 0 \times 10^{3}$
3	2	3	−2	1	2	2.7	2.9	0.65	$1.6552544122267435228875325600 5 \times 10^{5}$
3	2	3	−2	3	2	2.7	2.9	0.65	$1.3161858453611410146441229567 2 \times 10^{7}$
−2	−2	2	−2	−1	2	2.7	2.9	0.65	$2.9869654128578295059988954795 6 \times 10^{2}$
0	0	0	−2	−1	−1	2.7	2.9	0.65	1.5271059×10^{1}
0	0	0	−2	−1	1	2.7	2.9	0.65	$1.69867816033 \times 10^{1}$
0	0	0	−2	1	1	2.7	2.9	0.65	$8.0102940206259 \times 10^{1}$
0	0	0	−2	1	3	2.7	2.9	0.65	$4.057986194190158 \times 10^{2}$
0	0	0	−2	3	3	2.7	2.9	0.65	$7.59274487125250 \times 10^{3}$
0	0	0	−2	3	5	2.7	2.9	0.65	$8.3470410214165 \times 10^{4}$
0	0	0	−2	5	5	2.7	2.9	0.65	$3.7444633460214 \times 10^{6}$

A well-known difficulty associated with the application of Levin's u transformation is the severe loss of precision for higher values of k in Eq. (21). This point is illustrated for a representative example in Table I. No general algorithm is currently available which avoids this problem of precision loss for series summation using acceleration techniques, although a series transformation has been found that solves this problem for a large number of the I integrals satisfying $l, m, n \geq -1$ [23]. The Richardson extrapolation technique, which is often very effective for summing series with logarithmic convergence, also suffers from the same loss of precision problems. These problems can be circumvented by working with a multiple precision arithmetic routine in a Fortran code, but this is at the cost of more significant CPU resources.

Extensions of the present work are in progress in which alternative methods [39–41] to deal with the convergence accelerator precision problems are being attacked. The result presented in Eq. (11) is rather simple in structure and may prove to be a very good starting point for applying different convergence accelerator techniques. Judicious application of the approach developed in [23] may possibly lead to more effective convergence accelerator schemes for the evaluation of these difficult integrals.

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