Asymptotic-expansion method for the evaluation of correlated three-electron integrals

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(Received 5 July 1995)

An asymptotic-expansion method is presented for the evaluation of correlated three-electron integrals arising in Hylleraas-type variational calculations for lithium and other many-electron atoms. The method proves to be very efficient in accelerating the rate of convergence of an infinite series representation of the integrals. An analytic expression for the terms in the series is derived.

PACS number(s): 31.15.Ar, 31.25.Eb, 02.70−.C, 31.15.Pf

I. INTRODUCTION

Hylleraas-type basis sets, which include explicitly powers of the interelectronic distance $r_{12}=|\mathbf{r}_1-\mathbf{r}_2|$, [1] are well-established as providing the most accurate wave functions and energies in variational calculations for helium [2–4] and other three-body systems [5]. These calculations are particularly efficient owing to a simple closed-form expression for all the required correlated two-electron integrals [6].

The same methods can, in principle, be extended to lithium and beyond, but there is no longer a simple, closed-form expression for the most general integral of the form

$$I(j_1,j_2,j_3,j_{12},j_{23},j_{31};\alpha,\beta,\gamma)$$

$$=\int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 r_1^{j_1} r_2^{j_2} r_3^{j_3} r_{12}^{j_{12}} r_{23}^{j_{23}} r_{31}^{j_{31}} e^{-\alpha r_1-\beta r_2-\gamma r_3}\ , \quad (1)$$

involving correlations among all three particle pairs r_{12}, r_{23}, and r_{31}. The numerical summation of an infinite series is required if all three of the powers j_{12}, j_{23}, and j_{31} are odd numbers. For a given size of basis set, the calculation therefore becomes less efficient by several orders of magnitude relative to the two-electron (three-body) case, with the calculation of integrals being the rate-determining step. Also, the preservation of numerical accuracy becomes much more difficult.

Early work on the integral (1) with $j_\mu \geq -2$ and $j_{\mu\nu}\geq -1$ can be found in Refs. [7–13]. The main technique used by these authors (except Fromm and Hill) is to expand $r_{\mu\nu}$ in terms of individual coordinates r_μ and r_ν as well as Legendre polynomials. One way to avoid infinite summations is to place some restrictions on the choice of basis set so that at least one of the three powers in each integral is even [7,8,11,14]. However, such restrictions may seriously affect the rate of convergence of the basis set. King and Shoup [15] attempted to include all possible powers of r_μ and $r_{\mu\nu}$ such that

$$j_1+j_2+j_3+j_{12}+j_{23}+j_{31}\leq\Omega\ . \quad (2)$$

Since the number of integrals involved increases rapidly as Ω is enlarged, they were unable to proceed to large basis sets. Also, because of the time-consuming nature of the calculations, none of the nonlinear parameters in their basis sets was varied. The eigenvalues they obtained were only accurate to about 1 ppm. The best previous variational calculation in Hylleraas coordinates was done for the lithium ground state by McKenzie and Drake [16]. They performed a series of calculations for $\Omega\leq 7$, producing basis sets with up to 1134 terms. Nevertheless, the work was very time consuming, and was limited to the ground state. A generalization of integral (1) has been studied by Fromm and Hill [13]. Although a close form was obtained by them, problems of computational efficiency remain, and no application of their formula to lithium calculations has been reported.

The main purpose of this paper is to present an asymptotic-expansion method which reduces the time required to calculate even the most troublesome integrals by a factor of several hundreds, while preserving accuracy and numerical stability. It is essentially identical to a method used by Drake and Swainson [17] to perform sums over infinite sequences of states in their calculation of Bethe logarithms. The method has recently been successfully applied to the low-lying states of lithium [18], giving accuracies of a few parts in 10^{10} to 10^{11} for the nonrelativistic eigenvalues of the $2\,^2S$, $2\,^2P$, and $3\,^2D$ states. Thus, a major obstacle to the further progress has now been removed and large-scale high precision calculations for lithium atoms become feasible.

II. ASYMPTOTIC EXPANSION

A. Derivation

We begin with the expansion for the interelectron coordinate r_{12},

$$r_{12}^j=\sum_{q=0}^{L_1} P_q(\cos\theta_{12})\sum_{k=0}^{L_2} C_{jqk} r_<^{q+2k} r_>^{j-q-2k}\ , \quad (3)$$

derived by Perkins [10], where, for even values of j, $L_1=\frac{1}{2}j$, $L_2=\frac{1}{2}j-q$; for odd values of j, $L_1=\infty$, $L_2=\frac{1}{2}(j+1)$. Also in (3), $r_<=\min(r_1,r_2)$, $r_>=\max(r_1,r_2)$, and the coefficients are given by

$$C_{jqk}=\frac{2q+1}{j+2}\binom{j+2}{2k+1}\prod_{t=0}^{S_{qj}}\frac{2k+2t-j}{2k+2q-2t+1}\ , \quad (4)$$

where $S_{qj}=\min[q-1,\frac{1}{2}(j+1)]$. After expanding each of the $r_{\mu\nu}^{j_{\mu\nu}}$ in (1) and applying the addition theorem for spherical harmonics, the integral I can be simplified into its final form [10],

$$I=\sum_{q=0}^{\infty} T(q)\ , \quad (5)$$

with

$$T(q)=(4\pi)^3\sum_{k_{12}=0}^{L_{12}}\sum_{k_{23}=0}^{L_{23}}\sum_{k_{31}=0}^{L_{31}}\frac{1}{(2q+1)^2}C_{j_{12}qk_{12}}C_{j_{23}qk_{23}}C_{j_{31}qk_{31}}$$
$$\times[W(\tilde{j}_1+2q+2k_{12}+2k_{31},\ \tilde{j}_2+j_{12}-2k_{12}+2k_{23},\ \tilde{j}_3+j_{23}-2q-2k_{23}+j_{31}-2k_{31};\ \alpha,\beta,\gamma)$$
$$+W(\tilde{j}_1+2q+2k_{12}+2k_{31},\ \tilde{j}_3+j_{31}-2k_{31}+2k_{23},\ \tilde{j}_2+j_{12}-2q-2k_{12}+j_{23}-2k_{23};\ \alpha,\gamma,\beta)$$
$$+W(\tilde{j}_2+2q+2k_{12}+2k_{23},\ \tilde{j}_1+j_{12}-2k_{12}+2k_{31},\ \tilde{j}_3+j_{23}-2q-2k_{23}+j_{31}-2k_{31};\ \beta,\alpha,\gamma)$$
$$+W(\tilde{j}_2+2q+2k_{12}+2k_{23},\ \tilde{j}_3+j_{23}-2k_{23}+2k_{31},\ \tilde{j}_1+j_{12}-2q-2k_{12}+j_{31}-2k_{31};\ \beta,\gamma,\alpha)$$
$$+W(\tilde{j}_3+2q+2k_{23}+2k_{31},\ \tilde{j}_1+j_{31}-2k_{31}+2k_{12},\ \tilde{j}_2+j_{12}-2q-2k_{12}+j_{23}-2k_{23};\ \gamma,\alpha,\beta)$$
$$+W(\tilde{j}_3+2q+2k_{23}+2k_{31},\ \tilde{j}_2+j_{23}-2k_{23}+2k_{12},\ \tilde{j}_1+j_{12}-2q-2k_{12}+j_{31}-2k_{31};\ \gamma,\beta,\alpha)]\ , \tag{6}$$

where $L_{\mu\nu}=\frac{1}{2}(j_{\mu\nu}+1)$, and $\tilde{j}_i=j_i+2$, $i=1,2,3$. In (6), we have also assumed that all the $j_{\mu\nu}$ are odd integers; otherwise, I becomes a finite sum. W is a subsidiary integral defined by

$$W(l,m,n;\alpha,\beta,\gamma)=\int_0^\infty dx x^l e^{-\alpha x}\int_x^\infty dy y^m e^{-\beta y}\int_y^\infty dz z^n e^{-\gamma z}\ . \tag{7}$$

Traditionally, the W integral has been evaluated by applying several recursion relations, as outlined by Öhrn and Nordling [9]. However, as derived in the Appendix, the general analytic expression is

$$W(l,m,n;\alpha,\beta,\gamma)=\frac{l\,!}{(\alpha+\beta+\gamma)^{l+m+n+3}}\sum_{p=0}^{\infty}\frac{(l+m+n+p+2)!}{(l+1+p)!(l+m+2+p)}\left(\frac{\alpha}{\alpha+\beta+\gamma}\right)^p$$
$$\times{}_2F_1\left(1,l+m+n+p+3;l+m+p+3;\frac{\alpha+\beta}{\alpha+\beta+\gamma}\right), \tag{8}$$

with ${}_2F_1$ being the hypergeometric function. The above formula is valid for $l\geq 0$, $l+m+1\geq 0$, and $l+m+n+2\geq 0$. Since each term in (8) is positive, the series is numerically stable against roundoff errors. The hypergeometric functions may be accurately calculated using the backward recursion relation

$${}_2F_1(1,s+t;s;z)=1+\left(\frac{s+t}{s}\right)z\ {}_2F_1(1,s+t+1;s+1;z)\ . \tag{9}$$

The above recursion relation has also been tested and found to be numerically stable. The main advantage of (8) is its simplicity of form so that it can be easily implemented with the help of recursion relation (9). From (8), the rate of convergence of W is completely determined by the ratio

$$\frac{\alpha}{\alpha+\beta+\gamma}\ .$$

The asymptotic-expansion method follows from the asymptotic behavior of $T(q)$, as $q\to\infty$. From (4), the asymptotic behavior of C_{jqk} is

$$C_{jqk}\sim\frac{1}{q^{(j+1)/2}}\ , \tag{10}$$

and from (8), it can be seen that the W in (6) have the asymptotic dependence

$$W\sim\frac{1}{q^2} \tag{11}$$

by remembering that the dominating part of ${}_2F_1$ is 1. Finally, by combining (10) and (11) we obtain

$$T(q)\sim\frac{1}{q^\lambda},\quad q\to\infty\ , \tag{12}$$

where

$$\lambda=\frac{j_{12}+1}{2}+\frac{j_{23}+1}{2}+\frac{j_{31}+1}{2}+4\ . \tag{13}$$

The basic idea of the asymptotic-expansion method is to split the integral I from Eq. (5) into the two parts

$$I=I_{0,N}+I_{N+1,\infty}\ , \tag{14}$$

where

$$I_{0,N}=\sum_{q=0}^{N}T(q)\ , \tag{15}$$

$$I_{N+1,\infty}=\sum_{q=N+1}^{\infty}T(q)\ . \tag{16}$$

TABLE I. Convergence study of the integral $I(0,0,0,-1,-1,-1;1,1,1)$. $S_d(N)$ is the partial sum of the first N terms for the series expansion of the integral I, $S_a(N)$ is $S_d(N)$ with the asymptotic expansion included, $\Delta S_d = S_d(N) - S_d(N-1)$, and $\Delta S_a = S_a(N) - S_a(N-1)$.

N	$S_d(N)$	$\Delta S_d(N)$	$S_a(N)$	$\Delta S_a(N)$
7	684.034 879		684.113 411 762 670 353	
8	684.058 079	0.023 200	684.113 411 763 922 386	0.000 000 001 252 0
9	684.072 982	0.014 902	684.113 411 823 052 047	0.000 000 059 129 7
10	684.082 984	0.010 002	684.113 411 837 751 073	0.000 000 014 699 0
11	684.089 944	0.006 959	684.113 411 841 286 052	0.000 000 003 535 0
12	684.094 935	0.004 990	684.113 411 842 217 374	0.000 000 000 931 3
13	684.098 606	0.003 671	684.113 411 842 489 995	0.000 000 000 272 6
14	684.101 367	0.002 760	684.113 411 842 578 216	0.000 000 000 088 2
15	684.103 481	0.002 114	684.113 411 842 609 139	0.000 000 000 030 9
16	684.105 129	0.001 647	684.113 411 842 621 076	0.000 000 000 011 9
17	684.106 432	0.001 302	684.113 411 842 625 965	0.000 000 000 004 9
18	684.107 475	0.001 043	684.113 411 842 627 556	0.000 000 000 001 6
19	684.108 320	0.000 845	684.113 411 842 629 489	0.000 000 000 001 9
20	684.109 012	0.000 692	684.113 411 842 629 034	−0.000 000 000 000 5
21	684.109 585	0.000 572	684.113 411 842 629 034	0.000 000 000 000 0
Exact			684.113 411 842 629 911 836 172	
Fromm and Hill [a]			684.113 411 842 629 911 836	

[a]Reference [13].

Then $I_{0,N}$ can be calculated exactly, and, for N sufficiently large, the $T(q)$ terms contained in the remainder $I_{N+1,\infty}$ can be estimated from their asymptotic expansions

$$T(q)=\sum_{i=0}^{\infty}\frac{A_i}{q^{i+\lambda}} \tag{17}$$

for each q, with the leading power λ determined by Eq. (13). Equations (14)–(16) then give

$$I=I_{0,N}+\sum_{i=0}^{\infty}A_i\zeta_N(i+\lambda)\ , \tag{18}$$

where $\zeta_N(i)=\sum_{j=N+1}^{\infty}1/j^i$ is the Riemann zeta function with the first N terms subtracted. The $I_{N+1,\infty}$ term is thereby converted from a series converging as $1/i^{\lambda}$ to one converging as $1/(N+1)^{i+\lambda}$. The advantage is that only the first few A_i coefficients need be known for N sufficiently large since $\zeta_N(i+\lambda)\sim 1/(N+1)^{i+\lambda}$.

The main obstacle to the application of this procedure is that the A_i coefficients are either not known or difficult to calculate. However, they can be determined "on the spot" to sufficient accuracy from the calculation itself by the following strategy. Assume that for some suitably chosen integer Λ, the directly calculated $T(q)$ are given exactly by the truncated expansion

$$T(q)=\sum_{i=0}^{\Lambda}\frac{A_i}{q^{i+\lambda}}\ . \tag{19}$$

This assumption in fact quickly becomes true to machine precision for $q\geq q_{\min}$. If $T(q)$ is now calculated for $q=N-\Lambda,\ N-\Lambda+1,\ldots,N$, then Eq. (19) can be regarded as a system of $\Lambda+1$ linear equations in $\Lambda+1$ unknowns which can be solved for the A_i, $i=0,\ldots,\Lambda$. The final estimate of the integral is then

$$I=I_{0,N}+\sum_{i=0}^{\Lambda}A_i\zeta_N(i+\lambda). \tag{20}$$

The calculation proceeds by progressively increasing N until I no longer changes to machine accuracy. As Λ becomes larger, the N required for convergence becomes smaller; but eventually there is a tradeoff with the time required to solve for the A_i coefficients. The optimum values are approximately $\Lambda=7$ and $N=20$ for sixteen-digit precision.

B. Test calculations

Table I shows a convergence study for the integral $I(0,0,0,-1,-1,-1;1,1,1)$ which corresponds to $\lambda=4$ in (13), the most difficult integral in the variational eigenvalue calculations. Here we choose $\Lambda=7$, i.e., seven terms in the asymptotic expansion. Using double precision arithmetic (approximately 16 figures), the second column of Table I contains the values of $S_d(N)$ calculated from the direct summation of the series. Successive differences of these values are listed in the third column. The fourth column contains the values obtained by the asymptotic-expansion method. The corresponding successive differences are listed in the last column. The exact value listed in the table is evaluated in quadruple precision, and agrees with the benchmark calculation of Fromm and Hill [13]. It can be seen that at $N=21$, the results in the fourth column have converged to nearly the machine precision $\epsilon\approx 2.2\times 10^{-16}$, while the direct sum in the second column converges only to the fourth digit. This example demonstrates the dramatic improvement in the rate of convergence provided by the asymptotic-expansion technique. In fact, a direct summation can never exceed a relative

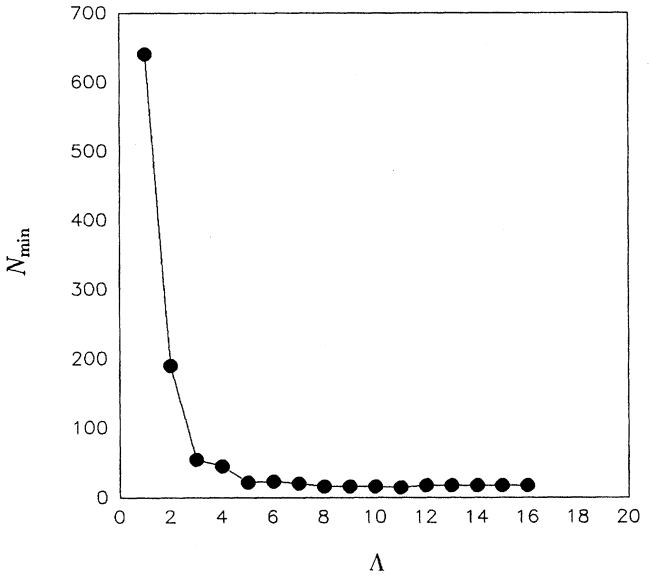

FIG. 1. Dependence of $N_{\min}$ on Λ for the integral $I(0,0,0,-1,-1,-1;1,1,1)$, where Λ is the number of terms contained in the asymptotic expansion and $N_{\min}$ is the minimum number of terms required to achieve a full convergence.

accuracy of 1.5×10^{-13} in double precision. This occurs at $N=6860$, where the $T(N)/I$ drop below the machine ϵ, and so adding more terms does not change I. At this level, the gain in speed by the asymptotic expansion method is about a factor of 400. Figure 1 shows the dependence of $N_{\min}$, the minimum value of N required to reach the final convergence, on Λ for the same integral. For $\Lambda=1$, 641 terms in (18) are required to obtain the final convergence. However, as Λ increases, $N_{\min}$ drops dramatically and approaches a stable value of about 17. Since this behavior is quite typical for integrals of this kind, one can simply fix the parameter Λ for the computation of a large body of integrals. In fact, in our lithium calculations [18], the global value of $\Lambda=7$ was just sufficient to calculate all the slowly convergent integrals, and it does no harm to more rapidly convergent integrals where a smaller value of Λ would be sufficient.

Other commonly used convergence acceleration techniques are the Levin u transformation and the Richardson extrapolation [19,20]. In the Levin u transformation, the partial sum of a slowly convergent series $S_n=\Sigma_{q=0}^{n}T(q)$ is transformed to the more rapidly convergent sequence of partial sums

$$u(k)=\frac{\sum_{q=0}^{k}(-1)^q\binom{k}{q}(q+1)^{k-2}S_qT(q)^{-1}}{\sum_{q=0}^{k}(-1)^q\binom{k}{q}(q+1)^{k-2}T(q)^{-1}}. \quad (21)$$

There is a similar expression for the Richardson extrapolation. Serious numerical cancellation may occur when k becomes large due to the existence of the oscillating factor $(-1)^q$. Typically, the accuracy of the u transformation increases with k up to an optimal value k_0 and then deteriorates quickly. This is clearly demonstrated in Table II, which lists the results of the evaluation of the integral $I(0,0,0,-1,-1,-1;1,1,1)$ in double precision. Relative to the direct summation, the u transformation does improve the rate of convergence for small values of k. However, the results rapidly deteriorate after reaching the optimal value at $k_0=13$, where the relative accuracy is only about 1.5×10^{-12}. Since k_0 depends strongly on the particular series being summed and cannot be predicted beforehand, the method is difficult to apply to large-scale calculations involving many different cases. As for the Richardson extrapolation, it is also subject to loss of significant figures. Our method, however, not only can achieve full convergence for a slowly convergent series, but also is insensitive to the choice of the number of terms in the asymptotic expansion.

TABLE II. Convergence study of the integral $I(0,0,0,-1,-1,-1;1,1,1)$ using the Levin u transformation.

k	$u(k)$	$u(k)-u(k-1)$
5	684.113 573 763 105	
6	684.113 429 363 967	−0.000 144 399 14
7	684.113 410 768 429	−0.000 018 595 54
8	684.113 411 504 931	0.000 000 736 50
9	684.113 411 839 111	0.000 000 334 18
10	684.113 411 847 795	0.000 000 008 68
11	684.113 411 843 377	−0.000 000 004 42
12	684.113 411 842 995	−0.000 000 000 38
13	684.113 411 842 431	−0.000 000 000 56
14	684.113 411 853 603	0.000 000 011 17
15	684.113 411 818 997	−0.000 000 034 61
16	684.113 411 766 733	−0.000 000 052 26
17	684.113 411 882 088	0.000 000 115 35
18	684.113 412 030 780	0.000 000 148 69
19	684.113 414 065 650	0.000 002 034 87
20	684.113 406 521 980	−0.000 007 543 67
21	684.113 418 297 312	0.000 011 775 33
22	684.113 489 777 282	0.000 071 479 97
23	684.113 511 820 949	0.000 022 043 67
24	684.114 315 563 275	0.000 803 742 33
25	684.119 174 405 598	0.004 858 842 32

III. SUMMARY

The asymptotic-expansion method presented here has been shown to decrease dramatically the time required for the calculation of three-electron integrals in Hylleraas coordinates. As a consequence, a major bottleneck in the development of variational calculations for lithiumlike systems has been removed. The technique itself is conceptually simple, numerically stable, and easy to implement. It can be applied to many other problems involving the summation of series converging asymptotically as $1/i^{\lambda}$. In addition, we have obtained an analytic expression for the W integral.

The asymptotic method may also be applied to the more singular integrals which arise in the calculation of relativistic corrections from the Breit interaction. Work along this direction is currently in progress.

ACKNOWLEDGMENT

Research support by the Natural Sciences and Engineering Research Council of Canada is gratefully acknowledged.

APPENDIX

In this appendix, we discuss the derivation of formula (8). After changing the order of integration, the W integral can be rewritten as

$$W=\int_0^\infty dz z^n e^{-\gamma z} T_2(z) , \tag{A1}$$

where

$$T_2(z)=\int_0^z dy y^m e^{-\beta y} T_1(y) \tag{A2}$$

with

$$T_1(y)=\int_0^y dx x^l e^{-\alpha x} . \tag{A3}$$

Using formula 6.5.12 of Ref. [21], $T_1(y)$ becomes

$$T_1(y)=\frac{y^{l+1}}{l+1} e^{-\alpha y} {}_1F_1(1;l+2;\alpha y) , \tag{A4}$$

where ${}_1F_1$ is the confluent hypergeometric function. Substituting $T_1(y)$ into (A2) and letting $\xi=y/z$, one has

$$T_2(z)=\frac{1}{l+1} z^{l+m+2} \int_0^1 d\xi \xi^{l+m+1} \times e^{-(\alpha+\beta)z\xi} {}_1F_1(1;l+2;\alpha z\xi) . \tag{A5}$$

Furthermore, expanding ${}_1F_1$ in (A5) according to its definition and performing the integration over ξ by the same formula mentioned above, $T_2(2)$ becomes

$$\begin{aligned} T_2(z) &= l! \sum_{p=0}^\infty \frac{\alpha^p}{(l+1+p)!} z^{l+m+2+p} \int_0^1 d\xi \ \xi^{l+m+1+p} e^{-(\alpha+\beta)z\xi} \\ &= l! \sum_{p=0}^\infty \frac{\alpha^p}{(l+1+p)!(l+m+p+2)} z^{l+m+2+p} e^{-(\alpha+\beta)z} {}_1F_1(1;l+m+p+3;(\alpha+\beta)z) . \end{aligned} \tag{A6}$$

Thus, W can be put into the form of

$$W=l! \sum_{p=0}^\infty \frac{\alpha^p}{(l+1+p)!(l+m+p+2)} \int_0^\infty dz \ z^{l+m+n+2+p} e^{-(\alpha+\beta+\gamma)z} {}_1F_1(1;l+m+p+3;(\alpha+\beta)z) . \tag{A7}$$

Finally, the application of formula 7.621(4) of Ref. [22] yields Eq. (8).

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