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Mathematical and computational science issues in high precision Hylleraas-configuration interaction variational calculations: I. Three-electron integrals

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Abstract

The most difficult integral arising in Hylleraas-configuration interaction (Hy-CI) calculations, the three-electron triangle integral, is discussed. We focus on recursive techniques at both the double precision and quadruple precision level of accuracy while trying to minimize the use of higher precision arithmetic. Also, we investigate the use of series acceleration to overcome problems of slow convergence of certain integrals defined by infinite series. We find that a direct + tail Levin u-transformation convergence acceleration overcomes problems that arise when using other convergence acceleration techniques, and is the best method for overcoming the slow convergence of the triangle integral. The question of calibrating an acceleration method is also discussed, as well as ways to improve our work.

1. Introduction

Frolov and Bailey have recently published [1] a scheme for evaluating few-body auxiliary functions and four-body integrals with extremely high accuracy using a sophisticated arbitrary multiple precision (MP) Fortran 90 package (MPFUN) developed by Bailey [2]. Some of these integrals also occur in attempting to obtain very precise energies for few electron atomic systems using the Hylleraas-configuration interaction (Hy-CI) formalism. Our Hy-CI employs a novel wavefunction, namely, a wavefunction with terms consisting of at most a single r_{ij} raised to the first power combined with a conventional non-orthogonal configuration interaction (CI) basis[3]. We have recently used this technique to determine nonrelativistic ground-state energies of helium and helium-like ions [3, 4]. We used this technique 30 years ago to determine energy levels of Li [5], Li^- [6] and Be [7, 8] much less accurately with

[3] Which eliminates some of the most difficult integrals Frolov and Bailey discuss.

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the supercomputers of that era. Here we discuss how to efficiently evaluate the only difficult integrals arising when using this technique in the more general case of N (number of electrons) $\geqslant 3$. We will be focusing on recursive techniques (section 3) at both the double precision (DP) and quadruple precision (QP)[4] level of accuracy while trying to minimize the use of higher precision arithmetic. In this sense the focus of this work is substantially different from that of Frolov and Bailey. Also, we investigate the use of series acceleration to overcome problems of slow convergence of certain integrals defined by infinite series (section 4).

Many of the details of the integrals which arise in an Hy-CI calculation of atomic systems have been discussed previously [9]. In this paper we discuss changes that we have made to our integral methodology in our most recent work [10]. As discussed in [9], all integrals can be expressed in terms of the standard Condon and Shortley coefficients (c^ks) [11, 9] and auxiliary functions A, V, W, and X. In this paper we update the treatment of V and W auxiliary functions to reflect changes we have made to most effectively use modern day computers to increase the size (number of terms) and accuracy of the calculations. We reserve treatment of X auxiliary functions to a future paper, but we note that our X functions are easier than the more general functions treated by Frolov and Bailey, a consequence of the restriction of the r_{ij} terms to a single r_{ij} raised to the first power (in contrast to Hy-r_{ij} calculations where products of r_{ij} terms in wavefunctions have to be dealt with).

Our emphasis on efficient methods for calculating these integrals arises because of how we handle the H matrix assembly problem, which is still the hardest part of a high precision atomic energy level calculation, especially for Be and beyond. In our energy calculations, we essentially multipass the assembly of Hamiltonian matrix elements, ending up after pass one with long lists of integrals needed, which we then sort by integral type, orbital type, nonlinear parameters, and so on so that integrals depending on the same types of auxiliary functions are effectively grouped together. To make the integral calculation efficient we need fast, stable methods for calculating large arrays of auxiliary functions from which large blocks (tens of thousands in some cases) of integrals can be calculated at one time. Recursive techniques for calculating these arrays are the only viable methods found for implementing this approach.

2. Hy-CI triangle integral evaluation

The three-electron r_{ij} integrals which arise in our Hy-CI calculations are of the form

$$I = \int \Omega_1(\mathbf{r}_1)\Omega_2(\mathbf{r}_2)\Omega_3(\mathbf{r}_3)R\,\mathrm{d}\mathbf{r}_1\,\mathrm{d}\mathbf{r}_2\,\mathrm{d}\mathbf{r}_3, \tag{1}$$

where R can be any of the following r_{ij} products,

$$r_{12}r_{13}, \quad r_{12}r_{13}^{-1}, \quad r_{12}r_{13}^{-1}r_{23},$$

and the Ω are 'charge distributions' made up of products of unnormalized Slater-type orbitals (STOs) $\phi(\mathbf{r})$

$$\phi_i(\mathbf{r}) = r^{n_i-1}\,\mathrm{e}^{-\alpha_i r}Y_{l_i}^{m_i}(\theta,\phi), \tag{2}$$

$$\Omega_i(\mathbf{r}) = \phi_i^*(\mathbf{r})\phi_i'(\mathbf{r}). \tag{3}$$

In equation (2), $Y_l^m(\theta,\phi)$ is a normalized spherical harmonic in the Condon and Shortley phase convention [11]. Of these r_{ij} integrals, the one arising when $R = r_{12}r_{13}^{-1}r_{23}$, the so-called 'triangle integral', stands out because its Legendre expansion is an *infinite* series requiring special treatment to achieve high precision without prohibitive computational costs. The

[4] When we refer to double, quadruple, or other precision it is with respect to a 32-bit word.

remaining two r_{ij} integrals, the ones when $R = r_{12}r_{13}$ and $R = r_{12}r_{13}^{-1}$, lead to short, finite expansions whose evaluation has been well covered in the literature and will not be discussed further here[5]. For a very thorough treatment of three-electron integrals over s-type STOs[6] (see [1–25] of the paper by Pelzl and King [12] and [16–40] in the review article by King [13]). Yan and Drake [14] treat the more general case of three-electron integrals over nonspherically symmetric STOs.

The triangle integrals which have to be evaluated in our Hy-CI calculations are therefore

$$\begin{aligned} I &= \langle \phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2)\phi_3(\mathbf{r}_3)|r_{12}r_{13}^{-1}r_{23}|\phi_1'(\mathbf{r}_1)\phi_2'(\mathbf{r}_2)\phi_3'(\mathbf{r}_3)\rangle \\ &= \int \Omega_1(\mathbf{r}_1)\Omega_2(\mathbf{r}_2)\Omega_3(\mathbf{r}_3)r_{12}r_{13}^{-1}r_{23}\,\mathrm{d}\mathbf{r}_1\,\mathrm{d}\mathbf{r}_2\,\mathrm{d}\mathbf{r}_3. \end{aligned} \tag{4}$$

Expanding the charge distributions $\Omega_i(\mathbf{r})$ as linear combinations of STOs $f_i(\mathbf{r}_i)$

$$f_i(\mathbf{r}) = r^{N_i-1}\,\mathrm{e}^{-w_i r}\,Y_{L_i}^{M_i}(\theta,\phi) \tag{5}$$

with $N_i = n_i + n_i' - 1$, $w_i = \alpha_i + \alpha_i'$, $L_i = |l_i - l_i'|, |l_i - l_i'|+2, \ldots, l_i + l_i' - 2, l_i + l_i'$, $M_i = m_i' - m_i$, I becomes

$$I = \delta(M_1 + M_2 + M_3, 0) \sum_{L_1,L_2,L_3} \prod_{i=1}^{3} \left\{(2L_i+1)^{\frac{1}{2}} c^{L_i}(l_i', m_i'; l_i, m_i)\right\} J(L_1, L_2, L_3), \tag{6}$$

where the c^{L_i} are standard Condon and Shortley coefficients (the so-called c^ks) [11, 9]. The factor $J(L_1, L_2, L_3)$ is given by

$$\begin{aligned} J(L_1, L_2, L_3) &= \frac{1}{(4\pi)^{3/2}} \int r_{12}r_{13}^{-1}r_{23} \prod_{i=1}^{3} \{f_i(\mathbf{r}_i)\,\mathrm{d}\mathbf{r}_i\} \\ &= \frac{1}{(4\pi)^{3/2}} \int r_1^{N_1-1} r_2^{N_2-1} r_3^{N_3-1} \frac{r_{12}r_{23}}{r_{13}} \exp(-w_1 r_1 - w_2 r_2 - w_3 r_3) \\ &\quad \times Y_{L_1}^{M_1}(1) Y_{L_2}^{M_2}(2) Y_{L_3}^{M_3}(3)\,\mathrm{d}\mathbf{r}_1\,\mathrm{d}\mathbf{r}_2\,\mathrm{d}\mathbf{r}_3. \end{aligned} \tag{7}$$

Inserting the Legendre expansions for r_{ij} and r_{ij}^{-1} we get

$$\begin{aligned} J(L_1, L_2, L_3) &= \sum_{q=0}^{\infty} \sum_{n_s=|q-L_1|}^{q+L_1} \sum_{n_u=\max(|q-L_3|,|n_s-L_2|)}^{\min(q+L_3,n_s+L_2)} \mathcal{A}(L_1, L_2, L_3, n_s, q, n_u) \\ &\quad \times \sum_{l=0}^{1} \sum_{n=0}^{1} B_l^{n_s,1} B_n^{n_u,1} \mathcal{R}(N_1, N_2, N_3, N_{12}(l), N_{13}(q), N_{23}(n)), \end{aligned} \tag{8}$$

with $N_{12}(l) = n_s + 1 - 2l$, $N_{13}(q) = q + 1$, $N_{23}(n) = n_u + 1 - 2n$. The B coefficients are $B_0^{m,1} = 1/(2m+3)$ and $B_1^{m,1} = -1/(2m-1)$, while

$$\begin{aligned} \mathcal{A}(L_1, L_2, L_3, n_s, q, n_u) &= \frac{1}{\{(2n_s+1)(2q+1)(2n_u+1)\}^{1/2}} \sum_{m_q} c^q(n_s, m_q + M_1; L_1, M_1) \\ &\quad \times c^{n_s}(n_u, m_q + M_1 + M_2; L_2, M_2) c^{n_u}(q, m_q; L_3, M_3) \end{aligned} \tag{9}$$

[5] We have discussed how we do these integrals in a previous paper [9].

[6] The STOs we use are defined fully in [9]. An s-type STO has $l = 0$, a p-type STO has $l = 1$, a d-type STO has $l = 2$, etc.

is a three-electron angular factor with m_q running from $\max[-q, -(n_s+M_1), -(n_u+M_1+M_2)]$ to $\min(q, n_s - M_1, n_u - M_1 - M_2)$. $\mathcal{R}$ is a special case of equation (32) of [9] and is

$$\begin{aligned}
&\mathcal{R}(N_1, N_2, N_3, N_{12}, N_{13}, N_{23}) \\
&\quad = \int r_1^{N_1+1} r_2^{N_2+1} r_3^{N_3+1} \frac{r_{12<}^{N_{12}+1} r_{13<}^{N_{13}-1} r_{23<}^{N_{23}+1}}{r_{12>}^{N_{12}} r_{13>}^{N_{13}} r_{23>}^{N_{23}}} \exp(-w_1 r_1 - w_2 r_2 - w_3 r_3)\, \mathrm{d}r_1\, \mathrm{d}r_2\, \mathrm{d}r_3 \\
&\quad = W(N_1 + N_{12} + N_{13} + 1, N_2 - N_{12} + N_{23} + 2, N_3 - N_{13} - N_{23} + 1; w_1, w_2, w_3) \\
&\qquad + W(N_1 + N_{12} + N_{13} + 1, N_3 - N_{13} + N_{23} + 2, N_2 + 1 - N_{12} - N_{23}; w_1, w_3, w_2) \\
&\qquad + W(N_2 + N_{12} + N_{23} + 3, N_1 - N_{12} + N_{13}, N_3 - N_{13} - N_{23} + 1; w_2, w_1, w_3) \\
&\qquad + W(N_2 + N_{12} + N_{23} + 3, N_3 - N_{23} + N_{13}, N_1 - N_{12} - N_{13} + 1; w_2, w_3, w_1) \\
&\qquad + W(N_3 + N_{13} + N_{23} + 1, N_1 + N_{12} - N_{13} + 2, N_2 + 1 - N_{12} - N_{23}; w_3, w_1, w_2) \\
&\qquad + W(N_3 + N_{13} + N_{23} + 1, N_2 + N_{12} - N_{23} + 2, N_1 - N_{12} - N_{13} + 1; w_3, w_2, w_1),
\end{aligned} \tag{10}$$

where $N_{12} \equiv N_{12}(l)$, $N_{13} \equiv N_{13}(q)$, $N_{23} \equiv N_{23}(n)$, and the auxiliary function W, whose efficient evaluation is the main focus of this paper, is defined in section 3 by equation (15).

Expanding equation (8) and substituting for the B coefficients, and then inserting the resulting expression for $J(L_1, L_2, L_3)$ into equation (6) leads to our final expression for I

$$I = \delta(M_1 + M_2 + M_3, 0) \sum_{q=0}^{\infty} A(q), \tag{11}$$

where

$$\begin{aligned}
A(q) = &\sum_{L_1,L_2,L_3} \prod_{i=1}^{3} \{(2L_i+1)^{1/2} c^{L_i}(l_i', m_i'; l_i, m_i)\} \\
&\times \sum_{n_s=|q-L_1|}^{q+L_1} \sum_{n_u=\max(|q-L_3|,|n_s-L_2|)}^{\min(q+L_3,n_s+L_2)} \mathcal{A}(L_1, L_2, L_3, n_s, q, n_u) \\
&\times \left[\frac{\mathcal{R}(N_1, N_2, N_3, n_s+1, q+1, n_u+1)}{(2n_s+3)(2n_u+3)} \right. \\
&- \frac{\mathcal{R}(N_1, N_2, N_3, n_s+1, q+1, n_u-1)}{(2n_s+3)(2n_u-1)} \\
&- \frac{\mathcal{R}(N_1, N_2, N_3, n_s-1, q+1, n_u+1)}{(2n_s-1)(2n_u+3)} \\
&\left. + \frac{\mathcal{R}(N_1, N_2, N_3, n_s-1, q+1, n_u-1)}{(2n_s-1)(2n_u-1)} \right].
\end{aligned} \tag{12}$$

If all orbitals are s-type, $L_1 = L_2 = L_3 = 0$ and the $A(q)$ reduce to

$$\begin{aligned}
A(q) = &\mathcal{A}(0, 0, 0, q, q, q) \\
&\times \left[\frac{\mathcal{R}(N_1, N_2, N_3, q+1, q+1, q+1)}{(2q+3)(2q+3)} - \frac{\mathcal{R}(N_1, N_2, N_3, q+1, q+1, q-1)}{(2q+3)(2q-1)} \right. \\
&\left. - \frac{\mathcal{R}(N_1, N_2, N_3, q-1, q+1, q+1)}{(2q-1)(2q+3)} + \frac{\mathcal{R}(N_1, N_2, N_3, q-1, q+1, q-1)}{(2q-1)(2q-1)} \right].
\end{aligned} \tag{13}$$

If in addition all orbitals are 1s-type, our I integral reduces (except for a factor) to the integral

$$\mathbf{Z}(w_1, w_2, w_3) = \int r_{12} r_{13}^{-1} r_{23} \exp(-w_1 r_1 - w_2 r_2 - w_3 r_3)\, \mathrm{d}\mathbf{r}_1\, \mathrm{d}\mathbf{r}_2\, \mathrm{d}\mathbf{r}_3 \tag{14}$$

that Remiddi has evaluated in closed form [15]. See also Sims and Hagstrom [10, 16] and Harris *et al* [17] for correction of some minor misprints in the original published formula [15]. We have found Remiddi's result extremely useful by providing exact answers with which to compare both our truncated expansions and the results of various series convergence acceleration attempts (see below).

Our I integral (equations (11) and (12)), of course, is a more general form than the Remiddi integral with N_is > 1 and non-s STOs. While parametric differentiation with respect to the w_is in equation (14) would generate closed form expressions for integrals with 1s2s, 2s2s etc charge distributions, thus far no convenient analytic expressions for the non-s charge distribution cases have been derived (although Fromm and Hill [18] suggested an elegant method for deriving such expressions). Even if such expressions existed actual implementation would be beyond the scope of the present investigation.

The angular terms $\mathcal{A}(L_1, L_2, L_3, n_s, q, n_u)$ in equation (12) present no real problems. For accurate work they do need to be calculated to greater than QP, but they can be precomputed in advance of the integral calculation, stored by orbital l quantum numbers and used multiple times. The $\mathcal{R}$ in equation (12) are the $\mathcal{R}(N_1, N_2, N_3, N_{12}, q, N_{23})$ given by equation (10), a sum over 6 $W_{fgh}(\alpha\beta\gamma)$ terms. The $W_{fgh}(\alpha\beta\gamma)$ terms will be considered in the following section while the question of the convergence of the $A(q)$ summation in equation (11) will be taken up in section 4.

3. Computation of the A, V, and W auxiliary functions

We now turn our attention to the W auxiliary functions in equation (10) along with two other auxiliary functions, A and V, used in the evaluation of the W functions. Here, f, g and h are integers, and α, β, and γ are real and positive. We supplement the definitions of the functions by giving sufficient conditions on the parameters f, g and h to ensure the convergence of the integrals. These supplementary conditions can be derived easily by inspection of the problematic integration regions which occur when the integration variables x, y, and z assume values close to zero.

$$W(fgh;\alpha\beta\gamma) \equiv W_{fgh}(\alpha\beta\gamma) = \int_0^\infty x^f \,\mathrm{e}^{-\alpha x}\,\mathrm{d}x \int_x^\infty y^g \,\mathrm{e}^{-\beta y}\,\mathrm{d}y \int_y^\infty z^h \mathrm{e}^{-\gamma z}\,\mathrm{d}z,$$
$$(f \geqslant 0,\ f+g \geqslant -1,\ f+g+h \geqslant -2) \tag{15}$$

$$V(mn;\alpha\beta) \equiv V_{mn}(\alpha\beta) = \int_0^\infty x^m \,\mathrm{e}^{-\alpha x}\,\mathrm{d}x \int_x^\infty y^n \,\mathrm{e}^{-\beta y}\,\mathrm{d}y, \qquad (m \geqslant 0, \quad m+n \geqslant -1) \tag{16}$$

$$A(n;\alpha) \equiv A_n(\alpha) = \int_0^\infty x^n \mathrm{e}^{-\alpha x}\,\mathrm{d}x = \frac{n!}{\alpha^{n+1}}, \qquad n \geqslant 0. \tag{17}$$

For the triangle integral there are two cases to consider, $W_{fgh}(\alpha\beta\gamma)$ for $f, g, h \geqslant 0$ and $f, g \geqslant 0, h < 0$. Only the $h < 0$ case presents any difficulties.

3.1. Recurrence relationships for $W_{fgh}(\alpha\beta\gamma)$ for $f, g, h \geqslant 0$

Recurrence relationships between the W auxiliary functions have been given by James and Coolidge [19] and Öhrn and Nordling [20], and included in our earlier integral paper [9].

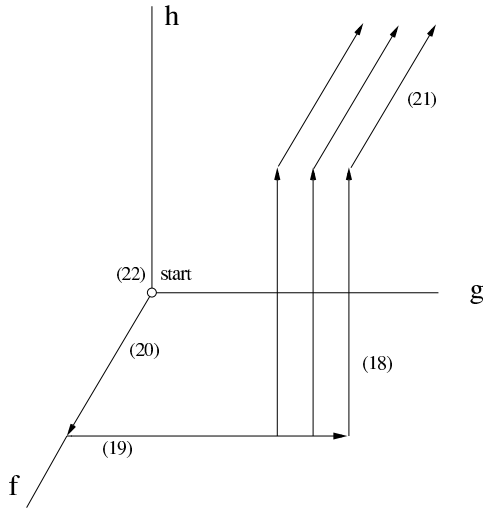

Figure 1. Recursion scheme for calculating $W_{fgh}(\alpha\beta\gamma)$ for $f, g, h \geqslant 0$.

$$W_{fgh}(\alpha\beta\gamma) = \gamma^{-1}[hW_{f,g,h-1}(\alpha\beta\gamma) + V_{f,g+h}(\alpha, \beta+\gamma)], \quad (f \geqslant 0,\ f+g \geqslant -1,\ f+g+h \geqslant -1) \tag{18}$$

$$W_{fgh}(\alpha\beta\gamma) = (\beta+\gamma)^{-1}[gW_{f,g-1,h}(\alpha\beta\gamma) + hW_{f,g,h-1}(\alpha\beta\gamma) + V_{f+g,h}(\alpha+\beta, \gamma)], \quad (f \geqslant 0,\ f+g \geqslant 0,\ f+g+h \geqslant -1) \tag{19}$$

$$W_{fgh}(\alpha\beta\gamma) = (\alpha+\beta+\gamma)^{-1}[fW_{f-1,g,h}(\alpha\beta\gamma) + gW_{f,g-1,h}(\alpha\beta\gamma) + hW_{f,g,h-1}(\alpha\beta\gamma)], \quad (f \geqslant 1,\ f+g \geqslant 0,\ f+g+h \geqslant -1) \tag{20}$$

$$W_{f-1,g,h}(\alpha\beta\gamma) = f^{-1}[\alpha W_{fgh}(\alpha\beta\gamma) + V_{f+g,h}(\alpha+\beta, \gamma)], \quad (f \geqslant 1,\ f+g \geqslant 0,\ f+g+h \geqslant -1) \tag{21}$$

$$W_{000}(\alpha\beta\gamma) = [(\alpha+\beta+\gamma)(\beta+\gamma)\gamma)]^{-1}. \tag{22}$$

Equations (18)–(22) enable one to calculate the W in a stable way using equation (22) as the starting point (see figure 1). Each leg of the path is labelled with the formula we use to raise/lower the corresponding index.

For checking the accuracy of the recursions the explicit finite sum of Frolov and Smith [21], equation (16), is useful:

$$W_{fgh}(\alpha\beta\gamma) = \sum_{\sigma=0}^{h} C_n^{\sigma} A_{\sigma}(\gamma) V_{f,g+h-\sigma}(\alpha+\beta+\gamma, \beta+\gamma) \tag{23}$$

where the C_n^{σ} are binomial coefficients, i.e., $C_n^m = \frac{n!}{m!(n-m)!}$.

3.2. Recurrence relationships for $V_{mn}(\alpha\beta)$ for $m, n \geqslant 0$

In the previous section, we also needed arrays of $V_{mn}(\alpha\beta)$ for $m, n \geqslant 0$. In equation (16), integration by parts using $e^{-\beta y}$ leads to [20]

$$V_{mn}(\alpha\beta) = \beta^{-1}[nV_{m,n-1}(\alpha\beta) + A_{m+n}(\alpha+\beta)], \qquad (m \geqslant 0, m+n \geqslant 0) \tag{24}$$

which is useful for raising the second index n. Equation (24) is obviously stable for $n \geqslant 0$. For $n = 0$ we get

$$V_{m0}(\alpha\beta) = \beta^{-1}[A_m(\alpha+\beta)], \qquad (m \geqslant 0). \tag{25}$$

Similarly, integrating by parts using $e^{-\alpha x}$ in equation (16) gives a recurrence relation for lowering the m index:

$$V_{m-1,n}(\alpha\beta) = m^{-1}[\alpha V_{mn}(\alpha\beta) + A_{m+n}(\alpha+\beta)], \qquad (m \geqslant 1, m+n \geqslant 0). \tag{26}$$

The above formulae lead to the following scheme for the efficient computation of $V_{mn}(\alpha\beta)$ when m and n are $\geqslant 0$: use equation (25) to get $V_{m0}(\alpha\beta)$ for $m = 0, \ldots, m_{\max}$, then use equation (24) for $m_{\max}$ to get all $V_{m_{\max},n}(\alpha\beta)$, followed by equation (26) to lower m from $m_{\max}$ down to 0 for each value of n. All coefficients enter with positive sign, hence it is a stable scheme.

For checking the accuracy of the $V_{mn}(\alpha\beta)$ recursions the explicit finite sum form of Frolov and Smith [21] can be used:

$$V_{mn}(\alpha\beta) = \sum_{\nu=0}^{n} C_n^{\nu} A_{m+n-\nu}(\alpha+\beta) A_{\nu}(\beta) \tag{27}$$

where the C_n^m are binomial coefficients. Equation (27) follows immediately from the parametric derivative representation of $V_{mn}(\alpha\beta)$, namely,

$$\begin{aligned} V_{mn}(\alpha\beta) &= \left(-\frac{\mathrm{d}}{\mathrm{d}\alpha}\right)^m \left(-\frac{\mathrm{d}}{\mathrm{d}\beta}\right)^n V_{00}(\alpha\beta) \\ &= \left(-\frac{\mathrm{d}}{\mathrm{d}\alpha}\right)^m \left(-\frac{\mathrm{d}}{\mathrm{d}\beta}\right)^n A_0(\beta) A_0(\alpha+\beta) \\ &= \left(-\frac{\mathrm{d}}{\mathrm{d}\beta}\right)^n A_0(\beta) A_m(\alpha+\beta) \end{aligned} \tag{28}$$

and the binomial theorem for differentiation. This calculation is obviously stable as there is no loss of precision due to differencing anywhere in the formulae.

3.3. Recurrence relationships for $W_{fgh}(\alpha\beta\gamma)$ for $f, g \geqslant 0, h < 0$

The calculation of $W_{fgh}(\alpha\beta\gamma)$ for $f, g \geqslant 0, h < 0$ presents some serious difficulties over the range of the f, g, h indices and α, β, γ arguments that arise in practical problems. The basic problem is that some of the recursion relations that must be used involve negative signs and are hence potentially unstable. There is no really good, stable recursion scheme starting with $W_{0,0,-1}(\alpha\beta\gamma)$, especially if more than double precision accuracy is needed, although earlier work along this line has been extensive [19, 20, 22–24, 9]. Our earlier scheme for evaluating these integrals was adopted by others, for example, [25], but it needs to be revised to meet present high precision requirements.

We have found, surprisingly, that if one starts out by calculating the integrals $W_{f_{\max},g,h_0}(\alpha\beta\gamma)$ for each $g = 0, \ldots, g_{\max}$ (where $f_{\max}$ and $g_{\max}$ are the maximum values needed for f and g, and h_0 is suitably chosen), then potentially unstable recursions in fact turn out to be stable (how we judge the accuracy of the W integrals will be explained towards the end of this section), and there is no real difficulty in generating the entire array from 'the top down', using only a relatively few starting W integral values. More to the point, suppose we want to calculate the array $W(0{:}\, f_{\max}, 0{:}\, g_{\max}, h_{\min}{:}\, -1)$.[7] For that, the following recursion scheme has proven to be remarkably effective:

[7] An array of values of $W_{f,g,h}(\alpha,\beta,\gamma)$ integrals for a fixed α,β,γ and f, g, and h taking on the values $f = 0, \ldots, f_{\max}$, $g = 0, \ldots, g_{\max}$, and $h = h_{\min}, \ldots, -1$.

(i) Calculate a starting function $W_{f_{max},g_{max},h_0}(\alpha\beta\gamma)$, using the stable Larsson summation (see below), where $h_{min} < h_0 < -1$ and with h_0 suitably chosen (see below).

(ii) Use equation (18) with $f = f_{max}$, $g = g_{max}$

$$W_{f_{max},g_{max},h}(\alpha\beta\gamma) = \gamma^{-1}[hW_{f_{max},g_{max},h-1}(\alpha\beta\gamma) + V_{f_{max},g_{max}+h}(\alpha, \beta+\gamma)], \quad (f \geqslant 0,\ f+g \geqslant -1,\ f+g+h \geqslant -1) \tag{29}$$

to raise h from h_0 up to the value -1. In spite of the fact that h is negative, this recursion is stable up to fairly large values of f_{max}(≈200–300), provided h_0 is appropriately chosen. We invert the above formula and use

$$W_{f_{max},g_{max},h-1}(\alpha\beta\gamma) = [\gamma W_{f_{max},g_{max},h}(\alpha\beta\gamma) - V_{f_{max},g_{max}+h}(\alpha, \beta+\gamma)]/h \tag{30}$$

to lower h down to the value h_{min}. Remarkably, this recursion also is stable. The final result after two steps, therefore, will be the vector (one-dimensional array) $W(f_{max}, g_{max}, h_{min} : -1)$.

(iii) Repeat (i) and (ii) for $g = g_{max} - 1, g_{max} - 2, \ldots, 1, 0$ giving one the subarray (two-dimensional array) $W(f_{max}, 0 : g_{max}, h_{min} : -1)$. Note that the existing V integral values may be used over again (which was the reason for starting with $g = g_{max}$).

(iv) Finally, complete the calculation by lowering the value of the f index down to its lowest allowed value $f = \max(0, |\, h \,| - g - 2)$ (recall that $f \geqslant 0$, $f+g \geqslant -1$, and $f+g+h \geqslant -2$ for the W auxiliary function to exist) for each g, h pair using the stable recursion equation (21)

$$W_{f-1,g,h}(\alpha\beta\gamma) = f^{-1}[\alpha W_{fgh}(\alpha\beta\gamma) + V_{f+g,h}(\alpha+\beta, \gamma)]. \tag{31}$$

This recursion is actually hyperstable in that it is possible to start out with W values not of full accuracy and after a few steps obtain fully accurate W values, provided of course that the V are fully accurate.

This is the scheme we use in practical calculations, although it is not the most efficient scheme since W functions are computed that never arise in actual triangle integrals. For example, $W_{f_{max},g,-1}$ will never arise in any triangle integral, although it is the starting element for the generation of the vector $W(0{:}\, f_{max}, g, -1)$. Furthermore, this is an integral that can result in exponent overflow for some argument values. A more efficient scheme would endeavour to avoid calculating such elements. For example, suppose we partition the $W(0 : f_{max}, 0 : g_{max}, h_{min} : -1)$ matrix using h_1 approximately midway between h_{min} and -1. Calculate $W(f_{max}, g, h_{min}{:}\, h_1)$ as outlined above, then lower f to get $W(f_1{:}\, f_{max}, g, h_1)$, where f_1 is the maximum value of f for this value of the indices g and h_1. Then raise the h index to get the vector $W(f_1, g, h_1 : -1)$ and finally lower f from f_{max} (case $h \leqslant h_1$) and f_1 (case $h \geqslant h_1$) using equation (31). In this manner calculating the subarray $W(f_1+1 : f_{max}, g, h_1+1 : -1)$ (which is never needed) can be avoided. Further partitioning of the W array is obviously possible with further savings. The limiting process here would be some sort of 'diagonal' recursion relating W_{fgh} to its neighbours $W_{f+1,g,h-1}$ and $W_{f-1,g,h+1}$ along with the associated V functions. We have looked at this process but have been unable to find a good starting point, since one will presumably have to recur in both directions along the diagonal.

The starting $W_{f_{max},g,h_0}(\alpha\beta\gamma)$, $g = 0, \ldots, g_{max}$ values in step (i) above can be calculated using the stable (sum of positive terms) summation formula derived many years ago by Larsson [24], equation (32), based on the work of Öhrn and Nordling [20],

$$W_{fgh}(\alpha\beta\gamma) = \sum_{\nu=1}^{M} \alpha^{\nu-1} \frac{f!}{(f+\nu)!} V_{f+g+\nu,h}(\alpha+\beta, \gamma) \tag{32}$$

for each g in the range $(0, g_{\max})$.[8] M depends on the values of f, g, h and the argument $(\alpha+\beta)/(\alpha+\beta+\gamma)$ and should be chosen large enough for convergence to occur, yet not too large. How does one choose h_0? In practice the simple rule $h_0 = h_{\min}/2$ works well for values of $h_{\min}$ not too negative. For $h_{\min}$ in the range (−200–80) the rule $\frac{3}{8}h_{\min}$ works fairly well. There is also a slight dependence on f and g that can usually be ignored.

The Larsson summation in equation (32) requires knowledge of the vector $V(f_{\max}+1{:}\,m_{\max}, h_0; \alpha+\beta, \gamma)$, where $m_{\max} = f_{\max} + g_{\max} + M$, and M depends on h_0 and the value of the parameter ratio $s = (\alpha+\beta)/(\alpha+\beta+\gamma)$ as well as, obviously, on the type of arithmetic being used (double precision (DP), quadruple precision (QP) or multiple precision (MP)). One first calculates $V(m_{\max}, h_0; \alpha+\beta, \gamma)$ and then uses equation (26) to lower the first index down to $f_{\max}+1$. For mid-range values of s and typical h_0 values M < 75, but as s approaches 1.0, M can be as large as 300.

In practice M is set to a value based on s (and other factors) that allows the series to converge in most cases. However, if the series still does not converge, a special coding option exists to sum the remainder of the series, but this time using MP arithmetic (the MP calculations are done using Richard Brent's multiple precision package [26]) to handle exponent overflow problems that might otherwise occur for large values of M).

The $V_{m_{\max},h_0}(\alpha+\beta, \gamma)$ value required to calculate $V(f_{\max}+1{:}\,m_{\max}, h_0; \alpha+\beta, \gamma)$ is calculated using another Larsson summation formula [24], (equation (34)):

$$\begin{aligned} V_{mn}(\alpha\beta) &= \sum_{\nu=1} \frac{\alpha^{\nu-1} m!}{(m+\nu)!} A_{m+n+\nu}(\alpha+\beta) \\ &= \alpha^{-1} A_{m+n}(\alpha+\beta)\left[\frac{m+n+1}{m+1}s + \frac{(m+n+1)(m+n+2)}{(m+1)(m+2)}s^2 + \cdots\right] \\ &= \frac{A_{m+n+1}(\alpha+\beta)}{(m+1)}\,{}_2F_1(1, m+n+2; m+2; s) \end{aligned} \tag{33}$$

where $s = \alpha/(\alpha+\beta)$ and ${}_2F_1(a, b; c; s)$ is the usual hypergeometric function [27]. The second form shows the behaviour of the series with respect to s, with convergence becoming very slow as s nears 1 and slower still if the ratio $(m+n)/m$ is close to 1 (which it may be since $m_{\max} \gg |h_0|$). On the other hand, for small s the summation length is largely independent of m and n. Any of the forms in equation (33) can be used depending on the circumstances. For convenience, over most of the range of s we just sum the series brute force. However, for $s < 0.3$ an expansion in $-z/(1-z)$ (see equation (15.3.4) in Abramowitz and Stegun [27]) is shorter and just as accurate as the canonical expansion. For $s > 0.9$ and the ratio of $(m+n+1)/(m+1)$ close to 1, we use the closed form expression due to McKoy [22]:

$$V_{m_{\max},-1}(\alpha\beta) = -A_{m_{\max}}(\alpha)\left[\ln(1-s) + \sum_{\nu=1}^{m_{\max}} (s^\nu/\nu)\right], \qquad s = \alpha/(\alpha+\beta) \tag{34}$$

followed by downward recursion using the reverse of equation (24)

$$V_{m,n-1}(\alpha\beta) = n^{-1}[\beta V_{mn}(\alpha\beta) - A_{m+n}(\alpha+\beta)], \qquad (m \geqslant 0, m+n \geqslant 0) \tag{35}$$

to lower the second index down to h_0. This recursion is in practice very stable up to large values of m for all allowed values of the second index. There is mild differencing in equation (34), which unfortunately increases with increasing m, so for this case we use extended precision (QP or MP) to calculate just the $V_{m,-1}(\alpha\beta)$ function and only if full machine precision is required.

An expansion in $(1-s)$ for use as s nears 1.0 can be obtained from equation (15.3.11) in Abramowitz and Stegun [27], namely

[8] Note that for most of our work g is in the range (0–20).

$$
\begin{aligned}
{}_2F_1(1, m+n+2; m+2; s) = &-\frac{(s-1)^{-n-1}s^{-m-1}\Gamma(m+2)\log(1-s)}{\Gamma(-n)\Gamma(m+n+2)} \\
&-(1-\delta(n,-1))\left[\frac{m+1}{n+1}\sum_{k=0}^{-n-2}\frac{(m+n+2)_k(1-s)^k}{(n+2)_k}\right] \\
&+(1-\delta(m,0))\left[(s-1)^{-n-1}\frac{\Gamma(m+2)}{\Gamma(m+n+2)}\right. \\
&\left.\times\sum_{k=0}^{\infty}\frac{(1-s)^k(m+1)_k(-n)_k(\psi^{(0)}(k+1)-\psi^{(0)}(k+m+1))}{k!(k-n-1)!}\right], \qquad (36)
\end{aligned}
$$

with $\Gamma(k)$, $(a)_k$ and $\psi(k)$ the usual gamma function, Pochhammer symbol, and logarithmic derivative of the gamma function, respectively. This complicated (and costly to implement) expression has several problems, including the fact that the first and third terms have opposite signs and the first sum contains alternating signs (both of which can lead to significant differencing). Only in the s-range (0.97–1.0) is this approach superior (and then not always) to the McKoy scheme, described above, which we use. See appendix B for further details regarding equation (36).

Following a suggestion by King [28, 29], we have also looked into evaluating the hypergeometric functions using Taylor series expansions about points $s = 0.8(0.002)1.0$ over a grid of m, n value pairs. A minimum of 1 function value and derivatives up to order 6 when $s < 0.9$, and a maximum 1 function value plus derivatives up to order 15 for $s > 0.9$ are required at the DP level of accuracy and approximately double this number when using QP. This approach is completely stable and a factor of 5–20 times faster than any of the methods mentioned above. The problem with this approach is obviously that the memory requirements can be quite large, depending on the number of m, n pairs involved (for example, anywhere from 2–32 Mb in our studies).

Finally we note that Frolov and Smith [21] and Drake and Yan [30] have both employed the hypergeometic form in equation (33) in their studies of the V and W integrals (Frolov and Smith's A_2 and A_3 integrals). In this connection, we note that Drake and Yan give an elegant backward recursion relation for evaluating ${}_2F_1(1, m+n+2; m+2; s)$:

$$
{}_2F_1(1, m+n+1; m+1; s) = 1 + \left(\frac{m+n+1}{m+1}\right) s\,{}_2F_1(1, m+n+2; m+2; s). \qquad (37)
$$

This relation is extremely simple to code, completely stable, is self starting (use 1.0), and for a given s the starting value of m depends essentially only on n. Unfortunately the number of iterations (hence the operation count) turns out to be very similar to the number of terms needed when using the defining series for ${}_2F_1(1, m+n+2; m+2; s)$.

Once one has $V(m_{\max}, h_0; \alpha+\beta, \gamma)$ in hand, the m index is lowered from $m_{\max}$ down to $(-h_0 - 1)$ using the stable recursion relation equation (26)

$$
V_{m-1,n}(\alpha\beta) = m^{-1}[\alpha V_{mn}(\alpha\beta) + A_{m+n}(\alpha+\beta)], \qquad (m \geqslant 1, m+n \geqslant 0). \qquad (38)
$$

This completes the calculation of the starting function $W_{f_{\max},g,h_0}(\alpha\beta\gamma)$.

The V functions in equations (29) and (30) are calculated by a scheme analogous to that used for the W, namely, calculate a starting function $V_{m_{\max},n_0}$ with n_0 carefully chosen, then recur up/down on n to get $V(m_{\max}, n_{\min} : -1)$ followed by downward recursion on m to its minimum allowed value of $(-n-1)$. The choice of n_0 turns out to be a bit more difficult than the choice of h_0 for the starting W function. However, we have been able to show that for m in the range (10–400), s in the range (0.01–0.97), and $(\alpha+\beta)$ in the range (1.0–300.0), we can find values of n_0 for a starting function $V(m_{\max}, n_0)$ which will allow us to generate

the V integrals needed in building the W-array from only one Larsson summation and stable recursion schemes. Further details are available on request from the authors.

Our recursion scheme is best illustrated with an example. Suppose we want the array $W(0:f_{\max}, 0:20, h_{\min}:-1)$, that is, with g in the range (0–20).

(i) Calculate $W(f_{\max}, 20, h_0)$ using the Larsson [24] summation given by equation (32). This is the hard part as the $V(m,n)$ series is usually slowly converging (and there may be overflow problems to avoid). But note that the V needed in this summation can be calculated by just one call to the routine which computes a fixed V using the Larsson-type summation described in equation (33) (or, in special cases, by McKoy's formula, equation (34)), followed by the stable recursion relation given by equation (35).

(ii) Raise the third index to get $W(f_{\max}, 20, h_0+1:-1)$ using equation (29). This is a stable recursion. Lower the third index to get $W(f_{\max}, 20, h_{\min}:h_0-1)$ using equation (30). This is also stable over the α, β, γ values we have tried. Repeat (i) and (ii) for another value of g. The Larsson summation will be easier this time as the same set of V can be used over again.

(iii) For each h in the range $(h_{\min}:-1)$ and for each g in the range (0–20) one can lower the first index to get $W(-h-1:f_{\max}, g, h)$ using the stable recursion formula equation (31).

So, for g in the range (0–20), which is typical for us, one only has to do 21 Larsson summations (non-trivial) followed by the usual recursion relations.

The accuracy of the W integrals is checked by comparing W values (the entire array or a specified subarray) calculated in QP with accurate 40 decimal digit MP values obtained using converged Larsson summation and outputting a table giving the number of integrals calculated versus binary bits of accuracy of the QP values. Ordinarily, only the W for small values of f, g, h need be checked in practice since these depend on the W for larger values of the indices through the various recursion equations. For example, we typically only check the subarray $W(0{:}8, 0{:}5, -6{:}-1)$ or perhaps a section along the diagonal $W(f_1{:}f+1+10, g, h_1{:}-1)$, for small values of h_1 and selected g values and where $f_1 = \max(0, -1-g, -2-g-|h|)$. As an additional test MP checks were made for the subarray $W(f_{\max-5}{:}f_{\max}, g, h_{\min}{:}1)$ to test the choice of h_0 and subsequent recursions to raise/lower h. The V were similarly compared with MP values and in much the same way. For the entire V and W arrays, 30 place agreement with the 40 decimal place MP results were routine.

Finally, one additional detail of the W-array calculation is worth mentioning. Floating point exponent overflow is an occasional problem whenever $(\alpha+\beta+\gamma)$ is small and f and h are large in magnitude. Although clever programming can handle problems of this sort, by far the easiest thing to do in practice is just scale the nonlinear parameters of W using the fact that

$$W_{fgh}(\alpha\beta\gamma) = s^{f+g+h+3} W_{fgh}(s\alpha, s\beta, s\gamma) \tag{39}$$

where s is the scale factor, which is most conveniently taken to be a power of two depending on the particular case (it being trival to multiply QP numbers in-line by powers of two). Hopefully the scaled W functions will behave more sensibly than the unscaled W. The cost of this scaling is, therefore, just one extra (trivial) multiplication for each W function calculated, a modest cost for the computational stability obtained. We have found this to be an extremely easy way to eliminate the exponent overflow problem.

4. Convergence acceleration

In tables 1 and 2 we have summarized the results obtained for the series expansion of a typical triangle integral given by equations (11) and (12) using the procedures described in section 3,

Table 1. Levin u-transform acceleration applied to the series expansion of the integral $I = \langle 1s(r_1)1s(r_2)1s(r_3)|r_{12}r_{13}^{-1}r_{23}|1s(r_1)1s''(r_2)1s(r_3)\rangle$, where $1s(r) = \exp(-0.9375r)$ and $1s''(r) = \exp(-3.6875r)$. In the notation of Remiddi this is the integral $Z(1.875, 4.625, 1.875)$ given in equation (14).

N	$I(N)$	Levin $(0, N)$
0	$0.26243\ 75873\ 41781\ 604 \times 10^{-2}$	
1	$0.26503\ 67394\ 61564\ 128 \times 10^{-2}$	
2	$0.26505\ 79473\ 16383\ 076 \times 10^{-2}$	
3	$0.26505\ 91749\ 37799\ 976 \times 10^{-2}$	
4	$0.26505\ 93291\ 00921\ 617 \times 10^{-2}$	
5	$0.26505\ 93590\ 49782\ 063 \times 10^{-2}$	
6	$0.26505\ 93667\ 68479\ 784 \times 10^{-2}$	
7	$0.26505\ 93691\ 95071\ 254 \times 10^{-2}$	
8	$0.26505\ 93700\ 79194\ 118 \times 10^{-2}$	$0.26505\ 93707\ 72107\ 87554\ 95682\ 74743 \times 10^{-2}$
9	$0.26505\ 93704\ 40200\ 502 \times 10^{-2}$	$0.26505\ 93707\ 72116\ 63440\ 45833\ 86022 \times 10^{-2}$
10	$0.26505\ 93706\ 01604\ 334 \times 10^{-2}$	$0.26505\ 93707\ 72116\ 21988\ 03288\ 33951 \times 10^{-2}$
11	$0.26505\ 93706\ 79306\ 139 \times 10^{-2}$	$0.26505\ 93707\ 72116\ 14894\ 71291\ 41561 \times 10^{-2}$
12	$0.26505\ 93707\ 19083\ 962 \times 10^{-2}$	$0.26505\ 93707\ 72116\ 15185\ 68254\ 40808 \times 10^{-2}$
13	$0.26505\ 93707\ 40532\ 094 \times 10^{-2}$	$0.26505\ 93707\ 72116\ 15250\ 20996\ 26353 \times 10^{-2}$
14	$0.26505\ 93707\ 52622\ 044 \times 10^{-2}$	$0.26505\ 93707\ 72116\ 15248\ 33212\ 49204 \times 10^{-2}$
15	$0.26505\ 93707\ 59703\ 982 \times 10^{-2}$	$0.26505\ 93707\ 72116\ 15247\ 74062\ 99741 \times 10^{-2}$
16	$0.26505\ 93707\ 63994\ 105 \times 10^{-2}$	$0.26505\ 93707\ 72116\ 15247\ 74993\ 62547 \times 10^{-2}$
17	$0.26505\ 93707\ 66671\ 112 \times 10^{-2}$	$0.26505\ 93707\ 72116\ 15247\ 75519\ 00254 \times 10^{-2}$
18	$0.26505\ 93707\ 68386\ 069 \times 10^{-2}$	$0.26505\ 93707\ 72116\ 15247\ 75517\ 63156 \times 10^{-2}$
19	$0.26505\ 93707\ 69510\ 860 \times 10^{-2}$	$0.26505\ 93707\ 72116\ 15247\ 75513\ 13851 \times 10^{-2}$
20	$0.26505\ 93707\ 70264\ 354 \times 10^{-2}$	$0.26505\ 93707\ 72116\ 15247\ 75513\ 08210 \times 10^{-2}$
21	$0.26505\ 93707\ 70778\ 867 \times 10^{-2}$	$0.26505\ 93707\ 72116\ 15247\ 75513\ 15893 \times 10^{-2}$
22	$0.26505\ 93707\ 71136\ 357 \times 10^{-2}$	$0.26505\ 93707\ 72116\ 15247\ 75512\ 97711 \times 10^{-2}$
	Procedure	I
	Remiddi 'exact' result	$0.26505\ 93707\ 72116\ 15247\ 75513\ 12672 \times 10^{-2}$
	$I(1)$ + Levin (2, 7)	$0.26505\ 93707\ 71028\ 69329\ 30647\ 87266 \times 10^{-2}$
	$I(1)$ + Levin (2, 12)	$0.26505\ 93707\ 72116\ 15155\ 44538\ 30885 \times 10^{-2}$
	$I(1)$ + Levin (2, 17)	$0.26505\ 93707\ 72116\ 15247\ 75216\ 36081 \times 10^{-2}$
	$I(1)$ + Levin (2, 22)	$0.26505\ 93707\ 72116\ 15247\ 75513\ 12900 \times 10^{-2}$
	$I(1)$ + Levin (2, 27)	$0.26505\ 93707\ 72116\ 15247\ 75513\ 12679 \times 10^{-2}$
	$I(2)$ + Levin (3, 8)	$0.26505\ 93707\ 71546\ 90581\ 96662\ 95490 \times 10^{-2}$
	$I(2)$ + Levin (3, 13)	$0.26505\ 93707\ 72116\ 15108\ 59017\ 54022 \times 10^{-2}$
	$I(2)$ + Levin (3, 18)	$0.26505\ 93707\ 72116\ 15247\ 76056\ 40655 \times 10^{-2}$
	$I(2)$ + Levin (3, 23)	$0.26505\ 93707\ 72116\ 15247\ 75513\ 12081 \times 10^{-2}$
	$I(2)$ + Levin (3, 28)	$0.26505\ 93707\ 72116\ 15247\ 75513\ 12671 \times 10^{-2}$
	$I(3)$ + Levin (4, 9)	$0.26505\ 93707\ 71846\ 06434\ 29947\ 87907 \times 10^{-2}$
	$I(3)$ + Levin (4, 14)	$0.26505\ 93707\ 72116\ 14785\ 52033\ 98432 \times 10^{-2}$
	$I(3)$ + Levin (4, 19)	$0.26505\ 93707\ 72116\ 15247\ 76077\ 76597 \times 10^{-2}$
	$I(3)$ + Levin (4, 24)	$0.26505\ 93707\ 72116\ 15247\ 75513\ 13088 \times 10^{-2}$
	$I(3)$ + Levin (4, 29)	$0.26505\ 93707\ 72116\ 15247\ 75513\ 12672 \times 10^{-2}$
	$I(4)$ + Levin (5, 10)	$0.26505\ 93707\ 71986\ 85529\ 15619\ 33481 \times 10^{-2}$
	$I(4)$ + Levin (5, 15)	$0.26505\ 93707\ 72116\ 14441\ 75105\ 49427 \times 10^{-2}$
	$I(4)$ + Levin (5, 20)	$0.26505\ 93707\ 72116\ 15247\ 74384\ 49217 \times 10^{-2}$
	$I(4)$ + Levin (5, 25)	$0.26505\ 93707\ 72116\ 15247\ 75513\ 22971 \times 10^{-2}$
	$I(4)$ + Levin (5, 30)	$0.26505\ 93707\ 72116\ 15247\ 75513\ 12672 \times 10^{-2}$

Table 2. Generalized (Hurwitz) zeta function acceleration applied to the series expansion of the integral $\langle 1s(r_1)1s(r_2)1s(r_3)|r_{12}r_{13}^{-1}r_{23}|1s(r_1)1s''(r_2)1s(r_3)\rangle$, where $1s(r) = \exp(-0.9375r)$ and $1s''(r) = \exp(-3.6875r)$. In the notation of Remiddi this is the integral $Z(1.875, 4.625, 1.875)$ given in equation (14).

N	$I(N)$	$I(N) + Z(8, N)$
10	$0.26505\,93706\,01604\,334 \times 10^{-2}$	$0.26505\,93707\,72114\,98348\,41908\,17171 \times 10^{-2}$
12	$0.26505\,93707\,19083\,962 \times 10^{-2}$	$0.26505\,93707\,72116\,13547\,76363\,87170 \times 10^{-2}$
14	$0.26505\,93707\,52622\,044 \times 10^{-2}$	$0.26505\,93707\,72116\,15173\,03512\,92726 \times 10^{-2}$
16	$0.26505\,93707\,63994\,105 \times 10^{-2}$	$0.26505\,93707\,72116\,15240\,48596\,20462 \times 10^{-2}$
18	$0.26505\,93707\,68386\,069 \times 10^{-2}$	$0.26505\,93707\,72116\,15246\,67337\,92125 \times 10^{-2}$
20	$0.26505\,93707\,70264\,354 \times 10^{-2}$	$0.26505\,93707\,72116\,15247\,54794\,42339 \times 10^{-2}$
30	$0.26505\,93707\,71994\,834 \times 10^{-2}$	$0.26505\,93707\,72116\,15247\,75470\,85112 \times 10^{-2}$
40	$0.26505\,93707\,72099\,009 \times 10^{-2}$	$0.26505\,93707\,72116\,15247\,75512\,55363 \times 10^{-2}$
50	$0.26505\,93707\,72112\,431 \times 10^{-2}$	$0.26505\,93707\,72116\,15247\,75513\,10544 \times 10^{-2}$
60	$0.26505\,93707\,72115\,089 \times 10^{-2}$	$0.26505\,93707\,72116\,15247\,75513\,12524 \times 10^{-2}$
70	$0.26505\,93707\,72115\,785 \times 10^{-2}$	$0.26505\,93707\,72116\,15247\,75513\,12656 \times 10^{-2}$
80	$0.26505\,93707\,72116\,006 \times 10^{-2}$	$0.26505\,93707\,72116\,15247\,75513\,12670 \times 10^{-2}$
84	$0.26505\,93707\,72116\,048 \times 10^{-2}$	$0.26505\,93707\,72116\,15247\,75513\,12671 \times 10^{-2}$
88	$0.26505\,93707\,72116\,076 \times 10^{-2}$	$0.26505\,93707\,72116\,15247\,75513\,12672 \times 10^{-2}$
100	$0.26505\,93707\,72116\,121 \times 10^{-2}$	
	Remiddi 'exact' result	$0.26505\,93707\,72116\,15247\,75513\,12672 \times 10^{-2}$

along with results obtained for three series acceleration methods. The integral chosen involves only 1s-orbitals so that direct comparison can be made with Remiddi's analytic result [15] for the all 1s orbital case. Nonlinear parameters used are typical of what one would use in an actual Be atom energy calculation. Orbital notation follows our earlier Be work [7].

The triangle integral expansion given by equations (11) and (12) is well known to converge slowly (see column 2 in both tables). Here $I(N)$ is the direct sum value of I when the series for I (given by equation (11)) is truncated at $q = N$. Convergence is logarithmic as shown by Larsson [24]. As can be seen from table 2, column 2, direct summation of the series can give full DP accuracy, but at the QP (30 decimal place) level direct summation is clearly not an attractive option (we are only at DP accuracy with 100 terms in the direct sum[9]). Hence the need for some sort of extrapolation/acceleration. A number of methods exist that attempt to accelerate the convergence, the most promising of which for this work seemed to be the Levin u-transform [32], generalized zeta function extrapolation [33, 34], and van Wijngaarden [35] transformation followed by Levin u-transformation. The respective details for all three of these methods are given in the appendix.

Pelzl and King [12] have applied the Levin u-transformation and the van Wijngaarden method to the related integral:

$$\mathbf{Z}(-1,-1,-1;w_1,w_2,w_3) = \int r_{12}^{-1}r_{13}^{-1}r_{23}^{-1}\exp(-w_1r_1 - w_2r_2 - w_3r_3)\,\mathrm{d}\mathbf{r}_1\,\mathrm{d}\mathbf{r}_2\,\mathrm{d}\mathbf{r}_3 \qquad (40)$$

which converges more slowly than the integral discussed here, obtaining good results at the DP and DP+ level of accuracy. Drake and Yan [30] have used the generalized zeta function extrapolation for the same integral with satisfactory results. Our results for the Levin and zeta function acceleration methods are shown in tables 1 and 2. The van Wijngaarden transformation is not a viable option since it involves 'looking ahead' on the series to calculate

[9] Frolov [31] has reported that QP accuracy requires about 12 000 terms.

additional $A(q)$ elements needed for the extrapolation and we have no way to efficiently calculate these additional elements without calculating all the intervening elements.

In table 1, column 2, we list $I(N), N = 0, \ldots, 22$, with $I(22)$ accurate only to 11 decimals. However, one should note the initial rapid convergence of the series, with $I(3)$ being accurate to five digits. Column 3 gives the results of a Levin u-transform acceleration using these 23 partial sum values (alternatively the 23 $A(q)$ values). Specifically, Levin (0, N) denotes the result for the integral I when Levin u-transform acceleration is applied to the sequence $A(q), q = 0, \ldots, N$. Also shown is the Remiddi 'exact' result (accurate to 30 decimal digits) from which we see that the Levin acceleration gives 25 to 26 place agreement with the exact answer. Although not shown in table 1, still larger Levin (0, N) transforms (i.e., for $N > 22$) actually give progressively worse results, a result which is well understood to be caused by differencing inherent in the Levin u-transform procedure. A similar result was noted by Drake and Yan [30] in their work. However, comparison with $I(22)$ indicates a remarkable 14 digits of accuracy gained by using the Levin procedure.

It is possible to do better still if we partition the series in equation (11) as follows:

$$I = I(K) + \sum_{q=K+1}^{N} A(q) \tag{41}$$

and then apply the Levin u-transform acceleration to the second factor, or 'tail' of the series. The results of this procedure, labelled

$$I(K) + \text{Levin}\,(K+1, N),$$

are given in table 1 also, for $K = 1, \ldots, 4$ and selected values of N (up to 30). It is seen that essentially full agreement with the Remiddi result is obtained for $K = 2, 3, 4$ and $N = K+26$, while the $K = 1$ case differs from the Remiddi result by only 7 in the 30th digit. The reason for the improved agreement is obvious. Since $I(K), k \geqslant 2$ is accurate to 5 digits and the $A(q)$ have all been computed to full accuracy, the erroneous digits in the Levin$(K+1, N)$ term, when added to $I(K)$, do not enter into the 30 digits of the final result. Comparing $I(30)$ from table 2 with $I(4)$ + Levin (5, 30) we see that 18 digits have been gained by the acceleration.

In table 2 we present the results of a generalized zeta function extrapolation/acceleration for this same integral. Column 2 gives the direct sum results $I(N)$ for selected values of N up to $N = 100$. Column 3 lists values of $I(N) + Z(8, N)$, where $Z(8, N)$ is the generalized zeta function estimate for the I-series 'tail' $\sum_{q=N+1}^{\infty} A(q)$. Essentially full QP accuracy (30 decimals) is obtained for $N \geqslant 80$. A $Z(7, N)$ extrapolation would work equally well here (see the appendix for details). Note that zeta function extrapolation does not appear to have the sort of inherent differencing errors one encounters with the Levin u-transform method. On the other hand, the expansion length N is approximately three times as long as for the tail Levin acceleration for the same QP level of accuracy, leading one to prefer Levin in practical calculations, with the zeta function extrapolation serving mainly as a check on the Levin result.

Whereas the 'cost' of calculating the W-array is spread over the cost of calculating maybe thousands of triangle integrals, each integral undergoing 'acceleration' incurs a separate, non-trivial fixed cost for the acceleration. For example, a Levin u-transform of the sequence $A(0), \ldots, A(N)$ requires $(5N + 2)$ floating point arithmetic operations. Thus, the $I(3)$ + Levin (4, 29) scheme requires $5 \times 25 + 2 = 127$ arithmetic operations. On the other hand, the $I(88) + Z(8, 88)$ zeta function acceleration, which gives the same result, requires $2(8 + 1)(8 + 2) = 180$ arithmetic operations. A $Z(7, 88)$ extrapolation would require 144 operations. Here again Levin u-transformation would seem to be the method of choice. Of course, if one does not need full QP accuracy, one can lower the 'sizes' of the extrapolations for both methods and reduce the per integral acceleration cost accordingly.

Table 3. Series acceleration applied to the expansion of the integral $\mathbf{Z}(N_1, N_2, N_3, w_1, w_2, w_3) = \int r_{12} r_{13}^{-1} r_{23} r_1^{N_1-1} r_2^{N_2-1} r_3^{N_3-1} \exp(-w_1 r_1 - w_2 r_2 - w_3 r_3)\, \mathrm{d}\mathbf{r}_1\, \mathrm{d}\mathbf{r}_2\, \mathrm{d}\mathbf{r}_3$.

N_1	N_2	N_3	ω_1	ω_2	ω_3	Procedure	I
1	1	2	1.875	1.875	1.875	$I(3) + L(4, 29)$	0.13082 09812 08397 73522 35202 82063
1	1	2	1.875	1.875	1.875	$I(88) + Z(8, 88)$	0.13082 09812 08397 73522 35202 82063
1	1	3	1.875	1.875	4.625	$I(3) + L(4, 29)$	$0.33721\ 55183\ 97029\ 92662\ 01726\ 35923 \times 10^{-2}$
1	1	3	1.875	1.875	4.625	$I(88) + Z(8, 88)$	$0.33721\ 55183\ 97029\ 92662\ 01726\ 35922 \times 10^{-2}$
3	3	3	1.875	1.875	4.625	$I(3) + L(4, 29)$	$0.60013\ 12193\ 11404\ 67291\ 98499\ 11050 \times 10^{-1}$
3	3	3	1.875	1.875	4.625	$I(88) + Z(8, 88)$	$0.60013\ 12193\ 11404\ 67291\ 98499\ 11051 \times 10^{-1}$
1	1	3	1.875	1.875	7.375	$I(3) + L(4, 29)$	$0.34451\ 77030\ 77120\ 20124\ 05543\ 27182 \times 10^{-3}$
1	1	3	1.875	1.875	7.375	$I(88) + Z(8, 88)$	$0.34451\ 77030\ 77120\ 20124\ 05543\ 27181 \times 10^{-3}$
1	2	3	1.875	1.875	7.375	$I(3) + L(4, 29)$	$0.84633\ 71300\ 85042\ 97747\ 68064\ 59143 \times 10^{-3}$
1	2	3	1.875	1.875	7.375	$I(88) + Z(8, 88)$	$0.84633\ 71300\ 85042\ 97747\ 68064\ 59142 \times 10^{-3}$
3	3	3	1.875	1.875	7.375	$I(3) + L(4, 29)$	$0.57815\ 58605\ 15428\ 39144\ 73631\ 36233 \times 10^{-2}$
3	3	3	1.875	1.875	7.375	$I(88) + Z(8, 88)$	$0.57815\ 58605\ 15428\ 39144\ 73631\ 36232 \times 10^{-2}$
3	3	5	1.875	1.875	7.375	$I(3) + L(4, 29)$	$0.32093\ 93187\ 20061\ 10583\ 85837\ 28259 \times 10^{-2}$
3	3	5	1.875	1.875	7.375	$I(88) + Z(8, 88)$	$0.32093\ 93187\ 20061\ 10583\ 85837\ 28260 \times 10^{-2}$
3	5	5	1.875	7.375	7.375	$I(3) + L(4, 29)$	$0.55456\ 45336\ 69859\ 54897\ 01541\ 65994 \times 10^{-6}$
3	5	5	1.875	7.375	7.375	$I(88) + Z(8, 88)$	$0.55456\ 45336\ 69859\ 54897\ 01541\ 65998 \times 10^{-6}$
3	5	7	1.875	7.375	7.375	$I(3) + L(4, 29)$	$0.64154\ 30023\ 06312\ 85317\ 08759\ 36157 \times 10^{-6}$
3	5	7	1.875	7.375	7.375	$I(88) + Z(8, 88)$	$0.64154\ 30023\ 06312\ 85317\ 08759\ 36158 \times 10^{-6}$

In table 3 we give values for a selection of triangle integrals over Ns orbitals computed using QP arithmetic corresponding to the integral

$$\mathbf{Z}(N_1, N_2, N_3, w_1, w_2, w_3) = \int r_{12} r_{13}^{-1} r_{23} r_1^{N_1-1} r_2^{N_2-1} r_3^{N_3-1} \exp(-w_1 r_1 - w_2 r_2 - w_3 r_3)\, \mathrm{d}\mathbf{r}_1\, \mathrm{d}\mathbf{r}_2\, \mathrm{d}\mathbf{r}_3. \quad (42)$$

This table shows that the $I(3)$ + Levin (4, 29) procedure works for QP accuracy in the calculations for Ns orbitals as well. In this table $L(4, 29) \equiv$ Levin (4, 29). Generalized zeta function extrapolation ($I(88) + Z(8, 88)$) is used as the 'exact' result for estimating the accuracy of the direct + tail Levin u-transforms for these integrals, since only in the all 1s-orbitals case can direct comparison with Remiddi's analytic result be made. Comparison with the Remiddi 'exact' value in table 2 indicates that comparison with the $I(8) + Z(8, 88)$ zeta function expansion is a good indicator of accuracy for these integrals. We judge these results to be accurate to essentially 30 digits. In practical calculations we use an $I(3)$ + Levin (4, 29) acceleration procedure for QP accuracy calculations for triangle integrals over Ns orbitals.

For non-s orbitals, the situation is more complicated. For all s orbitals, the series $A(q)$ in equations (11) and (12) is monotone decreasing starting with $A(0)$. Integrals of the form (ss, ss, $nln'l$), $l > 0$ behave similarly[10], since such integrals are easily shown to be proportional to the corresponding integral with $nln'l$ replaced by nsn's. But for integrals of the form (sl, ss, sl), l = p, d, f, the $A(q)$ series initially increases in value with the maximum occurring at $A(1)$ for p orbitals, $A(2)$ for d-orbitals, $A(3)$ for f orbitals, etc. This implies that logarithmic convergence will not obtain until further out in the series, meaning one must take a larger direct sum $I(K)$ before applying an appropriate tail Levin transform. That is, the acceleration procedure is now a function of the type of integral. This is shown in table 4,

[10] The notation for the integrals lists the orbitals in charge distribution form, orbitals for electrons 1, 2 and 3, respectively, separated by commas.

Table 4. Direct + tail Levin u-transform applied to the series expansion of the integrals $I = \langle\phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2)\phi_3(\mathbf{r}_3)|r_{12}r_{13}^{-1}r_{23}|\phi_1'(\mathbf{r}_1)\phi_2'(\mathbf{r}_2)\phi_3'(\mathbf{r}_3)\rangle$, where the s and non-s STOs $\phi_i(\mathbf{r})$ are defined in equation (2). 'Charge distrib' lists the orbitals used in the integrals in charge distribution form, the product of orbitals for electrons 1, 2 and 3, respectively, separated by commas. $\alpha = 3.6875$ for orbitals labelled with $''$ 0.9375 otherwise. ω_i is the sum of the α for electron i.

ω_1	ω_2	ω_3	Charge distrib	I
1.875	1.875	4.625	$(1s2\,p_0, 1s1s, 1s2\,p_0'')$	$0.10066\,84878\,43444\,84864\,63592\,909 \times 10^{-2}$
1.875	1.875	4.625	$(1s2\,p_0, 1s1s, 1s4\,p_0'')$	$0.11833\,16774\,13366\,58115\,19439\,408 \times 10^{-2}$
1.875	1.875	1.875	$(1s2\,p_0, 1s1s, 1s6\,p_0'')$	$0.25743\,89694\,78797\,30692\,11152\,245 \times 10^{-2}$
4.625	1.875	4.625	$(1s3\,d_0'', 1s1s, 1s3\,d_0'')$	$0.14346\,47386\,47689\,32252\,51073\,608 \times 10^{-4}$
4.625	1.875	4.625	$(1s3\,d_0'', 1s1s, 1s4\,d_0'')$	$0.14703\,92116\,35576\,65591\,18724\,228 \times 10^{-4}$
4.625	1.875	4.625	$(1s4\,d_0'', 1s1s, 1s4\,d_0'')$	$0.16231\,07687\,95971\,07033\,07366\,828 \times 10^{-4}$
4.625	1.875	4.625	$(1s4\,f_0'', 1s1s, 1s4\,f_0'')$	$0.90510\,72608\,44242\,71161\,49757\,6 \times 10^{-5}$
4.625	1.875	4.625	$(1s4\,f_0'', 1s1s, 1s5\,f_0'')$	$0.11374\,35574\,81047\,80859\,46671\,6 \times 10^{-4}$
4.625	1.875	4.625	$(1s5\,f_0'', 1s1s, 1s5\,f_0'')$	$0.15286\,81862\,39593\,07275\,31049\,5 \times 10^{-4}$
1.875	1.875	4.625	$(2\,p_0 2\,p_0, 1s1s, 2\,p_0 2\,p_0'')$	$0.98583\,53341\,16785\,59122\,05368\,963 \times 10^{-2}$
1.875	1.875	4.625	$(2\,p_0 2p_0, 1s1s, 2\,p_0 3\,p_0'')$	$0.11134\,31134\,51262\,35929\,64403\,064 \times 10^{-1}$
1.875	1.875	4.625	$(2\,p_0 2\,p_0, 1s1s, 3\,p_0 3\,p_0'')$	$0.15035\,21732\,19263\,87212\,62852\,604 \times 10^{-1}$
1.875	1.875	4.625	$(3\,d_0 3\,d_0, 1s1s, 3\,d_0 3\,d_0'')$	0.11449 39119 42576 97455 82583 88
1.875	1.875	4.625	$(3\,d_0 3\,d_0, 1s1s, 3\,d_0 4\,d_0'')$	0.18406 70664 81700 38830 73834 80
1.875	1.875	4.625	$(3\,d_0 3\,d_0, 1s1s, 4\,d_0 4\,d_0'')$	0.33719 54635 42604 81407 30305 24

where we list our best estimates for the values of a number of triangle integrals involving non-s type orbitals. It can be seen that the accuracy for integrals containing p orbitals is 28 digits, 27 digits for d orbitals, and 26 digits when f orbitals are used. We point out that (pp, ss, pp) type integrals have an estimated accuracy similar to that of (sd, ss, sd) integrals. This follows from the fact that pp charge distributions can be expanded in terms of ss and sd charge distributions, meaning that (pp, ss, pp) type integrals can be expressed in terms of (ss, ss, ss) and (sd, ss, sd) type integrals, from which one can infer the probable accuracy of any acceleration attempt. Similarly, (dd, ss, dd) can be expressed in terms of (ss, ss, ss), (sd, ss, sd) and (sg, ss, sg) type integrals.

Also, the accuracy of the non-s orbital integrals is not full QP accuracy. We have done extensive experimentation but have been unable to achieve QP accuracy or to understand why the accuracy of the series acceleration falls off as the orbital l value increases. Fortunately, in actual calculations these integrals do not need to be known to such high accuracy because they ordinarily enter into matrix elements that are less important in the energy calculation. Certainly, for the Be atom the (ss, ss, ss) type triangle integrals are far and away the most important. However we are still looking into the problem, especially with respect to calculating the $\mathcal{A}$ factors, more accurate zeta expansions (which we use to judge the tail Levin extrapolations), and perhaps using quad-double (QD) to get some 'known' values against which we can calibrate acceleration schemes.

For DP accuracy, table 1 suggests that either $I(1)$ + Levin (2, 12) or $I(2)$ + Levin (3, 13) accelerations will give full DP accuracy (when the $A(q)$ values are computed to (full) DP accuracy). And in table 2, $I(12) + Z(8, 12)$ also gives full DP accuracy. That is, 14 terms in the I expansion are required for DP accuracy using Levin acceleration while 13 terms are needed for the zeta function acceleration. For expansions of this length, many of the problems mentioned in section 3.3 no longer obtain, including exponent overflow or the need for QP arithmetic. Since both acceleration methods perform similarly at the DP level, both are made

available in our codes as user selected options. We also note that Levin (0,10) or Levin (0,11), which give essentially DP accuracy, are not attractive options as the $A(q)$ values must be calculated in QP arithmetic for the acceleration to work. Finally we note that the above observations are made with data from s orbital calculations. The problems with non-s orbitals affecting the accuracy of the QP calculation do not affect the DP calculation of non-s orbitals. These can be handled the same way as the all s orbital cases, except that we may need to go to $I(3)$ + Levin (4, 21) to compensate for the fact that the series is not monotone decreasing.

5. Discussion

The techniques we have discussed, which include doing integrals by blocks, recursive calculation of V and W, special techniques for slowly convergent regions, direct plus Levin u convergence acceleration, and minimizing the number of MP calculations are all important in any attempt to extend high precision calculations to Be and beyond (and probably for Li too). The W integrals have been discussed extensively in the past [19, 20, 22–24, 9, 36, 30, 21, 1], but no one has discussed them in the context of both accuracy (30 digits) and speed. Calculation of the W to QP accuracy is absolutely essential in order for the triangle integral direct sum to be Levin extrapolated.

It is also important to know how 'good' our extrapolated results really are, especially in the absence of any Remiddi style analytic results with which to calibrate an acceleration method. Certainly, agreement between Levin and Zeta function methods is one way to proceed, assuming there is a systematic pattern to the acceleration data. But we still have a problem in the non-s orbital cases where we have not been able to get as good a zeta extrapolation value as that given by tail Levin extrapolation. We are investigating larger zeta function extrapolations to get calibration values for the non-s cases. It may not be possible to get these two very different extrapolation schemes to agree (zeta and tail Levin), of course, in which case what we really need are analytic Remiddi style formulae. Or we could use the brute force methods of Frolov and Bailey [1] (Frolov and Bailey do not discuss the recursive evaluation of the vast majority of the W needed, a major part of this paper), there being little difference between an all s-orbital and an (sp, ss, sp) integral. We cannot be really certain of the non-s results beyond what is suggested by the 'pattern' of convergence, but the important all s-orbital case seems solved to QP accuracy. It is important to note that either acceleration scheme will give DP accuracy with no doubt whatsoever. With full DP accuracy, one can go a long way at the DP level. Specifically, we should have accurate enough integrals for a 10^{-9} uncertainty in the total energy.

There is considerable room for improving the W-array calculation. Specifically,

(i) Minimizing the calculation of W that are never used but arise because of the recursion used.

(ii) More use of mixed mode arithmetic, i.e., calculate early terms in the I-series in QP but the higher terms in DP.

(iii) Use of additional data types (beyond DP and QP) to essentially eliminate the need for MP. Note that the time consumed in MP code is negligible overall since only a very small number of W are calculated using Larsson summation and the rest of the W are calculated on average with one floating point multiply and 1 floating point add plus an integer divide (fast in QP) (or they are calculated in QP in the case of an DP accuracy calculation). Software support for a number of new data types for Fortran 90 has recently become available, including double precision with exponent (DPE), quadruple precision with exponent (QPE) (for handling the exponent overflow problem), quad–double precision

(QD), and quad–double with exponent (QDE). And triple–double (TD) and triple–double with exponent (TDE) are under development for general purpose MP [37].

(iv) It is important to tune the DP accuracy option for maximum speed, since the bulk of the time will be spent in this mode. The overhead associated with QP arithmetic is such that 'tuning' is not really feasible in practice.

The results of our convergence acceleration study can be summarized as follows: Levin u-transforms have problems because of alternating signs, zeta expansions are too long, and B-transforms, while they solve the sign problem, introduce another problem. The direct + tail Levin extrapolation used in this work largely overcomes all these problems.

The methods developed in this paper should be relevant to the calculation of the very difficult X functions arising in conventional Hy-r_{ij} calculations. And they should be relevant to the acceleration of the infinite series that arise in three and four-electron systems. A Larsson summation formula exists for the X function in terms of W functions, so that one can start a recursion scheme essentially identical to the one used here for the W. Of course, one needs lots of W but we have an efficient scheme to get them.

Finally, we point out that the three-electron triangle integrals discussed here have been the real bottleneck to highly accurate Hy-CI calculations. Now that this bottleneck has been removed, doing really accurate calculations on atoms with $N \geqslant 5$ becomes a real possibility. This is unlike the situation with Hy-r_{ij}, where there are considerable difficulties already at $N = 5$ due to the large number of five-electron integrals [38].

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Appendix A. Convergence acceleration methods

A.1. Levin u-transform

A Levin u-transformation [32] is perhaps the most widely known technique for accelerating logarithmically convergent series. Consider equation (11), written as

$$I = \sum_{q=0}^{\infty} A(q). \tag{A.1}$$

This becomes $I = \sum_k u_k$ with the Levin u-transformation given by

$$u_k = \frac{\sum_{j=0}^{k} c_j(k, A(j)) S_j}{\sum_{j=0}^{k} c_j(k, A(j))}. \tag{A.2}$$

In equation (A.2) S_j is a partial sum of I given by

$$S_j = \sum_{w=0}^{j} A(w) \tag{A.3}$$

and

$$c_j(k, A(j)) = (-1)^j C_j^k (j+1)^{k-2} A(j)^{-1} \tag{A.4}$$

with C_j^k the binomial coefficient given by

$$C_j^k = \frac{j!}{k!(k-j)!}. \tag{A.5}$$

Equation (A.2) is Levin's u-transformation. Note that the Levin u-transformation has coefficients that alternate in sign [39] which is responsible for the cancellation problems in the Levin scheme.

A.2. van Wijngaarden transform

If the series of interest

$$S_\infty = \sum_{w=0}^{\infty} A(w) \tag{A.6}$$

can be converted to a series of the form

$$S_\infty = \sum_{w=0}^{\infty} (-1)^w B(w) \tag{A.7}$$

followed by a Levin u-transform of the new series, then the alternating sign in the new series will cancel the alternating sign in equation (A.4) and the Levin 'differencing' problem essentially goes away.

Pelzl and King [12] were able to come up with an expression for the $B(w)$ which allowed them to apply convergence acceleration techniques in a very effective manner by eliminating the alternate sign problem. Jentschura, Mohr, Soff and Weniger [40], however, point out that the Pelzl–King transform is a rederivation of an older transform of van Wijngaarden [35], where

$$B(w) = \sum_{t=0}^{\infty} 2^t A(2^t(w+1) - 1). \tag{A.8}$$

The Pelzl–King function, as well as all the functions Jentschura *et al* consider, has first to be converted into an alternating series. This involves sampling of the complete series by directly (rather than recursively) calculating the terms with large index, as is seen from equation (A.8). Thus this transform cannot be used in our situation as this involves knowing terms in the expansion we do not have and cannot get in any reasonable manner. The reason the van Wijngaarden transform gives such good results, of course, is just this 'lookahead' feature, but it is also the feature that prevents it from being useful to us.

A.3. Generalized zeta function

Suppose one has the series

$$I = \sum_{s=0}^{\infty} A(s) = \sum_{s=0}^{N} A(s) + \sum_{s=N+1}^{\infty} A(s) \tag{A.9}$$

$$I = I(N) + \sum_{s=N+1}^{\infty} \frac{a(s)}{s^6}, \tag{A.10}$$

where the rate of convergence is geometric. Larsson [24] has shown that the triangle integral has a rate of convergence that has this asymptotic form for $A(s)$, $s \geqslant N+1$. If now we assume that the analytic functions $a(s)$ can be written

$$a(s) = \sum_{n=0}^{L} \frac{\alpha(n)}{s^n}, \tag{A.11}$$

then equation (A.10) becomes

$$I = I(N) + \sum_{N+1}^{\infty} \frac{1}{s^6} \sum_{n=0}^{L} \frac{\alpha(n)}{s^n} \tag{A.12}$$

$$= I(N) + \sum_{n=0}^{L} \alpha(n) \left(\sum_{s=N+1}^{\infty} \frac{1}{s^{n+6}} \right) \tag{A.13}$$

$$= I(N) + \sum_{n=0}^{L} \alpha(n) \zeta(n+6, N+1), \tag{A.14}$$

where $\zeta(n+6, N+1)$ is the generalized (Hurwitz) zeta function, which in this case is just $\zeta(n+6)$ minus the first N terms of the series. Observe that $\zeta(n+6, N+1) \approx \frac{1}{(N+1)^{n+6}}$. The rate of convergence therefore remains geometric but this rate can now be as large as desired by taking N large enough. To determine the constants $\alpha(n)$, $n = 0, 1, \ldots, L$ we use the last $(L+1)$ values of $A(s)$ in the series for I and assume that

$$A(s) = \sum_{n=0}^{L} \frac{\alpha(n)}{s^{n+6}}, \qquad s = N - L, \qquad N - L = 1, \ldots, N. \tag{A.15}$$

This is a linear system that can be solved for the $\alpha(n)$. Let $M_s(n) = \frac{1}{s^{n+6}}$ be the coefficient matrix. Then

$$\boldsymbol{A} = M\boldsymbol{\alpha} \qquad \boldsymbol{\alpha} = M^{-1}A \tag{A.16}$$

L should be picked first and foremost to get the best acceleration but also to minimize the cost of calculating the $\alpha(n)$ constants. In the present work $L = 8$ seemed to be optimum. Once a value of L has been decided on, the Hurwitz functions in equation (A.14) (whose computation is non-trivial) can be precomputed and entered into the program at compile time. And, of course, the $(L+1)$ by $(L+1)$ inverse matrix M^{-1} is a one time only calculation. Given M^{-1} and the Hurwitz function values, the per integral *cost* of a generalized zeta function acceleration is $2(L+1)(L+2)$ floating point operations, a not inconsiderable expense.

Note added in proof. Equation (36) and appendix B (below) are very recent developments aided by a referee's comments.

Appendix B. Comments on equation (36)

Both of the summations in equation (36) are of hypergeometric type and accordingly can be collapsed to simpler closed form using any of the modern computer algebra systems. Specifically, the second definite sum in equation (36) is reducible with a little prodding by either Mathematica or Maple to the following:

$$\frac{-\sum_{k=1}^{m} \frac{s^k}{k}}{s^{m+1}\Gamma(-n)} \tag{B.1}$$

Inserting this expression into equation (36) and collecting terms gives the simple closed form expression

$$
{}_2F_1(1, m+n+2; m+2; s) = -\frac{(s-1)^{-n-1}s^{-m-1}\Gamma(m+2)}{\Gamma(-n)\Gamma(m+n+2)}\left[\log(1-s) + \sum_{k=1}^{m}\frac{s^k}{k}\right]
$$
$$
-\frac{m+1}{n+1}\sum_{k=0}^{-n-2}\frac{(m+n+2)_k(1-s)^k}{(n+2)_k} \tag{B.2}
$$

which is valid for $n \leqslant -1$ if we adopt the convention that there is no sum when the upper limit is less than the lower limit. The similarity with the McKoy formula, equation (34), is obvious. We have been unable to reduce the remaining indefinite sum in equation (B.2) to a simpler form, although a number of different interesting expressions can be generated, all of which (unfortunately) contain essentially $(-n-1)$ terms. That is, no real simplification is obtained. On the other hand, we have *not* been able to show that a suitable 'closed form' expression for this sum is *not* possible. A detailed numerical comparison between equation (B.2) and the combination McKoy formula followed by recursion to lower n gives essentially identical results (with respect to accuracy and floating point operation counts). Finally, we point out that for large values of m and for s near 1.0 the summation form in equation (36) may in fact be computationally more efficient than its closed form counterpart.

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