Improvements on the application of convergence accelerators for the evaluation of some three-electron atomic integrals

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Convergence accelerator methods are employed to analyze some of the most difficult three-electron integrals that arise in atomic calculations. These integrals have an explicit dependence on the interelectronic coordinates, and take the form $\int r_1^i r_2^j r_3^k r_{23}^l r_{31}^m r_{12}^n \exp^{(-\alpha r_1-\beta r_2-\gamma r_3)} d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3$. The focus of the present investigation are the most difficult cases of the parameter set $\{i, j, k, l, m, n\}$. Several convergence accelerator techniques are studied, and a comparison presenting the relative effectiveness of each technique is reported. When the convergence accelerator approach is combined with specialized numerical quadrature methods, we find that the overall technique yields high-precision results and is fairly efficient in terms of computational resources. Difficulties associated with the standard numerical precision loss of convergence accelerator techniques are circumvented.

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I. INTRODUCTION

The progress on the calculation of a variety of properties for three-electron atomic systems has been significant over the past several years. Both the ground and low-lying excited states of the lithium atom have been the focus of much of the computational activity. There has also been renewed interest in high-precision spectroscopy of this system. Much of the recent progress, together with some of the earlier contributions, can be found in two recent reviews [1,2]. Hylleraas-type calculations have played an important role in many of the high-precision calculations. In this approach, the variational method is employed using basis sets that depend explicitly on the interelectronic coordinates r_{ij}. This choice has the advantage of reasonably rapid convergence of the energy and a number of other properties, but at the cost of more significant integration problems in comparison to what is obtained with a basis set of Slater-type orbitals with no r_{ij} factors present.

For the calculation of the energy and a variety of other properties, such as isotope shifts and hyperfine coupling constants, the integration problems have been substantially resolved. However, for some important properties, principally relativistic contributions to the energy or terms that arise in computing lower bounds for energy levels, there is significant opportunity to improve upon the existing results.

Using Hylleraas-type basis functions, the integration problem for a calculation of atomic three-electron S states reduces to the evaluation of integrals that take the form

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

where r_i denotes an electron-nuclear distance and r_{ij} is an electron-electron separation. It is known that a large class of integrals arising in the four-electron atomic problem using Hylleraas expansions can be reduced to the three-electron case [3]; this provides an added incentive to obtain highly efficient computational algorithms for the three-electron integrals. The integrals in Eq. (1) can be grouped according to the values taken by the parameter set $\{l, m, n\}$. In order of increasing complexity: (i) those integrals having $l, m, n \geqslant -1$, (ii) those integrals have one of the indices $\{l,m,n\} = -2$, with the other two indices $\geqslant -1$, (iii) and the most difficult case, two of the indices $= -2$. The indices $\{i, j, k\}$ are each $\geqslant -2$ (with some restrictions depending on the set $\{l, m, n\}$) and the orbital exponents $\{\alpha, \beta, \gamma\}$ are individually greater than zero.

An energy evaluation for an S state three-electron system by the Hylleraas method requires integrals in case (i). These have been the most extensively studied [4–15] and we do not consider this case at all in the present work. Case (ii) has received far less attention [16–22], and case (iii) has received very little study [18,19]. These latter cases are required for energy lower bound calculations [23,24] and for the calculation of relativistic components of the energy [25,26]. Cases (ii) and (iii) are the focus of the present study.

Progress on improving convergence acceleration techniques has been a topic of ongoing interest [27–41]. One objective of the present investigation is to determine, for the numerical problem under investigation, which of the common convergence accelerator techniques is the most robust. The principal deciding factor in determining this is the numerical precision obtained. A key feature of our computational strategy is a coupling of convergence accelerator methods with specialized numerical quadrature procedures.

II. THEORY

In what follows, we will assign $n = -2$. For case (ii) there are two subcases: l and m not both odd and $\geqslant -1$, l and m *both* odd. The former has received more attention, and is by far the easier integral to evaluate. Many of the integrals in this case can, in fact, be reduced to a sum of two-electron integrals [16]. Integrals with l and m *both* odd are treated by breaking the integral down to an infinite sum of contributions. The individual terms in the sum have been evaluated using different approaches [16–22]. There are two principal issues involved in the numerical computation of one of these integrals. These are the evaluation speed of the individual

terms in the sum, and the actual numerical summation process. Both issues are of concern in the present study. Computational efficiency is an important concern, since the number of integrals required in a high-precision atomic calculation is enormous, particularly when extensive optimization of nonlinear parameters is involved.

The term r_{12}^{-2} may be expanded in terms of Legendre polynomials, and takes the form [16,42,43]

$$\frac{1}{r_{12}^2}=\sum_{l=0}^{\infty}\left[\frac{2l+1}{2}\right]4^{-l}\Bigg[\ln\left|\frac{r_1+r_2}{r_1-r_2}\right|\sum_{\kappa=0}^{l} r_1^{2\kappa-l-1}r_2^{l-2\kappa-1} \times \sum_{\nu=0}^{\min[\kappa,l-\kappa]}(-4)^{\nu}\binom{l}{\nu}\binom{2l-2\nu}{l}\binom{l-2\nu}{\kappa-\nu} -2\sum_{\kappa=0}^{l-1} r_1^{-l+2\kappa}r_2^{l-2\kappa-2}\sum_{j=0}^{\min[\kappa,l-\kappa-1]}4^{j}\binom{l-2j-1}{\kappa-j} \times\sum_{\nu=0}^{j}\frac{(-1)^{\nu}\binom{l}{\nu}\binom{2l-2\nu}{l}}{2j-2\nu+1}\Bigg]P_l(\cos\theta_{12}), \tag{2}$$

where $\binom{a}{b}$ denotes a binomial coefficient. The appearance of the logarithm factor gives an indication that the evaluation of the individual contributions to the sum will be far from trivial, which indeed turns out to be the case, and also gives some clue that the overall rate of convergence for any series decomposition is not expected to be high. We will find it useful to utilize an equivalent expansion

$$r_{12}^{-2}=\sum_{w=0}^{\infty}\frac{(2w+1)}{2r_1r_2}Q_w\left[\frac{r_1^2+r_2^2}{2r_1r_2}\right]P_w(\cos\theta_{12}), \tag{3}$$

where Q_w denotes a Legendre function of the second kind, which leads to some simplifications over Eq. (2). For the other two factors r_{23}^l and r_{31}^m in Eq. (1), a standard Sack [44] expansion in terms of Legendre polynomials is employed

$$r_{31}^m=\sum_{w_1=0}^{\infty}R_{mw_1}(r_3,r_1)P_{w_1}(\cos\theta_{31}), \tag{4}$$

where $R_{mw_1}(r_3,r_1)$ denotes the Sack radial function. A similar expansion is employed for r_{23}^l.

A. The case $n=-2$, $l\geqslant -1$, $m\geqslant -1$

Inserting Eq. (3), the last result and the analogous expansion for r_{23}^l into Eq. (1), leads to

$$I\equiv I(i,j,k,l,m,-2,\alpha,\beta,\gamma) =\sum_{w=0}^{\infty}\sum_{w_1=0}^{\infty}\sum_{w_2=0}^{\infty}I_R(w,w_1,w_2)I_\Omega(w,w_1,w_2), \tag{5}$$

where I_Ω denotes the integral over the angular variables, and I_R is an integral over the radial variables. The angular integral can be written as

$$I_\Omega(w,w_1,w_2)=\int P_w(\cos\theta_{12})P_{w_1}(\cos\theta_{31})P_{w_2}(\cos\theta_{23}) \times d\Omega_1 d\Omega_2 d\Omega_3 =\frac{64\pi^3}{(2w+1)^2}\delta_{ww_1}\delta_{ww_2}\delta_{w_1w_2}, \tag{6}$$

where δ_{ij} denotes a Kronecker delta. Inserting this result into Eq. (5) leads to

$$I(i,j,k,l,m,-2,\alpha,\beta,\gamma)=64\pi^3\sum_{w=0}^{\infty}\frac{I_R(w,w,w)}{(2w+1)}. \tag{7}$$

To evaluate the integral over the radial coordinates, the expansion for the Sack radial function is employed

$$R_{lw}(r_2,r_3)=\sum_{p=0}^{\infty}a_{wlp}r_{23<}^{w+2p}r_{23>}^{l-w-2p}, \tag{8}$$

where $r_{23<}$ denotes $\min(r_2,r_3)$ and $r_{23>}$ designates $\max(r_2,r_3)$. The coefficient a_{wlp} is given by

$$a_{wlp}=\frac{(-\frac{l}{2})_w(w-\frac{l}{2})_p(-\frac{1}{2}-\frac{l}{2})_p}{(\frac{1}{2})_w p!(w+\frac{3}{2})_p}, \tag{9}$$

where $(m)_n$ denotes a Pochhammer symbol. On noting the property of the Pochhammer symbol

$$(-p)_q=0 \quad \text{for integer } p \text{ and } q>p, \tag{10}$$

then the p summation in Eq. (8) terminates at $p_{\max}$, where

$$p_{\max}=\begin{cases}\dfrac{l}{2}-w, & \text{for } l \text{ even}\\ \dfrac{(l+1)}{2}, & \text{for } l \text{ odd.}\end{cases} \tag{11}$$

If Eq. (8) and the analogous result for $R_{mw}(r_3,r_1)$ are substituted into Eq. (7), then

$$I(i,j,k,l,m,-2,\alpha,\beta,\gamma)$$

$$= 32\pi^3 \sum_{w=0}^{\infty} \frac{1}{(2w+1)} \sum_{p=0}^{p_{\max}} \sum_{q=0}^{q_{\max}} a_{wlp} a_{wmq} \times \int r_1^{i+1} r_2^{j+1} r_3^{k+2} r_{23<}^{w+2p} r_{23>}^{l-w-2p} \times r_{31<}^{w+2q} r_{31>}^{m-w-2q} Q_w[(2r_1 r_2)^{-1}(r_1^2+r_2^2)] \times \exp(-\alpha r_1 - \beta r_2 - \gamma r_3) dr_1 dr_2 dr_3, \quad (12)$$

where

$$q_{\max} = \begin{cases} \frac{m}{2} - w, & \text{for } m \text{ even} \\ \frac{(m+1)}{2}, & \text{for } m \text{ odd.} \end{cases} \quad (13)$$

On breaking the integration region appropriately, this last result simplifies to yield

$$I(i,j,k,l,m,-2,\alpha,\beta,\gamma)$$

$$\begin{aligned} &= 32\pi^3 \sum_{w=0}^{\infty} \frac{1}{(2w+1)} \sum_{p=0}^{p_{\max}} \sum_{q=0}^{q_{\max}} a_{wlp} a_{wmq} \{ W_{Q1}(w,k+2+2w+2p+2q,i+1+m-w-2q,j+1+l-w-2p,\gamma,\alpha,\beta) \\ &+ W_{Q1}(w,k+2+2w+2p+2q,j+1+l-w-2p,i+1+m-w-2q,\gamma,\beta,\alpha) \\ &+ W_{Q2}(w,i+1+w+2q,j+1+w+2p,k+2+l+m-2w-2p-2q,\alpha,\beta,\gamma) \\ &+ W_{Q2}(w,j+1+w+2p,i+1+w+2q,k+2+l+m-2w-2p-2q,\beta,\alpha,\gamma) \\ &+ W_{Q3}(w,i+1+w+2q,k+2+m+2p-2q,j+1+l-w-2p,\alpha,\gamma,\beta) \\ &+ W_{Q3}(w,j+1+w+2p,k+2+l+2q-2p,i+1+m-w-2q,\beta,\gamma,\alpha)\}, \end{aligned} \quad (14)$$

where

$$W_{Q1}(w,L,M,N,a,b,c) = \int_0^{\infty} x^L e^{-ax} dx \int_x^{\infty} y^M e^{-by} dy \int_y^{\infty} z^N e^{-cz} Q_w[(2yz)^{-1}(y^2+z^2)] dz, \quad (15)$$

$$W_{Q2}(w,L,M,N,a,b,c) = \int_0^{\infty} x^L e^{-ax} dx \int_x^{\infty} y^M e^{-by} Q_w[(2xy)^{-1}(x^2+y^2)] dy \int_y^{\infty} z^N e^{-cz} dz, \quad (16)$$

$$W_{Q3}(w,L,M,N,a,b,c) = \int_0^{\infty} x^L e^{-ax} dx \int_x^{\infty} y^M e^{-by} dy \int_y^{\infty} z^N e^{-cz} Q_w[(2xz)^{-1}(x^2+z^2)] dx. \quad (17)$$

We term these last three the W_Q integrals.

B. The case $n=-2$, $m=-2$

To arrive at a suitable formula for this case, we first note the use of an alternative expansion for r_{31}^{-2} as

$$r_{31}^{-2} = \sum_{w_2=0}^{\infty} r_{31<}^{w_2} r_{31>}^{-w_2-2} C_{w_2}^1(\cos\theta_{31}), \quad (18)$$

where $C_{w_2}^1(\cos\theta_{31})$ denotes a Gegenbauer polynomial. This alternative expansion is made for the factor r_{31}^{-2} because it leads to a simpler radial integral, but this is at the expense of a more complicated angular integral. If we use Eqs. (3), (18), and the Sack expansion for r_{23}^l,

$$I(i,j,k,l,-2,-2,\alpha,\beta,\gamma)$$

$$= \frac{1}{2} \sum_{w=0}^{\infty} \sum_{w_1=0}^{\infty} \sum_{w_2=0}^{\infty} \sum_{p=0}^{\infty} (2w+1) a_{wlp} S_R(w,w_1,w_2) \times S_\Omega(w,w_1,w_2), \quad (19)$$

where the angular integral S_Ω is

$$S_\Omega(w,w_1,w_2)=\int P_w(\cos\theta_{12})P_{w_1}(\cos\theta_{23})C^1_{w_2}(\cos\theta_{31}) \times d\Omega_1 d\Omega_2 d\Omega_3, \tag{20}$$

and the integral over the radial coordinates $S_R(w,w_1,w_2)$ is

$$S_R(w,w_1,w_2)=\int r_1^{i+1}r_2^{j+1}r_3^{k+2}r_{23<}^{w_1+2p}r_{23>}^{l-w_1-2p}r_{31<}^{w_2}r_{31>}^{-w_2-2} \times Q_w[(2r_1r_2)^{-1}(r_1^2+r_2^2)] \times \exp(-\alpha r_1-\beta r_2-\gamma r_3)dr_1dr_2dr_3. \tag{21}$$

To evaluate the integral over angular coordinates, choose the coordinate system such that

$$d\Omega_1 d\Omega_2 d\Omega_3 = \sin\theta_1 d\theta_1 d\phi_1 \sin\theta_{12} d\theta_{12} d\phi_{12} \sin\theta_{31} d\theta_{31} d\chi \tag{22}$$

with

$$\chi=\phi_{31}-\phi_{12}. \tag{23}$$

In this coordinate system the addition theorem for Legendre polynomials is

$$P_{w_1}(\cos\theta_{23})=P_{w_1}(\cos\theta_{12})P_{w_1}(\cos\theta_{31}) + \sum_{n=1}^{w_1}\frac{(w_1-n)!}{(w_1+n)!}P^n_{w_1}(\cos\theta_{12}) \times p^n_{w_1}(\cos\theta_{31})\cos n\chi. \tag{24}$$

Inserting Eq. (24) into Eq. (20) and integrating over θ_1, ϕ_1, ϕ_{12}, and χ, the finite sum of Eq. (24) vanishes and we are left with

$$\begin{aligned} S_\Omega(w,w_1,w_2) &= 16\pi^3\int_0^\pi P_w(\cos\theta_{12})P_{w_1}(\cos\theta_{12})\sin\theta_{12}d\theta_{12} \\ &\quad\times\int_0^\pi P_{w_1}(\cos\theta_{31})C^1_{w_2}(\cos\theta_{31})\sin\theta_{31}d\theta_{31} \\ &= \frac{32\pi^3}{2w+1}\delta_{ww_1}b_{w_1w_2}, \quad w_2\geqslant w_1, \text{ and } w_1+w_2 \text{ even}, \end{aligned} \tag{25}$$

where the coefficient $b_{w_1w_2}$ is given in terms of γ functions by

$$b_{w_1w_2}=\frac{\Gamma\left(\frac{w_2-w_1}{2}+\frac{1}{2}\right)\left(\frac{w_2+w_1}{2}\right)!}{\Gamma\left(\frac{w_2+w_1}{2}+\frac{3}{2}\right)\left(\frac{w_2-w_1}{2}\right)!}. \tag{26}$$

If the last two conditions in Eq. (25) are not met, the angular integral is zero.

Inserting Eq. (26) into Eq. (19) yields

$$\begin{aligned} I(i,j,k,l,-2,-2,\alpha,\beta,\gamma) &= 16\pi^3\sum_{\substack{w_2=0\\(w_1+w_2)\ \text{even}}}^{\infty}\sum_{w_1=0}^{w_2}b_{w_1w_2}\sum_{p=0}^{p_{\max}}a_{w_1lp} \\ &\quad\times\int r_1^{i+1}r_2^{j+1}r_3^{k+2}r_{23<}^{w_1+2p}r_{23>}^{l-w_1-2p}r_{31<}^{w_2}r_{31>}^{-w_2-2}Q_{w_1}[(2r_1r_2)^{-1}(r_1^2+r_2^2)] \\ &\quad\times\exp(-\alpha r_1-\beta r_2-\gamma r_3)dr_1dr_2dr_3, \end{aligned} \tag{27}$$

and $p_{\max}$ is given by Eq. (11) with w replaced by w_1. If the integration range is appropriately subdivided, then

$$\begin{aligned} I(i,j,k,l,-2,-2,\alpha,\beta,\gamma) &= 16\pi^3\sum_{\substack{w_2=0\\(w_1+w_2)\ \text{even}}}^{\infty}\sum_{w_1=0}^{w_2}b_{w_1w_2}\sum_{p=0}^{p_{\max}}a_{w_1lp}\{W_{Q1}(w_1,k+2+w_1+w_2+2p,i-1-w_2,j+1+l-w_1-2p,\gamma,\alpha,\beta) \\ &\quad+W_{Q1}(w_1,k+2+w_1+w_2+2p,j+1+l-w_1-2p,i-1-w_2,\gamma,\beta,\alpha) \\ &\quad+W_{Q2}(w_1,i+1+w_2,j+1+w_1+2p,k+l-w_1-w_2-2p,\alpha,\beta,\gamma) \\ &\quad+W_{Q2}(w_1,j+1+w_1+2p,i+1+w_2,k+l-w_1-w_2-2p,\beta,\alpha,\gamma) \end{aligned}$$

$$+W_{Q3}(w_1,i+1+w_2,k+w_1-w_2+2p,j+1+l-w_1-2p,\alpha,\gamma,\beta)$$
$$+W_{Q3}(w_1,j+1+w_1+2p,k+2+l+w_2-w_1-2p,i-1-w_2,\beta,\gamma,\alpha)\}. \quad (28)$$

The index l is $\geqslant -1$, subject to the constraint that $(i+j+k+l+4)\geqslant 0$, with combinations of the indices $\{i, j, k\}$ satisfying some additional constraints, in order that the integral is convergent. The barely convergent integrals for case (iii) do not arise in any applications with which we are familiar.

C. Simplification of the W_Q integrals

To evaluate the two key results obtained so far, Eqs. (14) and (28), it is necessary to be able to compute the integrals in Eqs. (15)–(17). Following an earlier approach for some related integrals [17] we proceed as follows. With the change of variables $x=uy$, $y=zt$, we have

$$W_{Q1}(w,L,M,N,a,b,c)=\mathcal{L}!\int_0^1 t^{L+M+1} \times Q_w[(2t)^{-1}(1+t^2)]f(t)dt, \quad (29)$$

where $\mathcal{L}=L+M+N+2$, and

$$f(t)=\int_0^1 \frac{u^L du}{(aut+bt+c)^{\mathcal{L}+1}}. \quad (30)$$

With the change of variables $x=yt$, $y=zu$,

$$W_{Q2}(w,L,M,N,a,b,c) = \mathcal{L}!\int_0^1 t^L Q_w[(2t)^{-1}(1+t^2)]g(t)dt, \quad (31)$$

where

$$g(t)=\int_0^1 \frac{u^{L+M+1}du}{(aut+bu+c)^{\mathcal{L}+1}}. \quad (32)$$

With the change of variables $x=zt$, $y=zu$, we have

$$W_{Q3}(w,L,M,N,a,b,c)=\mathcal{L}!\int_0^1 t^L Q_w[(2t)^{-1} \times(1+t^2)]h(t)dt, \quad (33)$$

where

$$h(t)=\int_0^1 \frac{u^M du}{t(at+bu+c)^{\mathcal{L}+1}}. \quad (34)$$

The key to an efficient evaluation of the W_Q integrals lies in part in setting up a fast and high precision determination of the functions $f(t)$, $g(t)$, and $h(t)$. The function $f(t)$ can be written in the following form:

$$f(t)=\frac{1}{(L+1)(at+bt+c)^{\mathcal{L}+1}} \times {}_2F_1(\mathcal{L}+1,1;L+2;(at+bt+c)^{-1}at), \quad (35)$$

where ${}_2F_1$ denotes a hypergeometric function. For $g(t)$ we have

$$g(t)=\frac{1}{(L+M+2)(at+b+c)^{\mathcal{L}+1}} \times {}_2F_1(\mathcal{L}+1,1;L+M+3;(at+b+c)^{-1}(at+b)), \quad (36)$$

and for $h(t)$

$$h(t)=\frac{1}{(L+N+2)}\left\{\frac{t^{M+1}}{(at+bt+c)^{\mathcal{L}+1}}\,{}_2F_1(\mathcal{L}+1,1; L+N+3;(at+c)(at+bt+c)^{-1})-\frac{1}{(at+b+c)^{\mathcal{L}+1}} \times {}_2F_1(\mathcal{L}+1,1;L+N+3;(at+c)(at+b+c)^{-1})\right\}. \quad (37)$$

Equation (37) can be rewritten in a form more suitable for computation in cases involving $M>-1$ as

$$h(t)=\frac{1}{(M+1)}\left\{\frac{1}{(at+b+c)^{\mathcal{L}+1}}\,{}_2F_1(\mathcal{L}+1,1;M+2; b(at+b+c)^{-1})-\frac{t^{M+1}}{(at+bt+c)^{\mathcal{L}+1}}\,{}_2F_1(\mathcal{L}+1,1; M+2;bt(at+bt+c)^{-1})\right\}. \quad (38)$$

A problematic case occurs for $h(t)$ when $M=-1$. When this situation arises, the following alternative formula is employed:

$$h(t)=\frac{1}{(at+c)^{L+N+2}}\left\{\ln\left[\frac{at+bt+c}{t(at+b+c)}\right]+\sum_{\kappa=0}^{L+N}\binom{L+N+1}{\kappa}\frac{(-b)^{L+N+1-\kappa}}{[\kappa-(L+N+1)]}\times\left[\frac{t^{L+N+1-\kappa}}{(at+bt+c)^{L+N+1-\kappa}}-\frac{1}{(at+b+c)^{L+N+1-\kappa}}\right]\right\}. \tag{39}$$

In Eq. (39) the standard summation convention $\Sigma_{\kappa=0}^{m}\{\}=0$ when $m<0$ is employed. The last equation has the potential to lead to significant figure loss, but in practical calculations given the likely ranges for the values $\{l,m,n\}$, this was not found to be a problem.

D. Moments of the Legendre functions of the second kind

The last integrals that require discussion are the moments of the Legendre functions of the second kind. These are needed for the numerical quadratures, which we detail in the following section. The required integrals are

$$\mathsf{M}(m,w)=\int_0^1 t^{m+w-1}Q_w[(2t)^{-1}(1+t^2)]dt \quad \text{for} \quad m\geqslant 0. \tag{40}$$

The Legendre functions of the second kind are expanded in a series, and after a little manipulation we obtain

$$\mathsf{M}(m,w)=\frac{1}{2^w}\sum_{\kappa=0}^{\lfloor w/2\rfloor}\frac{(-1)^\kappa(2w-2\kappa)!}{\kappa!(w-\kappa)!(w-2\kappa)!}\frac{1}{2^{w-2\kappa}}\sum_{n=0}^{w-2\kappa}\binom{w-2\kappa}{n}\int_0^1 t^{m+2w-2\kappa-2n-1}\ln\left(\frac{1+t}{1-t}\right)dt$$
$$-\sum_{\kappa=0}^{\lfloor (w-1)/2\rfloor}\frac{2(w-2\kappa)-1}{(2\kappa+1)!(w-\kappa)}\frac{1}{2^{w-2\kappa-1}}\sum_{n=0}^{\lfloor (w-2\kappa-1)/2\rfloor}\frac{(-1)^n(2w-4\kappa-2-2n)!}{n!(w-2\kappa-1-n)!(w-2\kappa-1-2n)!}$$
$$\times\frac{1}{2^{w-2\kappa-1-2n}}\sum_{\tau=0}^{w-2\kappa-1-2n}\binom{w-2\kappa-1-2n}{\tau}\frac{1}{(m+2w-2\kappa-2n-2\tau-1)}, \tag{41}$$

where the notation $\lfloor x\rfloor$ is used to designate the floor function; the greatest integer not larger than x. Methods to deal with the integrals involving a log factor that occur in the last equation have been discussed elsewhere [17]. An alternative approach to the evaluation of the moments employs the recursive scheme

$$\mathsf{M}(m,w)=\frac{2w-1}{2w}\{\mathsf{M}(m,w-1)+\mathsf{M}(m+2,w-1)\}-\frac{(w-1)}{w}\mathsf{M}(m+2,w-2), \tag{42}$$

which can be readily derived using the standard recursive formula for Legendre functions of the second kind.

The more complicated moments defined by

$$\mathsf{M}_\mathsf{L}(m,w)=\int_0^1 t^{m+w-1}Q_w[(2t)^{-1}(1+t^2)]\ln t\,dt, \quad \text{for} \quad m\geqslant 0, \tag{43}$$

are also required. They can be calculated by the recursive formula

$$\mathsf{M}_\mathsf{L}(m,w)=\frac{2w-1}{2w}\{\mathsf{M}_\mathsf{L}(m,w-1)+\mathsf{M}_\mathsf{L}(m+2,w-1)\}-\frac{(w-1)}{w}\mathsf{M}_\mathsf{L}(m+2,w-2), \tag{44}$$

and by taking advantage of the results

$$\mathsf{M}_\mathsf{L}(0,0)=-\frac{7\zeta(3)}{4}, \tag{45}$$

$$\mathsf{M}_\mathsf{L}(m,0)=\frac{1}{m}\left[\frac{\pi^2}{12}(2+(-1)^m)-\frac{[1-(-1)^m]}{m}\ln 2-\sum_{k=1}^{m}\frac{(m+k)[1-(-1)^{m+k}]}{k^2}\right],\ m\geqslant 1. \tag{46}$$

In Eq. (45) $\zeta(n)$ denotes the Riemann zeta function.

E. Modified moments involving the Legendre functions of the second kind

In order to carry out some of the specialized numerical quadratures discussed in the following section, it is necessary

to find an efficient scheme to evaluate the following modified moments:

$$\mathsf{M}_{\mathsf{m}}(j,w)=\frac{(j!)^2}{(2j)!}\int_0^1 P_j(2t-1)t^{w-1}Q_w[(2t)^{-1}(1+t^2)]dt. \tag{47}$$

By expanding the Legendre function of the first kind, the following result can be obtained:

$$\mathsf{M}_{\mathsf{m}}(j,w)=\frac{(j!)^2}{2^j(2j)!}\sum_{k=0}^{\lfloor j/2\rfloor}\alpha_{kj}\sum_{l=0}^{j-2k}\beta_{lkj}\mathsf{M}(j-2k-l,w), \tag{48}$$

where

$$\alpha_{kj}=\frac{(-1)^k(2j-2k)!}{k!(j-k)!(j-2k)!}, \tag{49}$$

$$\beta_{lkj}=\binom{j-2k}{l}(-1)^l 2^{j-2k-l}. \tag{50}$$

III. COMPUTATIONAL APPROACH

There have been significant advances in computer technology over the past couple of years. One of the principal advances has been the development of extremely inexpensive memory, relative to what existed just a few years back. This plays a pivotal role in how one might think about solving problems of the type explored in this work. Storing significant amounts of auxiliary functions (when they are not too costly to compute) is the underlying strategy of the numerical approach that we develop.

A. Specialized numerical quadrature

In Sec. II, the W_Q integrals were reduced to sets of one-dimensional quadratures. Some closed-form expressions for these integrals may be obtained [16], but their structure is not well suited to efficient computation. The approach given here is to employ a specialized Gaussian quadrature technique, which permits the required integrals to be rapidly evaluated to high precision. The essential approach is to approximate the integral by a compact sum

$$\int_0^1 s(x)V(x)dx\approx\sum_{i=1}^{N} s(x_i)\nu_i, \tag{51}$$

where $V(x)$ is a given weight function, and $\{x_i,\nu_i\}_{i=1}^N$ is a set of function evaluation points and corresponding weights. An effective procedure for choosing the points and weights involves first finding the set of polynomials that are orthogonal over the weight function V. As standard methods for performing this calculation are extremely ill conditioned, an alternative approach was employed, which lends itself to improved numerical stability. Sack and Donovan [45] (see also [46]) developed a method for finding the points and weights via a set of *modified* moments, which are the inner products of the weight function with the members of some set of orthogonal polynomials $\{\pi_j(x)\}_{j=0}^{2N-1}$. Wheeler [47] formulated an efficient recursive algorithm for implementing those results; the necessary details are concisely presented in [48].

In order to calculate the W_Q integrals to high precision, it is necessary to compute quadrature points and weights for the weight functions

$$V_{w1}(t)=t^{-1}Q_w[(2t)^{-1}(1+t^2)] \tag{52}$$

and

$$V_{w2}(t)=t^{-1}\ln(t)Q_w[(2t)^{-1}(1+t^2)]. \tag{53}$$

The second weight function is necessary because the logarithmic factor in Eq. (39) is poorly sampled by the quadrature sum in Eq. (52) for t near zero; inclusion of this term in the weight function eliminates the problem. If the orthogonal polynomials π_j are based on the shifted Legendre polynomials [49], then the necessary modified moments may be calculated by the formulas given in Sec. II E.

Using quadruple-precision arithmetic (with a 32-bit word), calculating the W_Q integrals to the maximum-attainable precision requires quadrature sums as large as $N=80$, although N as small as 30 is sufficient for many of the integrals. The quadrature size required depends primarily on w; at run time, values of N may be read from a small lookup table containing empirically determined optimal choices.

While Sack and Donovan's approach substantially improves numerical stability, some precision loss was still observed. However, the numerical instability can be alleviated by calculating the quadrature points and weights using a large number of digits in MATHEMATICA [50]. The values of $\{x_i,\nu_i\}_{i=1}^N$, which were stored in a table as a one-time calculation, were determined for both weight functions with w ranging between 0 and 53 and N between 30 and 80.

B. Efficient computation of auxiliary functions

A computationally swift implementation of numerical quadrature techniques for evaluating the W_Q integrals requires a rapid method for computing the auxiliary functions given in Eqs. (30), (32), and (34). Such a method, in turn, necessitates an efficient procedure for calculating the hypergeometric function ${}_2F_1(\alpha,1;\gamma;z)$ to high precision.

Standard series expansions for the hypergeometric function converge rather slowly for certain argument values. To avoid use of the standard series expansion, the ${}_2F_1$ function may be Taylor expanded about a large number of points $z_0\in[0,1)$ for a wide range of integer-valued α and γ. Calculation of a specific hypergeometric function value can then be performed by summing a Taylor series using the expansion coefficients corresponding to the nearest z_0. Since the power term $(z-z_0)^n$ approaches zero very rapidly with increasing n, only a small number of Taylor series terms need to be summed to achieve full precision. The expansion coefficients, which may be formulated in terms of specific hypergeometric function values, can be stored in a substantial lookup table.

As the auxiliary functions f, g, and h lie at the innermost loop of the I-integral calculation, the overall speed of the

TABLE I. Relative performance of some different convergence accelerator techniques on representative I integrals.

Convergence accelerator method	$I(i,j,k,l,m,-2,\alpha,\beta,\gamma)$
	$I(0,0,0,-1,-1,-2,0.65,2.9,2.7)$
Levin-u method	15.271 059 472 580 983 291 193
Levin-t' method	15.271 0
Wynn ρ method	15.271 059 472 580 983 29
Weniger (method 1)	15.27
Weniger (method 2)	15.271 0
	$I(1,1,-2,1,1,-2,2.7,2.7,2.7)$
Levin-u method	9.405 035 706 957 597 571 712 81
Levin-t' method	9.405 035 706 957
Wynn ρ method	9.405 035 706 957 597 571
Weniger (method 1)	9.405 035 706 9
Weniger (method 2)	9.405 035 706 957 5
	$I(1,1,2,3,3,-2,4.338,4.338,7.384)$
Levin-u method	$0.499\,366\,182\,632\,626\,760\,958\,228\,689\times10^{-2}$
Levin-t' method	$0.499\,366\,182\,632\,626\,760\times10^{-2}$
Wynn ρ method	$0.499\,366\,182\,632\,626\,760\times10^{-2}$
Weniger (method 1)	$0.499\,366\,182\,632\,626\times10^{-2}$
Weniger (method 2)	$0.499\,366\,182\,632\,626\,760\,95\times10^{-2}$

computation depends heavily on the degree to which they are optimized. Hence it is worthwhile to compute Taylor series coefficients for as many z_0 values as resources will allow. In particular, $z>0.95$ leads to a very slowly converging hypergeometric series, so tabling many coefficients in this region is particularly beneficial.

C. Application of convergence accelerator techniques

For the case where l and m are *not* both odd, Eq. (14) reduces to a finite series. However, when l and m are *both* odd, Eq. (14) is a logarithmically converging infinite series that behaves asymptotically as

$$I\sim\sum_k \frac{a_k}{k^n}, \tag{54}$$

where n may be at least as low as 3.5 for the worst case ($l=-1,m=-1$). Furthermore, Eq. (28) is an infinite series that converges logarithmically regardless of the value of l. Asymptotically, it also has the behavior of Eq. (54), where n

TABLE II. Sample values for the integrals $I(i,j,k,l,m,-2,\alpha,\beta,\gamma)$ for l and m taking odd integer values.

$I(i,j,k,l,m,-2,\alpha,\beta,\gamma)$	Integral value
$I(1,1,1,1,1,-2,2.7,2.7,2.7)$	7.187 646 245 091 837 752 640 509 647
$I(0,0,0,3,1,-2,0.65,2.9,2.7)$	$4.057\,986\,194\,190\,158\,421\,616\,751\,504\,88\times10^{2}$
$I(0,0,0,1,-1,-2,0.65,2.9,2.7)$	$1.698\,678\,160\,331\,952\,701\,523\,944\,364\times10^{1}$
$I(0,0,0,-1,-1,-2,0.65,2.9,2.7)$	$1.527\,105\,947\,258\,098\,329\,119\,351\,1\times10^{1}$
$I(2,1,1,3,3,-2,4.338,4.338,7.384)$	$4.993\,661\,826\,326\,267\,609\,582\,286\,897\times10^{-3}$
$I(1,1,1,-1,-1,-2,1,2,3)$	$1.539\,760\,693\,224\,313\,153\,271\,887\,8\times10^{1}$
$I(1,2,0,-1,-1,-2,2,1,3)$	$3.033\,016\,868\,423\,766\,832\,086\,433\times10^{1}$
$I(2,3,1,3,-1,-2,4,3,2)$	$1.231\,923\,984\,891\,346\,014\,701\,890\,064\,5\times10^{1}$
$I(0,0,0,1,1,-2,0.65,2.9,2.7)$	$8.010\,294\,020\,625\,911\,698\,150\,966\,029\,63\times10^{1}$
$I(0,0,0,1,1,-2,0.6,2.5,2.5)$	$2.035\,406\,498\,195\,068\,857\,011\,288\,410\,79\times10^{2}$
$I(-1,-1,-1,1,1,-2,0.65,2.9,2.7)$	$7.290\,827\,553\,016\,028\,983\,342\,145\,559\,48\times10^{1}$
$I(2,1,0,1,1,-2,1,1,1)$	$9.081\,208\,531\,877\,960\,030\,338\,360\,040\,9\times10^{5}$
$I(1,1,1,1,1,-2,1,1,1)$	$1.078\,827\,141\,800\,904\,545\,813\,023\,958\,4\times10^{6}$
$I(0,2,3,3,1,-2,1,2,3)$	$1.215\,736\,501\,201\,013\,767\,334\,217\,899\,17\times10^{4}$
$I(-2,-1,2,1,3,-2,1,1,1)$	$1.009\,981\,064\,833\,779\,122\,292\,237\,518\,028\times10^{8}$
$I(-1,-1,0,3,1,-2,1,1,1)$	$8.372\,981\,669\,415\,318\,211\,538\,998\,165\,739\times10^{5}$
$I(0,0,0,3,3,-2,0.65,2.9,2.7)$	$7.592\,744\,871\,252\,500\,069\,580\,632\,976\,73\times10^{3}$
$I(0,0,0,5,3,-2,0.65,2.9,2.7)$	$8.347\,041\,021\,416\,493\,583\,756\,762\,895\,244\times10^{4}$
$I(0,0,0,5,5,-2,0.65,2.9,2.7)$	$3.744\,463\,346\,021\,418\,929\,820\,423\,102\,579\times10^{6}$

TABLE III. Representative values for the integrals $I(i,j,k,l,m,-2,\alpha,\beta,\gamma)$ computed using higher precision arithmetic.

$I(i,j,k,l,m,-2,\alpha,\beta,\gamma)$	Integral value
$I(0,0,0,-1,-1,-2,0.65,2.9,2.7)$	$1.527\,105\,947\,258\,098\,329\,119\,350\,984\,727\,02\times10^{1}$
$I(1,1,1,-1,-1-2,1,2,3)$	$1.539\,760\,693\,224\,313\,153\,271\,888\,635\,230\,4\times10^{1}$
$I(0,0,0,1,1,-2,0.65,2.9,2.7)$	$8.010\,294\,020\,625\,911\,698\,150\,966\,029\,125\times10^{1}$
$I(-2,-1,2,1,3,-2,1,1,1)$	$1.009\,981\,064\,833\,779\,122\,292\,237\,518\,017\,0\times10^{8}$

takes on slightly smaller values than the aforementioned value. Direct summation of Eq. (14) is inefficient, while summation of Eq. (28) is not feasible. However, both of these series may be effectively summed via an appropriately chosen convergence accelerating transformation.

A number of well-known transformations were applied to these two series, with varying success. In addition to the Levin-u [30] and modified Levin-t [31,34], which we denote as Levin-t', the Wynn ρ algorithm [28,29,34] and two transforms presented by Weniger [34] were applied. These convergence accelerators are given by the following formulas. The Levin-u formula is

$$u_k=\frac{\Sigma_{j=0}^{k}c_{jk}(j+1)^{k-2}\dfrac{S_{j+1}}{A_{j+1}}}{\Sigma_{j=0}^{k}c_{jk}(j+1)^{k-2}\dfrac{1}{A_{j+1}}}, \tag{55}$$

the Levin-t' formula is

$$t'_k=\frac{\Sigma_{j=0}^{k}c_{jk}(j+1)^{k-1}\dfrac{S_{j+1}}{A_{j+2}}}{\Sigma_{j=0}^{k}c_{jk}(j+1)^{k-1}\dfrac{1}{A_{j+2}}}, \tag{56}$$

the Wynn ρ formula is

$$\rho_{k+1}^{(n)}=\rho_{k-1}^{(n+1)}+\frac{(k+1)}{\rho_k^{(n+1)}-\rho_k^{(n)}}, \tag{57}$$

with

$$\rho_{-1}^{(n)}=0,\quad \rho_0^{(n)}=S_n, \tag{58}$$

the Weniger (1) formula is

$$w_k^{(1)}=\frac{\Sigma_{j=0}^{k}c_{jk}(-j-1)_{k-1}\dfrac{S_{j+1}}{A_{j+1}}}{\Sigma_{j=0}^{k}c_{jk}(-j-1)_{k-1}\dfrac{1}{A_{j+1}}}, \tag{59}$$

and the Weniger (2) formula is

$$w_k^{(2)}=\frac{\Sigma_{j=0}^{k}c_{jk}(j+1)_{k-1}\dfrac{S_{j+1}}{A_{j+1}}}{\Sigma_{j=0}^{k}c_{jk}(j+1)_{k-1}\dfrac{1}{A_{j+1}}}, \tag{60}$$

where S_i is the ith partial sum of a series, A_i is the ith term of the series and $c_{jk}=(-1)^j\binom{k}{j}$.

It is important to note that Eq. (28) does not converge smoothly, due in part to the constraint that w_1+w_2 must be even. In order to achieve adequate performance from convergence acceleration, one must form a new sequence of terms $\{A_0+A_1,A_2+A_3,\ldots\}$ that exhibits improved characteristics. A slight increase in precision is also obtained when applying this procedure to Eq. (14), at the cost of a small increase in CPU requirements.

TABLE IV. Representative values for the integrals $I(i,j,k,l,-2,-2,\alpha,\beta,\gamma)$.

$I(i,j,k,l,-2,-2,\alpha,\beta,\gamma)$	Integral value
$I(0,0,0,4,-2,-2,0.65,2.9,2.7)$	$7.370\,751\,717\,424\,573\,837\times10^{1}$
$I(0,0,0,6,-2,-2,0.65,2.9,2.7)$	$4.912\,247\,149\,187\,431\,890\times10^{2}$
$I(5,5,0,4,-2,-2,6.52,6.52,1.42)$	$2.648\,011\,637\,084\,397\,34\times10^{-2}$
$I(1,7,3,4,-2,-2,1.42,6.52,6.52)$	$1.775\,862\,983\,358\,494\,38\times10^{-2}$
$I(0,0,0,4,-2,-2,6.52,3.97,3.97)$	$1.239\,128\,937\,797\,144\,948\,1\times10^{-1}$
$I(2,3,1,4,-2,-2,6.52,3.97,3.97)$	$2.417\,774\,258\,610\,491\,439\times10^{-2}$
$I(3,1,2,4,-2,-2,0.65,2.9,2.7)$	$3.696\,961\,214\,545\,992\,677\times10^{3}$
$I(2,2,2,4,-2,-2,0.65,2.9,2.7)$	$2.076\,347\,965\,560\,003\,099\times10^{3}$
$I(2,7,3,4,-2,-2,0.65,2.9,2.7)$	$9.284\,583\,074\,893\,533\,1\times10^{5}$
$I(2,3,1,6,-2,-2,0.65,2.9,2.7)$	$3.875\,442\,706\,643\,971\,86\times10^{4}$
$I(5,5,5,2,-2,-2,0.65,2.9,2.7)$	$2.340\,828\,566\,557\,067\,17\times10^{6}$
$I(1,1,1,5,-2,-2,0.65,2.9,2.7)$	$7.604\,960\,853\,694\,618\,83\times10^{2}$

Several representative *I*-integral values are provided in Table I, which demonstrate the maximum level of precision obtained by each method. No more than 23 partial sums (21 for paired series) were provided as input to each transformation. Superior results were obtained using the Levin-*u* transformation. The maximum level of precision obtained from Eq. (55) increases up to a specific value of the index *k*, after which it rapidly deteriorates. The optimal value of *k* when applying the Levin-*u* transformation to Eq. (14) ranges between 18 and 24, and depends on the values of *l* and *m*. The optimal *k* value for the *u* transformation applied to Eq. (28) remains fixed at 25.

IV. RESULTS AND DISCUSSION

An inspection of the results presented in Table I reveals that the Levin-*u* convergence accelerator is the most robust of the techniques examined. In a practical calculation where the *I* integrals are encountered, limited CPU resources can be efficiently devoted to a determination of the optimal method to employ for each individual integral. A more effective computational strategy is to group integrals by particular classes, with appropriate ranges of the indices $\{i, j, k, l, m, n\}$ specified, and then use the most robust convergence accelerator technique for that class of integrals. For the particular cases examined in the present work, the Levin-*u* technique proves to be superior. For particular cases, all the convergence accelerators give reasonably satisfactory agreement with one another.

In Table II we tabulate a representative sample of the case (ii) integrals. For the most slowly convergent cases, those with $l=-1$, $m=-1$, at least 25 digits of precision have been obtained. For other entries, as many as 31 digits of precision are obtained, which essentially represent the maximum precision possible working in quadruple precision with a 32-bit word length. Since results for a wide range of case (ii) integrals with odd *l* and *m* can be obtained with close to or at machine precision, further improvements in the numerical evaluation of these integrals is most likely to be achieved by fine tuning the code to obtain small gains in computational speed.

The precision reported for the results in Table II has been checked by doing independent calculations using Bailey's [51] multiple precision FORTRAN conversion packages. A small sample of higher-precision values is tabulated in Table III. These values are extremely useful as reference points to check the precision of the standard quadruple precision calculations. Using Bailey's multiple precision packages to produce a standard FORTRAN add-on module for an atomic code would not be a practical consideration, because of the very slow speed of the multiple precision calculations.

Table IV presents a sample of values for the case (iii) integrals. Here the precision is somewhat decreased from the case (ii) results presented in Table II, with about 17–19 digits of precision being obtained. This is a significant improvement over the results obtained in two previous publications [18,19], where approximately 12–14 digits of precision have been reported.

V. CONCLUSION

In summary, a fairly efficient procedure has been presented for the numerical evaluation of a class of three-electron atomic integrals, which yields high-precision results in a fairly fast computational scheme. With some additional tabling of the auxiliary functions, enhancement to the speed of evaluation could be obtained. Convergence accelerators play a critical role in evaluating the slowly converging sums that are obtained in the analysis.

Probably a number of the techniques discussed here can be applied to some of the much more difficult one-center four-electron integrals of similar structure to those of the present work. This topic is under investigation.

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