Calculation of some integrals for the atomic three-electron problem

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An analysis is presented for the evaluation of integrals of the form $\int r_1^i r_2^j r_3^k r_{23}^{-2} r_{31}^m r_{12}^n e^{-\alpha r_1 - \beta r_2 - \gamma r_3} d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3$ which arise in the determination of certain properties for atomic three-electron systems. All convergent integrals with $i \geq -2$, $j \geq -2$, $k \geq -2$, $m \geq -1$, and $n \geq -1$ are discussed. These integrals are solved by reduction to one-dimensional quadratures of the form $\int_0^1 f(x)w(x)\,dx$, where $w(x)$ is one of the four functions $\ln[(1+x)/(1-x)]$, $x^{-1}\ln[(1+x)/(1-x)]$, $\ln[(1+x)/(1-x)]\ln(x^{-1})$, and $x^{-1}\ln[(1+x)/(1-x)]\ln(x^{-1})$, and $f(x)$ is a well-behaved function on the interval [0,1]. The polynomials, which are mutually orthogonal over the interval [0,1] for each of the preceding four weight functions $w(x)$, are determined. These polynomials allow specialized numerical quadrature calculations to be performed, which leads to an efficient algorithm for evaluation of the above integrals.

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I. INTRODUCTION

The integral defined by

$$I(i,j,k,l,m,n,\alpha,\beta,\gamma) = \int r_1^i r_2^j r_3^k r_{23}^l r_{32}^m r_{12}^n e^{-\alpha r_1 - \beta r_2 - \gamma r_3} d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 \; , \quad (1)$$

where r_i is the electron-nuclear coordinate and r_{ij} is the interelectronic separation, occurs in several contexts for the three-electron atomic problem [1–8]. Evaluation of certain relativistic contributions and the determination of lower bounds for energy levels involve these integrals, when a Hylleraas-type expansion is employed for the wave function.

Special cases of the above integral have received attention in the literature. The most difficult cases occur for $l=-2$. For $l=-2$, the case $m=0$ and $n=0$ being well studied, as the two-electron integrals contained in Eq. (1), are those required for the evaluation of relativistic contributions and lower bounds in the two-electron problem [9–12]. A generalization of Eq. (1) has been discussed in the literature [13] for the cases $l,m,n, \geq -1$.

In a recent investigation [14] one of the present authors succeeded in evaluating some of the I integrals for the case $l=-2$. That work should be consulted for additional references and theoretical background.

The focus of this investigation is the reduction of the I integrals to a form suitable for numerical quadrature techniques. Because many I integrals may occur in the course of a single atomic calculation, efficiency of the evaluation technique becomes a critical concern. Specialized quadrature procedures are developed to yield an effective approach to the evaluation of the I integrals.

II. REDUCTION OF I TO THREE-DIMENSIONAL INTEGRALS

Two expansions for the interelectronic coordinates are required. r_{12}^{-2} can be expanded as [14]

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

A slightly modified version of Eq. (2) has been given by Pauli and Kleindienst [15]. The standard summation convention $\sum_{k=n}^{m}=0$ when $m<n$, is employed throughout this work. $\binom{a}{b}$ denotes a binomial coefficient. The Sack formula [16] for the expansion of r_{31}^m is

$$r_{31}^m = \sum_{p=0}^{\infty} R_{mp}(r_3,r_1) P_p(\cos\theta_{31}) \; , \quad (3)$$

where $P_p(\cos\theta_{31})$ are the Legendre polynomials and $R_{mp}(r_3,r_1)$ denotes the radial functions. If Eqs. (2) and (3) and the analogous Sack expansion for r_{23}^n are inserted in Eq. (1), then the I integral simplifies to

$$I(i,j,k,-2,m,n,\alpha,\beta,\gamma)=\int \sum_{p=0}^{\infty}\sum_{l_1=0}^{\infty}\sum_{l=0}^{\infty}\left[\frac{2l+1}{2}\right]4^{-l}P_l(\cos\theta_{23})r_1^i r_2^j r_3^k e^{-\alpha r_1-\beta r_2-\gamma r_3}$$
$$\times R_{mp}(r_3,r_1)R_{nl_1}(r_1,r_2)P_p(\cos\theta_{31})P_{l_1}(\cos\theta_{12})$$
$$\times\Bigg\{\sum_{\kappa=0}^{l} r_2^{-l-1+2\kappa}r_3^{l-1-2\kappa}\ln\left|\frac{r_2+r_3}{r_2-r_3}\right| \times\sum_{v=0}^{\min[\kappa,l-\kappa]}(-4)^v\begin{bmatrix} l\\ v\end{bmatrix}\begin{bmatrix} 2l-2v\\ l\end{bmatrix}\begin{bmatrix} l-2v\\ \kappa-v\end{bmatrix}$$
$$-2\sum_{\kappa=0}^{l-1} r_2^{-l+2\kappa}r_3^{l-2\kappa-2}\times\sum_{j=0}^{\min[\kappa,l-\kappa-1]}4^j\begin{bmatrix} l-2j-1\\ \kappa-j\end{bmatrix}\times\sum_{v=0}^{j}\frac{(-1)^v\begin{bmatrix} l\\ v\end{bmatrix}\begin{bmatrix} 2l-2v\\ l\end{bmatrix}}{2j-2v+1}\Bigg\}d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 . \tag{4}$$

$$I_\Omega=\int P_l(\cos\theta_{23})P_p(\cos\theta_{31})P_{l_1}(\cos\theta_{12})d\Omega_1 d\Omega_2 d\Omega_3 \tag{5}$$

which can be evaluated on employing the standard expansion of the Legendre polynomials

$$P_l(\cos\theta_{31})=\frac{4\pi}{2l+1}\sum_{M=-l}^{l}Y_{lM}^*(\theta_3,\phi_3)Y_{lM}(\theta_1,\phi_1) , \tag{6}$$

to yield

$$I_\Omega=\frac{64\pi^3}{(2l+1)^2}\delta_{l_1 p}\delta_{l l_1}\delta_{pl} , \tag{7}$$

where δ_{ij} is the Kronecker delta. To simplify the notation set

$$F(l,\kappa)=\sum_{v=0}^{\min[\kappa,l-\kappa]}(-4)^v\begin{bmatrix} l\\ v\end{bmatrix}\begin{bmatrix} 2l-2v\\ l\end{bmatrix}\begin{bmatrix} l-2v\\ \kappa-v\end{bmatrix} \tag{8}$$

and

$$G(l,\kappa)=2\sum_{j=0}^{\min[\kappa,l-\kappa-1]}4^j\begin{bmatrix} l-2j-1\\ \kappa-j\end{bmatrix}\sum_{v=0}^{j}\frac{(-1)^v\begin{bmatrix} l\\ v\end{bmatrix}\begin{bmatrix} 2l-2v\\ l\end{bmatrix}}{2j-2v+1} . \tag{9}$$

The functions $F(l,\kappa)$ and $G(l,\kappa)$ defined in Eqs. (8) and (9) are independent of the arguments of any particular I integral, so the most efficient computational procedure is to compute and store arrays for both functions. This actually becomes a necessary approach for odd-m odd-n I integrals. For these cases F and G functions involving large arguments are required. Equations (8) and (9) are not stable for standard numerical evaluation for these cases. This difficulty was solved by evaluating the F and G arrays using exact arithmetic (with MATHEMATICA [17]), and then converting to floating decimal point values suitable for input to our Fortran code. The results were checked by direct calculation using multiple precision arithmetic. Lüchow and Kleindienst [18] have just published an investigation of some of the properties of the functions G and F.

Inserting Eqs. (7)–(9) into Eq. (4) yields

$$I(i,j,k,-2,m,n,\alpha,\beta,\gamma)=32\pi^3\sum_{l=0}^{\infty}\frac{4^{-l}}{(2l+1)}\int R_{ml}(r_3,r_1)R_{nl}(r_1,r_2)r_1^{i+2}r_2^{j+2}r_3^{k+2}e^{-\alpha r_1-\beta r_2-\gamma r_3}$$
$$\times\left\{\sum_{\kappa=0}^{l}r_2^{-l-1+2\kappa}r_3^{l-1-2\kappa}\ln\left|\frac{r_2+r_3}{r_2-r_3}\right|F(l,\kappa)-\sum_{\kappa=0}^{l-1}r_2^{-l+2\kappa}r_3^{l-2\kappa-2}G(l,\kappa)\right\}dr_1dr_2dr_3\ . \tag{10}$$

Equation (10) can be simplified to

$$I(i,j,k,-2,m,n,\alpha,\beta,\gamma)=32\pi^3\sum_{w=0}^{\infty}\frac{4^{-w}(-m/2)_w(-n/2)_w}{(2w+1)[(1/2)_w]^2}\sum_{s=0}^{\infty}a_{wns}\sum_{t=0}^{\infty}a_{wmt}[R_1(i,j,k,m,n,w,s,t,\alpha,\beta,\gamma)$$
$$+R_2(i,j,k,m,n,w,s,t,\alpha,\beta,\gamma)]\ , \tag{11}$$

where

$$R_1=\sum_{\kappa=0}^{l}F(l,\kappa)\{W_{L_1}(i+2+2l+2s+2t,j+1+n-2l-2s+2\kappa,k+1+m-2t-2\kappa,\alpha,\beta,\gamma)$$
$$+W_{L_1}(i+2+2l+2s+2t,k+1+m-2t-2\kappa,j+1+n-2l-2s+2\kappa,\alpha,\gamma,\beta)$$
$$+W_{L_2}(k+1+2l+2t-2\kappa,j+1+2s+2\kappa,i+2+m+n-2l-2s-2t,\gamma,\beta,\alpha)$$
$$+W_{L_2}(j+1+2s+2\kappa,k+1+2l+2t-2\kappa,i+2+m+n-2l-2t-2s,\beta,\gamma,\alpha)$$
$$+W_{L_3}(j+1+2s+2\kappa,i+2+n+2t-2s,k+1+m-2t-2\kappa,\beta,\alpha,\gamma)$$
$$+W_{L_3}(k+1+2l+2t-2\kappa,i+2+m+2s-2t,j+1+n-2l-2s+2\kappa,\gamma,\alpha,\beta)\}\ , \tag{12}$$

$$R_2=-\sum_{\kappa=0}^{l-1}G(l,\kappa)\{W(i+2+2l+2t+2s,j+2+n-2l-2s+2\kappa,k+m-2t-2\kappa,\alpha,\beta,\gamma)$$
$$+W(j+2+2s+2\kappa,i+2+n+2t-2s,k+m-2t-2\kappa,\beta,\alpha,\gamma)$$
$$+W(k+2t+2l-2\kappa,j+2+2s+2\kappa,i+2+m+n-2l-2t-2s,\gamma,\beta,\alpha)$$
$$+W(i+2+2l+2s+2t,k+m-2t-2\kappa,j+2+n-2l-2s+2\kappa,\alpha,\gamma,\beta)$$
$$+W(j+2+2s+2\kappa,k+2l+2t-2\kappa,i+2+m+n-2l-2s-2t,\beta,\gamma,\alpha)$$
$$+W(k+2l+2t-2\kappa,i+2+m+2s-2t,j+2+n-2l-2s-2\kappa,\gamma,\alpha,\beta)\}\ , \tag{13}$$

and

$$W(L,M,N,a,b,c)=\int_0^{\infty}x^Le^{-ax}dx\int_x^{\infty}y^Me^{-by}dy\int_y^{\infty}z^Ne^{-cz}dz\ , \tag{14}$$

$$W_{L_1}(L,M,N,a,b,c)=\int_0^{\infty}x^Le^{-ax}dx\int_x^{\infty}y^Me^{-by}dy\int_y^{\infty}z^Ne^{-cz}\ln\left|\frac{z+y}{z-y}\right|dz\ , \tag{15}$$

$$W_{L_2}(L,M,N,a,b,c)=\int_0^{\infty}x^Le^{-ax}\int_x^{\infty}y^Me^{-by}\ln\left|\frac{y+x}{y-x}\right|dy\int_y^{\infty}z^Ne^{-cz}dz\ , \tag{16}$$

$$W_{L_3}(L,M,N,a,b,c)=\int_0^{\infty}x^Le^{-ax}dx\int_x^{\infty}y^Me^{-by}dy\int_y^{\infty}z^Ne^{-cz}\ln\left|\frac{z+x}{z-x}\right|dz\ . \tag{17}$$

The coefficient a_{wns} in Eq. (11) is defined by

$$a_{wns}=\frac{(w-n/2)_s(-\frac{1}{2}-n/2)_s}{s!(w+\frac{3}{2})_s} \tag{18}$$

and $(m)_n$ denotes the Pochhammer symbol. Efficient methods exist [4] for the evaluation of the W integrals defined in Eq. (14).

III. SIMPLIFICATION OF THE W_L INTEGRALS

The W_L integrals defined in Eqs. (15)–(17) can be evaluated analytically for certain values of L, M, and N. However, for most negative values of these parameters, the integrals, despite their relatively simple appearance, become rather difficult to resolve in a form that is stable for numerical evaluation. Efficient evaluation of these integrals is paramount to the usefulness of Eq. (11), particularly for the case when m and n are *both* odd. In this case the lead summation in Eq. (11) does not terminate. The second and third summations both terminate at finite values for m and n even or odd, based on the properties of the Pochhammer symbols [see Eq. (18)].

The approach adopted below is to convert each of the W_L integrals to an essentially similar set of one-dimensional integrals. These are then evaluated by specialized numerical quadrature procedures.

A. W_{L_1} integrals

The W_{L_1} integral converges for

$$L \geq 0 , \tag{19}$$

$$L+M \geq -2 , \tag{20}$$

$$L+M+N \geq -2 . \tag{21}$$

The constants a, b, and c appearing in Eqs. (14)–(17) are greater than 0. With a suitable change of variable, Eq. (15) can be recast as

$$W_{L_1}(L,M,N,a,b,c)=q!\int_0^1 t^{L+M+1}\ln\left[\frac{1+t}{1-t}\right]dt \times\int_0^1\frac{w^L dw}{(awt+bt+c)^{q+1}} \tag{22}$$

with

$$q=L+M+N+2 . \tag{23}$$

Equation (22) can be simplified to yield several different expressions. The most convenient form, for reasons that will be apparent in Sec. IV, is to retain the distinct factor t^{L+M+1}. By differentiating with respect to a parameter in the second integral, the following result is obtained:

$$W_{L_1}(L,M,N,a,b,c)=q!\int_0^1 t^{L+M+1}\ln\left[\frac{1+t}{1-t}\right]f(t)dt \tag{24}$$

with

$$f(t)=\frac{(-1)^q}{(bt+c)^{q+1}}\left\{\frac{(-1)^L\begin{bmatrix}L\\q\end{bmatrix}}{\epsilon^{L+1}}\left[\ln(1+\epsilon)+\sum_{j=1}^{L}\frac{(-\epsilon)^j}{j}\right]+\sum_{k=\max[1,q-L]}^{q}\frac{(-1)^k}{k(q-k)!(L-q+k)!}\sum_{j=0}^{k-1}\frac{(L+k-j-1)!}{(k-j-1)!(1+\epsilon)^{j+1}}\right\} \tag{25}$$

and

$$\epsilon=\frac{at}{bt+c} , \tag{26}$$

where $\binom{L}{q}$ is a binomial coefficient and

$$\begin{bmatrix}L\\q\end{bmatrix}=0 \quad \text{for } L<q \tag{27}$$

has been employed. The function $f(t)$ is well behaved for all values of t on the interval $[0,1]$. For small values of t, separate evaluation and combination of the factors $\ln(1+\epsilon)$ and $\sum_{j=1}^{L}(-\epsilon)^j/j$ leads to significant figure loss, particularly for large values of L. In such cases, these two factors can be combined by appropriate expansion of the term $\ln(1+\epsilon)$. When large negative arguments for the W_{L_1} integral are encountered, a superior approach to the evaluation of $f(t)$ is to utilize the following result:

$$f(t)=\begin{cases}\dfrac{\epsilon^{L+1}}{(\epsilon+1)^L(L+1)} & \text{for } M+N+1=0\\[2ex] \dfrac{L!}{q![(a+b)t+c]^{q+1}}\displaystyle\sum_{j=0}^{\infty}\frac{(j+q)!}{(j+L+1)!(1+\epsilon^{-1})^j} & \\ \text{for } M+N+1<0 . & \end{cases} \tag{28}$$

With appropriate programming, the calculation of factorial terms can be entirely avoided in the evaluation of Eq. (28).

B. W_{L_2} integrals

The conditions for convergence of the W_{L_2} integral are

$$L \geq -1 , \tag{29}$$

$$L+M \geq -1 , \tag{30}$$

$$L+M+N \geq -2 . \tag{31}$$

With a change in integration variables Eq. (16) can be simplified to yield

$$W_{L_2}(L,M,N,a,b,c) =q!\int_0^1\ln\left[\frac{1+t}{1-t}\right]t^L dt\int_0^1\frac{w^{L+M+1}dw}{(awt+bw+c)^{q+1}} \tag{32}$$

and q is given in Eq. (23). Evaluation of the second integral in Eq. (32) leads to

$$W_{L_2}(L,M,N,a,b,c)=\frac{q!}{c^{N+1}a^{L+M+2}}\int_0^1 t^L \ln\left[\frac{1+t}{1-t}\right] g(t)dt \tag{33}$$

with

$$g(t)=\frac{1}{(t+b/a)^{L+M+2}}\sum_{j=0}^{L+M+1}{}' \begin{bmatrix} L+M+1 \\ j \end{bmatrix} (-1)^j \left[\delta_{N+1+j,0}\ln\left[\frac{\beta+1}{\beta}\right]+\frac{1}{N+1+j}\left\{1-\left[\frac{\beta}{\beta+1}\right]^{N+1+j}\right\}\right] \tag{34}$$

and

$$\beta=c(at+b)^{-1}, \tag{35}$$

and the prime on the summation in Eq. (34) signifies that the second term involving the factor $(N+1+j)^{-1}$ is omitted if $N+1+j=0$. By inspection, $g(t)$ is observed to be well behaved for all values of t on the interval [0,1]. For large values of $L+M+1$ and large negative values of N [a situation which arises for m and n both odd in Eq. (1)], Eq. (33) can be cast into a more suitable form for numerical evaluation:

$$g(t)=\frac{(c/a)^{N+1}}{[t+(b+c)/a]^{q+1}}\frac{p!}{q!}\sum_{j=0}^{\infty}\frac{(j+q)!}{(j+p+1)!(1+\beta)^j}, \tag{36}$$

where $p=L+M+1$. $N<0$ implies $p+1>q$ so Eq. (36) provides a stable procedure for evaluating $g(t)$ for large negative values of N.

C. W_{L_3} integral

The W_{L_3} integral converges for

$$L\geq -1, \tag{37}$$

$$L+M\geq -2, \tag{38}$$

$$L+M+N\geq -2. \tag{39}$$

This integral is most conveniently treated by considering two cases: (i) $M\geq 0$ and (ii) $M<0$. With a change of integration variable Eq. (17) simplifies to

$$W_{L_3}(L,M,N,a,b,c)=q!\int_0^1 x^L dx\int_0^1\frac{y^{L+M+1}\ln[(1+xy)/(1-xy)]}{(axy+by+c)^{q+1}}dy=q!\int_0^1\ln\left[\frac{1+t}{1-t}\right]t^L dt\int_t^1\frac{w^M dw}{(at+bw+c)^{q+1}} \tag{40}$$

on using the transformation formula

$$\int_0^\alpha dy\int_y^\alpha f(x,y)dx=\int_0^\alpha dx\int_0^x f(x,y)dy . \tag{41}$$

Equation (40) can be simplified to yield

$$W_{L_3}(L,M,N,a,b,c)=\frac{q!}{b^{q+1}}\int_0^1\ln\left[\frac{1+t}{1-t}\right]t^L h_1(t)dt \tag{42}$$

with

$$h_1(t)=\frac{1}{\gamma^{L+N+2}}\sum_{j=0}^{M}{}'(-1)^j\begin{bmatrix} M \\ j\end{bmatrix}\left\{\delta_{L+N+j+2,0}\ln\left[\frac{\gamma+1}{\gamma+t}\right]+\frac{1}{(L+N+j+2)}\left[\frac{\gamma}{\gamma+1}\right]^{L+N+j+2}\left[\left[\frac{\gamma+1}{\gamma+t}\right]^{L+N+j+2}-1\right]\right\} \tag{43}$$

with

$$\gamma=\frac{at+c}{b}, \tag{44}$$

and the prime on the summation signifies the term involving $(L+N+j+2)^{-1}$ is omitted if $L+N+j+2=0$. $h_1(t)$ is well behaved for all values of t on the interval [0,1].

For case (ii) with $M<0$, Eq. (40) can be transformed by differentiation with respect to a parameter, to the form

$$W_{L_3}(L,M,N,a,b,c)=\frac{(-1)^M}{b^{q+1}}\left\{\frac{(L+N+1)!}{(-M-1)!}\left[\int_0^1\ln\left[\frac{1+t}{1-t}\right]\ln t\, t^L\gamma^{-L-N-2}dt+\int_0^1\ln\left[\frac{1+t}{1-t}\right]t^L\ln\left[\frac{1+\gamma}{t+\gamma}\right]\gamma^{-L-N-2}dt\right]+\int_0^1\ln\left[\frac{1+t}{1-t}\right]t^{L+M+1}h_2(t)dt\right\} \tag{45}$$

with

$$h_2(t)=\gamma^{-L-N-2}\left\{\frac{(L+N+1)!}{(-M-1)!}\sum_{i=1}^{-M-1}\frac{(-\gamma)^i(t^i-1)t^{-M-1-i}}{i}\right.$$
$$+\frac{1}{(-M-1)!}\sum_{k=1}^{q}\begin{bmatrix}q\\k\end{bmatrix}(-\gamma)^k(L+N+1-k)!\left[(-1)^{k-1}(k-1)!\{(1+\gamma)^{-k}-(t+\gamma)^{-k}\}t^{-M-1}\right.$$
$$\left.\left.+\gamma^{-k}\sum_{i=k}^{-M-1}\frac{(-\gamma)^i(i-1)!}{(i-k)!}(t^i-1)t^{-M-1-i}\right]\right\} \tag{46}$$

and γ is defined in Eq. (44). By inspection, $h_2(t)$ is well behaved for all values of t on the interval [0,1].

IV. EVALUATION OF THE W_L INTEGRALS

Equations (24), (33), (42), and (45) represent the basic results for the evaluation of the W_L integrals. The structure of the integrands are not very suitable for standard numerical quadrature. For example, a 32-point Gauss-Legendre quadrature of

$$\int_0^1 \ln\left[\frac{1+x}{1-x}\right]dx$$

yields the result 1.385 696, while a 384-point Gauss-Legendre quadrature leads to the result 1.386 290 090. Neither value is in very close agreement to the exact result of $2\ln 2 = 1.386\,294\,36\ldots$. One can, of course, resort to interval disection techniques, but these are likely to be ineffective. The reason for these poor results is obvious: the integrand is a rather slowly converging series, and a great number of terms are required to yield an accurate result. A close inspection of the final results for the W_L integrals will make it clear that the integrands can be more of a problem than the illustrative example just discussed above. For W_{L_1}, $(L+M+1)$ may equal -1, in which case the integrand has the basic form $t^{-1}\ln[(1+t)/(1-t)]$ [$f(t)$ does not affect this behavior], which means additional care would be needed in any quadrature approach as $t\to 0$. A similar situation arises for the case when $L=-1$ for W_{L_2} [see Eq. (33)], and for W_{L_3} when $M\geq 0$ [see Eq. (42)]. The W_{L_3} integral for the case $M<0$ involves integrands like $\ln[(1+t)/(1-t)]$, $t^{-1}\ln[(1+t)/(1-t)]$, $\ln[(1+t)/(1-t)]\ln t$, and $t^{-1}\ln[(1+t)/(1-t)]\ln t$. The latter three integrands will all require considerable additional care in the region $t\to 0$. From the preceding comments, it should be apparent that a conventional quadrature scheme is likely to be particularly ineffective.

The final results for the W_L integrals can be cast into a form depending on one of the following integrals:

$$\int_0^1 \ln\left[\frac{1+t}{1-t}\right]F_1(t)dt ,$$

$$\int_0^1 \ln\left[\frac{1+t}{1-t}\right]t^{-1}F_2(t)dt ,$$

$$\int_0^1 \ln\left[\frac{1+t}{1-t}\right]\ln(t^{-1})F_3(t)dt ,$$

$$\int_0^1 \ln\left[\frac{1+t}{1-t}\right]t^{-1}\ln(t^{-1})F_4(t)dt ,$$

where $F_i(t)$, $i=1$–4, are well-behaved functions with no singular behavior on the interval [0,1]. These integrals can be very efficiently evaluated by finding the set of polynomials which are orthogonal on the interval [0,1] with the weight functions

$$w_1(t)=\ln\left[\frac{1+t}{1-t}\right] , \tag{47}$$

$$w_2(t)=t^{-1}\ln\left[\frac{1+t}{1-t}\right] , \tag{48}$$

$$w_3(t)=\ln\left[\frac{1+t}{1-t}\right]\ln(t^{-1}) , \tag{49}$$

$$w_4(t)=t^{-1}\ln\left[\frac{1+t}{1-t}\right]\ln(t^{-1}) . \tag{50}$$

We are not aware of any discussion of these polynomials in the literature. Standard sources do not provide any quadrature points for the above functions, though a remark in one text [19] gives a hint of the difficulty to be expected working with the simple weight function $\ln(x^{-1})$.

The polynomials were determined using the recurrence relation

$$p_0(t)=1 , \tag{51}$$

$$p_{i+1}(t)=\left[t-\frac{\langle p_i(t)t|p_i(t)\rangle}{\langle p_i(t)|p_i(t)\rangle}\right]p_i(t) - \frac{\langle p_i(t)|p_i(t)\rangle}{\langle p_{i-1}(t)|p_{i-1}(t)\rangle}p_{i-1}(t), \quad i\geq 1 , \tag{52}$$

where

$$\langle p_i(t)|p_i(t)\rangle=\int_0^1 w_j(t)[p_i(t)]^2dt \tag{53}$$

and $w_j(t)$ is one of the four weight functions given in Eqs. (47)–(50).

The recurrence scheme given above is well known to have numerical limitations [20]. There is potential for *considerable* loss of significant figures in determination of the coefficients of the polynomials. An initial double precision test calculation followed by an extended precision calculation involving $w_1(t)$ on a Vax mainframe gave poor results. The problem for $w_1(t)$ was initially resolved by evaluating the polynomials analytically using the symbolic algebra capabilities of MATHEMATICA [17].

The moments of each weight function are required for the evaluation of the inner products $\langle p_i | p_i \rangle$. The results employed are

$$\int_0^1 x^m \ln\left[\frac{1+x}{1-x}\right] dx = \left\{[1+(-1)^m]\ln 2 + 2\sum_{i=1}^{[(m+1)/2]} \frac{1}{m-2i+2}\right\}(1+m)^{-1} \quad \text{for } m \geq 0\ , \tag{54}$$

where $[(m+1)/2]=(m+1)/2$ if m is odd and $m/2$ if m is even.

$$\int_0^1 x^m \ln\left[\frac{1+x}{1-x}\right] x^{-1} dx$$

is evaluated using Eq. (54) and for $m=0$ the result

$$\int_0^1 x^{-1} \ln\left[\frac{1+x}{1-x}\right] dx = \frac{\pi^2}{4} \tag{55}$$

is employed. Also

$$\int_0^1 x^m \ln\left[\frac{1+x}{1-x}\right] \ln(x^{-1}) dx = -(m+1)^{-1}\left\{\frac{\pi^2}{12}[2-(-1)^m] - \frac{1+(-1)^m}{(m+1)}\ln 2 - \frac{1}{m+1}\sum_{n=1}^{m+1}\frac{(m+n+1)[1+(-1)^{m+n}]}{n^2}\right\} \quad \text{for } m \geq 0\ . \tag{56}$$

$$\int_0^1 x^m \ln\left[\frac{1+x}{1-x}\right] x^{-1}\ln(x^{-1}) dx$$

is evaluated from Eq. (56), and for $m=0$

$$\int_0^1 \frac{\ln[(1+x)/(1-x)]\ln(x^{-1})dx}{x} = \frac{7\zeta(3)}{4} \tag{57}$$

where $\zeta(n)$ is the Riemann zeta function.

The polynomial coefficients become extremely complex very quickly. Analytic expressions for the first few polynomials can be obtained from the authors. To speed up the calculations, the coefficients of the polynomials were determined numerically, using the variable precision option of MATHEMATICA. Once the polynomials were found, the abscissas x_i of the N-point quadrature and the corresponding weight w_i were determined by standard procedures [21]. As a check on the x_i and w_i values, the integrals in Eqs. (54)–(57) were evaluated by quadrature on a Cray YMP in double precision. The results were found to be in excellent agreement with the analytical results (the relative error was typically $\sim 10^{-28}$). The required integrals were then evaluated using the standard formula

$$\int_0^1 F_1(x)\ln\left[\frac{1+x}{1-x}\right] dx = \sum_{i=1}^{N} F_1(x_i) w_i \tag{58}$$

with similar results for the other integrals discussed above.

V. RESULTS

The polynomial determinations and the evaluation of the x_i and w_i for each polynomial were initially carried out on a PS/2 (model 70) personal computer with no math coprocessor. The calculations were somewhat slow on the PS/2 and it became necessary to continue the problem on a RISC/6000 work station. Even on this machine the calculations were rather slow for the evaluation of the polynomial associated with the fourth weight function, due in part to the result for the zeroth moment, Eq. (57). Some trial and error experimentation was necessary to find the appropriate number of digits of precision to carry in the calculations, in order to accurately determine the x_i and w_i values. The values of x_i and w_i may have applications in a number of problems, and have therefore been submitted to the Physics Auxiliary Publication Service [22].

To show how effective these specialized quadratures are, results for the evaluation of some representative W_L integrals are shown in Table I as a function of the number of quadrature points. Table II gives a selection of values of the W_L integrals, with some additional difficult cases considered.

A few representative I integrals are tabulated in Table III based on the use of Eq. (11). To show the convergence of the w summation in Eq. (11), six examples are illustrated in Table IV where the values of the sum after each value of w are indicated. All the results reported in Tables II–IV were calculated with the quadrature point

TABLE I. Values for some W_L integrals as a function of the number of quadrature points.

Number of quadrature points	$W_{L_1}(1,2,4,2.7,2.9,0.65)$	$W_{L_1}(0,-2,1,2.7,2.9,0.65)$	$W_{L_1}(4,-2,-3,2.7,2.9,0.65)$
10	6.350 817 $\times 10^{-1}$	6.788 721 $\times 10^{-1}$	5.598 422 712 $\times 10^{-3}$
20	6.348 287 386 $\times 10^{-1}$	6.788 781 252 781 $\times 10^{-1}$	5.598 422 539 226 05 $\times 10^{-3}$
30	6.348 291 500 2168 $\times 10^{-1}$	6.788 781 252 876 741 5385 $\times 10^{-1}$	5.598 422 539 225 546 490 99 $\times 10^{-3}$
40	6.348 291 500 611 4396 $\times 10^{-1}$	6.788 781 252 876 741 687 272 684 $\times 10^{-1}$	5.598 422 539 225 546 490 045 482 27 $\times 10^{-3}$
50	6.348 291 500 611 447 850 657 $\times 10^{-1}$	6.788 781 252 876 741 687 272 915 726 $\times 10^{-1}$	5.598 422 539 225 546 490 045 480 648 $\times 10^{-3}$
60	6.348 291 500 611 447 850 745 661 094 $\times 10^{-1}$	6.788 781 252 876 741 687 272 915 726 $\times 10^{-1}$	5.598 422 539 225 546 490 045 480 649 $\times 10^{-3}$
80	6.348 291 500 611 447 850 745 662 590 $\times 10^{-1}$	6.788 781 252 876 741 687 272 915 724 $\times 10^{-1}$	5.598 422 539 225 546 490 045 480 650 $\times 10^{-3}$
100	6.348 291 500 611 447 850 745 662 590 $\times 10^{-1}$	6.788 781 252 876 741 687 272 915 724 $\times 10^{-1}$	5.598 422 539 225 546 490 045 480 646 $\times 10^{-3}$
	$W_{L_2}(1,2,4,2.7,2.9,0.65)$	$W_{L_2}(-1,2,1,2.7,2.9,0.65)$	$W_{L_2}(4,-2,-3,2.7,2.9,0.65)$
10	1.855 658 619 312 4	1.520 882 775 346 809 65 $\times 10^{-1}$	7.809 352 399 028 916 77 $\times 10^{-3}$
20	1.855 658 619 309 307 602 118 614 971	1.520 882 775 346 824 131 371 213 040 $\times 10^{-1}$	7.809 352 399 028 919 648 248 914 499 $\times 10^{-3}$
30	1.855 658 619 309 307 602 118 614 967	1.520 882 775 346 824 131 371 213 040 $\times 10^{-1}$	7.809 352 399 028 919 648 248 914 499 $\times 10^{-3}$
40	1.855 658 619 309 307 602 118 614 965	1.520 882 775 346 824 131 371 213 040 $\times 10^{-1}$	7.809 352 399 028 919 648 248 914 499 $\times 10^{-3}$
50	1.855 658 619 309 307 602 118 614 962	1.520 882 775 346 824 131 371 213 040 $\times 10^{-1}$	7.809 352 399 028 919 648 248 914 499 $\times 10^{-3}$
60	1.855 658 619 309 307 602 118 614 962	1.520 882 775 346 824 131 371 213 040 $\times 10^{-1}$	7.809 352 399 028 919 648 248 914 499 $\times 10^{-3}$
80	1.855 658 619 309 307 602 118 614 965	1.520 882 775 346 824 131 371 213 039 $\times 10^{-1}$	7.809 352 399 028 919 648 248 914 499 $\times 10^{-3}$
100	1.855 658 619 309 307 602 118 614 962	1.520 882 775 346 824 131 371 213 039 $\times 10^{-1}$	7.809 352 399 028 919 648 248 914 498 $\times 10^{-3}$
	$W_{L_3}(1,2,4,2.7,2.9,0.65)$	$W_{L_3}(-1,2,1,2.7,2.9,0.65)$	$W_{L_3}(1,-2,1,2.7,2.9,0.65)$
10	2.590 197 $\times 10^{-1}$	4.234 636 $\times 10^{-2}$	3.520 643 $\times 10^{-2}$
20	2.589 557 73 $\times 10^{-1}$	4.234 775 365 7 $\times 10^{-2}$	3.519 533 469 63 $\times 10^{-2}$
30	2.589 554 750 3 $\times 10^{-1}$	4.234 775 371 119 720 $\times 10^{-2}$	3.519 533 467 796 302 $\times 10^{-2}$
40	2.589 554 749 988 807 7 $\times 10^{-1}$	4.234 775 371 119 757 562 00 $\times 10^{-2}$	3.519 533 467 796 299 064 376 74 $\times 10^{-2}$
50	2.589 554 749 988 800 732 04 $\times 10^{-1}$	4.234 775 371 119 757 562 158 853 45 $\times 10^{-2}$	3.519 533 467 796 299 064 370 313 935 $\times 10^{-2}$
70	2.589 554 749 988 800 731 967 377 608 $\times 10^{-1}$	4.234 775 371 119 757 562 158 853 952 $\times 10^{-2}$	3.519 533 467 796 299 064 370 313 919 $\times 10^{-2}$
90	2.589 554 749 988 800 731 967 377 608 $\times 10^{-1}$	4.234 775 371 119 757 562 158 853 952 $\times 10^{-2}$	3.519 533 467 796 299 064 370 313 916 $\times 10^{-2}$
	$W_{L_3}(0,-2,1,2.7,2.9,0.65)$	$W_{L_3}(-1,-1,2,2.7,2.9,0.65)$	$W_{L_3}(200,-100,-100,5.4,5.4,1.3)$
10	2.967 674 05 $\times 10^{-1}$	1.134 395 0	3.97 $\times 10^{-7}$
20	2.967 668 681 42 $\times 10^{-1}$	1.134 291 802 309 7	2.951 $\times 10^{-7}$
30	2.967 668 681 357 287 04 $\times 10^{-1}$	1.134 291 802 078 768 939	2.947 411 26 $\times 10^{-7}$
40	2.967 668 681 357 286 921 366 07 $\times 10^{-1}$	1.134 291 802 078 768 448 255 36	2.947 411 151 082 793 $\times 10^{-7}$
50	2.967 668 681 357 286 921 365 870 227 $\times 10^{-1}$	1.134 291 802 078 768 448 254 383 650	2.947 411 151 082 751 414 529 0 $\times 10^{-7}$
70	2.967 668 681 357 286 921 365 870 225 $\times 10^{-1}$	1.134 291 802 078 768 448 254 383 649	2.947 411 151 082 751 414 528 879 $\times 10^{-7}$
90	2.967 668 681 357 286 921 365 870 224 $\times 10^{-1}$	1.134 291 802 078 768 448 254 383 649	2.947 411 151 082 751 414 528 881 61 $\times 10^{-7}$

TABLE II. Some W_L integrals involving negative arguments. All integrals are evaluated using $a=2.7$, $b=2.9$, and $c=0.65$ and the quadrature point set employed is (100, 100, 100, 90).

Type	L	M	N	Integral value
W_{L_1}	0	−2	0	1.083 879 599 898 198 513 257 178 293
W_{L_1}	2	−3	−1	$1.250\,010\,973\,399\,807\,433\,307\,142\,399\times10^{-1}$
W_{L_1}	1	−3	1	$3.062\,696\,750\,071\,622\,728\,513\,911\,399\times10^{-1}$
W_{L_2}	−1	0	2	4.208 102 671 056 596 251 692 555 269
W_{L_2}	−1	2	0	$6.907\,359\,995\,821\,510\,518\,498\,717\,951\times10^{-2}$
W_{L_2}	−1	2	3	2.400 459 131 058 917 517 788 881 101
W_{L_3}	−1	0	2	$2.764\,499\,740\,806\,429\,169\,877\,617\,486\times10^{-1}$
W_{L_3}	−1	1	−2	$2.037\,462\,701\,111\,799\,221\,300\,890\,409\times10^{-1}$
W_{L_3}	3	−1	2	$6.227\,779\,185\,629\,390\,790\,392\,624\,846\times10^{-3}$
W_{L_3}	0	−1	2	$1.102\,428\,636\,266\,714\,271\,801\,334\,512\times10^{-1}$
W_{L_3}	0	−1	−1	$1.660\,849\,370\,085\,631\,845\,528\,907\,460\times10^{-1}$
W_{L_3}	0	−2	0	$4.705\,557\,080\,602\,339\,931\,684\,159\,418\times10^{-1}$
W_{L_3}	1	−3	0	$3.073\,732\,135\,871\,503\,739\,127\,446\,372\times10^{-1}$
W_{L_3}	−1	−1	3	3.543 868 845 554 504 664 788 125 473
W_{L_3}	−1	−1	0	$9.876\,051\,123\,075\,226\,886\,136\,545\,810\times10^{-1}$

set {100,100,100,90}; 100 points employed for the first weight function, 100 for the second, etc.

VI. DISCUSSION

The key observation to be made from the results of Table I is the extremely rapid convergence of the W_L integral values as the number of quadrature points is increased. In several cases (particularly for W_{L_2}), approximately 27 digits of precision are obtained with only 20 quadrature points. All the results reported in Table I were matched with the values computed by independent methods which yield, in certain cases, a smaller number of digits of precision. Typically 16–23 digits of precision were found to match between the different methods of calculation.

The fast convergence for many of the W_L integrals is tied to two factors. The logarithmic terms have a poor representation as a polynomial expansion, but this problem is entirely avoided by the nature of the specialized quadrature procedures employed. The rate of convergence for a particular W_L integral is thus determined by how well the functions $f(t)$, $g(t)$, $h_1(t)$, and $h_2(t)$ can be represented by a polynomial expansion. Since none of these functions have any singularities on the interval [0,1], a very good polynomial representation is possible, subject to the values of the arguments for each particular integral. For large negative values of M or N, the above functions are less likely to be accurately approximated by polynomials of short length. In these cases, a large number of quadrature points are necessary to obtain an accurate value for the integral.

The W_{L_1} results reported in Table II were evaluated using Eq. (25). A large number of additional W_L integral test cases were examined. A focus of the effort was the examination of integrals involving large negative arguments for M and N (up to −200). These are the most difficult cases, but are extremely important for the evalu-

TABLE III. Values of $I(i,j,k,l,m,n,\alpha,\beta,\gamma)$ computed using Eq. (11).

i	j	k	l	m	n	α	β	γ	I
0	0	0	−2	0	0	2.5	3.0	0.6	$2.625\,998\,889\,298\,125\,422\,146\,962\,8\times10^{-1}$
0	0	0	−2	4	6	2.5	3.0	0.6	$4.509\,905\,007\,964\,538\,011\times10^{6}$
0	0	0	−2	6	6	2.5	3.0	0.6	$3.333\,172\,436\,048\,289\,562\,605\,531\,173\times10^{8}$
−2	−2	4	−2	2	2	2.5	3.0	0.6	$3.761\,971\,636\,531\,376\,663\,166\,128\,677\times10^{6}$
−1	−2	2	−2	2	4	2.5	3.0	0.6	$1.590\,374\,828\,884\,498\,105\,225\,072\,180\times10^{5}$
0	0	0	−2	−1	0	2.5	3.0	0.6	$1.611\,019\,909\,354\,640\,984\,938\,494\,180\times10^{1}$
0	0	1	−2	−1	2	2.5	3.0	0.6	$6.017\,750\,485\,629\,056\,093\,536\,290\,760\times10^{1}$
1	2	3	−2	1	2	2.5	3.0	0.6	$6.833\,815\,746\,120\,315\,435\,488\,530\,589\times10^{4}$
−2	2	2	−2	−1	2	2.5	3.0	0.6	$7.555\,096\,795\,290\,167\,516\,269\,164\,257\times10^{2}$
−1	−1	3	−2	5	4	2.5	3.0	0.6	$1.105\,739\,136\,640\,783\,062\,978\,512\,954\times10^{9}$
1	−2	1	−2	1	2	2.5	3.0	0.6	$4.141\,831\,292\,273\,281\,421\,100\,703\,936\times10^{3}$
−2	−1	1	−2	−1	2	2.5	3.0	0.6	$1.056\,402\,594\,446\,466\,865\,747\,747\,807\times10^{2}$

TABLE IV. Evaluation of I integrals for some representative odd-m odd-n cases. The convergence is shown as a function of the w summation index of Eq. (11).

w	(1,1,1,−2,1,1, 2.7,2.7,2.7)	(−1,−1,−1,−2,1,1, 2.7,2.9,0.65)	(0,0,0,−2,1,3, 2.7,2.9,0.65)	(0,0,0,−2,1,1, 2.5,2.5,0.6)	(0,0,0,−2,−1,1, 2.7,2.9,0.65)	(0,0,0,−2,−1,−1, 2.7,2.9,0.65)
0	6.940 94	71.539 9	383.964 9	198.929 8	17.831 1	14.02
1	7.183 64	72.889 7	406.040 2	203.475 0	17.044 4	14.89
2	7.187 27	72.906 6	405.804 4	203.534 7	16.998 7	15.09
3	7.187 576	72.907 982	405.799 142	203.539 6	16.990 6	15.17
4	7.187 628	72.908 198	405.798 704	203.540 37	16.988 4	15.21
5	7.187 639 9	72.908 250	405.798 639	203.540 55	16.987 6	15.23
6	7.187 643 7	72.908 265	405.798 624 9	203.540 61	16.987 2	15.24
7	7.187 645 1	72.908 270 9	405.798 621 3	203.540 633	16.987 03	15.25
8	7.187 645 7	72.908 273 2	405.798 620 1	203.540 641	16.986 94	15.25
9	7.187 645 9	72.908 274 3	405.798 619 73	203.540 645	16.986 88	15.25
10	7.187 646 08	72.908 274 8	405.798 619 56	203.540 647	16.986 85	15.257
11	7.187 646 14	72.908 275 12	405.798 619 49	203.540 648 3	16.986 83	15.260
12	7.187 646 18	72.908 275 28	405.798 619 457	203.540 648 9	16.986 82	15.261
13	7.187 646 205	72.908 275 37	405.798 619 440	203.540 649 2	16.986 81	15.263
14	7.187 646 219	72.908 275 42	405.798 619 431	203.540 649 4	16.986 802	15.264
15	7.187 646 227	72.908 275 458	405.798 619 426	203.540 649 6	16.986 797	15.265
16	7.187 646 233	72.908 275 480	405.798 619 423	203.540 649 6	16.986 794	15.265
17	7.187 646 236	72.908 275 494	405.798 619 422	203.540 649 7	16.986 791	15.265 9
18	7.187 646 239	72.908 275 504	405.798 619 420 8	203.540 649 72	16.986 789	15.266 5
19	7.187 646 240 4	72.908 275 511	405.798 619 420 2	203.540 649 75	16.986 788	15.266 9
20	7.187 646 241 6	72.908 275 516	405.798 619 419 8	203.540 649 77	16.986 787	15.267 3
21	7.187 646 242 4	72.908 275 519	405.798 619 419 6	203.540 649 78	16.986 786	15.267 6
22	7.187 646 243 1	72.908 275 521 9	405.798 619 419 4	203.540 649 79	16.986 785	15.267 9
23	7.187 646 243 5	72.908 275 523 8	405.798 619 419 30	203.540 649 80	16.986 784 7	15.268 2
24	7.187 646 243 9	72.908 275 525 2	405.798 619 419 22	203.540 649 80	16.986 784 2	15.268 4
25	7.187 646 244 11	72.908 275 526 2	405.798 619 419 16	203.540 649 80	16.986 783 8	15.268 6
26	7.187 646 244 31	72.908 275 527 0	405.798 619 419 13	203.540 649 808	16.986 783 5	15.268 8
27	7.187 646 244 46	72.908 275 527 6	405.798 619 419 098	203.540 649 810	16.986 783 3	15.268 9
28	7.187 646 244 58	72.908 275 528 11	405.798 619 419 078	203.540 649 812	16.986 783 0	15.269 1
29	7.187 646 244 677	72.908 275 528 49	405.798 619 419 063	203.540 649 813	16.986 782 9	15.269 2
30	7.187 646 244 751	72.908 275 528 79	405.798 619 419 052 1	203.540 649 814 4	16.986 782 7	15.269 3
40	7.187 646 245 028	72.908 275 529 90	405.798 619 419 019 7	203.540 649 818 6	16.986 781 97	15.270 07
50	7.187 646 245 074 6	72.908 275 530 091	405.798 619 419 016 52	203.540 649 819 3	16.986 781 75	15.270 42
60	7.187 646 245 086 0	72.908 275 530 137	405.798 619 419 016 00	203.540 649 819 42	16.986 781 68	15.270 61
70	7.187 646 245 089 5	72.908 275 530 151	405.798 619 419 015 890	203.540 649 819 47	16.986 781 64	15.270 73
80	7.187 646 245 090 8	72.908 275 530 156 0	405.798 619 419 015 859	203.540 649 819 49	16.986 781 627	15.270 806
90	7.187 646 245 091 30	72.908 275 530 158 1	405.798 619 419 015 848 7	203.540 649 819 50	16.986 781 618	15.270 858
100	7.187 646 245 091 55	72.908 275 530 159 1	405.798 619 419 015 845 0	203.540 649 819 503	16.986 781 613	15.270 896
110	7.187 646 245 091 68	72.908 275 530 159 64	405.798 619 419 015 843 5	203.540 649 819 504	16.986 781 610	15.270 924
120	7.187 646 245 091 74	72.908 275 530 159 90	405.798 619 419 015 842 83	203.540 649 819 505 5	16.986 781 608 1	15.270 946
130	7.187 646 245 091 778	72.908 275 530 160 05	405.798 619 419 015 842 52	203.540 649 819 506 0	16.986 781 606 8	15.270 962
140	7.187 646 245 091 799	72.908 275 530 160 135	405.798 619 419 015 842 36	203.540 649 819 506 31	16.986 781 605 91	15.270 976
150	7.187 646 245 091 812	72.908 275 530 160 187	405.798 619 419 015 842 28	203.540 649 819 506 51	16.986 781 605 29	15.270 986

ation of I integrals with m and n both odd. Effective evaluation of these integrals required the alternative forms for $f(t)$ and $g(t)$ given in Eqs. (28) and (36). The final entry shown in Table I is representative of the observed convergence behavior when large negative arguments are involved. Clearly, in this example (and in many other test cases examined) a large number of quadrature points are necessary to obtain an accurate value of the integral.

The most difficult I integrals to compute are those involving odd-m and odd-n values. The w summation in Eq. (11) is nonterminating in this case. Table IV illustrates the convergence for some examples of this type as a function of the w summation index. The poorest convergence is observed for the $m=-1$, $n=-1$ integral, with approximately 6–7 digits of precision obtained after 150 terms have been employed in the sum. In contrast, the case $m=1$, $n=3$ has converged to approximately 19 digits of precision using 150 terms.

In summary, a viable procedure has been presented to evaluate some of the more difficult integrals arising in certain aspects of the atomic three-electron problem. Extensions of the approach to more complicated integrals are being explored.

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$$\sum_{\nu=0}^{k-j}\frac{(-1)^\nu\binom{l_{12}}{\nu}\binom{2l_{12}-2\nu}{l_{12}}}{2k-2j-2\nu+1}=0$$

with $0\le l_{12}<\infty$, $0\le k\le l_{12}-1$, $0\le j\le k$. An earlier paper [E. O. Steinborn and E. Filter, Theoret. Chim. Acta. **38**, 261 (1975)] gives a formula for r_{12}^{-2}, but in a form that does not appear particularly useful for numerical calculations.
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