Evaluation of some integrals for the atomic three-electron problem using convergence accelerators

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An analysis is presented for the evaluation of atomic integrals of the form
\[ \int r_1^{i} r_2^{j} r_3^{k} r_3^{l} e^{-\alpha r_1 - \beta r_2 - \gamma r_3} dr_1 dr_2 dr_3. \]
General formulas are worked out for the cases (i) \( l = -2, \ m \geq -1, \ n \geq -1 \), and (ii) \( l = -2, \ m = -2 \). A series solution for both cases is obtained. The Levin u transformation and the Richardson extrapolation techniques are employed to obtain a reasonable number of digits of precision for the integral with minimum CPU requirements.

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I. INTRODUCTION

The purpose of this paper is to present an evaluation scheme for the integrals
\[ I = I(i,j,k,l,m,n,\alpha,\beta,\gamma) \]
\[ = \int r_1^{i} r_2^{k} r_3^{l} e^{-\alpha r_1 - \beta r_2 - \gamma r_3} dr_1 dr_2 dr_3. \] (1)

For the situation where \( l \geq -1, \ m \geq -1, \) and \( n \geq -1 \) a considerable literature exists describing effective evaluation approaches [1–8]. These integrals arise in the determination of various properties for three-electron atomic systems when a Hylleraas-type basis set is employed [9–12]. The focus of this paper is to consider the cases (i) \( l = -2, \ m \geq -1, \) and \( n \geq -1 \); and (ii) \( l = -2, \ m = -2, \) and \( n \geq -1 \). These integrals are required for the calculation of certain relativistic corrections and also in the evaluation of particular lower-bound formulas, when a Hylleraas wave function is used to describe a three-electron system. Much less attention has been directed towards the aforementioned two cases [13–15].

Previous work on integrals with \( l = -2 \) has employed the Sack [16] expansion for the interelectronic coordinate. Employing this expansion leads to a simple angular integration with the complexity of the integral evaluation tied up in the radial integral. In this investigation, a different approach is taken. The factors \( r_j^{l-2} \) are expanded in such a way that the resulting radial integrals are simpler to evaluate, while this is at the expense of a more complicated angular-integration problem. The next two sections give the analysis for the two cases mentioned above, and Sec. IV deals with the numerical evaluation of the formulas obtained in Secs. II and III.

II. THE CASE \( l = -2, \ m \geq -1, \ n \geq -1 \)

The analysis presented below is general and applies for integrals with \( i \geq -2, \ j \geq -2, \ k \geq -2, \ l = -2, \ m \geq -1, \) and \( n \geq -1 \). The most difficult subcase arises for \( m \) and \( n \) both odd. For integrals with one or both of \( m \) and \( n \) even, more effective evaluation procedures have been presented elsewhere [13,14].

To evaluate Eq. (1) the following two expansions are employed [16,17]:
\[ r_{23}^{-2} = \sum_{w_1=0}^{w_1} \frac{r_{23}^{w_1}}{r_{23}^{w_1+2}} C_{w_1}^{l} (\cos \theta_{23}) , \] (2)
\[ r_{13}^{m} = \sum_{w_2=0}^{\infty} R_{m w_2} (r_1, r_3) P_{w_2} (\cos \theta_{13}) . \] (3)

Equation (3) is the Sack expansion for the interelectronic coordinate. \( R_{m w_2} (r_1, r_3) \) denotes a radial function and \( P_{w_2} (\cos \theta_{13}) \) is a Legendre polynomial. In Eq. (2) \( r_{23} < \) denotes the lesser of \( r_{23} \) and \( r_{23} > \) designates the larger of \( r_{23} \). \( C_{w_1}^{l} (\cos \theta_{23}) \) represents a Gegenbauer polynomial. If Eqs. (2) and (3) and an analogous expression for \( r_{12}^{l} \) are inserted into Eq. (1), then
\[ I = \sum_{w_1=0}^{\infty} \sum_{w_2=0}^{\infty} \sum_{w_3=0}^{\infty} I_R (w_1, w_2, w_3) I_A (w_1, w_2, w_3) , \] (4)
where the angular integral is
\[ I_A (w_1, w_2, w_3) = \int C_{w_1}^{l} (\cos \theta_{23}) P_{w_2} (\cos \theta_{13}) P_{w_3} (\cos \theta_{12}) \times d \Omega_1 d \Omega_2 d \Omega_3 \] (5)
and the radial integral is
\[ I_R (w_1, w_2, w_3) \equiv I_R (w_1, w_2, w_3, i, j, k, l, m, n, \alpha, \beta, \gamma) \]
\[ = \int r_1^{i} r_2^{j} r_3^{k} e^{-\alpha r_1 - \beta r_2 - \gamma r_3} dr_1 dr_2 dr_3 . \] (6)

The evaluation of \( I_A \) is now considered. Expressing \( P_{w_1} (\cos \theta_{13}) \) and \( P_{w_3} (\cos \theta_{12}) \) as \( C_{w_1}^{l/2} (\cos \theta_{13}) \) and \( C_{w_3}^{l/2} (\cos \theta_{12}) \), respectively, and employing the addition
Theorem for the Gegenbauer polynomials [18] allows $I_A$ to be separated into a product of integrals in the variables $\{\theta_i, \phi_i\}, i = 1 \rightarrow 3$. The resulting integrals can be readily evaluated, but the final expression is rather complex. The key observation to obtaining a simple formula for $I_A$ is to employ the following expansion for the Gegenbauer polynomials:

$$C_{w_1}^1(x) = \sum_{k=0}^{w_1} b_{w_1,k} P_k(x).$$

(7)

The expansion coefficients $b_{w_1,k}$ are given by

$$b_{w_1,k} = \frac{2k+1}{2} \int_{-1}^{1} P_k(x) C_{w_1}^1(x) dx,$$

(8)

a result obtained by multiplying both sides of Eq. (7) by $P_j(x)$ (for $0 \leq j \leq w_1$) and integrating over $[-1, 1]$. Equation (8) can be rewritten as

$$b_{w_1,k} = \frac{2k+1}{2} \int_{0}^{\pi/2} \sin \theta C_{w_1}^1(\cos \theta) C_{k/2}^1(\cos \theta) d\theta$$

$$= \frac{2k+1}{2} A(1; w_1, 1; k, \frac{1}{2}),$$

(9)

where the $A$ integral is discussed in the Appendix. Inserting Eq. (7) (with $x = \cos \theta_2$) into Eq. (5) leads to

$$I_A(w_1, w_2, w_3) = \sum_{k=0}^{w_1} b_{w_1,k} \int P_k(\cos \theta_2) P_{w_2}(\cos \theta_3) P_{w_3}(\cos \theta_1)$$

$$\times d\Omega_1 d\Omega_2 d\Omega_3.$$

(10)

On expanding each Legendre polynomial in terms of spherical harmonics, the following result is obtained:

$$I_A(w_1, w_2, w_3) = \frac{(4\pi)^3}{(2w_2+1)^2} \sum_{k=0}^{w_1} b_{w_1,k} \delta_{k w_2} \delta_{w_2 w_3},$$

(11)

where $\delta_{jk}$ denotes a Kronecker delta. Since

$$w_2 > w_1 \implies I_A = 0,$$

(12)

Eq. (4) can be simplified to

$$I = \sum_{w_1=0}^{\infty} \sum_{w_2=0}^{w_1} I_R(w_1, w_2) I_A(w_1, w_2),$$

(13)

with

$$I_A(w_1, w_2) = \frac{(4\pi)^3}{(2w_2+1)^2} b_{w_1,w_2}$$

$$= \left\{ \begin{array}{ll}
2^{1/2(w_1+w_2+12)} \pi \sum_{\tau=0}^{\tau_{\text{max}}} \frac{(w_1 - \tau)!}{(w_2 - 1/2)!} \left( -2 \right)^\tau \left( \frac{w_1-w_2}{2} - \tau \right) \left( \frac{w_1+w_2+1-2\tau}{2} \right) & \text{for } w_1 + w_2 \text{ even and } w_1 \geq w_2, \\
0 & \text{for } w_1 + w_2 \text{ odd or } w_1 > w_2,
\end{array} \right.$$ 

(14)

and Eqs. (9) and (A11) have been employed in Eq. (11). In Eq. (14)

$$\tau_{\text{max}} = \min \left[ \left\lceil \frac{w_1}{2} \right\rceil, \left\lceil \frac{w_1-w_2}{2} \right\rceil \right],$$

where the standard convention $\lceil x/2 \rceil = x/2$ if $x$ is even and $(x-1)/2$ if $x$ is odd, has been employed.

To evaluate the radial integral in Eq. (6) (with $w_3 = w_3$) the Sack formulas for the $R$ functions are employed. These take the form

$$R_{nw_k}(r_1, r_2) = \sum_{r=0}^{\infty} a_{w_1, w_2, w_3}^r 2^{w_2+2q} n^{w_2-2q}$$

(16)

with

$$a_{w_2} = \left( \begin{array}{c}
-\frac{u}{2} \\
-\frac{1}{2}
\end{array} \right)_r \left( \begin{array}{c}
-\frac{u}{2} \\
\frac{1}{2}
\end{array} \right)_r,$$

(17)

and $(k)_r$ denotes a Pochhammer symbol. If Eqs. (15) and (16) are inserted into Eq. (6), then

$$I_R(w_1, w_2) = \sum_{p=0}^{\infty} a_{w_1, w_2, w_3}^p \int_{r_1 < 0}^{r_1 < \infty} r_1^{w_1+2p} m^{-w_2-2p}$$

$$\times \int_{r_2 < 0}^{r_2 < \infty} r_2^{w_2+2q} n^{-w_3-2q} e^{-\alpha r_1 - \beta r_2 - \gamma r_3} dr_1 dr_2 dr_3.$$

(18)

If the integration range in Eq. (18) is broken up according to $0 \leq r_i \leq r_j \leq r_k$, then Eq. (18) simplifies to
\[
I_R(w_1, w_2) = \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} a_{w_2mp} a_{w_2nq} \times \left\{ W(w_1 + w_2 + 2p + k + 2, w_2 - w_1 + 1 + 2w_2 - 2p - 2q, \gamma, \beta, \alpha) \\
+ W(w_1 + w_2 + 2p + k + 2, 2q + p + m + i + 2, n + j - w_1 - w_2 - 2q, \gamma, \alpha, \beta) \\
+ W(2w_2 + 2p + 2q + i + 2, w_1 - w_2 - 2p + m + k + 2, n + j - w_1 - w_2 - 2q, \gamma, \alpha, \beta) \\
+ W(2w_2 + 2p + 2q + j + 2, w_1 - w_2 - 2q + n + j + 2, m + k - w_1 - w_2 - 2p, \alpha, \beta, \gamma) \\
+ W(w_1 + w_2 + 2q + j + 2, 2p - 2q + n + i + 2, m + k - w_1 - w_2 - 2p, \beta, \alpha, \gamma) \\
+ W(w_1 + w_2 + 2q + j + 2, w_2 - w_1 + 2p + k, n + m + 1 + 2w_2 - 2p - 2q, \beta, \gamma, \alpha) \right\}, \quad (19)
\]

where

\[
W(L, M, N, a, b, c) = \int_0^\infty \int_0^\infty \int_0^\infty x^L e^{-ax} dx \int_0^\infty \int_0^\infty y^M e^{-by} dy \int_0^\infty \int_0^\infty z^N e^{-cz} dz. \quad (20)
\]

The \( W \) integrals in Eq. (20) have been discussed extensively in the literature and efficient algorithms are available for their evaluation [1,2,19,20].

Eqs. (13), (14), and (19) thus represent the required solution of the integral. Our attention is now turned to the summation limits occurring in Eqs. (13) and (19).

Because of the following result for the Poisson symbol

\[
(-k)_{i=0} = 0, \quad l > k \text{ for integer } k, \quad (21)
\]

the \( p \) summation terminates at \((m + 1)/2\) if \( m \) is odd and \( m/2 - w_2 \) if \( m \) is even. Similarly the \( q \) summation terminates at \((n + 1)/2\) for odd \( n \) and \( n/2 - w_2 \) for even \( n \). These conditions follow from the definition of \( a_{iwv} \) given in Eq. (17). The \( w_2 \) summation in Eq. (13) terminates at one of the following values:

\[
\begin{align*}
& w_1, \quad m \text{ and } n \text{ both odd,} \\
& \min \left\{ \frac{w_1 + m}{2}, \frac{w_2 + m}{2} \right\}, \quad m \text{ even,}
\end{align*}
\]

The last three conditions follow from the definition of \( a_{iwv} \) given in Eq. (17). The \( w_1 \) summation is nonterminating.

III. THE CASE \( I = -2, m = -2 \)

Inserting Eq. (2) and the analogous expression for \( r_{13}^{-2} \) into Eq. (1), as well as the Sack expansion for \( r_{12}^{-2} \), leads to the result

\[
I = \sum_{w_1=0}^{\infty} \sum_{w_2=0}^{\infty} \sum_{w_3=0}^{\infty} I_R(w_1, w_2, w_3) I_A(w_1, w_2, w_3), \quad (22)
\]

where

\[
I_A(w_1, w_2, w_3) = \int \left( \cos \theta_{23} \right) C_{w_2}^L \left( \cos \theta_{31} \right) P_{w_1} \left( \cos \theta_{12} \right) \times d \Omega_1 d \Omega_2 d \Omega_3 \quad (23)
\]

and

\[
I_R(w_1, w_2, w_3) = \int r_1^{i+2} r_2^{j+2} r_3^{k+2} r_{13}^{w_1} r_{23}^{w_1} r_{31}^{w_1} r_{12}^{w_1} r_{21}^{w_1} r_{31}^{w_1} \ di dr_1 dr_2 dr_3. \quad (24)
\]

To simplify Eq. (23), Eq. (7) is employed for each Gegenbauer polynomial; the result is

\[
I_A(w_1, w_2, w_3) = \sum_{j=0}^{w_1} \sum_{k=0}^{w_2} b_{w_1} b_{w_2} \int P_j \left( \cos \theta_{23} \right) P_k \left( \cos \theta_{31} \right) P_{w_1} \left( \cos \theta_{12} \right) d \Omega_1 d \Omega_2 d \Omega_3
\]

\[
= \frac{(4\pi)^3}{(2w_3 + 1)^2} \sum_{j=0}^{w_1} \sum_{k=0}^{w_2} b_{w_1} b_{w_2} \delta_{jw_3} \delta_{kw_3}, \quad (25a)
\]

and the \( b \) coefficient is given in Eq. (9). The radial integral in Eq. (24) can be evaluated by employing the expansion for the Sack \( R \) function; the result is

\[
= \frac{(4\pi)^3}{(2w_3 + 1)^2} b_{w_1} b_{w_2} b_{w_3}, \quad (25b)
\]
where the $W$ integral is defined in Eq. (20).

Equations (22), (25), and (26) constitute the solution of the $l = -2$, $m = -2$ case. The $q$ summation terminates at $(n + 1)/2$ if $n$ is odd or $n/2 - w_3$ if $n$ is even [see Eqs. (17) and (21)]. The $w_3$ summation in Eq. (22) terminates at min$\{w_1, w_2\}$ if $n$ is odd and min$\{w_1, w_2, n/2\}$ if $n$ is even. The first part of each condition results from the result

$$I_A = 0 \text{ if } w_3 > w_1 \text{ or } w_3 > w_2,$$

which follows directly from Eq. (25a). The second constraint involving $n/2$ follows from the coefficient $a_{w, nq}$ in Eq. (26). The $w_1$ and $w_2$ summations are both nonterminating. Equation (26) is valid for $n \geq -1$. Additional constraints are required on $i$, $j$, and $k$. These may be found from the conditions required for the convergence of the $W$ integral in Eq. (20), that is, $L \geq 0$, $L + M \geq -1$, and $L + M + N \geq -2$. This leads to the requirement that $i + j + k + 3 \geq 0$.

IV. NUMERICAL EVALUATION STRATEGIES

The evaluation of Eqs. (13), (14), and (19) is considered first. The function $I_A(w_1, w_2)$ [Eq. (14)] is independent of any of the arguments $i, j, k, m, n, \alpha, \beta, \gamma$, so this function need only be evaluated once. In the present work Eq. (14) was calculated analytically using the symbolic package MATHEMATICA [21], and the final expressions evaluated numerically. In a similar fashion, an array for the $a$ coefficients appearing in Eq. (19) was constructed in MATHEMATICA. The constraint given in Eq. (14) that $w_1 + w_2$ must be even simplifies the calculations considerably. For the case when $m$ and $n$ are both odd, which is the one of principle interest in this work, the summation limit of the $w_3$ sum in Eq. (13) is $w_1$. However, in practical calculations, this limit can be replaced by a cutoff of the summation as the terms $I_R(w_1, w_3)$ become increasingly small. This particular simplification was not needed in the approach employed in this study.

Equation (13) is not suitable for direct numerical evaluation, particularly if a large number of digits of precision are required. The key expansion employed for $r_3^2$ [Eq. (2)] is deceptive in one sense. An alternative expansion in terms of Legendre polynomials can be written, but the radial factor now involves a logarithmic function of $r_3$ and $r_3$ [13,14,22]. This logarithmic behavior must be imbedded in the series expansion of Eq. (13), so a slow conver-
It should therefore be clear from the combination of results, Eq. (33) and in particular Eq. (35), that a direct summation strategy is not feasible.

In place of a direct summation approach, two convergence acceleration techniques were applied to Eq. (13). The first acceleration method employed was Levin’s u transformation [23,24]. This is widely regarded as a very effective procedure to accelerate a series with logarithmic convergence characteristics [25,26]. This transformation has been applied in other atomic and two-center integration problems [15,27].

A sequence of partial sums are defined,

\[ S_n = \sum_{w=0}^{n} A_w, \]

and these converge to some limit \( S \). Then an improved approximation to the sum is given by

\[ u_k = \sum_{j=0}^{k} (-1)^j \binom{k}{j} (j! + 1)^{k-2} S_j A_j^{-1} \]

where \( \binom{k}{j} \) denotes a binomial coefficient. A well-known difficulty associated with Eq. (37) is that serious cancellation errors occur when \( k \) becomes large [27,28].

The series expansion of Eq. (13) shows it to be composed of two monotonically decreasing series, one for \( w_1 \) even, the other for \( w_1 \) odd. Since the \( A_n \) values for the separate series are significantly different in size, a direct application of Eq. (37) is not expected to be very satisfactory, and that turns out to be true for the test cases examined. However, if Eq. (13) is split as

\[ I = \sum_{w_1=0}^{\infty} A_{w_1} + \sum_{w_1=1}^{\infty} A_{w_1} \]

and the u transformation applied separately to each series in Eq. (38), then a fairly significant improvement in convergence is obtained. The other important factor is that this improvement is obtained for only a modest number of terms in each series in Eq. (38). Some representative test cases are presented in Table I. The principal drawback of the application of the u transformation is that the number of digits of precision obtained for the sum is critically tied to the computer precision available. All the results reported in this work were carried out on a Cray YMP in double precision.

The Richardson extrapolation technique [29] was also tested on Eq. (13). As for the previous technique, this was also applied to Eq. (13) in the form of Eq. (38). The Richardson extrapolation is given by

\[ S_0 = \sum_{k=0}^{N} \frac{S_{n+k}((n+k)N(-1)^{k+N}}{k!(N-k)!}, \]

where \( S_0 \) is an approximation to the total sum in Eq. (13). The results of a representative test case are shown in Table II, where \( S_0 \) is presented as a function of \( N \) and \( n \). The Richardson technique is also subject to the loss of numerical precision (for higher \( N, n \) values) similar to that found for Levin’s u transformation.

Evaluation of the I integral for the case \( l = -2, m = -2 \) by direct summation of the series in Eq. (22) is not viable. Because of the presence of two factors \( r_{ij}^{-2} \) and \( r_{jk}^{-2} \) there is a product logarithmic dependence (in the variables \( r_i + r_j \) and \( r_j + r_k \) imbedded in the series given by Eq. (22). For this reason, a direct summation of the series will not be feasible.

The Levin u transformation was applied to evaluate Eq. (22). Suppose the cutoff for the \( w_1 \) and \( w_2 \) summations in Eq. (22) is denoted by \( N \). Then it proves to be most useful to restructure Eq. (22) in the form

\[ \sum_{w_1=0}^{N} \sum_{w_2=0}^{N} f(w_1, w_2) \]

where \( f(w_1, w_2) \) can be identified as the sum over \( w_1 \) in Eq. (22). The even condition on \( w \) in Eq. (40) follows directly from the product of the \( b \) coefficients given in Eq. (25b) and from Eq. (14). The Levin u transformation was applied to the sum over \( w \) in Eq. (40). Table III presents a couple of representative test cases showing the nature of the convergence obtained using Levin’s transformation. Table IV collects some additional test values. The first four entries included in Table IV have been reported by Luchow and Kleindienst [15], though to a smaller number of digits of precision. Generally 13 to 14 digits of precision are obtained from the application of the Levin u transformation to Eq. (40). The level of precision starts to fall significantly for values of \( k \) higher than those reported in Table III. This was found for all the entries reported in Table IV as well.

V. DISCUSSION

The results from the application of the Levin u transformation shown in Table I indicate that approximately 16 to 17 digits of precision have been obtained. The optimum value of \( k \) appears to be around \( k = 22 \). The possibility of convergence to an incorrect value was excluded by computing several of the test cases by an independent method and also by employing the Richardson extrapolation technique.

The precision starts to drop off after the optimal \( k \) value is reached. The precision of the results reported in Table I is limited by the substantial round off that occurs in the use of Eq. (37). This problem could be avoided in part by the use of a multiprecision arithmetic package.

Particularly noteworthy is the convergence of the case \( m = -1, n = -1 \). It is extremely difficult to evaluate integrals of this form to even a modest number of digits of precision by any other available procedure.

The Richardson extrapolation also performs fairly well. The test case reported in Table II agrees with the value found using the Levin u transformation to approxi-
<table>
<thead>
<tr>
<th>$k$</th>
<th>$I(1, 1, 1, -2, 1, 1, 2, 7, 2, 7, 2, 7)$</th>
<th>$I(0, 0, 0, -2, 1, 3, 2, 7, 2, 9, 0.65)$</th>
<th>$I(0, 0, 0, -2, -1, 1, 2, 7, 2, 9, 0.65)$</th>
<th>$I(0, 0, 0, -2, -1, -1, 2, 7, 2, 9, 0.65)$</th>
<th>$I(2, 1, 1, -2, 3, 3, 7, 3, 84, 4, 338, 4, 338)$</th>
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<tr>
<td>2</td>
<td>7.100</td>
<td>400.736</td>
<td>16.779</td>
<td>15.056</td>
<td>4.943 [−3]</td>
</tr>
<tr>
<td>5</td>
<td>7.188 316</td>
<td>405.737 494</td>
<td>16.986</td>
<td>15.270</td>
<td>4.994 [532 [−3]</td>
</tr>
</tbody>
</table>

L PORRAS AND FREDERICK W KING
### TABLE II. Results for the Richardson extrapolation [Eq. (39)] applied to the integral \( I(0,0,0,-2,-1,1,2,7,9,0.65) \).

<table>
<thead>
<tr>
<th>( n )</th>
<th>( N = 2 )</th>
<th>( N = 4 )</th>
<th>( N = 6 )</th>
<th>( N = 8 )</th>
<th>( N = 10 )</th>
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<tbody>
<tr>
<td>1</td>
<td>15.070</td>
<td>15.263</td>
<td>15.270 89</td>
<td>15.271 057 07</td>
<td>15.271 059 450</td>
</tr>
<tr>
<td>5</td>
<td>15.255</td>
<td>15.270 85</td>
<td>15.271 057 53</td>
<td>15.271 059 459</td>
<td>15.271 059 472 519</td>
</tr>
<tr>
<td>9</td>
<td>15.267 07</td>
<td>15.271 033</td>
<td>15.271 059 333</td>
<td>15.271 059 472 016</td>
<td>15.271 059 472 579 63</td>
</tr>
<tr>
<td>13</td>
<td>15.269 48</td>
<td>15.271 053 19</td>
<td>15.271 059 452</td>
<td>15.271 059 472 525</td>
<td>15.271 059 472 580 907</td>
</tr>
<tr>
<td>17</td>
<td>15.270 28</td>
<td>15.271 057 41</td>
<td>15.271 059 467 84</td>
<td>15.271 059 472 572 13</td>
<td>15.271 059 472 580 976</td>
</tr>
</tbody>
</table>

### TABLE III. Convergence of some integrals as a function of \( k \) for the Levin \( u \) transformation applied to Eq. (40).

<table>
<thead>
<tr>
<th>( k )</th>
<th>( I(0,0,0,-2,-2,2,7,9,0.65) )</th>
<th>( I(0,0,0,-2,-6,2,7,9,0.65) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>59.19</td>
<td>41.54</td>
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<td>42.20</td>
</tr>
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### TABLE IV. Some \( I \) integrals evaluated from Eq. (40).

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<th>( j )</th>
<th>( k )</th>
<th>( l )</th>
<th>( m )</th>
<th>( n )</th>
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<th>( \beta )</th>
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<td>6.52</td>
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<td>-2</td>
<td>4</td>
<td>3.97</td>
<td>3.97</td>
<td>6.52</td>
<td>2.417 774 258 610 ( \times 10^{-2} )</td>
</tr>
<tr>
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<td>-2</td>
<td>4</td>
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<td>2.9</td>
<td>0.65</td>
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<tr>
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<td>-2</td>
<td>4</td>
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<td>2.9</td>
<td>0.65</td>
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<tr>
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<td>-2</td>
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<td>2.9</td>
<td>0.65</td>
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<td>-2</td>
<td>2</td>
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<td>2.9</td>
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<td>1</td>
<td>1</td>
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<td>-2</td>
<td>5</td>
<td>2.7</td>
<td>2.9</td>
<td>0.65</td>
<td>7.604 960 853 694 ( \times 10^{5} )</td>
</tr>
</tbody>
</table>
mately 16 digits of precision. The other integrals evaluated by the Richardson approach yielded a similar level of precision.

For the more difficult case of \( l = -2, m = -2 \), the Levin \( u \) transformation also does a particularly satisfactory job at producing a converged value for the integrals. The optimum value of \( k \) for these cases appears to be around \( k = 26 \).

A particularly significant feature of the present work is that both techniques employed to evaluate Eq. (38) are computationally fast. The acceleration techniques avoid the problem of having to deal with some rather difficult integration problems. These procedures are feasible for application to large scale \( ab \) initio calculations.

ACKNOWLEDGMENTS

Support from the National Science Foundation (Grant No. PHY-9300863) and the Camille and Henry Dreyfus Foundation are appreciated. Cray Research, Inc. is thanked for a generous grant of supercomputer time. Financial support for the visit of I.P. from the Junta de Andalucia, Spain, is greatly appreciated.

APPENDIX

In the appendix we consider the evaluation of the integral

\[
A(\alpha; m, \mu; n, \nu) = \int_0^\pi \sin^\alpha \theta C_m^\mu(\cos \theta) C_n^\nu(\cos \theta) d\theta
\]

\[
= \int_{-1}^1 (1-x^2)^{(\alpha-1)/2} C_m^\mu(x) C_n^\nu(x) dx
\]  

(A1)

The case \( \mu = \gamma = \alpha/2 \) is the standard orthogonality condition for the Gegenbauer polynomials.

If \( m + n \) is odd then \( A = 0 \). Equation (A1) is recast as

\[
A = \int_{-1}^1 (1-x^2)^{(\alpha-1)/2} C_m^\mu(x) q(x) dx
\]  

(A2)

with

\[
q(x) = (1-x^2)^{\alpha/2 - \mu} C_n^\nu(x)
\]  

(A3)

If \( \alpha - 2\mu \) is even and \( \geq 0 \), then \( q(x) \) is a polynomial of degree \( x - 2\mu + n \). For the case \( \alpha - 2\mu + n < m \), \( A = 0 \). This follows from the well-known result in the theory of orthogonal polynomials that

\[
\int_a^b w(x) p_n(x) q(x) dx = 0
\]  

(A4)

where \( p_n(x) \) is an orthogonal polynomial on the interval \([a, b]\) with weight function \( w(x) \) and \( q(x) \) is a polynomial of degree less than \( n \).

If \( \alpha - 2\mu + n \geq m \), then substituting the Rodrigues formula for \( C_m^\mu(x) \) [30],

\[
C_m^\mu(x) = \frac{1}{a_m^{\mu}} (1-x^2)^{\mu + 1/2} \frac{d^m}{dx^m} ((1-x^2)^{\mu + m - 1/2})
\]  

(A5)

with

\[
a_m^{\mu} = (-2)^m m! \Gamma(2\mu) \Gamma(m + \mu + \frac{1}{2}) \Gamma(m + \mu + 2\mu)
\]  

(A6)

into Eq. (A2), yields, on integration by parts,

\[
A = \frac{(-1)^m}{a_m^{\mu}} \int_{-1}^1 (1-x^2)^{\mu + m - 1/2} \frac{d^m q(x)}{dx^m} dx
\]  

(A7)

From Eq. (A3) \( q(x) \) is evaluated to be

\[
q(x) = \sum_{\sigma = 0}^{\infty} (-1)^\sigma \left\{ \sum_{\rho = 0}^{\infty} \frac{(-1)^\rho \Gamma(n + n - \tau)}{\Gamma(n + n - \rho) \Gamma(n - 2\tau)!} x^{n + 2\sigma - 2\tau} \right\}
\]  

(A8)

Inserting this expression for \( q(x) \) into Eq. (A7) leads to a sum of \( \beta \) functions. The final result is

\[
A(\alpha; m, \mu, n, \nu) = \frac{1 + (-1)^m + n}{4\mu m! \Gamma(\mu)} \sum_{\sigma = \sigma_{\text{min}}}^{\alpha - 2\mu} \left\{ \frac{1}{(-4)^\sigma} \right\}
\]

\[
\times \sum_{\tau = 0}^{\tau_{\text{max}}} \frac{(-1)^\tau \Gamma(n + n - \tau)(n + 2\sigma - 2\tau)!}{\Gamma(n - 2\tau)! \Gamma(n - 2\sigma + \tau)} \left( \frac{n - m}{2} + \sigma + \tau \right)^{\mu + \sigma - \tau + 1}
\]  

(A9)

with

\[
\sigma_{\text{min}} = \max \left\{ 0, \frac{m - n}{2} \right\},
\]

\[
\tau_{\text{max}} = \min \left\{ \frac{n}{2}, \frac{n - m}{2} + \sigma \right\}
\]  

(A10)

The duplication formula for the \( \Gamma \) function has been employed to obtain the final result given in Eq. (A9).

If \( \alpha - 2\mu \) is odd or less than 0, then the above procedure could be repeated if \( \alpha - 2\nu \) is even and \( \geq 0 \), because of the symmetric nature of \( A \) with respect to the interchange \( m \leftrightarrow n \) and \( \mu \leftrightarrow \nu \). If neither condition on \( \alpha - 2\mu \) or \( \alpha - 2\nu \) is satisfied, a formula involving a double sum can be obtained by employing explicit expansions for both Gegenbauer polynomials \( C_m^\mu(x) \) and \( C_n^\nu(x) \).

The special case of \( A \) required in Eq. (9) is \( A(1; \nu, 1; k, \frac{1}{2}) \). The condition \( \nu + k \) even must hold; otherwise \( A = 0 \). Because of the factor \( \delta_{\nu \nu + 1} \) in Eq. (11), the condi-
tion \( w_1 + w_2 \) even emerges in Eq. (14). With the substitutions \( \alpha = 1, m = k, \mu = 1/2, n = w_1, \nu = 1 \) in Eq. (A9), the following result is obtained:

\[
A(1; w_1, 1; k, \tau) = \sqrt{\pi} \sum_{\tau=0}^{\tau_{\text{max}}} (-1)^{\tau}(w_1 - \tau) \Gamma \left( \frac{w_1 - k}{2} - \tau \right) \Gamma \left( \frac{w_1 + k}{2} - \tau + \frac{1}{2} \right) , \tag{A11}
\]

with

\[
\tau_{\text{max}} = \min \left( \frac{w_1}{2}, \frac{w_1 - k}{2} \right) .
\]

For the cases \( \alpha - 2\mu \geq 0 \) and even, or \( \alpha - 2\nu \geq 0 \) and even, the procedure employed above leads to a more efficient formula than the use of explicit expansions for both Gegenbauer polynomials. For the particular case of interest just discussed, the number of terms required for expansion of both Gegenbauer polynomials is

\[
\begin{vmatrix} m/2 \ 2 \\ n/2 \ 2 \end{vmatrix} = \begin{vmatrix} w_1/2 \ 2 \\ k/2 \ 2 \end{vmatrix} ,
\]

while from Eq. (A11) the number of terms is governed by

\[
\tau_{\text{max}} = \min \left( \frac{w_1}{2}, \frac{w_1 - k}{2} \right) .
\]

There will be considerable reduction in computational effort for the latter case when \( w_1 \) and \( k \) are both large.

[13] F. W. King, Phys. Rev. A 44, 7108 (1991). In this paper, after the Sec. IV heading, the condition on \( m \) and \( n \) should read \( m \geq -1, n \geq -1 \).
[14] F. W. King, K. J. Dykema, and A. Lund, Phys. Rev. A 46, 5406 (1992). Three typographical errors have surfaced in this work; in Eq. (1) \( r_{\text{max}} \) should read \( \tau_{\text{max}} \); the second factor \(-2x\) in the last line of Eq. (13) should read \(+2x\). In Eq. (51) add \( p_i(t) = i - \langle p_0(t) \rangle^2 \langle p_0(t) \rangle^{-1} \).
[21] MATHEMATICA is a software package available from Wolfram Research, Inc. in Illinois.