Recurrence Formulas for Fully Exponentially Correlated Four-Body Wavefunctions

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Formulas are presented for the recursive generation of four-body integrals in which the integrand consists of arbitrary integer powers ($\geq -1$) of all the interparticle distances $r_{ij}$, multiplied by an exponential containing an arbitrary linear combination of all the $r_{ij}$. These integrals are generalizations of those encountered using Hylleraas basis functions, and include all that are needed to make energy computations on the Li atom and other four-body systems with a fully exponentially correlated Slater-type basis of arbitrary quantum numbers. The only quantities needed to start the recursion are the basic four-body integral first evaluated by Fromm and Hill, plus some easily evaluated three-body “boundary” integrals. The computational labor in constructing integral sets for practical computations is less than when the integrals are generated using explicit formulas obtained by differentiating the basic integral with respect to its parameters. Computations are facilitated by using a symbolic algebra program (maple) to compute array index pointers and present syntactically correct fortran source code as output; in this way it is possible to obtain error-free high-speed evaluations with minimal effort. The work can be checked by verifying sum rules the integrals must satisfy.

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I. INTRODUCTION

As long ago as 1929, Hylleraas [1] presented a computation of the electronic structure of the He atom showing that a basis of explicitly correlated wavefunctions provided a far more efficient representation of that system than was available from a conventional orbital basis. What has come to be known as a Hylleraas atomic basis consists of functions, each of which is a product of exponentials in the electron-nuclear distances (often kept identical for all basis members) to which is appended a product of powers of both the electron-nuclear and the electron-electron distances. Hylleraas-basis computations of the electronic structure and properties of two-electron systems (i.e. the He isoelectronic series) have by now been successfully carried out to great precision by the inclusion of up to several thousand terms in a basis-set expansion. Representative results are those of Yan and Drake [2, 3].

An alternative to the traditional Hylleraas expansion is the use of basis functions that have correlation in the exponential, i.e. in which both the electron-nuclear and electron-electron distances appear exponentially. This type of basis exhibits (at modest expansion lengths) an even more efficient representation of two-electron problems than does the original Hylleraas basis, and has in addition the theoretical advantage that, because it provides similar descriptions of all the particle pairs, it is also applicable to so-called nonadiabatic systems in which all three particles have comparable mass. Extensive computations of two-electron systems in these exponentially correlated bases have been reported by a number of investigators; representative of this work is a contribution by Frolov and Smith [4].

Calculations in the Hylleraas, the exponentially correlated, and other bases (e.g. containing logarithmic terms [5]) have now been carried out, at least for the neutral He atom, to truly extreme accuracy. The situation has been summarized recently by Schwartz [6].

A related line of endeavor has been to search for wavefunctions which yield optimum results when restricted to highly compact forms. Moderate success in this direction has been obtained using a basis that takes full cognizance of the asymptotic and other limiting behavior of the wavefunction [2]; a greater degree of quantitative success has been achieved for the He isoelectronic series by careful optimization of four-term exponentially correlated functions [8, 9].

Part of the reason for the great success with three-body (two-electron) problems has been that the necessary integrals for both Hylleraas and ex-
ponentially correlated functions are relatively simple, and the organization of the integral computations has been facilitated by the existence of recursive procedures [10] enabling integrals of the form

$$\Gamma_{n_1,n_2,n_12}(\alpha, \beta, \gamma) = \int \frac{d\mathbf{r}_1 d\mathbf{r}_2}{16\pi^2} r_1^{n_1-1} r_2^{n_2-1} r_{12}^{n_{12}-1} \times e^{-\alpha r_1 - \beta r_2 - \gamma r_{12}}$$

for $n_1, n_2, n_{12}$ to be constructed systematically from those of smaller $n_1, n_2, n_{12}$. Here $r_i$ is the magnitude of $\mathbf{r}_i$ and $r_{ij} \equiv |\mathbf{r}_i - \mathbf{r}_j|$.

The situation becomes drastically different for problems containing more than three particles. Historically, integrals for fully exponentially correlated wavefunctions were regarded as intractable, while the corresponding integrals for Hylleraas wavefunctions could only be evaluated by writing the pre-exponential powers of the inter-electron coordinates as spherical-harmonic expansions [11]. Thus far, the most accurate studies of a four-body system, the Li atom, have used the Hylleraas basis set. A good survey of the current situation is in a review by King [12], to which should be added a recent paper by Puchalski and Remiddi [17] that reports a more accurate Li computation than those discussed by King.

A major advance for four-body systems occurred when Fromm and Hill [14] presented in 1987 a closed formula for the basic exponentially correlated integral

$$I_0(u_1, u_2, u_3, w_1, w_2, w_3) = \int \frac{d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3}{64\pi^3} \times e^{-w_1 r_1 - w_2 r_2 - w_3 r_3 - u_1 r_1 - u_2 r_2 - u_3 r_3}$$

for $r_1, r_2, r_3$ to be differentiated with respect to the $w_i$ and $u_i$ to introduce pre-exponential powers of the $r_i$ and $r_{ij}$, the lack of $u_i$ dependence in the Remiddi formula made such an approach unavailable there. This difficulty was removed when Pachucki, Puchalski, and Remiddi [18] published a set of recurrence relations enabling arbitrary increases to all the pre-exponential powers in four-body Hylleraas integrals. While Pachucki et al. indicated that the extension of their results to the fully exponentially correlated case would be “of great interest”, they did not consider that problem in their work.

The present work builds upon a preliminary study by the present author [19] which presented some identities (which could be characterized as sum rules) connecting four-body exponentially correlated integrals with contiguous pre-exponential powers. The main result of the present communication is a family of recurrence formulas which enable construction of exponentially correlated integrals with arbitrary pre-exponential powers, starting from the basic integral, Eq. (2), and “boundary” integrals involving fewer than four particles. It thus constitutes a generalization of the valuable result of Pachucki et al.

While the integrals explicitly discussed in this paper [i.e., those represented by Eq. (3)] involve only the interparticle distances and are therefore independent of the coordinates needed to describe the overall angular dependence of a four-body wavefunction, it was pointed out by Fromm and Hill [14] that if spherical-harmonic angular functions are included, integration over their coordinates can be carried out, leaving resultant forms that can be identified as cases of Eq. (3). Details of this reduction have been addressed in previous work by the present author [20, 21], so that in principle the technology to address $P, D, \ldots$ states is complete. However, the evaluation of the angular contributions to the kinetic-energy matrix elements is complicated when expressed in terms of the interparticle coordinates, and there is room for further analysis to identify straightforward methods for treating these states.

II. PROBLEM FORMULATION

The integrals that are the subject of this study are of the general form

$$f_{n_1,n_2,n_3,m_1,m_2,m_3}(u_1, u_2, u_3, w_1, w_2, w_3) = \int \frac{d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3}{64\pi^3} r_1^{m_1-1} r_2^{m_2-1} r_3^{m_3-1} \times e^{-w_1 r_1 - w_2 r_2 - w_3 r_3 - u_1 r_1 - u_2 r_2 - u_3 r_3}$$

and can be interpreted as describing the interaction of one particle (Particle 0), at the origin of the coordinate system, with three others (1,2,3) at
the respective positions \( r_i \). The integrals \( f \) therefore have not only the symmetry corresponding to renumberings of Particles 1, 2, and 3, but also that resulting from rewriting Eq. \( \text{(3)} \) to place a particle other than Particle 0 at the coordinate origin. Specifically, the renumbering of 1–3 yields the identities

\[
\begin{align*}
  f_{n_1,n_3,m_1,m_2,m_3}(u_1, u_2, u_3, w_1, w_2, w_3) &= \\
  f_{n_2,n_3,m_1,m_2,m_3}(u_2, u_1, u_3, w_2, w_1, w_3) &= \\
  f_{n_3,n_1,m_1,m_2,m_3}(u_3, u_1, u_2, w_3, w_1, w_2) &= \\
  f_{n_1,n_3,m_2,m_1,m_2}(u_1, u_3, u_2, w_1, w_3, w_2) &= \\
  f_{n_2,n_3,m_3,m_1,m_2}(u_2, u_3, u_1, w_2, w_3, w_1) &= \\
  f_{n_3,n_2,m_3,m_1,m_2}(u_3, u_1, u_2, w_1, w_2, w_3) =
\end{align*}
\]

The placement of a particle other than Particle 0 at the coordinate origin yields the additional relations

\[
\begin{align*}
  f_{n_1,n_2,n_3,m_1,m_2,m_3}(u_1, u_2, u_3, w_1, w_2, w_3) &= \\
  f_{m_1,m_2,n_1,n_2,m_3}(w_1, u_1, u_2, u_3, w_2, w_3) &= \\
  f_{m_1,n_2,m_3,n_1,m_2}(w_1, u_2, u_3, u_1, w_2, w_3) &= \\
  f_{m_1,m_2,m_3,n_2,n_3}(w_1, u_2, u_3, u_1, w_2, w_3) &= \\
  f_{n_1,m_2,n_3,m_1,n_2}(u_1, u_2, w_3, w_1, u_2, w_3) =
\end{align*}
\]

and the complete symmetry of the \( f \) is the 24-element group (isomorphic with that of the 6-j symbol) that is the direct product of the symmetry operations identified in Eqs. \((4)\) and \((5)\). Notice that the parameter set \( (u_1, u_2, u_3) \) does not have the same symmetry properties as \( (w_1, w_2, w_3) \); the \( u_i \) relate to \( r_{jk} \) that form a triangle, while the \( w_i \) relate to \( r_i \) that form a star.

An important consequence of the symmetry relations is that it is only necessary to derive one key recurrence formula, which we choose to be that which increases the index \( n_1 \) from those of a reference set. Formulas for the advancement of all the other indices can then be obtained by an appeal to symmetry.

It is convenient, following Pachucki et al, to define a shell of integrals as those with a common value of \( N \equiv m_1 + m_2 + m_3 + n_1 + n_2 + n_3 \) and refer to \( N \) as the shell index. We shall find that the key recurrence formula relates one integral in the shell of index \( N+1 \) to a number of integrals in shells of index \( N \) or less, so a systematic procedure for generating integrals in shell \( N+1 \) will involve the prior generation of all integrals in the shells with indices \( \leq N \).

Because the number of parameters and indices is rather large, increased compactness and clarity in the exposition can be achieved by the judicious use of notational conventions. We therefore introduce the notion of a reference index set \( n_1, n_2, n_3, m_1, m_2, m_3 \) and adopt the convention that when ambiguity will not thereby result, indices having their reference values will be omitted. We also suppress the parameters \( u_i \) and \( w_i \) whenever possible. Thus, for example,

\[
\begin{align*}
  f & \equiv f_{n_1,n_2,n_3,m_1,m_2,m_3} , \\
  f_{n_2+1,m_3-1} & \equiv f_{n_1,n_2+1,n_3,m_1,m_2,m_3-1} , \\
  f_{n_1+1,m_3=1} & \equiv f_{n_1+1,n_2,n_3,m_1,m_2,1} .
\end{align*}
\]

The recurrence formula we shall derive is most directly formulated in a notation in which the boundary integrals entering the formula are identified as degenerate cases of the \( f \). Accordingly, using a notation introduced by Pachucki et al, we define

\[
\begin{align*}
  f_{s,n_2,n_3,m_1,m_2,m_3} = \int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 \frac{4\pi\delta(\mathbf{r}_{23})}{64\pi^3} & \times \left( \frac{r_1^{m_1-1} r_2^{m_2-1} r_3^{m_3-1}}{r_1^{n_1-1} r_2^{n_2-1} r_3^{n_3-1}} \right) & \\
  & \times e^{-w_1 r_1 - w_2 r_2 - w_3 r_3 - u_2 r_{12} - u_3 r_{13} - u_1 r_{23}} .
\end{align*}
\]

Note that in Eq. \((9)\), the asterisk indicates the presence of \( 4\pi\delta(\mathbf{r}_{23}) \) in place of \( r_{23}^{n_1-1} \exp(-u_1 r_{23}) \). Other placements of the asterisk correspond to making this substitution with respect to other \( r_{ij} \) or \( r_i \). The notational convention of the preceding paragraph also applies to these degenerate \( f \), so, for example,

\[
\begin{align*}
  f_{n_3+1,m_1=s} & \equiv f_{n_1,n_2,n_3+1,s,m_2,m_3} .
\end{align*}
\]

### III. Recurrence Formula

We present here the key recurrence formula, deferring its detailed derivation to Section [V]. This formula, for \( f_{n_1+1,n_2,n_3,m_1,m_2,m_3} \), written in terms of the reference indices \( n_1, n_2, n_3, m_1, m_2, m_3 \) and therefore denoted simply \( f_{n_1+1} \), takes the deceptively simple form

\[
\begin{align*}
  f_{n_1+1} = \frac{C_1 X_1 + C_2 X_2 + C_3 X_3}{D} .
\end{align*}
\]
The coefficients $C_1$, $C_2$, $C_3$, and $D$ are independent of the index values and are given by

$$C_1 = u_1(\mu_2^2 - 4u_2^2u_3^2),$$

$$C_2 = u_2(2u_2^2\mu_{12} - \mu_{13}\mu_{23}),$$

$$C_3 = u_3(2u_2^2\mu_{13} - \mu_{12}\mu_{23}),$$

$$D = 2u_2u_3(u_2^2\mu_{23} + u_2^2\mu_{13} + u_2^2\mu_{12} - \mu_{12}\mu_{13}\mu_{23} - 4u_1^2u_2^2u_3^2),$$

where the new quantities $\mu_{ij}$ are

$$\mu_{12} = u_1^2 + u_2^2 - u_3^2,$$

$$\mu_{13} = u_1^2 + u_3^2 - u_2^2,$$

$$\mu_{23} = u_2^2 + u_3^2 - u_1^2.$$

The numerator quantities $X_i$ in Eq. (11) depend on the reference index set and on the $f$ from shells of index $\leq N$, thereby imparting the recursive property. The $X_i$ have the following explicit form, in which the $jk$ sum is over the two ordered pairs in which $j$ and $k$ are the members of $(1,2,3)$ other than $i$, and $\delta_p$ is unity if $p = 0$ and zero otherwise:

$$X_i = 2u_ju_k(n_i + n_j + n_k + 1)f - njnk\left[2u_if_{n_i+1,n_j-1,n_k-1} - (2n_i + n_j + n_k)f_{n_j-1,n_k-1}\right]$$

$$+ \sum_{jk} \left\{ m_j(m_j - 1)[u_jf_{n_k+1,m_j-2} - n_jf_{n_j-1,n_k+1,m_j-2}] + 2n_iu_i[u_jf_{n_i-1,n_k+1} - n_jf_{n_j-1,n_k-1,n_k+1}]$$

$$- n_i(n_i - 1)[u_jf_{n_i-2,n_k+1} - n_jf_{n_i-2,n_j-1,n_k+1}] - 2m_jw_j[u_jf_{n_i+1,m_j-1} - n_jf_{n_j-1,n_k+1,m_j-1}]$$

$$+ n_jw_k[2u_if_{n_j-1,n_k-1} - (2n_i + n_j + 2n_k + 1)f_{n_j-1}] + n_j\mu_{ik}f_{n_j-1,n_k+1}$$

$$- \delta_{m_j}[u_jf_{n_k+1,m_j=\ast} - n_jf_{n_j-1,n_k+1,m_j=\ast}] + \delta_{n_i}[u_jf_{n_i=\ast,n_k+1} - n_jf_{n_i=\ast,n_j-1,n_k+1}] \right\}. \quad (19)$$

The last line of Eq. (19) contains boundary integrals of the type introduced at Eq. (9). As shown in Appendix B, these terms can be written in terms of the three-body integrals $\Gamma_{n_1,n_2,n_3}(\alpha, \beta, \gamma)$ given in Eq. (10). We have

$$f_{s,n_2,n_3,m_1,m_2,m_3} =$$

$$\Gamma_{m_1,m_2+m_3-1,n_2+n_3-1}(w_1, w_2+w_3, u_2+u_3), \quad (20)$$

$$f_{n_1,n_2,n_3,m_1,m_2,\ast} =$$

$$\Gamma_{m_1+n_2-1,n_1+m_2-1,n_3}(w_1+u_2, u_1+w_2, u_3), \quad (21)$$

and further formulas obtainable by simultaneous permutation of the $u_i, u_i, m_i$, and $n_i$.

The expressions given above provide a formal route to all $f$ of shells with $N > 0$ from the single basic $N = 0$ four-body integral $f_{00000} = I_0$ and various three-body integrals $\Gamma$. To make this paper self-contained, recursive formulas for the $\Gamma$ are included in Appendix B, and evaluation of the basic integral $I_0$ is treated in Appendix C.

The recursive scheme outlined above will fail when the quantity $D$ or any of its permutational analogs are zero, a condition that occurs if any of the $u_i$ or $w_i$ vanish. The methods reported here are therefore not directly applicable to the Hylleraas basis (in which all the $u_i$ are zero); that case is more appropriately handled by the formulas of Pachucki et al.

**IV. NUMERICAL EVALUATION**

It is considerably more complicated than it may at first appear to make actual calculations based on the recursive process defined in the preceding section. Nevertheless, the recursive process turns out to be less cumbersome than procedures that depend upon the explicit evaluation of high-order derivatives of the basic integral presented as Eq. (2).
The applications we presently contemplate involve the use of basis sets that can mimic the $1s^22s$ ground-state electronic structure of the Li atom, and therefore require computations at least as far as the shell of integrals with $N = 8$. To reach the integrals needed from the $N = 8$ shell requires the evaluation of approximately 700 integrals, and it is desirable to carry out the computations in a way that does not include an unacceptable level of organizational overhead.

The actual approach we employed was to use MAPLE [22] to do the index arithmetic needed to write each specific instance of Eq. (11) in a form requiring no index computations, following which we arranged to have these equations output in a form fully compliant with FORTRAN-95 language specifications and involving no nested loops. These procedures may seem to be overkill until it is recognized that index computations may require nearly an order of magnitude more computer time than the subsequent formation of the recurrence formulas.

Grouping the FORTRAN formulas into sets with the same shell index, we were then able to carry out the recursive computations in a permissible order. This strategy caused the generation, through the $N = 8$ shell, of nearly 10,000 lines of error-free code. To avoid an excessive accumulation of round-off error, all the FORTRAN computations were carried out in quadruple-precision floating point, and checked for adherence to the sum rules reported in earlier work [19]. The final integral values were generally found consistent to at least double-precision accuracy. We note that for the problems for which the methods of this paper are appropriate, it would not be cost-prohibitive to carry out the arithmetic operations with even higher-precision arithmetic.

V. DERIVATION OF RECURRENCE FORMULA

Following Pachucki et al. [18], we introduce a set of integrals $G$, of definition

$$G_{n_1,n_2,n_3,m_1,m_2,m_3} = \int \frac{dk_1 dk_2 dk_3}{8\pi^6} \times (k_1^2 + u_1^2)^{-n_1} (k_2^2 + u_2^2)^{-n_2} (k_3^2 + u_3^2)^{-n_3} \times (k_{23}^2 + u_1^2)^{m_1} (k_{13}^2 + u_2^2)^{m_2} (k_{12}^2 + u_3^2)^{m_3}. \quad (22)$$

The relation between $G$ and the integrals $\Gamma$ and $f$, respectively introduced at Eqs. (11) and (13), is discussed in Appendix A; results needed here are Eqs. (A9)-(A11) and their permutational analogs.

Continuing the path of Pachucki et al, we consider the following integral, which can be shown to vanish by application of Gauss’s theorem:

$$I_g = \int \frac{dk_1 dk_2 dk_3}{8\pi^6} \times \nabla_1 \cdot \left[ \frac{k_1}{(k_1^2 + u_1^2)(k_2^2 + u_2^2)(k_3^2 + u_3^2)} \times \frac{1}{(k_{23}^2 + u_1^2)(k_{13}^2 + u_2^2)(k_{12}^2 + u_3^2)} \right]. \quad (23)$$

Carrying out the operations implied by the integrand and identifying the result in terms of the $G$ (a process that requires the use of identities such as $2k_1 \cdot k_2 = k_1^2 + k_2^2 - k_{12}^2$), we reach

$$I_g = 2u_1^2 G_{211111} + (u_1^2 - u_3^2 + u_2^2) G_{111112} + (u_1^2 - u_2^2 + u_3^2) G_{111112} - G_{111111} - G_{011112} - G_{011121} + G_{101112} + G_{110121} = 0. \quad (24)$$

At this point it is convenient to modify Eq. (23) to a symmetry-equivalent equation by interchanging $u_2 \leftrightarrow u_2$, $u_3 \leftrightarrow u_3$, $n_2 \leftrightarrow m_2$, $n_3 \leftrightarrow m_3$, thereby obtaining

$$2u_1^2 G_{211111} + \mu_{12} G_{121111} + \mu_{13} G_{112111} - G_{111111} - G_{012111} + G_{112011} + G_{121110} = 0. \quad (25)$$

We now replace the $G$ by their equivalents in terms of $f$, using formulas from Appendix A. After multiplying through by the factor needed to clear all variables from the denominators, Eq. (25) becomes

$$2u_1 u_2 u_3 f_{100000} + \mu_{12} u_3 f_{010000} + \mu_{13} u_2 f_{001000} = \hat{X}_1, \quad (26)$$

where

$$\hat{X}_1 = 2u_1 u_2 u_3 f_{000000} + u_3 (f_{100000} - f_{010000}) + u_2 (f_{010000} - f_{001000}). \quad (27)$$

Our next step is to apply to both sides of Eq. (26) the differentiation operator

$$D = \prod_{i=1}^{3} \left( -\frac{\partial}{\partial u_i} \right)^{n_i} \left( -\frac{\partial}{\partial w_i} \right)^{m_i},$$
after which we define the reference index values to be \((n_1, n_2, n_3, m_1, m_2, m_3)\). Looking at Eq. (3), we see that differentiation of \(f\) with respect to \(u_i\) (or \(w_i\)) will cause its index \(n_i\) (or \(m_i\)) to be increased by unity. Therefore, the left hand side of the resulting equation will contain one term in which the differentiations are all applied to the function \(f_{100000}\); this term will have the same coefficient as the \(f_{100000}\) term of Eq. (29) and, in terms of the reference index values, \(f_{100000}\) becomes \(f_{n_1+1}\). Similar observations apply to \(f_010000\) and \(f_{001000}\). There will also be additional terms that result when one or more of the left-hand-side differentiations are applied to the coefficients \(2u_1u_2u_3, \mu_1u_2u_3, \text{or } \mu_1u_3u_2\). We transpose these terms to the right hand side and combine them with the result of differentiating \(X_1\).

When \(D\) is applied to \(X_1\), we encounter differentiations of quantities such as \(f_{100000}\). Keeping in mind that \(f_{100000}\) does not depend upon \(u_1\) but depends exponentially on the other \(u_i\) and \(w_i\), we see that \(Df_{100000}\) will vanish unless \(n_1 = 0\), and nonzero values of the other \(n_i\) and \(m_i\) will result in incrementation of the non-asterisked indices. This lack of \(n_1\) dependence leads to the introduction of a factor \(\delta_{n_1}\) in the differentiation. Corresponding observations apply to the other terms containing asterisks.

Based on the analysis of the preceding two paragraphs, the application of \(D\) to Eq. (29) can be seen to yield the first of the three equations shown below. The second and third of these equations follow by permutation of the indices in the first equation.

\[
\begin{align*}
2u_1u_2u_3f_{n_1+1} + \mu_1u_2u_3f_{n_1+1} + \mu_1u_3u_2f_{n_1+1} &= X_1, \\
\mu_1u_2u_3f_{n_1+1} + 2u_1u_2u_3f_{n_1+1} + \mu_2u_3u_1f_{n_1+1} &= X_2, \\
\mu_1u_2u_3f_{n_1+1} + \mu_2u_3u_1f_{n_1+1} + 2u_1u_2u_3f_{n_1+1} &= X_3.
\end{align*}
\]

The \(X_i\) have the values given in Eq. (19).

Finally, we solve the equation set, Eq. (28). Applying Cramer’s Rule, we get for \(f_{n_1+1}\):

\[
f_{n_1+1} = \frac{1}{\hat{D}} \begin{vmatrix} X_1 & \mu_1u_2u_3 & \mu_1u_3u_2 \\ X_2 & 2u_1u_2u_3 & \mu_2u_3u_1 \\ X_3 & \mu_2u_3u_1 & 2u_1u_2u_3 \end{vmatrix}, \quad (29)
\]

with

\[
\hat{D} = \begin{vmatrix} 2u_1u_2u_3 & \mu_1u_2u_3 & \mu_1u_3u_2 \\ \mu_1u_2u_3 & 2u_1u_2u_3 & \mu_2u_3u_1 \\ \mu_1u_3u_2 & \mu_2u_3u_1 & 2u_1u_2u_3 \end{vmatrix} \quad (30)
\]

Expanding the determinants and dividing the numerator and denominator of Eq. (29) by \(-u_1\), we obtain the expression for \(f_{n_1+1}\) shown in Eq. (11), with \(C_1, D_2, C_3, \text{ and } D\) as given in Eqs. (12–15). We need not exhibit solutions for \(f_{n_2+1}\) or \(f_{n_3+1}\) because they can be reached by permutation of the indices in the expression for \(f_{n_1+1}\).

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**APPENDIX A: FOURIER REPRESENTATION FORMULAS**

The formulas in section V have forms that depend crucially on the Fourier-representation forms of four-body integrals of the generic type

\[
L = \int \frac{dr_1 dr_2 dr_3}{64\pi^3} h_{23}(r_{23})h_{13}(r_{13})h_{12}(r_{12})h_1(r_1)h_2(r_2)h_3(r_3)
\]

\[
= \int \frac{dr_1 dr_2 dr_3}{64\pi^3} \int dq_1 dq_2 dq_3 dq_4 dq_5 dq_6 \frac{(2\pi)^6}{(2\pi)^6} h_{23}^T(q_1)h_{13}^T(q_2)h_{12}^T(q_3)h_1^T(q_4)h_2^T(q_5)h_3^T(q_6)
\]

\[
\times \exp \left( \frac{i}{2} \left[ q_1 \cdot (r_2 - r_3) + q_2 \cdot (r_3 - r_1) + q_3 \cdot (r_1 - r_2) + q_4 \cdot r_1 - q_5 \cdot r_2 - q_6 \cdot r_3 \right] \right).
\]

(A1)

Here \(h(r)\) is a direct-space function and \(h^T(q)\) is its Fourier transform. The transform pairs needed here are

\[
h(r) = \frac{e^{-i\mathbf{r} \cdot \mathbf{r}}}{r}, \quad h^T(q) = \frac{4\pi}{q^2 + t^2}, \quad (A2)
\]

\[
h(r) = \delta(r), \quad h^T(q) = 1. \quad (A3)
\]

Performing now the \(r_i\) integrations, which are all of the generic type

\[
\int e^{iq \cdot r} dr = (2\pi)^3 \delta(q), \quad (A4)
\]
and then evaluating the integrals over \( q_4, q_5, \) and \( q_6 \), we find

\[
L = \int \frac{dq_1 dq_2 dq_3}{2^{15} \pi^{12}} h_T^{23}(q_1) h_T^{12}(q_2) h_T^{13}(q_3)
\times h_T^{1}(q_23) h_T^{2}(q_13) h_T^{3}(q_12),
\]

(A5)

where \( q_{ij} = |q_i - q_j| \).

We now insert into \( L \) as given by Eq. (A5), factors \( h^T \) of the form in Eq. (A2), with the result that \( L \) becomes equal to the integral \( G_{111111} \) as defined in Eq. (22). In addition, we can insert the corresponding functions \( h \) into the direct-space form in Eq. (A1), thereby also identifying \( L \) as \( f_{000000} \), defined in Eq. (3). Equating these forms for \( L \), we reach

\[
G_{111111} = f_{000000}.
\]

(A6)

Next, we consider the result when we evaluate \( L \) taking \( h_{23} \) and \( h_{23}^T \) of the form in Eq. (A3), with the other \( h \) and \( h^T \) continuing as instances of Eq. (A2). We then have, from Eq. (A6),

\[
L = \frac{G_{011111}}{4\pi}.
\]

Alternatively, the direct-space formula for this \( L \) can be identified as \( f_{000000}/4\pi \), where the asterisk-containing form is the degenerate form introduced at Eq. (9). Equating these alternate forms for \( L \), we have

\[
G_{011111} = f_{*00000}.
\]

(A7)

Similar operations can be carried out if \( L \) is evaluated taking Eq. (A3) for \( h_3 \) and \( h_3^T \), with Eq. (A2) for the other \( h \) and \( h^T \). The result is

\[
G_{111110} = f_{0000*}.
\]

(A8)

Now, differentiating both sides of Eqs. (A7) and (A8) with respect to \( u_2 \), we obtain the following results needed in the main text:

\[
G_{021111} = \frac{f_{*10000}}{2u_2},
\]

(A9)

\[
G_{121110} = \frac{f_{01000*}}{2u_2}.
\]

(A10)

Finally, we need the result of differentiating Eq. (A6) with respect to \( u_1 \):

\[
G_{211111} = \frac{f_{10000}}{2u_1}.
\]

(A11)

APPENDIX B: THREE-BODY INTEGRALS

In order to carry out the recursive process defined by Eq. (19), we will need to evaluate integrals of the form introduced in Eq. (9). Carrying out the \( r_3 \) integrations, two such integrals reduce to the three-body integrals

\[
f_{*,n_2,n_3,m_1,m_2,m_3} = \int \frac{dr_1 dr_2}{16\pi^2} r_1^{m_1} r_2^{m_2 + n_3 - 2}
\times \exp[-(w_1 + w_3) r_1 - (u_1 + w_2) r_2 - u_3 r_1 r_2],
\]

(B1)

\[
f_{u_1,n_2,n_3,m_1,m_2,*} = \int \frac{dr_1 dr_2}{16\pi^2} r_1^{m_1 + n_2 - 2} r_2^{m_2 - n_3 - 2}
\times \exp[-(w_1 + w_2) r_1 - (u_1 + w_3) r_2 - u_3 r_1 r_2],
\]

(B2)

These integrals can be respectively identified as

\[
\Gamma_{m_1,m_2,m_3 - 1,n_2,n_3 - 1}(w_1, w_2 + w_3, u_2 + u_3),
\]

\[
\Gamma_{m_1 + n_2 - 1,n_1 + m_2 - 1,n_3}(w_1 + u_2, u_1 + w_2, u_3),
\]

as shown in Eq. (21) of the main text.

The asterisked \( f \) needed for the present work are equivalent to \( \Gamma \) in which no more than one of the indices is negative (with the only negative value \(-1\)). The recursive methods most often used for evaluating \( \Gamma \) do not directly permit advancement of an index from \(-1\); we also note that \( \Gamma \) is invariant with respect to simultaneous permutation of its indices and arguments. We may therefore identify the \( \Gamma \) needed here as falling into two cases: (1) \( \Gamma_{m_1,n_2,n_12} \) with all indices non-negative, and (2) \( \Gamma_{-1,n_2,n_12} \) with \( n_2 \) and \( n_{12} \) non-negative.

For the first case, the recursive process can start from \( \Gamma_{000} \), which by direct integration is found to have the value

\[
\Gamma_{000}(\alpha, \beta, \gamma) = \frac{1}{(\alpha + \beta)(\alpha + \gamma)(\beta + \gamma)},
\]

(B3)

which we rewrite

\[
\Gamma_{000}(\alpha, \beta, \gamma) = \frac{B_{000}(\alpha, \beta, \gamma)}{\alpha + \beta},
\]

(B4)

\[
B_{000}(\alpha, \beta, \gamma) = \frac{A_{000}(\alpha, \beta, \gamma)}{\alpha + \gamma},
\]

(B5)

\[
A_{000}(\alpha, \beta, \gamma) = \frac{1}{\beta + \gamma}.
\]

(B6)

We now introduce

\[
D_{n_1 n_2 n_{12}} = \left( -\frac{\partial}{\partial \alpha}\right)^{n_1} \left( -\frac{\partial}{\partial \beta}\right)^{n_2} \left( -\frac{\partial}{\partial \gamma}\right)^{n_{12}},
\]

(B7)
and apply the recursive procedure of Sack, Roothaan, and Kolos [10], leading to the following formulas:

\[
\Gamma_{n_1 n_2 n_3} = D_{n_1 n_2 n_3} \Gamma_{000} = \frac{1}{\alpha + \beta} \left[ n_1 \Gamma_{n_1-1, n_2, n_3} + n_2 \Gamma_{n_1, n_2-1, n_3} + B_{n_1 n_2 n_3} \right], \quad (B8)
\]

\[
B_{n_1 n_2 n_3} = D_{n_1 n_2 n_3} B_{000} = \frac{1}{\alpha + \gamma} \left[ n_1 B_{n_1-1, n_2, n_3} + n_2 B_{n_1, n_2-1, n_3} + A_{n_1 n_2 n_3} \right], \quad (B9)
\]

\[
A_{n_1 n_2 n_3} = D_{n_1 n_2 n_3} A_{000} = \frac{\delta_{n_1} (n_2 + n_3)!}{(\alpha + \gamma)^{n_1 + n_2 + 1}}. \quad (B10)
\]

It is a computationally stable procedure to evaluate first array \(A\), then \(B\), and finally \(\Gamma\).

For the second case, namely the integrals \(\Gamma_{-1, n_2 n_3}\), a starting formula, again by direct integration, is

\[
\Gamma_{-1,0,0}(\alpha, \beta, \gamma) = \frac{\ln(\alpha + \beta) - \ln(\alpha + \gamma)}{\beta^2 - \gamma^2}. \quad (B11)
\]

If \(\beta - \gamma\) is not too small, one can proceed by a variant of the procedure of Sack et al. Writing the recurrence formulas become

\[
\Gamma_{-1, n_2 n_3} = \frac{1}{\beta + \gamma} \left[ n_2 \Gamma_{-1, n_2-1, n_3} + n_3 \Gamma_{-1, n_2 n_3-1} + G_{n_2 n_3} \right], \quad (B15)
\]

\[
G_{n_2 n_3} = \frac{1}{\beta - \gamma} \left[ n_2 G_{n_2-1, n_3} - n_3 G_{n_2 n_3-1} + K_{n_2 n_3} \right], \quad (B16)
\]

\[
K_{n_2 n_3} = \delta_{n_2} \delta_{n_3} K_{00} - \frac{\delta_{n_2} (1 - \delta_{n_2}) (n_2 - 1)!}{(\alpha + \beta)^{n_2}} + \frac{\delta_{n_3} (1 - \delta_{n_3}) (n_3 - 1)!}{(\alpha + \gamma)^{n_3}}. \quad (B17)
\]

For \(\beta - \gamma\) small, it is more advisable to introduce \(x = \frac{1}{2}(\beta + \gamma), y = \frac{1}{2}(\beta - \gamma)\), to write

\[
G_{0,0} = \frac{\ln(\alpha + x + y) - \ln(\alpha + x - y)}{2y}, \quad (B18)
\]

and to expand in powers of \(y\). The result is

\[
G_{0,0} = \sum_{k=0}^{\infty} \frac{y^{2k}}{(2k + 1)(\alpha + x)^{2k+1}}. \quad (B19)
\]

Differentiation of Eq. (B19) leads to the expansion

\[
G_{n_2 n_3} = \frac{1}{n_2 + n_3 + 1} + \frac{n_2 - n_3}{2} y + \frac{(n_2 - n_3)^2 + n_2 + n_3 + 2}{2(n_2 + n_3 + 3)} y^2 + \ldots \]

\[
\] which can then be inserted into Eq. (B15).

**APPENDIX C: BASIC INTEGRAL \(I_0\)**

The integral \(I_0\), defined in Eq. (2), is needed to start the recursive process. As discussed in [11, 13, 16], the evaluation depends upon whether the quantity \(\sigma\) is real, where

\[
\sigma^2 = u_1^2 u_2^2 u_3^2 + u_1^2 u_2^2 u_3^2 + u_2^2 u_1 u_3^2 + u_2^2 u_1 u_3^2
\]

\[
+ u_2^2 u_1 u_3^2 + u_2^2 u_1 u_3^2 + u_2^2 u_1 u_3^2 + u_2^2 u_1 u_3^2
\]

\[
+ u_2^2 u_1 u_3^2 + u_2^2 u_1 u_3^2 + u_2^2 u_1 u_3^2 + u_2^2 u_1 u_3^2. \quad (C1)
\]
For real \( \sigma \), \( I_0 \) is given by

\[
I_0 = \frac{1}{4\sigma} \left[ -2 \sum_{i=1}^{3} v \left( \frac{\Gamma_i}{\sigma} \right) + \sum_{i,j=0}^{3} v \left( \frac{\gamma^{(i)}_j}{\sigma} \right) + \frac{\pi^2}{2} \right],
\]

where

\[
v(z) = \text{sign}(z) \left[ -\frac{1}{4} \ln^2 \left| 1 - z \right| - \frac{\pi^2}{12} + \text{Li}_2 \left( \frac{1-|z|}{2} \right) + \frac{1}{2} \ln^2 \left( \frac{1+|z|}{2} \right) \right],
\]

and \( \text{Li}_2(z) \) is the dilogarithm (see Formula 27.7.1 of [23]; also Lewin [24]). Both the logarithm and \( \text{Li}_2 \) are multiple-valued, but, contrary to the original formulation that required branch tracking [1], Eq. (C2) can be evaluated straightforwardly with all functions assigned their principal values.

\[
\Gamma_i = \left[ w_i^2 + (u_j + u_k)(w_j + w_k) \right] u_j + u_k + w_j + w_k
\]

The four \( \gamma^{(0)}_j \) are

\[
\gamma^{(0)}_0 = 2u_1u_2u_3 + u_1\mu_{23} + u_2\mu_{13} + u_3\mu_{12},
\]

\[
\gamma^{(0)}_1 = -2u_1u_2u_3 - u_1\mu_{23} + u_2\mu_{13} + u_3\mu_{12},
\]

\[
\gamma^{(0)}_2 = -2u_1u_2u_3 + u_1\mu_{23} - u_2\mu_{13} + u_3\mu_{12},
\]

\[
\gamma^{(0)}_3 = -2u_1u_2u_3 + u_1\mu_{23} + u_2\mu_{13} - u_3\mu_{12},
\]

where \( \mu_{ij} \) are as defined in Eqs. (16)–(18). The \( \gamma^{(i)}_j \) with \( i \neq 0 \) can be obtained from \( \gamma^{(0)}_j \) by, for \( i = 1 \), the simultaneous permutation \( u_2 \leftrightarrow u_w \)

and \( u_3 \leftrightarrow w_3 \); for \( i = 2 \), \( u_1 \leftrightarrow w_1 \) and \( u_3 \leftrightarrow w_3 \); and for \( i = 3 \), \( u_1 \leftrightarrow w_1 \) and \( u_2 \leftrightarrow w_2 \). This recipe produces the \( \gamma^{(i)}_j \) with a different indexing than in earlier work, but the value of \( I_0 \) is not affected thereby.

There is a problem with the numerical evaluation of \( I_0 \) when the parameters \( w_i \) and \( u_i \) exactly or approximately satisfy certain relationships; these situations and methods for the avoidance of numerical instability have been discussed elsewhere [12,16].

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