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REGULAR ARTICLE

Atomic three- and four-body recurrence formulas and related summations

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Abstract A new recursive procedure is reported for the evaluation of certain three-body integrals involving exponentially correlated atomic orbitals. The procedure is more rapidly convergent than those reported earlier. The formulas are relevant to ab initio electronic-structure computations on three- and four-body systems. They also illustrate techniques that are useful in the evaluation of summations involving binomial coefficients.

Keywords Three-body integrals · Binomial summations · Exponentially correlated orbitals

1 Introduction

For electronic-structure computations involving exponentially correlated orbitals in atomic systems, it is convenient to generate the necessary integrals using recurrence formulas. For three-body systems, the integrals in question have the generic form

$$\Gamma_{n_1,n_2,n_{12}}(\alpha,\beta,\gamma) = \frac{1}{16\pi^2} \times \int r_1^{n_1-1} r_2^{n_2-1} r_{12}^{n_{12}-1} \mathrm{e}^{-\alpha r_1-\beta r_2-\gamma r_{12}} d^3\mathbf{r}_1 d^3\mathbf{r}_2, \tag{1}$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ (with respective magnitudes r_1 and r_2) are measured from a common origin (ordinarily the position of one of the three particles), $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$, and the integration is over all values of $\mathbf{r}_1$ and $\mathbf{r}_2$. Though it may not at first be obvious, the integral in Eq. (1) is symmetric under all simultaneous permutations of its arguments and indices; such permutations merely correspond to renumberings of the particles, including the choice of the particle defining the coordinate origin.

Conventional three-body energy computations require the integrals $\Gamma_{n_1,n_2,n_{12}}$ for a set of nonnegative integer values of n_1, n_2, and n_{12}. Even for $n_1 = n_2 = n_{12} = 0$ these integrals are nonsingular, as can be seen by writing them in terms of the relative coordinates r_1, r_2, and r_{12}, and noting that the volume element (after integrating out the angular coordinates) is proportional to $r_1 r_2 r_{12}\, dr_1 dr_2 dr_{12}$. A general discussion of these three-body integrals can be found in Ref. [1].

The $\Gamma_{n_1,n_2,n_{12}}$ can be generated recursively, starting from

$$\Gamma_{0,0,0}(\alpha,\beta,\gamma) = \frac{1}{(\alpha+\beta)(\alpha+\gamma)(\beta+\gamma)} \tag{2}$$

and using a procedure developed by Sack et al. [2]. That procedure involves the following formulas, in which the Γ, B, and A are assumed to have arguments α, β, γ,

Dedicated to the memory of Professor Isaiah Shavitt and published as part of the special collection of articles celebrating his many contributions.

The work of Isaiah Shavitt on ab initio atomic and molecular structure theory was characterized by careful attention to the details of the underlying mathematics and to its development into forms that permitted accurate digital computation. It is in that spirit that this contribution is dedicated to his memory.

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$$\Gamma_{n_1,n_2,n_{12}} = \frac{1}{\alpha+\beta}\left[n_1\Gamma_{n_1-1,n_2,n_{12}} + n_2\Gamma_{n_1,n_2-1,n_{12}} + B_{n_1,n_2,n_{12}}\right], \tag{3}$$

$$B_{n_1,n_2,n_{12}} = \frac{1}{\alpha+\gamma}\left[n_1 B_{n_1-1,n_2,n_{12}} + n_{12}B_{n_1,n_2,n_{12}-1} + A_{n_1,n_2,n_{12}}\right], \tag{4}$$

$$A_{n_1,n_2,n_{12}} = \frac{\delta_{n_1}(n_2+n_{12})!}{(\beta+\gamma)^{n_2+n_{12}+1}}, \tag{5}$$

where $\delta_n = 1$ if $n = 0$ and zero otherwise. It is computationally stable to compute first the array A, then B, and finally Γ.

For some atomic properties, and also in connection with four-body recurrence schemes (vide infra) the Γ are needed with one index equal to -1 but with the others nonnegative, e.g., $\Gamma_{-1,n_2,n_{12}}$. Integrals of this type are convergent, but the recurrence scheme using Eqs. (3)–(5) cannot be used to increase an index of Γ from -1. One method for recursive evaluation of these $\Gamma_{-1,n_2,n_{12}}$ has been presented both by the present author's research group [1] and by Korobov [3]; another method with more rapid convergence is developed in the present communication.

Recursive methods have also been reported for exponentially correlated four-body atomic systems, where the integrals have the generic form

$$\begin{aligned} &I_{n_1,n_2,n_3,m_1,m_2,m_3}(u_1,u_2,u_3,w_1,w_2,w_3) \\ &= \frac{1}{64\pi^3}\int r_1^{m_1-1}r_2^{m_2-1}r_3^{m_3-1}r_{23}^{n_1-1}r_{13}^{n_2-1}r_{12}^{n_3-1} \\ &\times e^{-w_1r_1-w_2r_2-w_3r_3-u_1r_{23}-u_2r_{13}-u_3r_{12}}\, d^3\mathbf{r}_1 d^3\mathbf{r}_2 d^3\mathbf{r}_3. \end{aligned} \tag{6}$$

The integrals described by Eq. (6) are invariant under particle permutations, which include not only permutations of the indices 1, 2, 3 but also changes in the coordinate origin, which correspond to permutations of the type ($w_2 \leftrightarrow u_2$, $w_3 \leftrightarrow u_3$, $n_2 \leftrightarrow m_2$, $n_3 \leftrightarrow m_3$). The symmetry group, isomorphic with that of the 6-j symbols, is the direct product of the six-member group of permutations of (1, 2, 3) and the four-member group of origin changes. The net result is that any one of the six indices of I can be brought to the first index position.

Recurrence formulas for the so-called Hylleraas basis (in which the parameters u_i are zero) were published in 2004 by Pachucki et al. [4]; that work was extended by the present author in 2009 [5] to handle full exponential correlation (general values of all the u_i and w_i). Both these sets of four-body recurrence formulas require an initial integral $I_{0,0,0,0,0,0}$ and various "boundary terms" of the form

$$\begin{aligned} I_{*,n_2,n_3,m_1,m_2,m_3} &= \frac{1}{64\pi^3}\int 4\pi\delta(\mathbf{r}_{23})r_1^{m_1-1}r_2^{m_2-1}r_3^{m_3-1}r_{13}^{n_2-1}r_{12}^{n_3-1} \\ &\times e^{-w+_1r_1-w_2r_2-w_3r_3-u_2r_{13}-u_3r_{12}}\, d^3\mathbf{r}_1 d^3\mathbf{r}_2 d^3\mathbf{r}_3. \end{aligned} \tag{7}$$

The asterisk, introduced for this purpose in Ref. [4], indicates that $r_{23}^{n_1-1}\exp(-u_1r_{23})$ is to be replaced by $4\pi\delta(r_{23})$. Insertion of this Dirac delta function enables the integral of Eq. (7) to be reduced to a three-body integral of the type defined in Eq. (1):

$$\begin{aligned} I_{*,n_2,n_3,m_1,m_2,m_3}(,u_2,u_3,w_1,w_2,w_3) &= \Gamma_{m_1,m_2+m_3-1,n_2+n_3-1} \\ &(w_1, w_2+w_3, u_2+u_3). \end{aligned} \tag{8}$$

The vacant first argument of the above I reflects the fact that this integral does not depend on the parameter u_1. When used for four-body recursion, the integrals of Eq. (8) appear only under conditions such that at least one of $m_2 + m_3$ and $n_2 + n_3$ is positive, so the integrals $\Gamma_{\sigma,\mu,\nu}$ will have indices that are nonnegative, except for at most one index of value -1.

The initial integral, $I_{0,0,0,0,0,0}$, can be evaluated in closed form; a formula for it was first presented by Fromm and Hill [6]. Improvements in the Fromm–Hill formula to illuminate its singularity structure and facilitate its computation were subsequently provided by the present author [7].

The recursive four-body formulas increased the importance of having good recursive methods for the three-body exponentially correlated integrals with one index equal to -1. An additional method for dealing with these integrals was briefly sketched by the present author [5], but the material there presented gave neither a full description of the formula nor its method of derivation. The present communication provides the missing derivation and discusses a class of finite summations that are relevant thereto.

2 Recurrence formulas for $\Gamma(-1, n_2, n_{12})$

A starting point for evaluation of $\Gamma(-1, n_2, n_{12})$ is the formula [1] for $\Gamma(-1, 0, 0)$:

$$\Gamma_{-1,0,0}(\alpha,\beta,\gamma) = \frac{1}{\beta^2-\gamma^2}\left[\ln(\alpha+\beta) - \ln(\alpha+\gamma)\right]. \tag{9}$$

We cannot use the procedure of Sack et al. to increase the index -1, but we can use that procedure on the other indices:

$$\Gamma_{-1,n_2,n_{12}} = \frac{1}{\beta+\gamma}\left[n_2\Gamma_{-1,n_2-1,n_{12}} + n_{12}\Gamma_{-1,n_2,n_{12}-1} + G_{n_2,n_{12}}\right] \tag{10}$$

Here $G_{n_2,n_{12}}$ has definition

$$G_{n_2,n_{12}} = \left(-\frac{\partial}{\partial\beta}\right)^{n_2}\left(-\frac{\partial}{\partial\gamma}\right)^{n_{12}} G_{0,0}, \tag{11}$$

with

$$G_{0,0} = \frac{\ln(\alpha+\beta) - \ln(\alpha+\gamma)}{\beta-\gamma}. \tag{12}$$

We have examined several alternative possibilities for the evaluation of $G_{n_2,n_{12}}$. If $|\beta-\gamma|$ is not too small, one can use a variant of the procedure of Sack *et al*, corresponding to the recurrence formula

$$G_{n_2,n_{12}} = \frac{1}{\beta-\gamma}\left[n_2 G_{n_2-1,n_{12}} - n_{12}G_{n_2,n_{12}-1} + K_{n_2,n_{12}}\right], \tag{13}$$

with

$$K_{n_2,n_{12}} = \delta_{n_2}\delta_{n_{12}}[\ln(\alpha+\beta) - \ln(\alpha+\gamma)] - \frac{\delta_{12}(1-\delta_{n_2})(n_2-1)!}{(\alpha+\beta)^{n_2}} + \frac{\delta_2(1-\delta_{n_{12}})(n_{12}-1)!}{(\alpha+\gamma)^{n_{12}}}. \tag{14}$$

Here $\delta_n = 1$ if $n = 0$ and zero otherwise. The use of Eq. (14) is, however, limited by the fact that the formula for $G_{n_2,n_{12}}$ becomes numerically unstable as $\beta-\gamma$ approaches zero. One way of overcoming this difficulty, noted by Korobov [3], is to use downward recursion in n_2 or n_{12}, starting from a $G_{n_2,n_{12}}$ that is deemed negligible.

The alternative approach of Ref. [1] starts by writing $G_{0,0}$ as the following expansion:

$$\begin{aligned} G_{0,0} &= \frac{1}{\beta-\gamma}[\ln(\alpha+\beta) - \ln(\alpha+\gamma)] \\ &= -\frac{1}{\beta-\gamma}\ln\left[\frac{(\alpha+\beta)-(\beta-\gamma)}{\alpha+\beta}\right] \\ &= \sum_{\mu=1}^{\infty}\frac{1}{\mu}\frac{(\beta-\gamma)^{\mu-1}}{(\alpha+\beta)^{\mu}}. \end{aligned} \tag{15}$$

Applying the operator $(-\partial/\partial\gamma)^{n_{12}}$ to Eq. (15), we get

$$G_{0,n_{12}} = \sum_{\mu>n_{12}}\frac{(\mu-1)!}{\mu(\mu-n_{12}-1)!}\frac{(\beta-\gamma)^{\mu-n_{12}-1}}{(\alpha+\beta)^{\mu}}. \tag{16}$$

We rewrite this equation in a form that causes the summation to start from zero:

$$G_{0,n_{12}} = \sum_{\mu=0}^{\infty}\frac{(\mu+n_{12})!}{(\mu+n_{12}+1)\mu!}\frac{(\beta-\gamma)^{\mu}}{(\alpha+\beta)^{\mu+n_{12}+1}}. \tag{17}$$

Then, applying $(-\partial/\partial\beta)^{n_2}$ and using Leibniz' formula for repeated differentiation of a product, we first obtain

$$G_{n_2,n_{12}} = \sum_{j=0}^{n_2}(-1)^j\binom{n_2}{j}\sum_{\mu\geq j}\frac{(\mu+n_{12}+n_2-j)!}{(\mu+n_{12}+1)(\mu-j)!} \times \frac{(\beta-\gamma)^{\mu-j}}{(\alpha+\beta)^{\mu+n_{12}+n_2-j+1}}. \tag{18}$$

We next replace μ by $j+k$ and note that the range of k is $(0,\infty)$. Also interchanging the order of the summations, Eq. (18) becomes

$$G_{n_2,n_{12}} = \sum_{k=0}^{\infty}\frac{(n_2+n_{12}+k)!}{k!}\frac{(\beta-\gamma)^k}{(\alpha+\beta)^{n_2+n_{12}+k+1}} \times \sum_{j=0}^{n_2}(-1)^j\binom{n_2}{j}\frac{1}{n_{12}+j+k+1}. \tag{19}$$

The j summation is addressed in Appendix 1; its value, from Eq. (40), is

$$\sum_{j=0}^{n_2}(-1)^j\binom{n_2}{j}\frac{1}{n_{12}+j+k+1} = \frac{n_2!(n_{12}+k)!}{(n_2+n_{12}+k+1)!}. \tag{20}$$

Inserting this result, we reach

$$G_{n_2,n_{12}} = \sum_{k=0}^{\infty}\frac{n_2!(n_{12}+k)!}{k!(n_2+n_{12}+k+1)}\frac{(\beta-\gamma)^k}{(\alpha+\beta)^{n_2+n_{12}+k+1}}. \tag{21}$$

It is evident that the variable involved in the expansion is the dimensionless quantity $\tau = (\beta-\gamma)/(\alpha+\beta)$. This approach is functionally equivalent to that of Korobov and will therefore have the same convergence characteristics. However, if Korobov's formulas are to be used, it should be noted that many are in error by a factor of 2.

For some purposes, it is desirable to have a more symmetric expansion, which we can achieve by defining $x = (\beta+\gamma)/2$, $y = (\beta-\gamma)/2$, and arranging for the expansion variable to be $y/(\alpha+x)$. With that set of variables, we have

$$G_{0,0} = \frac{\ln(\alpha+x+y) - \ln(\alpha+x-y)}{2y}. \tag{22}$$

By a procedure similar to that used in Eq. (15), we can bring $G_{0,0}$ to the form

$$G_{0,0} = \sum_{k=0}^{\infty} \frac{y^{2k}}{(2k+1)(\alpha+x)^{2k+1}}. \tag{23}$$

We now seek to construct the $G_{n_2,n_{12}}$ by applying Eq. (11). To do so, we note that

$$-\frac{\partial}{\partial\beta} = -\frac{1}{2}\left(\frac{\partial}{\partial x} + \frac{\partial}{\partial y}\right), \tag{24}$$

$$-\frac{\partial}{\partial\gamma} = -\frac{1}{2}\left(\frac{\partial}{\partial x} - \frac{\partial}{\partial y}\right). \tag{25}$$

When these formulas are inserted in Eq. (11), we have, for the case $n_2 \geq n_{12}$,

$$G_{n_2,n_{12}} = \frac{(-1)^{n_2+n_{12}}}{2^{n_2+n_{12}}}\left(\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2}\right)^{n_{12}}\left(\frac{\partial}{\partial x} + \frac{\partial}{\partial y}\right)^{n_2-n_{12}} G_{0,0}. \tag{26}$$

Applying binomial expansions to the compound factors in Eq. (26),

$$G_{n_2,n_{12}} = \frac{(-1)^{n_2+n_{12}}}{2^{n_2+n_{12}}}\sum_{\mu=0}^{n_{12}}(-1)^{\mu}\binom{n_{12}}{\mu}\left(\frac{\partial}{\partial x}\right)^{2n_{12}-2\mu}\left(\frac{\partial}{\partial y}\right)^{2\mu} \times \sum_{\nu=0}^{n_2-n_{12}}\left(\frac{\partial}{\partial x}\right)^{n_2-n_{12}-\nu}\left(\frac{\partial}{\partial y}\right)^{\nu}\sum_{k=0}^{\infty}\frac{y^{2k}}{(2k+1)(\alpha+x)^{2k+1}}. \tag{27}$$

When we carry out the indicated differentiations, we note that nonzero contributions only result when $k \geq \mu$, so we change the summation variable k to $j+\mu$, with $j \geq 0$. Evaluation of Eq. (27) then takes the form

$$G_{n_2,n_{12}} = \sum_{j=0}^{\infty}\sum_{\nu=0}^{n_2-n_{12}}\sum_{\mu=0}^{n_{12}}\frac{(-1)^{\mu+\nu}}{2^{n_2+n_{12}}}\binom{n_{12}}{\mu}\binom{n_2-n_{12}}{\nu} \times \frac{(2j+n_2+n_{12}-\nu)!}{(2j-\nu)!(2j+2\mu+1)}\,\frac{y^{2j-\nu}}{(\alpha+x)^{n_2+n_{12}+2j-\nu+1}}. \tag{28}$$

The summation over μ can now be evaluated. As shown in Appendix 1 at Eq. (41), we have

$$\sum_{\mu=0}^{n_{12}}(-1)^{\mu}\binom{n_{12}}{\mu}\frac{1}{2j+2\mu+1} = \frac{n_{12}!}{2}\frac{1}{(j+\frac{1}{2})_{n_{12}+1}}. \tag{29}$$

The notation $(a)_n$ denotes the Pochhammer symbol, with definition $(a)_0 = 1$, $(a)_1 = a$, $(a)_2 = a(a+1)$, $(a)_n = a(a+1)\cdots(a+n-1)$ for integers $n > 2$. Alternatively,

$$(a)_p = \frac{\Gamma(a+p)}{\Gamma(a)}. \tag{30}$$

The use of Eq. (29) enables us to rewrite the formula for $G_{n_2,n_{12}}$ as

$$G_{n_2,n_{12}} = \frac{n_{12}!}{2^{n_2+n_{12}+1}}\sum_{j=0}^{\infty}\sum_{\nu=0}^{n_2-n_{12}}(-1)^{\nu}\binom{n_2-n_{12}}{\nu} \times \frac{(2j-\nu+n_2+n_{12})!}{(2j-\nu)!(j+\frac{1}{2})_{n_{12}+1}}\,\frac{y^{2j-\nu}}{(\alpha+x)^{n_2+n_{12}+2j-\nu+1}}. \tag{31}$$

The summation in Eq. (31) can now be reorganized to a form that exhibits it as a power series in $y/(\alpha+x)$. To do so, set $2j-\nu=\sigma$, with $\sigma = 0,1,2,\ldots$. We must then restrict ν to nonnegative integers of the same parity as σ, and can write

$$G_{n_2,n_{12}} = \frac{n_{12}!}{2^{n_2}(\alpha+x)^{n_2+n_{12}+1}} \times \sum_{\sigma=0}^{\infty}(-1)^{\sigma}\frac{(n_2+n_{12}+\sigma)!}{\sigma!}S(n_2,n_{12},\sigma)\left(\frac{y}{\alpha+x}\right)^{\sigma}, \tag{32}$$

with

$$S(n_2,n_{12},\sigma) = \sum_{\nu_\sigma}\binom{n_2-n_{12}}{\nu} \times \frac{1}{(\sigma+\nu+1)(\sigma+\nu+3)\cdots(\sigma+\nu+2n_{12}+1)}. \tag{33}$$

The notation ν_σ indicates that ν must be restricted to integers of the same parity as σ.

To proceed further, we need to evaluate the summation S. The evaluation requires a significant number of steps. The result, developed in Appendix 2, takes the form

$$S(n_2,n_{12},\sigma) = \frac{(-1)^{\sigma}2^{n_2}n_2!}{(n_2+n_{12}+1)!}F(n_2+1,-\sigma;n_2+n_{12}+2;2). \tag{34}$$

The quantity $F(a,b;c;x)$ is a hypergeometric function, sometimes written ${}_2F_1(a,b;c;x)$, with definition

$${}_2F_1(a,b;\,c;\,x) = \sum_{j=0}^{\infty}\frac{(a)_j\,(b)_j}{(c)_j\,j!}\,x^j. \tag{35}$$

The quantities $(p)_j$ are Pochhammer symbols, defined after Eq. (29). For a general discussion of the functions ${}_2F_1$, see

Table 1 Coefficients in the expansion of $G_{n_2,n_{12}}$, Eq. (37)

$C_0 = 1$
$C_1 = (\Delta n)$
$C_2 = (\Delta n)^2 + (\Sigma n) + 2$
$C_3 = (\Delta n)^3 + [3(\Sigma n) + 8](\Delta n)$
$C_4 = (\Delta n)^4 + [6(\Sigma n) + 20](\Delta n)^2 + 3(\Sigma n)^2 + 18(\Sigma n) + 24$
$C_5 = \Delta n)^5 + [10(\Sigma n) + 40](\Delta n)^3 + [15(\Sigma n)^2 + 110(\Sigma n) + 184](\Delta n)$
$C_6 = (\Delta n)^6 + [15(\Sigma n) + 70](\Delta n)^4 + [45(\Sigma n)^2 + 390(\Sigma n) + 784](\Delta n)^2 + 15(\Sigma n)^3 + 180(\Sigma n)^2 + 660(\Sigma n) + 720$
$C_7 = (\Delta n)^7 + [21(\Sigma n) + 112](\Delta n)^5 + [105(\Sigma n)^2 + 1050(\Sigma n) + 2464](\Delta n)^3 + [105(\Sigma n)^3 + 1470(\Sigma n)^2 + 6384(\Sigma n) + 8448](\Delta n)$

Here $(\Sigma n) = n_2 + n_{12}$ and $(\Delta n) = n_2 - n_{12}$

Ref. [8]. Despite the appearance of Eq. (34), $S(n_2, n_{12}, \sigma)$ is not really transcendental; with the parameter values given in that equation S reduces to a rational fractional form, so the notation of that equation simply provides a convenient and compact way of specifying the coefficients in the expansion in Eq. (32). With this formula for S, the expansion for $G_{n_2,n_{12}}$ becomes

$$G_{n_2,n_{12}} = \frac{n_2!\, n_{12}!}{(n_2 + n_{12} + 1)!} \frac{1}{(\alpha + x)^{n_2+n_{12}+1}} \sum_{\sigma=0}^{\infty} \frac{(n_2 + n_{12} + \sigma)!}{\sigma!} \times F(n_2 + 1, -\sigma; n_2 + n_{12} + 2; 2) \left(\frac{y}{\alpha + x}\right)^{\sigma}. \tag{36}$$

We repeat the definitions: $x = (\beta + \gamma)/2$, $y = (\beta - \gamma)/2$. The expansion given by Eq. (36) should reflect the symmetry of the expansion variable; if we interchange $n_2 \leftrightarrow n_{12}$ and simultaneously interchange $\beta \leftrightarrow \gamma$, the value of G should not change. This invariance can be demonstrated using properties of the hypergeometric function; it can also be seen from the explicit forms of the expansion coefficients. Writing

$$G_{n_2,n_{12}} = \frac{n_2!\, n_{12}!}{(\alpha + x)^{n_2+n_{12}+1}} \sum_{\sigma=0}^{\infty} \frac{(-1)^{\sigma} C_{\sigma}}{\sigma!\,(n_2 + n_{12} + \sigma + 1)} \left(\frac{y}{\alpha + x}\right)^{\sigma}, \tag{37}$$

the first eight C_σ are given in Table 1. The C_σ have, under the interchange $n_2 \leftrightarrow n_{12}$, the parity of σ. Since y also has this parity under $\beta \leftrightarrow \gamma$, the individual terms in the expansion of $G_{n_2,n_{12}}$ according to Eq. (37) also exhibit its overall symmetry.

When $\beta - \gamma$ is small, the expansion of Eq. (37) converges more rapidly than that of Eq. (21) due to the fact that the expansion parameter in Eq. (37) is half as large as that in Eq. (21). Moreover, as already pointed out, truncated forms of Eq. (37) yield identical values under symmetry interchange, but the same is not true of Eq. (21). We present in Table 2 one numerical example that illustrates these observations.

Table 2 Computations of $G_{n_2,n_{12}}$ for $\alpha = 8.0$, $\beta = 2.0$, $\gamma = 3.0$, using Eqs. (21) or (37) at various truncations.

	Eq. (21)	Eq. (37)
4 terms		
$G_{2,3}(\alpha, \beta, \gamma)$	$1.4418\,19048 \times 10^{-6}$	$1.4412\,84145 \times 10^{-6}$
$G_{3,2}(\alpha, \gamma, \beta)$	1.4411 92027	1.4412 84145
6 terms		
$G_{2,3}(\alpha, \beta, \gamma)$	1.4412 92139	1.4412 82326
$G_{3,2}(\alpha, \gamma, \beta)$	1.4412 81243	1.4412 82326
8 terms		
$G_{2,3}(\alpha, \beta, \gamma)$	1.4412 82476	1.4412 82319
$G_{3,2}(\alpha, \gamma, \beta)$	1.4412 82307	1.4412 82319
Exact result	1.4412 82319	1.4412 82319

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Appendix 1: Some binomial sums

Starting from the equation

$$F(m,n) = \int_0^1 x^m (1 - x^2)^n \,\mathrm{d}x = \sum_{\mu=0}^{n} \binom{n}{\mu} (-1)^{\mu} \int_0^1 x^{2u+m} \,\mathrm{d}x = \sum_{\mu=0}^{n} \binom{n}{\mu} \frac{(-1)^{\mu}}{m + 1 + 2\mu}, \tag{38}$$

we evaluate $F(m,n)$ by identifying it as a beta function:

$$F(m,n)=\frac{1}{2}\,B\left(\frac{m+1}{2},\,n+1\right)=\frac{\Gamma(\frac{1}{2}[m+1])\Gamma(n+1)}{2\Gamma(\frac{1}{2}[2n+m+3])}=\frac{n!}{2(\frac{1}{2}[m+1])_{n+1}}. \tag{39}$$

For definition of the beta function and a derivation of Eq. (39), see Ref. [9]. Note also that the notation $(a)_p$ denotes a Pochhammer symbol, defined immediately after Eq. (29).

Expressions of the form $F(m,n)$ are used twice in the main text. Setting $n=n_2$ and $m=2n_{12}+2k+1$, Eqs. (38) and (39) correspond to

$$F(m,n)=\sum_{\mu=0}^{n_2}\binom{n_2}{\mu}\frac{(-1)^\mu}{2(n_{12}+\mu+k+1)}=\frac{\Gamma(n_{12}+k+1)\,n_2!}{2\Gamma(n_2+n_{12}+k+2)}=\frac{(n_{12}+k)!\,n_2!}{2(n_2+n_{12}+k+1)!}, \tag{40}$$

Equivalent to Eq. (20).

Setting $n=n_{12}$ and $m=2j$,

$$F(m,n)=\sum_{\mu=0}^{n_{12}}\binom{n_{12}}{\mu}\frac{(-1)^\mu}{2j+1+2\mu}=\frac{n_{12}!}{2(j+\frac{1}{2})_{n_{12}+1}}, \tag{41}$$

Equivalent to Eq. (29).

Appendix 2: Evaluation of $S(n_2,n_{12},\sigma)$

Our starting point for the evaluation of $S(n_2,n_{12},\sigma)$, defined in Eq. (32), is to write it as an iterated integral. To avoid unnecessary notational complexity, we make the temporary definitions $n=n_2-n_{12}$, $m=n_{12}$. Thus,

$$S(n_2,n_{12},\sigma)=\sum_{\nu_\sigma}\binom{n}{\nu}\times\frac{1}{(\sigma+\nu+1)(\sigma+\nu+3)\cdots(\sigma+\nu+2m+1)}=\underbrace{\int_0^1 dz_m\,z_m\int_0^{z_m}dz_{m-1}\,z_{m-1}\int_0^{z_{m-1}}\cdots\int_0^{z_2}dz_1\,z_1\int_0^{z_1}dz}_{m+1*\iota\nu\tau\epsilon\gamma\rho\alpha\lambda\sigma}\times\sum_{\nu_\sigma}\binom{n}{\nu}z^{\sigma+\nu}. \tag{42}$$

Remembering that the index ν_σ is to take only values of the same parity as σ, we evaluate the summation in Eq. (42), obtaining

$$g(z)=\sum_{\nu_\sigma}\binom{n}{\nu}z^{\sigma+\nu}=\frac{z^\sigma}{2}\left[(1+z)^n+(-1)^\sigma(1-z)^n\right]. \tag{43}$$

We now insert the right-hand side of Eq. (43) into Eq. (42), also reversing the integration order, reaching

$$S(n_2,n_{12},\sigma)=\int_0^1 dz\,g(z)\int_z^1 dz_1\,z_1\int_{z_1}^1\cdots\int_{z_{m-1}}^1 dz_m\,z_m. \tag{44}$$

We now integrate (from right to left) over the z_i. The z_m integration yields $(1-z_{m-1}^2)/2$; that over z_{m-1} produces $(1-z_{m-2}^2)^2/(2\cdot 2^2)$; further integrations over z_{m-2} through z_1 give the overall result $(1-z^2)^m/2^m m!$. Equation (44) is thereby reduced to

$$S(n_2,n_{12},\sigma)=\frac{1}{2^{m+1}m!}\int_0^1 dz\,z^\sigma(1-z^2)^m\times\left[(1+z)^n+(-1)^\sigma(1-z)^n\right]=\frac{1}{2^{m+1}m!}\int_0^1 dz\,z^\sigma\left[(1+z)^{n+m}(1-z)^m+(-1)^\sigma(1+z)^m(1-z)^{n+m}\right]. \tag{45}$$

We continue by writing z^σ as its expansion in powers of either $(1+z)$ or $(1-z)$, i.e., as one of

$$z^\sigma=\sum_{j=0}^{\sigma}(-1)^{\sigma-j}\binom{\sigma}{j}(1+z)^j=\sum_{j=0}^{\sigma}(-1)^j\binom{\sigma}{j}(1-z)^j. \tag{46}$$

We insert these expressions into Eq. (45) in a way that leads to

$$S(n_2,n_{12},\sigma)=\frac{(-1)^\sigma}{2^{m+1}m!}\sum_{j=0}^{\sigma}(-1)^j\binom{\sigma}{j}\times\int_0^1 dz\left[(1+z)^{n+m+j}(1-z)^m+(1-z)^{n+m+j}(1+z)^m\right]. \tag{47}$$

We next process Eq. (47) by carrying out $n+m+j$ integrations by parts, repeatedly differentiating the factors that were originally at powers $n+m+j$ and integrating the other factors. At each step the boundary (integrated) terms vanish. The differentiations produce (for each term) a factor $(n+m+j)!$, while the integrations generate (in the denominator) the product $(m+1)(m+2)\cdots(2m+n+j)$. At each step the (-1) from the integration by parts cancels against a similar quantity from the integration or differentiation of the $(1-z)$ factor. The overall result is

$$S(n_2,n_{12},\sigma)=\frac{(-1)^{\sigma}}{2^{m+1}m!}\sum_{j=0}^{\sigma}(-1)^{j}\binom{\sigma}{j}\frac{(n+m+j)!\,m!}{(n+2m+j)!}\times\int_0^1 dz\left[(1-z)^{n+2m+j}+(1+z)^{n+2m+j}\right]. \tag{48}$$

The integral in Eq. (48) has the value $2^{n+2m+j+1}/(n+2m+j+1)$. Inserting that value, canceling $m!$, expanding the binomial coefficient, and replacing n and m by the quantities they represent, we have

$$S(n_2,n_{12},\sigma)=(-1)^{\sigma}2^{n_2}\sum_{j=0}^{\sigma}\frac{(-1)^{j}\sigma^{j}}{(\sigma-j)!}\frac{(n_2+j)!}{(n_2+n_{12}+j+1)!}\frac{2^{j}}{j!}. \tag{49}$$

Converting to Pochhammer symbols, Eq. (49) becomes

$$S(n_2,n_{12},\sigma)=\frac{(-1)^{\sigma}2^{n_2}n_2!}{(n_2+n_{12}+1)!}\sum_{j=0}^{\sigma}(-\sigma)_j\frac{(n_2+1)_j}{(n_2+n_{12}+2)_j}\frac{2^{j}}{j!}. \tag{50}$$

Because $(-\sigma)_j$ vanishes for $j>\sigma$, we can extend the summation in Eq. (50) to infinity, thereby causing the sum to correspond to the definition of a hypergeometric function; compare with Eq. (35). The result then reduces to Eq. (34).

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