

Chapman–Enskog solutions to arbitrary order in Sonine polynomials IV: Summational expressions for the diffusion- and thermal conductivity-related bracket integrals

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ABSTRACT

The Chapman–Enskog solutions of the Boltzmann equations provide a basis for the computation of important transport coefficients for both simple gases and gas mixtures. These coefficients include the viscosity, the thermal conductivity, and the diffusion coefficient. In a preceding paper on simple gases, we have shown that the use of higher-order Sonine polynomial expansions enables one to obtain results of arbitrary precision that are free of numerical error. In two subsequent papers, we have extended our original simple gas work to encompass binary gas mixture computations of the viscosity, thermal conductivity, diffusion, and thermal diffusion coefficients to high-order. In all of this previous work we retained the full dependence of our solutions on the molecular masses, the molecular sizes, the mole fractions, and the intermolecular potential model via the omega integrals up to the final point of solution via matrix inversion. The elements of the matrices to be inverted are, in each case, determined by appropriate combinations of bracket integrals which contain, in general form, all of the various dependencies. Since accurate, explicit, general expressions for bracket integrals are not available in the literature beyond order 3, and since such general expressions are necessary for any extensive program of computations of the transport coefficients involving Sonine polynomial expansions to higher orders, we have investigated alternative methods of constructing appropriately general bracket integral expressions that do not rely on the term-by-term, expansion and pattern matching techniques that we developed for our previous work. It is our purpose in this paper to report the results of our efforts to obtain useful, alternative, general expressions for the bracket integrals associated with the diffusion- and thermal conductivity-related Chapman–Enskog solutions for gas mixtures. Specifically, we have obtained such expressions in summational form that are conducive to use in high-order transport coefficient computations for arbitrary gas mixtures and have computed and reported explicit expressions for all of the orders up to 5.

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1. Introduction

The Chapman–Enskog solutions of the Boltzmann equations provide a basis for the computation of important transport coefficients for both simple gases and gas mixtures [1–15]. The use of Sonine polynomial expansions for the Chapman–Enskog solutions was first suggested by Burnett [16] and has become the general method for obtaining the transport coefficients due to the relatively rapid convergence of this series [1–8,16]. While it has been found that relatively, low-order expansions (of order 4) can provide reasonable accuracy in computations of the transport

coefficients (to about 1 part in 1000), most existing computer codes do not use these solutions beyond order 2 or order 3 as the relevant expressions rapidly become increasingly complex and have not been available as general, explicit expressions in terms of arbitrary potential model (via the omega integrals) in the past. Recently, our investigations of simple gases and gas mixtures [17–20] have allowed us to pursue Chapman–Enskog solutions to relatively high orders computationally using *Mathematica*® and, thus, accurate, completely general, expressions have been obtained and used by us up to order 60 for the viscosity-related bracket integrals and up to order 70 for the diffusion- and thermal conductivity-related bracket integrals. We note that our initial work focused on the generation of the necessary bracket integral expressions via a method suggested in Chapman and Cowling [1] that is best described as a term-by-term, expansion

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and pattern matching technique. Since this method is relatively expensive in a computational sense due to the size of the higher-order bracket integral expressions, and since the size and complexity of the general expressions for the bracket integrals for gas mixtures makes them impractical to report explicitly in the open literature beyond the lowest orders even when organized into compact form, it is clearly desirable to have an alternative means of generation for the needed general bracket integral expressions that is both more compact and less cumbersome to implement as increasingly higher orders of approximation are employed in computations of the transport coefficients. Thus, in this paper, we report on the results of our efforts to develop a set of completely general expressions for the bracket integrals necessary to obtain Chapman–Enskog diffusion and thermal conductivity solutions up to any arbitrary order and which we have been able to present as compact summational representations that are straightforward to implement efficiently in a variety of different computational environments. In the following sections we describe the basic relationships relevant to the Chapman–Enskog solutions for diffusion and thermal conductivity, the role of the bracket integrals in these solutions, the details of our derivation of alternative, summational, expressions for the diffusion- and thermal conductivity-related bracket integrals, and explicit, precomputed expressions for the bracket integrals up to order 5 for use in existing computer codes where such are needed but have not previously been available beyond order 2 or order 3.

2. The basic relationships

Following the work and notations of Chapman and Cowling [1], as used in our previous work [19], we note that for binary gas mixtures the diffusion, the thermal diffusion, and the thermal conductivity coefficients may be expressed to some order of approximation, m , in terms of Sonine polynomial expansions as:

$$[D_{12}]_m = \frac{1}{2} x_1 x_2 \left(\frac{2kT}{m_0} \right)^{1/2} d_0^{(m)}, \quad (1)$$

$$[D_T]_m = -\frac{5}{4} x_1 x_2 \left(\frac{2kT}{m_0} \right)^{1/2} (x_1 M_1^{-1/2} d_1^{(m)} + x_2 M_2^{-1/2} d_{-1}^{(m)}), \quad (2)$$

$$[\lambda]_m = -\frac{5}{4} kn \left(\frac{2kT}{m_0} \right)^{1/2} (x_1 M_1^{-1/2} a_1^{(m)} + x_2 M_2^{-1/2} a_{-1}^{(m)}), \quad (3)$$

respectively, where $x_1 = n_1/n$ and $x_2 = n_2/n$ are the component mixture fractions, n_1 and n_2 are the component number densities with $n = n_1 + n_2$ being the total number density of the mixture, m_1 and m_2 are the component molecular masses with $m_0 = m_1 + m_2$, k is Boltzmann's constant, T is the temperature, $M_1 = m_1/m_0$, $M_2 = m_2/m_0$, and in which the quantities $d_0^{(m)}$, $d_{-1}^{(m)}$, $d_1^{(m)}$, $a_{-1}^{(m)}$, and $a_1^{(m)}$ are expansion coefficients determined by solving the following systems of algebraic equations:

$$\sum_{p=-m}^{+m} d_p a_{pq} = \delta_q, \quad (4)$$

$$\sum_{\substack{p=-m \\ p \neq 0}}^{+m} a_p a_{pq} = \alpha_q \quad (q \neq 0), \quad (5)$$

in which:

$$\delta_0 = \frac{3}{2n} \left(\frac{2kT}{m_0} \right)^{1/2}, \quad \delta_q = 0 \quad (q \neq 0), \quad (6)$$

$$\alpha_{-1} = -\frac{15}{4} \frac{n_2}{n^2} \left(\frac{2kT}{m_2} \right)^{1/2}, \quad \alpha_1 = -\frac{15}{4} \frac{n_1}{n^2} \left(\frac{2kT}{m_1} \right)^{1/2}, \quad (7)$$

and:

$$\alpha_q = 0 \quad (q \neq \pm 1). \quad (8)$$

We note that we have dropped the superscript (m) on the expansion coefficients $d_p^{(m)}$ and $a_p^{(m)}$ as is done in Chapman and Cowling. In matrix notation, these systems of equations may be written as:

$$\mathbf{Dd} = \boldsymbol{\delta} \quad \text{and} \quad \mathbf{Aa} = \boldsymbol{\alpha}, \quad (9)$$

where one has:

$$\mathbf{D} = \begin{bmatrix} a_{-m-m} & \cdots & a_{-m-1} & a_{-m0} & a_{-m1} & \cdots & a_{-mm} \\ \vdots & & \vdots & \vdots & \vdots & & \vdots \\ a_{-1-m} & \cdots & a_{-1-1} & a_{-10} & a_{-11} & \cdots & a_{-1m} \\ a_{0-m} & \cdots & a_{0-1} & a_{00} & a_{01} & \cdots & a_{0m} \\ a_{1-m} & \cdots & a_{1-1} & a_{10} & a_{11} & \cdots & a_{1m} \\ \vdots & & \vdots & \vdots & \vdots & & \vdots \\ a_{m-m} & \cdots & a_{m-1} & a_{m0} & a_{m1} & \cdots & a_{mm} \end{bmatrix}, \quad (10)$$

$$\mathbf{d} = \begin{bmatrix} d_{-m} \\ \vdots \\ d_{-1} \\ d_0 \\ d_1 \\ \vdots \\ d_m \end{bmatrix}, \quad \text{and} \quad \boldsymbol{\delta} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \delta_0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad (11)$$

and:

$$\mathbf{A} = \begin{bmatrix} a_{-m-m} & \cdots & a_{-m-1} & a_{-m1} & \cdots & a_{-mm} \\ \vdots & & \vdots & \vdots & & \vdots \\ a_{-1-m} & \cdots & a_{-1-1} & a_{-11} & \cdots & a_{-1m} \\ a_{1-m} & \cdots & a_{1-1} & a_{11} & \cdots & a_{1m} \\ \vdots & & \vdots & \vdots & & \vdots \\ a_{m-m} & \cdots & a_{m-1} & a_{m1} & \cdots & a_{mm} \end{bmatrix}, \quad (12)$$

$$\mathbf{a} = \begin{bmatrix} a_{-m} \\ \vdots \\ a_{-1} \\ a_1 \\ \vdots \\ a_m \end{bmatrix}, \quad \text{and} \quad \boldsymbol{\alpha} = \begin{bmatrix} 0 \\ \vdots \\ \alpha_{-1} \\ \alpha_1 \\ \vdots \\ 0 \end{bmatrix}, \quad (13)$$

for the diffusion and thermal conductivity problems, respectively, and where, as the order of the expansion, m , increases in each case, the matrices build outward from their centers in the manner indicated. Thus, to obtain the needed expansion coefficients, $d_0^{(m)}$, $d_{-1}^{(m)}$, $d_1^{(m)}$, $a_{-1}^{(m)}$, and $a_1^{(m)}$, and hence the diffusion, thermal diffusion, and thermal conductivity coefficients for a given order of the expansions, one need only generate the $[(2m+1) \times (2m+1)]$ and $[(2m) \times (2m)]$ matrices of Eqs. (10) and (12) and invert them.

The matrix elements, a_{pq} , in Eqs. (10) and (12) are constructed from combinations of bracket integrals containing the appropriate Sonine polynomials from the expansions used. Specifically, since it is straightforward to show for any (p, q) that $a_{pq} = a_{qp}$, one has that:

$$a_{pq} = a_{qp} = x_1^2 \left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_1^2) \mathcal{C}_1 \right]_1 + x_1 x_2 \left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_1^2) \mathcal{C}_1 \right]_{12}, \quad (14)$$

$$a_{p-q} = a_{-qp} = x_1 x_2 \left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_2^2) \mathcal{C}_2 \right]_{12}, \quad (15)$$

$$a_{-pq} = a_{q-p} = x_1 x_2 \left[S_{3/2}^{(p)}(\mathcal{C}_2^2) \mathcal{C}_2, S_{3/2}^{(q)}(\mathcal{C}_1^2) \mathcal{C}_1 \right]_{21}, \quad (16)$$

$$a_{-p-q} = a_{-q-p} = x_2^2 \left[S_{3/2}^{(p)}(\mathcal{C}_2^2) \mathcal{C}_2, S_{3/2}^{(q)}(\mathcal{C}_2^2) \mathcal{C}_2 \right]_2 + x_1 x_2 \left[S_{3/2}^{(p)}(\mathcal{C}_2^2) \mathcal{C}_2, S_{3/2}^{(q)}(\mathcal{C}_2^2) \mathcal{C}_2 \right]_{21}, \quad (17)$$

where:

$$S_m^{(n)}(x) = \sum_{p=0}^n \frac{(m+n)(n-p)}{(p)!(n-p)!} (-x)^p = \sum_{p=0}^n \frac{(m+n)!}{(p)!(n-p)!(m+p)!} (-x)^p \\ = \sum_{p=0}^n \frac{\Gamma(m+n+1)}{\Gamma(p+1)\Gamma(n-p+1)\Gamma(m+p+1)} (-x)^p, \quad (18)$$

(with $S_m^{(0)}(x) = 1$ and $S_m^{(1)}(x) = m+1-x$) are numerical multiples (un-normalized) of the Sonine polynomials originally used in the Kinetic Theory of Gases by Burnett [16], in which $\mathcal{C}_i = (m_i/2kT)^{1/2} \mathbf{c}_i$ are dimensionless, pre-collision, peculiar molecular velocities, $\mathbf{c}_i = \mathbf{c}_i - \mathbf{c}_0$ are the dimensional, pre-collision, peculiar molecular velocities, $\mathbf{c}_i$ are the pre-collision molecular velocities, and $\mathbf{c}_0 = M_1 x_1 \mathbf{c}_1 + M_2 x_2 \mathbf{c}_2$ is the mean mass velocity of the mixture. Here, one needs to be aware that the notation $(m+n)_{(n-p)}$ used by Chapman and Cowling in Eq. (18) is not the standard Pochhammer notation employed later in this work although it is related to it. From the definitions used in the bracket integral notation, it follows that Eqs. (17) and (16) are essentially identical to Eqs. (14) and (15), respectively, with the only difference being the interchange of the subscripts 1 and 2 representing the different components of the mixture. Thus, in general, the complete Chapman–Enskog solutions for both diffusion and thermal conductivity for binary gas mixtures require the evaluation of only three types of bracket integrals:

$$\left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_1^2) \mathcal{C}_1 \right]_1, \quad (19)$$

$$\left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_2^2) \mathcal{C}_2 \right]_{12}, \quad (20)$$

and:

$$\left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_1^2) \mathcal{C}_1 \right]_{12}. \quad (21)$$

Here, however, we note an observation made in our previous work [19] that, of the three required bracket integrals shown in Eqs. (19)–(21), the application of some simple combinatorial rules allows one to generate expressions for the bracket integrals of Eqs. (19) and (20) from an appropriate expression for the bracket integral of Eq. (21) if such is known. Thus, it is the derivation of such an expression for the bracket integral of Eq. (21) which could be said to be the most important goal of this paper. However, in terms of complexity, we have found it convenient to first pursue independently the derivation of an expression for the bracket integral of Eq. (20) before attempting the corresponding derivation for the bracket integral of Eq. (21). Both of these derivations are detailed below and the similarities between them are obvious. Our use of the resulting expressions for the bracket integrals of Eqs. (20) and (21) to

generate a similar expression for the bracket integral of Eq. (19) according to the appropriate combinatorial rule is a relatively minor exercise which is presented at the end of this paper. While all of the above expressions for binary gas mixtures are readily generalized for use with arbitrary mixtures by replacing the (1, 2) indexing scheme associated specifically with binary mixtures to a more general (i, j) indexing scheme, in what follows we retain the (1, 2) indexing scheme initially used by Chapman and Cowling as it improves (in our opinion) the clarity of the derivations. Of great importance in this work is the requirement that we have placed on our results that they continue to exhibit the full set of general dependencies of the bracket integrals on the molecular masses and the omega integrals, $\Omega_{12}^{(\ell)}(r)$, that we have retained in our previous recent work [17–20] and which is the most significant factor contributing to the utility of this recent body of work. The omega integrals are defined as:

$$\Omega_{12}^{(\ell)}(r) \equiv \left(\frac{kT}{2\pi m_0 M_1 M_2} \right)^{1/2} \int_0^\infty \exp(-g^2) g^{(2r+3)} \phi_{12}^{(\ell)}(g) dg, \quad (22)$$

with:

$$\phi_{12}^{(\ell)}(g) \equiv 2\pi \int_0^\pi [1 - \cos^\ell(\chi)] b db, \quad (23)$$

and contain all of the dependencies relating to the specific intermolecular potential model that is employed. Here, χ is the angle between the pre-collision ($\mathbf{g} = \mathbf{c}_2 - \mathbf{c}_1$) and post collision ($\mathbf{g}' = \mathbf{c}_2' - \mathbf{c}_1'$) relative velocities and is a function of the impact parameter, b , and the dimensionless pre-collision, relative velocity of the two colliding molecules, $g \equiv (m_0 M_1 M_2 / 2kT)^{1/2} \mathbf{g}$. As a brief aside, we note here that it is often considered convenient to define the omega integrals in terms of a simple scaling factor, $\sigma_{12} = \frac{1}{2}(\sigma_1 + \sigma_2)$, which is, in the most general of terms, only a convenient, arbitrarily chosen length within some range where the impact parameter is significant. Expressed in this manner, the omega integrals are then [1]:

$$\Omega_{12}^{(\ell)}(r) = \frac{1}{2} \sigma_{12}^2 \left(\frac{2\pi kT}{m_0 M_1 M_2} \right)^{1/2} W_{12}^{(\ell)}(r), \quad (24)$$

where:

$$W_{12}^{(\ell)}(r) \equiv 2 \int_0^\infty \exp(-g^2) g^{(2r+3)} \\ \times \int_0^\pi [1 - \cos^\ell(\chi)] (b/\sigma_{12}) d(b/\sigma_{12}) dg. \quad (25)$$

Note that when only one species is present, Eqs. (24) and (25) reduce to the following simple gas expressions:

$$\Omega_1^{(\ell)}(r) = \sigma_1^2 \left(\frac{\pi kT}{m_1} \right)^{1/2} W_1^{(\ell)}(r), \quad (26)$$

with:

$$W_1^{(\ell)}(r) = 2 \int_0^\infty \exp(-g^2) g^{(2r+3)} \\ \times \int_0^\pi [1 - \cos^\ell(\chi)] (b/\sigma_1) d(b/\sigma_1) dg. \quad (27)$$

In Eqs. (24)–(27), σ_1 is an arbitrary scale length associated with collisions between like molecules of type 1 while σ_{12} is associated

with collisions between unlike molecules of types 1 and 2. These scale lengths are commonly associated with some concept of the molecular diameters depending upon the specific details of the intermolecular potential model that is employed.

3. Derivation of summational representations for the bracket integrals

We begin our derivations at the point in Chapman and Cowling [1] where the evaluation of the six integrations in the bracket integrals that are unrelated to the intermolecular interaction model being employed are first considered. We note that Chapman and Cowling make use of the following relationships for the Sonine polynomials:

$$\left(\frac{S}{s}\right)^{(m+1)} \exp(-xS) = (1-s)^{(-m-1)} \exp(-xs/(1-s)) = \sum_{n=0}^{\infty} s^n S_m^{(n)}(x), \quad (28)$$

and:

$$\left(\frac{T}{t}\right)^{(m+1)} \exp(-xT) = (1-t)^{(-m-1)} \exp(-xt/(1-t)) = \sum_{n=0}^{\infty} t^n S_m^{(n)}(x), \quad (29)$$

where $S = s/(1-s)$ and $T = t/(1-t)$, to express the bracket in terms of the coefficients of expansions in the arbitrarily introduced variables, s and t . Thus, it is possible after following Chapman and Cowling to obtain the following expressions for the bracket integrals of Eqs. (20) and (21), respectively:

$$\left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_2^2) \mathcal{C}_2\right]_{12} = \text{coeff}[s^p t^q] \text{ in } \left(\frac{ST}{st}\right)^{5/2} \pi^{-3} \iiint [H_{12}(0) - H_{12}(\chi)] g b \, db \, d\epsilon \, dg, \quad (30)$$

and:

$$\left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_1^2) \mathcal{C}_1\right]_{12} = \text{coeff}[s^p t^q] \text{ in } \left(\frac{ST}{st}\right)^{5/2} \pi^{-3} \iiint [H_1(0) - H_1(\chi)] g b \, db \, d\epsilon \, dg. \quad (31)$$

Note that the retention of a single g in Eqs. (30) and (31) (as opposed to g) is not a typographical error but, rather, is the exact notation used by Chapman and Cowling. Then, one can express the χ -dependent portions of the RHS bracketed integrals of Eqs. (30) and (31) as:

$$\begin{aligned} \left(\frac{ST}{st}\right)^{5/2} (M_1 M_2)^{-1/2} \pi^{-3/2} H_{12}(\chi) &= \exp(-g^2) \sum_r \sum_n \{2M_1 M_2 st \\ &\times [1 - \cos(\chi)]\}^r \left(\frac{g^{2r}}{r!}\right) (M_2 s + M_1 t)^n \left\{ (n+1) S_{r+1/2}^{(n+1)}(g^2) \right. \\ &\left. + [1 - \cos(\chi)] g^2 S_{r+3/2}^{(n)}(g^2) \right\}, \end{aligned} \quad (32)$$

and:

$$\begin{aligned} \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_1(\chi) &= \exp(-g^2) \sum_r \sum_n \{st[M_1^2 + M_2^2 \\ &+ 2M_1 M_2 \cos(\chi)]\}^r \left(\frac{g^{2r}}{r!}\right) \{M_2(s+t) \\ &- (M_2 - M_1)st\}^n \left\{ M_1(n+1) S_{r+1/2}^{(n+1)}(g^2) \right. \\ &\left. + [M_1 + M_2 \cos(\chi)] g^2 S_{r+3/2}^{(n)}(g^2) \right\}, \end{aligned} \quad (33)$$

which are Eqs. (9.32, 5) and (9.4, 12), respectively, in Chapman and Cowling. In both of these cases, the coefficient of $[s^p t^q]$ yields a polynomial in powers of g^2 and $\cos(\chi)$ that is multiplied by $\exp(-g^2)$ and in which each term is some function of the molecular masses via M_1 and M_2 . The χ -independent portions of the RHS bracketed integrals of Eqs. (30) and (31) are obtained by the simple expedient of setting $\chi = 0$ in Eqs. (32) and (33) which then yields overall terms in the combined polynomials involving $[1 - \cos(\chi)]$. Thus, after completion of the six integrations not related to the intermolecular potential model, including the integrations over ϵ and the directions of g , it is possible to express the bracket integrals of Eqs. (30) and (31) as:

$$\begin{aligned} \left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_2^2) \mathcal{C}_2\right]_{12} &= 8\pi^{1/2} M_2^{(p+1)} M_1^{(q+1)} \int \int \exp(-g^2) \\ &\times \sum_{r,\ell} A_{pq\ell} g^{(2r+2)} [1 - \cos^\ell(\chi)] g b \, db \, dg \\ &= 8M_2^{(p+1)} M_1^{(q+1)} \sum_{r,\ell} A_{pq\ell} \Omega_{12}^{(\ell)}(r), \end{aligned} \quad (34)$$

and:

$$\begin{aligned} \left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_1^2) \mathcal{C}_1\right]_{12} &= 8\pi^{1/2} \int \int \exp(-g^2) \\ &\times \sum_{r,\ell} A'_{pq\ell} g^{(2r+2)} [1 - \cos^\ell(\chi)] g b \, db \, dg \\ &= 8 \sum_{r,\ell} A'_{pq\ell} \Omega_{12}^{(\ell)}(r), \end{aligned} \quad (35)$$

where the omega integrals have been defined in Eqs. (22) and (23). Here, we note that our initial work followed the prescription implied by Chapman and Cowling [1] for determination of the coefficients, $A_{pq\ell}$ and $A'_{pq\ell}$. According to Chapman and Cowling:

“Explicit expressions for $[A_{pq\ell}]$ and $[A'_{pq\ell}]$ can be obtained from [Eqs. (32) and (33)] using [Eq. (18)] for $S_m^{(n)}(x)$. In view of the complication of these expressions it is, however, better in practice to calculate any desired values of $[A_{pq\ell}]$ and $[A'_{pq\ell}]$ directly from [Eqs. (32) and (33)].”

The prescription implied by this statement is that one should expand Eqs. (32) and (33) directly in powers of s and t using the binomial theorem, collect terms containing identical powers of $[s^p t^q]$ to identify the omega integrals that are present, and then consolidate the coefficients of each to create the needed expressions for each of the (p, q) bracket integrals and their associated a_{pq} matrix elements. In general, this process works fine for lower-order expansions; particularly where one is required to do the algebra by hand, and is readily accomplished to much higher orders of

expansion by using *Mathematica*® to do the necessary algebra and pattern matching. However, at sufficiently high an order, the computational overhead associated with performing these operations on extremely large and complex expressions causes the process to become very inefficient in terms of the time required to determine the matrix elements. Thus, we return to the above quote by Chapman and Cowling and consider the alternative prescription that they have indicated which would be expected to yield general expressions for the bracket integrals much more conducive to efficient computations; particularly in computational environments employing more traditional languages and programming structures (such as FORTRAN or C++).

We return now to Eqs. (30) and (31). As we have pointed out, it is technically only necessary to actually derive an alternative expression for the coefficients $A'_{pq\ell}$ in Eq. (35) as the coefficients $A_{pq\ell}$ in Eq. (34) can then be determined from the $A'_{pq\ell}$ expression thus derived. In practice, however, an expression for $A_{pq\ell}$ is easier to derive due to its less complex dependence on the molecular masses. Therefore, $A_{pq\ell}$ is addressed first followed by $A'_{pq\ell}$. With both of these coefficients determined, the bracket integrals of Eqs. (20) and (21) are fully specified in the most general possible terms and may be combined in the appropriate manner to yield the most general possible expression for the simple gas bracket integral of Eq. (19). Then, with all three of the bracket integrals of Eqs. (19) and (21) thus specified, general expressions for the a_{pq} matrix elements may be constructed according to Eqs. (14)–(17) if one wishes. At this point, evaluation of the general matrix elements for specific values of the parameters and inversion of the coefficient matrices to obtain the expansion coefficients $d_0^{(m)}$, $d_1^{(m)}$, $d_2^{(m)}$, $a_1^{(m)}$, and $a_2^{(m)}$ is an extremely rapid process provided that values of the necessary omega integrals exist in pre-computed form to the necessary degree of precision for the specific intermolecular potential model being employed.

4. Derivation of a summational representation for the H_{12} bracket integral

First, consider the bracket integral type:

$$\left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_2^2) \mathcal{C}_2 \right]_{12}, \quad (36)$$

which we refer to here as the H_{12} bracket integral. Following Eq. (30), this may be determined by specifying the coefficient of $[s^p t^q]$ in the expansion of Eq. (32). As a first step one may rewrite Eq. (32) in the following slightly more convenient form:

$$\begin{aligned} \left(\frac{ST}{st} \right)^{5/2} \pi^{-3/2} H_{12}(\chi) &= (M_1 M_2)^{1/2} \exp(-g^2) \sum_{i=0}^{\infty} \sum_{n=0}^{\infty} (M_1 M_2)^i s^i t^n \\ &\times \frac{2^i}{(i)!} [1 - \cos(\chi)]^i (g^2)^i (M_2 s + M_1 t)^n \\ &\times \left\{ (n+1) S_{i+1/2}^{(n+1)}(g^2) \right. \\ &\left. + [1 - \cos(\chi)] g^2 S_{i+3/2}^{(n)}(g^2) \right\}. \end{aligned} \quad (37)$$

Now, one consolidates the Sonine polynomials using the definition of Eq. (18) which can be expressed as:

$$S_{z+1/2}^{(n)}(x) = \sum_{p=0}^n \frac{(-x)^p}{(p)!(n-p)! 4^{(n-p)}} \frac{(2n+2z+2)!(p+z+1)!}{(2p+2z+2)!(n+z+1)!}, \quad (38)$$

where we note that we have used the following property of the Gamma function:

$$\Gamma\left(n + \frac{1}{2}\right) = \frac{(2n)!}{4^n (n)!} \Gamma\left(\frac{1}{2}\right). \quad (39)$$

From Eq. (38), one may obtain:

$$\begin{aligned} S_{i+1/2}^{(n+1)}(g^2) &= \sum_{\eta=0}^{(n+1)} \frac{(-1)^\eta (g^2)^\eta}{(\eta)!(n+1-\eta)!} \\ &\times \frac{(2i+2n+4)!(i+\eta+1)!}{(2i+2\eta+2)!(i+n+2)!} \frac{4^\eta}{4^{(n+1)}}, \end{aligned} \quad (40)$$

and:

$$\begin{aligned} g^2 S_{i+3/2}^{(n)}(g^2) &= - \sum_{\eta=0}^{(n+1)} \frac{\eta (-1)^\eta (g^2)^\eta}{(\eta)!(n+1-\eta)!} \\ &\times \frac{(2i+2n+4)!(i+\eta+1)!}{(2i+2\eta+2)!(i+n+2)!} \frac{4^\eta}{4^{(n+1)}}. \end{aligned} \quad (41)$$

After this substitution, one can factor out the common terms in the two summations and combine them into a single summation as:

$$\begin{aligned} &\left\{ (n+1) S_{i+1/2}^{(n+1)}(g^2) + [1 - \cos(\chi)] g^2 S_{i+3/2}^{(n)}(g^2) \right\} \\ &= \sum_{\eta=0}^{(n+1)} \frac{(-1)^\eta (g^2)^\eta}{(\eta)!(n+1-\eta)!} \frac{(2i+2n+4)!(i+\eta+1)!}{(2i+2\eta+2)!(i+n+2)!} \\ &\times \frac{4^\eta}{4^{(n+1)}} \{ (n+1) - \eta [1 - \cos(\chi)] \}. \end{aligned} \quad (42)$$

Now, one can write:

$$\begin{aligned} &\left(\frac{ST}{st} \right)^{5/2} \pi^{-3/2} H_{12}(\chi) \\ &= (M_1 M_2)^{1/2} \exp(g^2) \sum_{i=0}^{\infty} \sum_{n=0}^{\infty} (M_1 M_2)^i s^i t^n \\ &\times \frac{2^i}{(i)!} [1 - \cos(\chi)]^i (M_2 s + M_1 t)^n \\ &\times \sum_{\eta=0}^{(n+1)} \frac{(-1)^\eta (g^2)^{(\eta+i)}}{(\eta)!(n+1-\eta)!} \frac{4^\eta}{4^{(n+1)}} \frac{(2i+2n+4)!}{(2i+2\eta+2)!} \\ &\times \frac{(i+\eta+1)!}{(i+n+2)!} [(n+1-\eta) + \eta \cos(\chi)]. \end{aligned} \quad (43)$$

To extract the summation over s , one first substitutes the binomial expansion:

$$(M_2 s + M_1 t)^n = \sum_{j=0}^n \binom{n}{j} M_2^j s^j M_1^{(n-j)} t^{(n-j)}, \quad (44)$$

where the $\binom{n}{j}$ are the binomial coefficients, such that:

$$\begin{aligned} &\left(\frac{ST}{st} \right)^{5/2} \pi^{-3/2} H_{12}(\chi) \\ &= (M_1 M_2)^{1/2} \exp(-g^2) \sum_{i=0}^{\infty} \sum_{n=0}^{\infty} (M_1 M_2)^i s^i t^n \\ &\times \frac{2^i}{(i)!} [1 - \cos(\chi)]^i \sum_{j=0}^n \binom{n}{j} M_2^j s^j M_1^{(n-j)} t^{(n-j)} \\ &\times \sum_{\eta=0}^{(n+1)} \frac{(-1)^\eta (g^2)^{(\eta+i)}}{(\eta)!(n+1-\eta)!} \frac{4^\eta}{4^{(n+1)}} \frac{(2i+2n+4)!}{(2i+2\eta+2)!} \end{aligned}$$

$$\begin{aligned}
& \times \frac{(i+\eta+1)!}{(i+n+2)!} [(n+1-\eta) + \eta \cos(\chi)] \\
& = (M_1 M_2)^{1/2} \exp(-g^2) \sum_{i=0}^{\infty} \sum_{n=0}^{\infty} \frac{2^i}{(i)!} [1 - \cos(\chi)]^i \\
& \quad \times \sum_{j=0}^n \binom{n}{j} M_2^{(j+i)} s^{(j+i)} M_1^{(n-j+i)} t^{(n-j+i)} \\
& \quad \times \sum_{\eta=0}^{(n+1)} \frac{(-1)^\eta (g^2)^{(\eta+i)}}{(\eta)!(n+1-\eta)!} \frac{4^\eta}{4^{(n+1)}} \frac{(2i+2n+4)!}{(2i+2\eta+2)!} \\
& \quad \times \frac{(i+\eta+1)!}{(i+n+2)!} [(n+1-\eta) + \eta \cos(\chi)]. \quad (45)
\end{aligned}$$

Then, shifting the j index one has that:

$$\begin{aligned}
& \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_{12}(\chi) \\
& = (M_1 M_2)^{1/2} \exp(-g^2) \sum_{i=0}^{\infty} \sum_{n=0}^{\infty} \frac{2^i}{(i)!} [1 - \cos(\chi)]^i \\
& \quad \times \sum_{j=i}^{(n+1)} \binom{n}{j-i} M_2^j s^j M_1^{(n-j+2i)} t^{(n-j+2i)} \\
& \quad \times \sum_{\eta=0}^{(n+1)} \frac{(-1)^\eta (g^2)^{(\eta+i)}}{(\eta)!(n+1-\eta)!} \frac{4^\eta}{4^{(n+1)}} \frac{(2i+2n+4)!}{(2i+2\eta+2)!} \\
& \quad \times \frac{(i+\eta+1)!}{(i+n+2)!} [(n+1-\eta) + \eta \cos(\chi)] \\
& = (M_1 M_2)^{1/2} \exp(-g^2) \sum_{i=0}^{\infty} \sum_{n=0}^{\infty} \sum_{j=i}^{(n+1)} s^j \frac{2^i}{(i)!} \\
& \quad \times [1 - \cos(\chi)]^i \binom{n}{j-i} M_2^j M_1^{(n-j+2i)} t^{(n-j+2i)} \\
& \quad \times \sum_{\eta=0}^{(n+1)} \frac{(-1)^\eta (g^2)^{(\eta+i)}}{(\eta)!(n+1-\eta)!} \frac{4^\eta}{4^{(n+1)}} \frac{(2i+2n+4)!}{(2i+2\eta+2)!} \\
& \quad \times \frac{(i+\eta+1)!}{(i+n+2)!} [(n+1-\eta) + \eta \cos(\chi)]. \quad (46)
\end{aligned}$$

Now, from Figs. 1 and 2 it can be seen that:

$$\sum_{i=0}^{\infty} \sum_{n=0}^{\infty} \sum_{j=i}^{(n+1)} = \sum_{j=0}^{\infty} \sum_{i=0}^j \sum_{n=j-i}^{\infty}. \quad (47)$$

Thus:

$$\begin{aligned}
& \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_{12}(\chi) \\
& = (M_1 M_2)^{1/2} \exp(-g^2) \sum_{j=0}^{\infty} s^j \sum_{i=0}^j \sum_{n=j-i}^{\infty} \frac{2^i}{(i)!} \\
& \quad \times [1 - \cos(\chi)]^i \binom{n}{j-i} M_2^j M_1^{(n-j+2i)} t^{(n-j+2i)} \\
& \quad \times \sum_{\eta=0}^{(n+1)} \frac{(-1)^\eta (g^2)^{(\eta+i)}}{(\eta)!(n+1-\eta)!} \frac{4^\eta}{4^{(n+1)}} \frac{(2i+2n+4)!}{(2i+2\eta+2)!} \\
& \quad \times \frac{(i+\eta+1)!}{(i+n+2)!} [(n+1-\eta) + \eta \cos(\chi)], \quad (48)
\end{aligned}$$

and one need only let $j \rightarrow p$ to obtain the coefficient of s^p , i.e.:

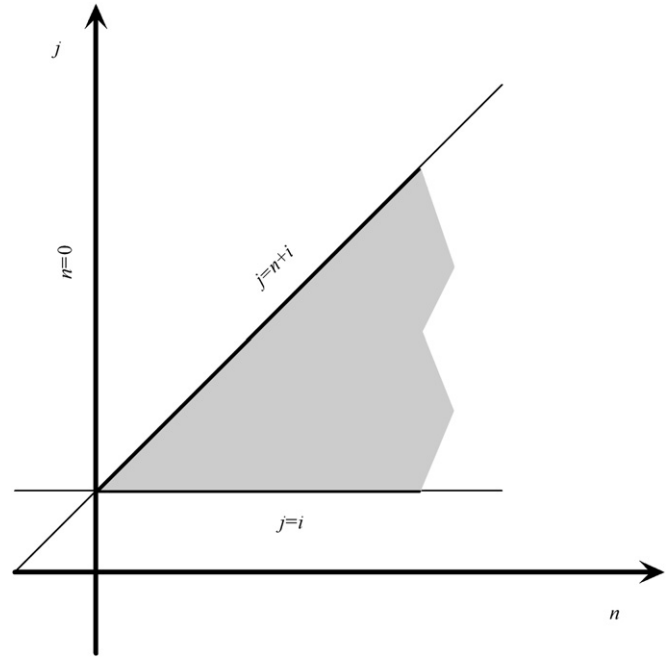


Fig. 1. The geometry of the summational transformation: $\sum_{n=0}^{\infty} \sum_{j=i}^{(n+1)} = \sum_{j=i}^{\infty} \sum_{n=j-i}^{\infty}$.

$$\begin{aligned}
& \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_{12}(\chi) \\
& = (M_1 M_2)^{1/2} \exp(-g^2) \sum_{p=0}^{\infty} s^p \sum_{i=0}^p \sum_{n=(p-i)}^{\infty} t^{(n-p+2i)} \\
& \quad \times \frac{2^i}{(i)!} [1 - \cos(\chi)]^i \binom{n}{p-i} M_2^p M_1^{(n-p+2i)} \\
& \quad \times \sum_{\eta=0}^{(n+1)} \frac{(-1)^\eta (g^2)^{(\eta+i)}}{(\eta)!(n+1-\eta)!} \frac{4^\eta}{4^{(n+1)}} \frac{(2i+2n+4)!}{(2i+2\eta+2)!} \\
& \quad \times \frac{(i+\eta+1)!}{(i+n+2)!} [(n+1-\eta) + \eta \cos(\chi)]. \quad (49)
\end{aligned}$$

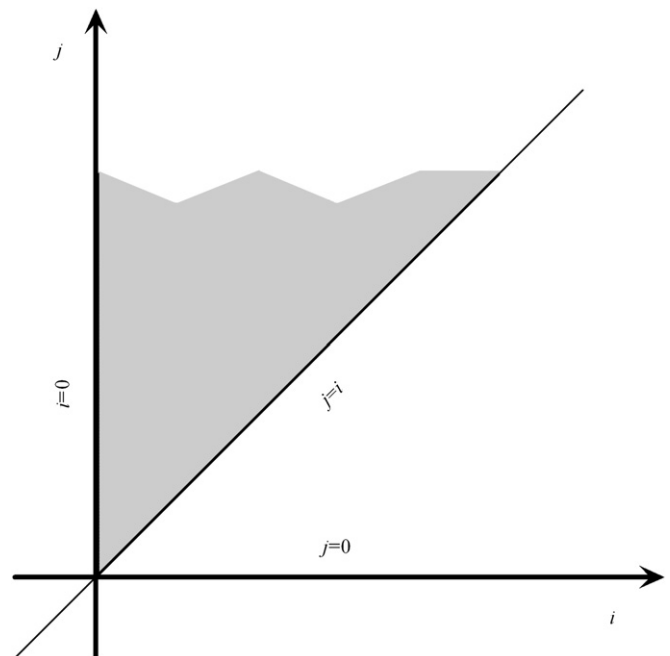


Fig. 2. The geometry of the summational transformation: $\sum_{i=0}^{\infty} \sum_{j=i}^{\infty} = \sum_{j=0}^{\infty} \sum_{i=0}^j$.

Next, to extract the summation over t , one shifts the n index such that:

$$\begin{aligned}
 & \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_{12}(\chi) \\
 &= (M_1 M_2)^{1/2} \exp(-g^2) \sum_{p=0}^{\infty} s^p \sum_{i=0}^p \sum_{n=i}^{\infty} t^n \\
 & \quad \times \frac{2^i}{(i)!} [1 - \cos(\chi)]^i \binom{p+n-2i}{p-i} M_2^p M_1^n \\
 & \quad \times \sum_{\eta=0}^{p+n+1-2i} \frac{(-1)^\eta (g^2)^{(\eta+i)}}{(\eta)!(p+n+1-2i-\eta)!} \\
 & \quad \times \frac{(2(p+n+2-i))!}{(2i+2\eta+2)!} \frac{(i+\eta+1)!}{(p+n+2-i)!} \\
 & \quad \times \frac{4^\eta}{4^{(p+n+1-2i)}} [(p+n+1-2i-\eta) + \eta \cos(\chi)]. \quad (50)
 \end{aligned}$$

Here, from Fig. 3, one has that:

$$\sum_{i=0}^p \sum_{n=i}^{\infty} = \sum_{n=0}^{\infty} \sum_{i=0}^{\min[p,n]}. \quad (51)$$

Thus:

$$\begin{aligned}
 & \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_{12}(\chi) \\
 &= (M_1 M_2)^{1/2} \exp(-g^2) \sum_{p=0}^{\infty} s^p \sum_{n=0}^{\infty} t^n \sum_{i=0}^{\min[p,n]} \\
 & \quad \times \frac{2^i}{(i)!} [1 - \cos(\chi)]^i \binom{p+n-2i}{p-i} M_2^p M_1^n \\
 & \quad \times \sum_{\eta=0}^{p+n+1-2i} \frac{(-1)^\eta (g^2)^{(\eta+i)}}{(\eta)!(p+n+1-2i-\eta)!} \\
 & \quad \times \frac{(2(p+n+2-i))!}{(2i+2\eta+2)!} \frac{(i+\eta+1)!}{(p+n+2-i)!} \\
 & \quad \times \frac{4^\eta}{4^{(p+n+1-2i)}} [(p+n+1-2i-\eta) + \eta \cos(\chi)], \quad (52)
 \end{aligned}$$

and one need only let $n \rightarrow q$ to obtain the coefficient of t^q , i.e.:

$$\begin{aligned}
 & \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_{12}(\chi) \\
 &= \sum_{p=0}^{\infty} s^p \sum_{q=0}^{\infty} t^q M_2^{(p+1/2)} M_1^{(q+1/2)} \exp(-g^2) \\
 & \quad \times \sum_{i=0}^{\min[p,q]} [1 - \cos(\chi)]^i \frac{2^i (p+q-2i)!}{(i)!(p-i)!(q-i)!} \\
 & \quad \times \sum_{\eta=0}^{p+q+1-2i} \frac{(-1)^\eta (g^2)^{(\eta+i)}}{(\eta)!(p+q+1-2i-\eta)!} \\
 & \quad \times \frac{(2(p+q+2-i))!}{(2(i+\eta+1))!} \frac{(i+\eta+1)!}{(p+q+2-i)!} \\
 & \quad \times \frac{4^\eta}{4^{(p+q+1-2i)}} [(p+q+1-2i-\eta) + \eta \cos(\chi)]. \quad (53)
 \end{aligned}$$

To extract the $\cos(\chi)$ summation, one must first factor out powers of the $\cos(\chi)$ from the last term as a summation over Kronecker deltas [21] in the following manner:

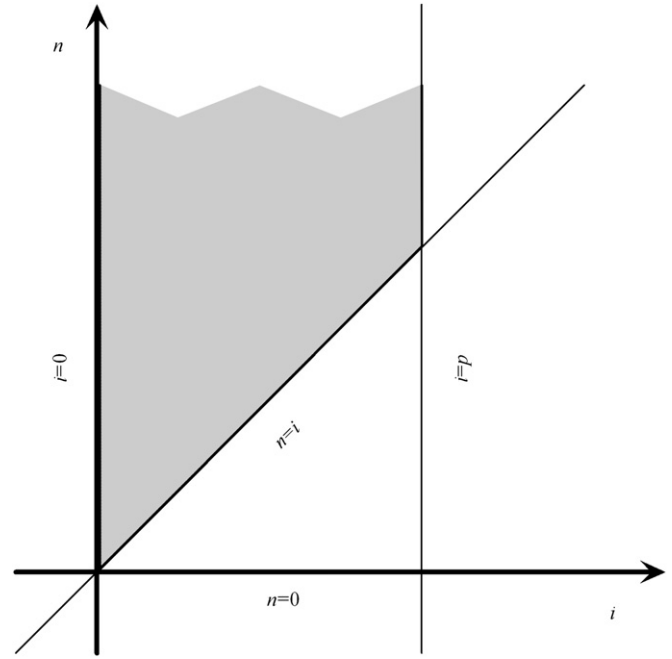


Fig. 3. The geometry of the summational transformation: $\sum_{i=0}^p \sum_{n=i}^{\infty} = \sum_{n=0}^{\infty} \sum_{i=0}^{\min[p,n]}$.

$$\begin{aligned}
 & \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_{12}(\chi) \\
 &= \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} [s^p t^q] M_2^{(p+1/2)} M_1^{(q+1/2)} \exp(-g^2) \\
 & \quad \times \sum_{i=0}^{\min[p,q]} [1 - \cos(\chi)]^i \frac{2^i (p+q-2i)!}{(i)!(p-i)!(q-i)!} \\
 & \quad \times \sum_{\eta=0}^{p+q+1-2i} \frac{(-1)^\eta (g^2)^{(\eta+i)}}{(\eta)!(p+q+1-2i-\eta)!} \\
 & \quad \times \frac{(2(p+q+2-i))!}{(2(i+\eta+1))!} \frac{(i+\eta+1)!}{(p+q+2-i)!} \frac{4^\eta}{4^{(p+q+1-2i)}} \\
 & \quad \times \sum_{j=0}^1 \cos^j(\chi) [(p+q+1-2i-\eta)\delta_{j,0} + \eta\delta_{j,1}]. \quad (54)
 \end{aligned}$$

Substitution of the binomial expansion:

$$[1 - \cos(\chi)]^i = \sum_{k=0}^i \binom{i}{k} (-1)^k \cos^k(\chi), \quad (55)$$

then yields:

$$\begin{aligned}
 & \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_{12}(\chi) = \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} [s^p t^q] M_2^{(p+1/2)} M_1^{(q+1/2)} \exp(-g^2) \\
 & \quad \times \sum_{i=0}^{\min[p,q]} \sum_{k=0}^i \sum_{j=0}^1 \cos^{(j+k)}(\chi) \binom{i}{k} (-1)^k \\
 & \quad \times \frac{2^i (p+q-2i)!}{(i)!(p-i)!(q-i)!} \sum_{\eta=0}^{p+q+1-2i} \frac{(-1)^\eta (g^2)^{(\eta+i)}}{(\eta)!(p+q+1-2i-\eta)!} \frac{(2(p+q+2-i))!}{(2(i+\eta+1))!} \\
 & \quad \times \frac{(i+\eta+1)!}{(p+q+2-i)!} \frac{4^\eta}{4^{(p+q+1-2i)}} \\
 & \quad \times [(p+q+1-2i-\eta)\delta_{j,0} + \eta\delta_{j,1}], \quad (56)
 \end{aligned}$$

which, following a shift of the j index, becomes:

$$\begin{aligned} \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_{12}(\chi) &= \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} [s^p t^q] M_2^{(p+1/2)} M_1^{(q+1/2)} \exp(-g^2) \\ &\times \sum_{i=0}^{\min[p,q]} \sum_{k=0}^i \sum_{j=k}^{(k+1)} \cos^j(\chi) \\ &\times \frac{(-1)^k 2^i (p+q-2i)!}{(k)!(i-k)!(p-i)!(q-i)!} \sum_{\eta=0}^{(p+q+1-2i)} \\ &\times \frac{(-1)^\eta (g^2)^{(\eta+i)}}{(\eta)!(p+q+1-2i-\eta)!} \frac{(2(p+q+2-i))!}{(2(i+\eta+1))!} \\ &\times \frac{(i+\eta+1)!}{(p+q+2-i)!} \frac{4^\eta}{4^{(p+q+1-2i)}} \\ &\times \left[(p+q+1-2i-\eta) \delta_{kj} + \eta \delta_{k,(j-1)} \right]. \quad (57) \end{aligned}$$

Now, from Figs. 4 and 5, one has that:

$$\sum_{i=0}^{\min[p,q]} \sum_{k=0}^i \sum_{j=k}^{(k+1)} = \sum_{j=0}^{\min[p,q]+1} \sum_{i=\max[0,(j-1)]}^{\min[p,q]} \sum_{k=\max[0,(j-1)]}^{\min[j,i]}, \quad (58)$$

such that:

$$\begin{aligned} \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_{12}(\chi) &= \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} [s^p t^q] M_2^{(p+1/2)} M_1^{(q+1/2)} \exp(-g^2) \\ &\times \sum_{j=0}^{(\min[p,q]+1)} \cos^j(\chi) \sum_{i=\max[0,(j-1)]}^{\min[p,q]} \sum_{k=\max[0,(j-1)]}^{\min[j,i]} \\ &\times \frac{(-1)^k 2^i (p+q-2i)!}{(k)!(i-k)!(p-i)!(q-i)!} \sum_{\eta=0}^{(p+q+1-2i)} \\ &\times \frac{(-1)^\eta (g^2)^{(\eta+i)}}{(\eta)!(p+q+1-2i-\eta)!} \frac{(2(p+q+2-i))!}{(2(i+\eta+1))!} \\ &\times \frac{(i+\eta+1)!}{(p+q+2-i)!} \frac{4^\eta}{4^{(p+q+1-2i)}} \\ &\times \left[(p+q+1-2i-\eta) \delta_{kj} + \eta \delta_{k,(j-1)} \right], \quad (59) \end{aligned}$$

and one need only let $j \rightarrow \ell$ to obtain the coefficient of $\cos^\ell(\chi)$, i.e.:

$$\begin{aligned} \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_{12}(\chi) &= \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} [s^p t^q] M_2^{(p+1/2)} M_1^{(q+1/2)} \exp(-g^2) \\ &\times \sum_{\ell=0}^{(\min[p,q]+1)} \cos^\ell(\chi) \sum_{i=\max[0,(\ell-1)]}^{\min[p,q]} \sum_{k=\max[0,(\ell-1)]}^{\min[\ell,i]} \\ &\times \frac{(-1)^k 2^i (p+q-2i)!}{(k)!(i-k)!(p-i)!(q-i)!} \sum_{\eta=0}^{(p+q+1-2i)} \\ &\times \frac{(-1)^\eta (g^2)^{(\eta+i)}}{(\eta)!(p+q+1-2i-\eta)!} \frac{(2(p+q+2-i))!}{(2(i+\eta+1))!} \\ &\times \frac{(i+\eta+1)!}{(p+q+2-i)!} \frac{4^\eta}{4^{(p+q+1-2i)}} \\ &\times \left[(p+q+1-2i-\eta) \delta_{k,\ell} + \eta \delta_{k,(\ell-1)} \right]. \quad (60) \end{aligned}$$

Here, note that the full integration involves the difference $[H_{12}(0) - H_{12}(\chi)]$ which yields terms containing $[1 - \cos^\ell(\chi)]$. When $\ell=0$, this quantity is identically zero and, hence, without loss of generality, one may neglect the lowest term of the summation over

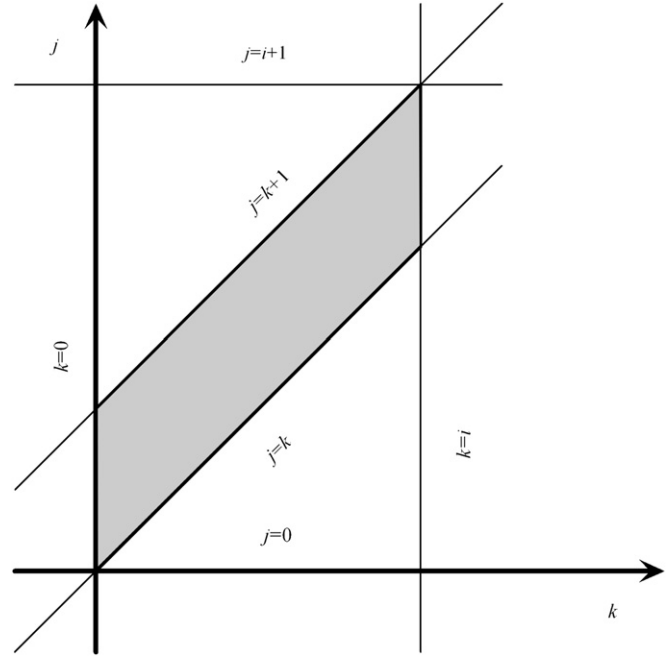


Fig. 4. The geometry of the summational transformation: $\sum_{k=0}^i \sum_{j=k}^{(k+1)} = \sum_{j=0}^{i+1} \sum_{k=\max[0,(j-1)]}^{\min[j,i]}$.

ℓ and express the limits of the ℓ summation accordingly as has been done in what follows.

Lastly, one needs to extract the (g^2) summation. Shifting the η index yields:

$$\begin{aligned} \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} [H_{12}(0) - H_{12}(\chi)] &= \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} [s^p t^q] M_2^{(p+1/2)} M_1^{(q+1/2)} \exp(-g^2) \end{aligned}$$

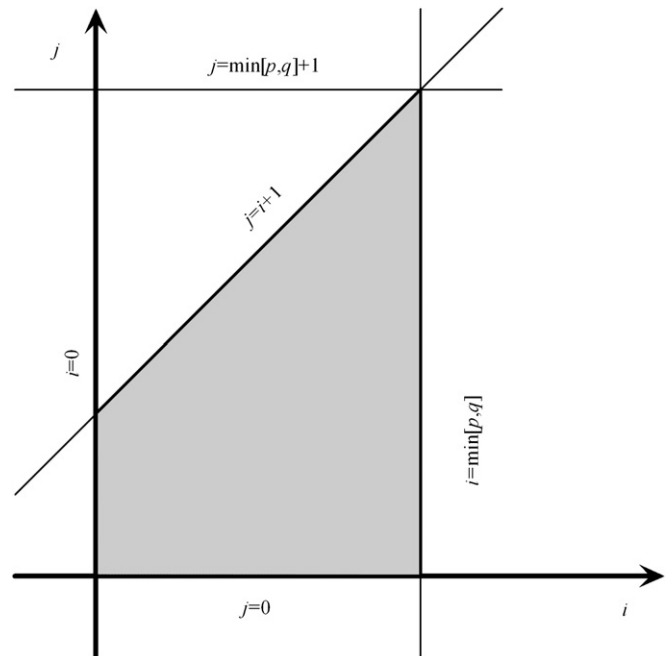


Fig. 5. The geometry of the summational transformation: $\sum_{i=0}^{\min[p,q]} \sum_{j=0}^{(i+1)} = \sum_{j=0}^{\min[p,q]+1} \sum_{i=\max[0,(j-1)]}^{\min[p,q]}$.

$$\begin{aligned}
& \times \sum_{\ell=1}^{(\min[p,q]+1)} [1 - \cos^\ell(\chi)] \sum_{i=\max[0,(\ell-1)]}^{\min[p,q]} \sum_{\eta=i}^{(p+q+1-i)} \\
& \times (g^2)^\eta \frac{8^i (p+q-2i)!}{(p-i)!(q-i)!} \frac{(-1)^{(\eta-i)}}{(\eta-i)!(p+q+1-i-\eta)!} \\
& \times \frac{(2(p+q+2-i))!}{(2(\eta+1))!} \frac{(\eta+1)!}{(p+q+2-i)!} \frac{4^{(\eta)}}{4^{(p+q+1)}} \\
& \times \sum_{k=\max[0,(\ell-1)]}^{\min[\ell,i]} \frac{(-1)^k}{(k)!(i-k)!} \\
& \times [(p+q+1-i-\eta)\delta_{k,\ell} + (\eta-i)\delta_{k,(\ell-1)}], \quad (61)
\end{aligned}$$

where it can be seen from Fig. 6 that:

$$\sum_{i=\max[0,(\ell-1)]}^{\min[p,q]} \sum_{\eta=i}^{(p+q+1-i)} = \sum_{\eta=\max[0,(\ell-1)]}^{(p+q+1-\max[0,(\ell-1)])} \sum_{i=\max[0,(\ell-1)]}^{\min[p,q,\eta,(p+q+1-\eta)]} \quad (62)$$

Thus:

$$\begin{aligned}
& \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} [H_{12}(0) - H_{12}(\chi)] \\
& = \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} [s^p t^q] M_2^{(p+1/2)} M_1^{(q+1/2)} \exp(-g^2) \\
& \times \sum_{\ell=1}^{(\min[p,q]+1)} [1 - \cos^\ell(\chi)] \sum_{\eta=\max[0,(\ell-1)]}^{(p+q+1-\max[0,(\ell-1)])} \\
& \times (g^2)^\eta \sum_{i=\max[0,(\ell-1)]}^{\min[p,q,\eta,(p+q+1-\eta)]} \frac{8^i (p+q-2i)!}{(p-i)!(q-i)!} \frac{4^\eta}{4^{(p+q+1)}} \\
& \times \frac{(-1)^{(\eta-i)}}{(\eta-i)!(p+q+1-i-\eta)!} \frac{(2(p+q+2-i))!}{(2(\eta+1))!} \\
& \times \frac{(\eta+1)!}{(p+q+2-i)!} \sum_{k=\max[0,(\ell-1)]}^{\min[\ell,i]} \frac{(-1)^k}{(k)!(i-k)!} \\
& \times [(p+q+1-i-\eta)\delta_{k,\ell} + (\eta-i)\delta_{k,(\ell-1)}], \quad (63)
\end{aligned}$$

and one need only let $\eta \rightarrow r$ to obtain the coefficient of $(g^2)^r$, i.e.:

$$\begin{aligned}
& \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} [H_{12}(0) - H_{12}(\chi)] \\
& = \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} [s^p t^q] M_2^{(p+1/2)} M_1^{(q+1/2)} \exp(-g^2) \\
& \times \sum_{\ell=1}^{(\min[p,q]+1)} [1 - \cos^\ell(\chi)] \sum_{r=\max[0,(\ell-1)]}^{(p+q+1-\max[0,(\ell-1)])} (g^2)^r \\
& \times \sum_{i=\max[0,(\ell-1)]}^{\min[p,q,r,(p+q+1-r)]} \frac{8^i (p+q-2i)!}{(p-i)!(q-i)!} \frac{4^r}{4^{(p+q+1)}} \\
& \times \frac{(-1)^{(r-i)}}{(r-i)!(p+q+1-r-i)!} \frac{(r+1)!}{(2r+2)!} \\
& \times \frac{(2(p+q+2-i))!}{(p+q+2-i)!} \sum_{k=\max[0,(\ell-1)]}^{\min[\ell,i]} \frac{(-1)^k}{(k)!(i-k)!} \\
& \times [(p+q+1-r-i)\delta_{k,\ell} + (r-i)\delta_{k,(\ell-1)}]. \quad (64)
\end{aligned}$$

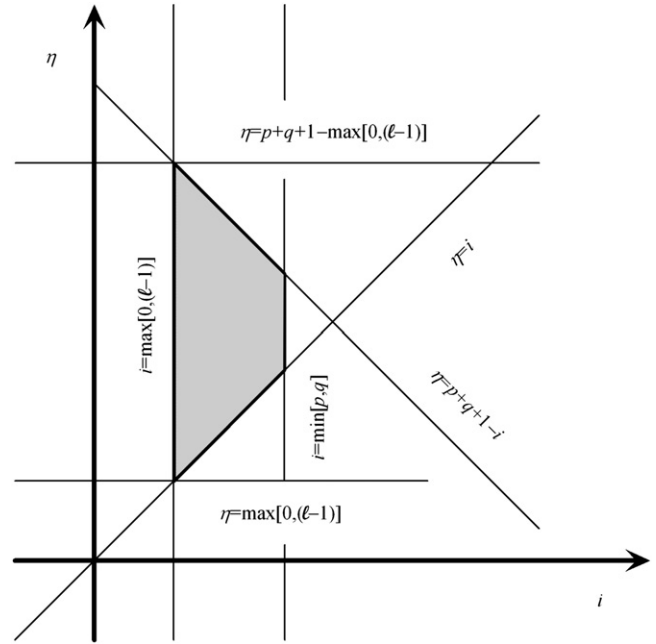


Fig. 6. The geometry of the summational transformation: $\sum_{i=\max[0,(\ell-1)]}^{\min[p,q]} \sum_{\eta=i}^{(p+q+1-i)} = \sum_{\eta=\max[0,(\ell-1)]}^{(p+q+1-\max[0,(\ell-1)])} \sum_{i=\max[0,(\ell-1)]}^{\min[p,q,\eta,(p+q+1-\eta)]}$.

From this, after integration of the coefficient of $[s^p t^q]$ over ε and the directions of g , one has that:

$$\begin{aligned}
& [S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_2^2) \mathcal{C}_2]_{12} = 8 M_2^{(p+1/2)} M_1^{(q+1/2)} \\
& \times \sum_{\ell=1}^{(\min[p,q]+1)} \sum_{r=\max[0,(\ell-1)]}^{(p+q+1-\max[0,(\ell-1)])} A_{pqr\ell} \Omega_{12}^{(\ell)}(r), \quad (65)
\end{aligned}$$

where:

$$\Omega_{12}^{(\ell)}(r) \equiv \iint \pi^{1/2} \exp(-g^2) g^{(2r+2)} [1 - \cos^\ell(\chi)] g b \, db \, dg, \quad (66)$$

are the omega integrals, and:

$$\begin{aligned}
A_{pqr\ell} & = \sum_{i=\max[0,(\ell-1)]}^{\min[p,q,r,(p+q+1-r)]} \frac{8^i (p+q-2i)!}{(p-i)!(q-i)!} \frac{4^r}{4^{(p+q+1)}} \\
& \times \frac{(-1)^{(r-i)}}{(r-i)!(p+q+1-r-i)!} \frac{(r+1)!}{(2r+2)!} \\
& \times \frac{(2(p+q+2-i))!}{(p+q+2-i)!} \sum_{k=\max[0,(\ell-1)]}^{\min[\ell,i]} \frac{(-1)^k}{(k)!(i-k)!} \\
& \times [(p+q+1-r-i)\delta_{k,\ell} + (r-i)\delta_{k,(\ell-1)}]. \quad (67)
\end{aligned}$$

Now, note that some simplification may be achieved in the above expressions by taking advantage of the fact that, since $\ell \geq 1$, one always has $\max[0, (\ell-1)] = (\ell-1)$. Thus, it is equivalent to write:

$$\begin{aligned}
& [S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_2^2) \mathcal{C}_2]_{12} \\
& = 8 M_2^{(p+1/2)} M_1^{(q+1/2)} \sum_{\ell=1}^{(\min[p,q]+1)} \sum_{r=(\ell-1)}^{(p+q+2-\ell)} A_{pqr\ell} \Omega_{12}^{(\ell)}(r), \quad (68)
\end{aligned}$$

with:

$$A_{pqr\ell} = \sum_{i=(\ell-1)}^{\min[p,q,r,(p+q+1-r)]} \frac{8^i (p+q-2i)!}{(p-i)!(q-i)!} \frac{4^r}{4^{(p+q+1)}} \times \frac{(-1)^{(r-i)}}{(r-i)!(p+q+1-r-i)!} \frac{(r+1)!}{(2r+2)!} \times \frac{(2(p+q+2-i))!}{(p+q+2-i)!} \sum_{k=(\ell-1)}^{\min[\ell,i]} \frac{(-1)^k}{(k)!(i-k)!} \times \left[(p+q+1-r-i)\delta_{k,\ell} + (r-i)\delta_{k,(\ell-1)} \right]. \quad (69)$$

Further, when $r = (\ell - 1)$ it follows that $i = k = r$ and one has that $\{(p+q+1-i-r)\delta_{k,\ell} + (r-i)\delta_{k,(\ell-1)}\} = 0$ such that the lowest term of the r summation may be neglected, i.e.:

$$\left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_2^2) \mathcal{C}_2 \right]_{12} = 8M_2^{(p+1/2)} M_1^{(q+1/2)} \times \sum_{\ell=1}^{\min[p,q+1]} \sum_{r=\ell}^{(p+q+2-\ell)} A_{pqr\ell} Q_{12}^{(\ell)}(r). \quad (70)$$

5. Derivation of a summational representation for the H_1 bracket integral

Next, consider the bracket integral type:

$$\left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_1^2) \mathcal{C}_1 \right]_{12}, \quad (71)$$

which we refer to here as the H_1 bracket integral. Following Eq. (31), one has that this bracket integral may be determined by specifying the coefficient of $[s^p t^q]$ in the expansion of Eq. (33). Expressing Eq. (33) more conveniently, one may write:

$$\left(\frac{ST}{st} \right)^{5/2} \pi^{-3/2} H_1(\chi) = \exp(-g^2) \sum_{i=0}^{\infty} \sum_{n=0}^{\infty} s^i t^n \times \left\{ M_1^2 + M_2^2 + 2M_1 M_2 \cos(\chi) \right\}^i \times (g^2)^i [(i)!]^{-1} \{ M_2(s+t) - (M_2 - M_1)st \}^n \times \left\{ M_1(n+1) S_{i+1/2}^{(n+1)}(g^2) + [M_1 + M_2 \cos(\chi)] g^2 S_{i+3/2}^{(n)}(g^2) \right\} + [M_1 + M_2 \cos(\chi)] g^2 S_{i+3/2}^{(n)}(g^2). \quad (72)$$

Again, the Sonine polynomials are consolidated using the definition of Eq. (18) such that:

$$\left\{ M_1(n+1) S_{i+1/2}^{(n+1)}(g^2) + [M_1 + M_2 \cos(\chi)] g^2 S_{i+3/2}^{(n)}(g^2) \right\} = \sum_{\eta=0}^{(n+1)} \frac{(-1)^\eta (g^2)^\eta}{(\eta)!(n+1-\eta)!} \frac{(2i+2n+4)!}{(2i+2\eta+2)!} \frac{(i+\eta+1)!}{(i+n+2)!} \times \frac{4^\eta}{4^{(n+1)}} \{ M_1(n+1) - \eta[M_1 + M_2 \cos(\chi)] \} = \sum_{\eta=0}^{(n+1)} \frac{(-1)^\eta (g^2)^\eta}{(\eta)!(n+1-\eta)!} \frac{(2i+2n+4)!}{(2i+2\eta+2)!} \frac{(i+\eta+1)!}{(i+n+2)!} \times \frac{4^\eta}{4^{(n+1)}} [M_1(n+1-\eta) - M_2 \eta \cos(\chi)], \quad (73)$$

so that one has:

$$\left(\frac{ST}{st} \right)^{5/2} \pi^{-3/2} H_1(\chi) = \exp(-g^2) \sum_{i=0}^{\infty} \sum_{n=0}^{\infty} s^i t^n 2^i M_1^i M_2^i [F + \cos(\chi)]^i [(i)!]^{-1}$$

$$\times M_2^n \{ [1 + Gt]s + t \}^n \sum_{\eta=0}^{(n+1)} \frac{(-1)^\eta (g^2)^\eta}{(\eta)!(n+1-\eta)!} \times \frac{(2i+2n+4)!}{(2i+2\eta+2)!} \frac{(i+\eta+1)!}{(i+n+2)!} \times \frac{4^\eta}{4^{(n+1)}} [M_1(n+1-\eta) - M_2 \eta \cos(\chi)], \quad (74)$$

where $F = (M_1^2 + M_2^2)/2M_1 M_2$ and $G = (M_1 - M_2)/M_2$.

To extract the summation over s , one first substitutes the binomial expansion:

$$\{ [1 + Gt]s + t \}^n = \sum_{j=0}^n \binom{n}{j} [1 + Gt]^j s^{(n-j)}, \quad (75)$$

such that:

$$\left(\frac{ST}{st} \right)^{5/2} \pi^{-3/2} H_1(\chi) = \exp(-g^2) \sum_{i=0}^{\infty} \sum_{n=0}^{\infty} \sum_{j=0}^n s^{(i+j)} t^{(i+n-j)} 2^i M_1^i M_2^i M_2^n \times [F + \cos(\chi)]^i [(i)!]^{-1} \binom{n}{j} [1 + Gt]^j \sum_{\eta=0}^{(n+1)} \frac{(-1)^\eta (g^2)^\eta}{(\eta)!(n+1-\eta)!} \frac{(2i+2n+4)!}{(2i+2\eta+2)!} \frac{(i+\eta+1)!}{(i+n+2)!} \times \frac{4^\eta}{4^{(n+1)}} [M_1(n+1-\eta) - M_2 \eta \cos(\chi)]. \quad (76)$$

Then, shifting the j index one has that:

$$\left(\frac{ST}{st} \right)^{5/2} \pi^{-3/2} H_1(\chi) = \exp(-g^2) \sum_{i=0}^{\infty} \sum_{n=0}^{\infty} \sum_{j=i}^{(n+1)} s^j t^{(2i+n-j)} 2^i M_1^i M_2^i M_2^n \times [F + \cos(\chi)]^i [(i)!]^{-1} \binom{n}{j-i} [1 + Gt]^{(j-i)} \sum_{\eta=0}^{(n+1)} \frac{(-1)^\eta (g^2)^\eta}{(\eta)!(n+1-\eta)!} \frac{(2i+2n+4)!}{(2i+2\eta+2)!} \frac{(i+\eta+1)!}{(i+n+2)!} \times \frac{4^\eta}{4^{(n+1)}} [M_1(n+1-\eta) - M_2 \eta \cos(\chi)]. \quad (77)$$

As before, from Figs. 1 and 2, one can apply the expression from Eq. (47) such that:

$$\left(\frac{ST}{st} \right)^{5/2} \pi^{-3/2} H_1(\chi) = \exp(-g^2) \sum_{j=0}^{\infty} s^j \sum_{i=0}^j \sum_{n=(j-i)}^{\infty} t^{(2i+n-j)} 2^i M_1^i M_2^i M_2^n \times [F + \cos(\chi)]^i [(i)!]^{-1} \binom{n}{j-i} [1 + Gt]^{(j-i)} \sum_{\eta=0}^{(n+1)} \frac{(-1)^\eta (g^2)^\eta}{(\eta)!(n+1-\eta)!} \frac{(2i+2n+4)!}{(2i+2\eta+2)!} \frac{(i+\eta+1)!}{(i+n+2)!} \times \frac{4^\eta}{4^{(n+1)}} [M_1(n+1-\eta) - M_2 \eta \cos(\chi)], \quad (78)$$

and one need only let $j \rightarrow p$ to obtain the coefficient of s^p , i.e.:

$$\begin{aligned} & \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_1(\chi) \\ &= \exp(-g^2) \sum_{p=0}^{\infty} s^p \sum_{i=0}^p \sum_{n=(p-i)}^{\infty} t^{(2i+n-p)} 2^i M_1^i M_2^i M_2^n \\ & \quad \times [F + \cos(\chi)]^i [(i)!]^{-1} \binom{n}{(p-i)} [1 + Gt]^{(p-i)} \sum_{\eta=0}^{(n+1)} \\ & \quad \times \frac{(-1)^\eta (g^2)^{(\eta+i)}}{(\eta)!(n+1-\eta)!} \frac{(2i+2n+4)! (i+\eta+1)!}{(2i+2\eta+2)! (i+n+2)!} \\ & \quad \times \frac{4^\eta}{4^{(n+1)}} [M_1(n+1-\eta) - M_2\eta \cos(\chi)]. \end{aligned} \quad (79)$$

Now, to extract the summation over t , one substitutes the binomial expansion:

$$[1 + Gt]^{(p-i)} = \sum_{w=0}^{(p-i)} \binom{p-i}{w} G^w t^w, \quad (80)$$

such that:

$$\begin{aligned} & \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_1(\chi) \\ &= \exp(-g^2) \sum_{p=0}^{\infty} s^p \sum_{i=0}^p \sum_{w=0}^{(p-i)} \sum_{n=(p-i-w)}^{\infty} t^{(2i+n-p+w)} 2^i \\ & \quad \times M_1^i M_2^i M_2^n [F + \cos(\chi)]^i \frac{G^w}{(i)!} \binom{n}{(p-i)} \binom{p-i}{w} \\ & \quad \times \sum_{\eta=0}^{(n+1)} \frac{(-1)^\eta (g^2)^{(\eta+i)}}{(\eta)!(n+1-\eta)!} \frac{(2i+2n+4)! (i+\eta+1)!}{(2i+2\eta+2)! (i+n+2)!} \\ & \quad \times \frac{4^\eta}{4^{(n+1)}} [M_1(n+1-\eta) - M_2\eta \cos(\chi)]. \end{aligned} \quad (81)$$

Then, after shifting the n index, one has:

$$\begin{aligned} & \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_1(\chi) \\ &= \exp(-g^2) \sum_{p=0}^{\infty} s^p \sum_{i=0}^p \sum_{w=0}^{(p-i)} \sum_{n=(w+i)}^{\infty} t^{2i} 2^i M_1^i M_2^i \\ & \quad \times M_2^{(p+n-2i-w)} [F + \cos(\chi)]^i \binom{p+n-2i-w}{(p-i)} \\ & \quad \times \binom{p-i}{w} \frac{G^w (p+n+1-2i-w)}{(i)!} \sum_{\eta=0}^{\infty} (g^2)^{(\eta+i)} \\ & \quad \times \frac{(-1)^\eta}{(\eta)!(p+n+1-2i-\eta-w)!} \frac{(i+\eta+1)!}{(2i+2\eta+2)!} \\ & \quad \times \frac{(2(p+n+2-i)-2w)!}{(p+n+2-i-w)!} \frac{4^\eta}{4^{(p+n+1-2i-w)}} \\ & \quad \times [M_1(p+n+1-2i-\eta-w) - M_2\eta \cos(\chi)]. \end{aligned} \quad (82)$$

From Figs. 3 and 7 one has that:

$$\sum_{i=0}^p \sum_{w=0}^{(p-i)} \sum_{n=(w+i)}^{\infty} = \sum_{n=0}^{\infty} \sum_{i=0}^{\min[p,n]} \sum_{w=0}^{\min[(p-i),(n-i)]}, \quad (83)$$

such that:

$$\begin{aligned} & \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_1(\chi) \\ &= \exp(-g^2) \sum_{p=0}^{\infty} s^p \sum_{n=0}^{\infty} t^n \sum_{i=0}^{\min[p,n]} \sum_{w=0}^{\min[(p-i),(n-i)]} 2^i M_1^i \end{aligned}$$

$$\begin{aligned} & \times M_2^i M_2^{(p+n-2i-w)} [F + \cos(\chi)]^i \binom{p+n-2i-w}{(p-i)} \\ & \times \binom{p-i}{w} \frac{G^w (p+n+1-2i-w)}{(i)!} \sum_{\eta=0}^{\infty} (g^2)^{(\eta+i)} \\ & \times \frac{(-1)^\eta}{(\eta)!(p+n+1-2i-\eta-w)!} \frac{(i+\eta+1)!}{(2i+2\eta+2)!} \\ & \times \frac{(2(p+n+2-i)-2w)!}{(p+n+2-i-w)!} \frac{4^\eta}{4^{(p+n+1-2i-w)}} \\ & \times [M_1(p+n+1-2i-\eta-w) - M_2\eta \cos(\chi)], \end{aligned} \quad (84)$$

and one need only let $n \rightarrow q$ to obtain the coefficient of t^q , i.e.:

$$\begin{aligned} & \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_1(\chi) \\ &= \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} [s^p t^q] \exp(-g^2) \sum_{i=0}^{\min[p,q]} \sum_{w=0}^{\min[(p-i),(q-i)]} 2^i M_1^i \\ & \quad \times M_2^i M_2^{(p+q-2i-w)} [F + \cos(\chi)]^i \binom{p+q-2i-w}{(p-i)} \\ & \quad \times \binom{p-i}{w} \frac{G^w (p+q+1-2i-w)}{(i)!} \sum_{\eta=0}^{\infty} (g^2)^{(\eta+i)} \\ & \quad \times \frac{(-1)^\eta}{(\eta)!(p+q+1-2i-\eta-w)!} \frac{(i+\eta+1)!}{(2i+2\eta+2)!} \\ & \quad \times \frac{(2(p+q+2-i)-2w)!}{(p+q+2-i-w)!} \frac{4^\eta}{4^{(p+q+1-2i-w)}} \\ & \quad \times [M_1(p+q+1-2i-\eta-w) - M_2\eta \cos(\chi)]. \end{aligned} \quad (85)$$

To extract the $\cos(\chi)$ summation, one must first factor out powers of the $\cos(\chi)$ from the last term as a summation over Kronecker deltas in the same manner as was done previously, i.e.:

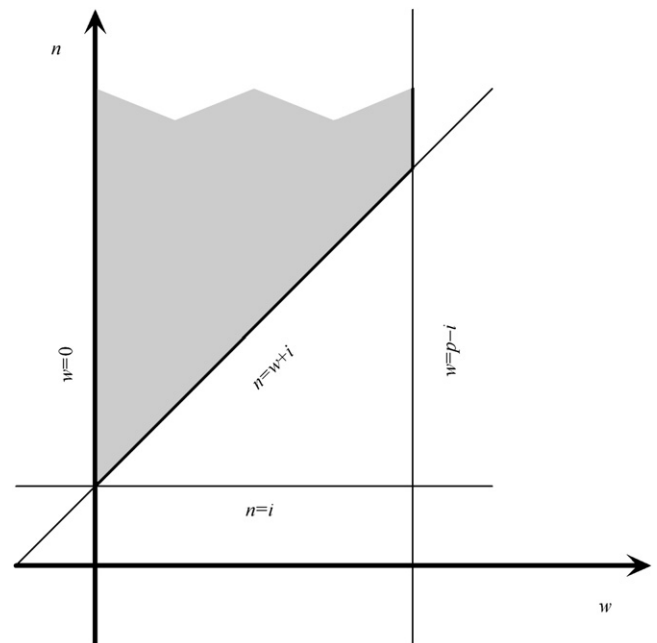


Fig. 7. The geometry of the summational transformation: $\sum_{w=0}^{(p-i)} \sum_{n=w+i}^{\infty} = \sum_{n=i}^{\infty} \sum_{w=0}^{\min[(p-i),(n-i)]}$.

$$\begin{aligned}
& \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_1(\chi) \\
&= \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} [s^p t^q] \exp(-g^2) \sum_{i=0}^{\min[p,q]} \sum_{w=0}^{\min[(p-i),(q-i)]} 2^i M_1^i \\
&\quad \times M_2^i M_2^{(p+q-2i-w)} [F + \cos(\chi)]^i \binom{p+q-2i-w}{p-i} \\
&\quad \times \binom{p-i}{w} \frac{G^w}{(i)!} \sum_{\eta=0}^{p+q+1-2i-w} (g^2)^{(\eta+i)} \\
&\quad \times \frac{(-1)^\eta}{(\eta)!(p+q+1-2i-\eta-w)!} \frac{(i+\eta+1)!}{(2i+2\eta+2)!} \\
&\quad \times \frac{(2(p+q+2-i)-2w)!}{(p+q+2-i-w)!} \frac{4^\eta}{4^{(p+q+1-2i-w)}} \sum_{j=0}^1 \cos^j(\chi) \\
&\quad \times [M_1(p+q+1-2i-\eta-w)\delta_{j,0} - M_2\eta\delta_{j,1}].
\end{aligned} \tag{86}$$

Substitution of the binomial expansion:

$$[F + \cos(\chi)]^i = \sum_{k=0}^i \binom{i}{k} F^{(i-k)} \cos^k(\chi), \tag{87}$$

then yields:

$$\begin{aligned}
& \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_1(\chi) \\
&= \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} [s^p t^q] \exp(-g^2) \sum_{i=0}^{\min[p,q]} \sum_{k=0}^i \sum_{j=0}^1 \cos^{(j+k)}(\chi) \\
&\quad \times \sum_{w=0}^{\min[(p-i),(q-i)]} 2^i M_1^i M_2^i M_2^{(p+q-2i-w)} \\
&\quad \times F^{(i-k)} \binom{p+q-2i-w}{p-i} \binom{p-i}{w} \\
&\quad \times \binom{i}{k} \frac{G^w}{(i)!} \sum_{\eta=0}^{p+q+1-2i-w} (g^2)^{(\eta+i)} \\
&\quad \times \frac{(-1)^\eta}{(\eta)!(p+q+1-2i-\eta-w)!} \frac{(i+\eta+1)!}{(2i+2\eta+2)!} \\
&\quad \times \frac{(2(p+q+2-i)-2w)!}{(p+q+2-i-w)!} \frac{4^\eta}{4^{(p+q+1-2i-w)}} \\
&\quad \times [M_1(p+q+1-2i-\eta-w)\delta_{j,0} - M_2\eta\delta_{j,1}],
\end{aligned} \tag{88}$$

which, following a shift of the j index, becomes:

$$\begin{aligned}
& \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_1(\chi) \\
&= \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} [s^p t^q] \exp(-g^2) \sum_{i=0}^{\min[p,q]} \sum_{k=0}^i \sum_{j=k}^{(k+1)} \cos^j(\chi) \\
&\quad \times \sum_{w=0}^{\min[(p-i),(q-i)]} 2^i M_1^i M_2^i M_2^{(p+q-2i-w)} \\
&\quad \times F^{(i-k)} \binom{p+q-2i-w}{p-i} \binom{p-i}{w} \\
&\quad \times \binom{i}{k} \frac{G^w}{(i)!} \sum_{\eta=0}^{p+q+1-2i-w} (g^2)^{(\eta+i)} \\
&\quad \times \frac{(-1)^\eta}{(\eta)!(p+q+1-2i-\eta-w)!} \frac{(i+\eta+1)!}{(2i+2\eta+2)!}
\end{aligned}$$

$$\begin{aligned}
& \times \frac{(2(p+q+2-i)-2w)!}{(p+q+2-i-w)!} \frac{4^\eta}{4^{(p+q+1-2i-w)}} \\
& \times [M_1(p+q+1-2i-\eta-w)\delta_{k,j} - M_2\eta\delta_{k,(j-1)}].
\end{aligned} \tag{89}$$

Again using Eq. (58) obtained from Figs. 4 and 5, yields:

$$\begin{aligned}
& \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_1(\chi) \\
&= \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} [s^p t^q] \exp(-g^2) \sum_{j=0}^{(\min[p,q]+1)} \cos^j(\chi) \sum_{i=\max[0,(j-1)]}^{\min[p,q]} \\
&\quad \times \sum_{k=\max[0,(j-1)]}^{\min[j,i]} \sum_{w=0}^{\min[(p-i),(q-i)]} 2^i M_1^i M_2^i M_2^{(p+q-2i-w)} \\
&\quad \times F^{(i-k)} \binom{p+q-2i-w}{p-i} \binom{p-i}{w} \\
&\quad \times \binom{i}{k} \frac{G^w}{(i)!} \sum_{\eta=0}^{p+q+1-2i-w} (g^2)^{(\eta+i)} \\
&\quad \times \frac{(-1)^\eta}{(\eta)!(p+q+1-2i-\eta-w)!} \frac{(i+\eta+1)!}{(2i+2\eta+2)!} \\
&\quad \times \frac{(2(p+q+2-i)-2w)!}{(p+q+2-i-w)!} \frac{4^\eta}{4^{(p+q+1-2i-w)}} \\
&\quad \times [M_1(p+q+1-2i-\eta-w)\delta_{k,j} - M_2\eta\delta_{k,(j-1)}],
\end{aligned} \tag{90}$$

and one need only let $j \rightarrow \ell$ to obtain the coefficient of $\cos^\ell(\chi)$, i.e.:

$$\begin{aligned}
& \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} H_1(\chi) \\
&= \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} [s^p t^q] \exp(-g^2) \sum_{\ell=0}^{(\min[p,q]+1)} \cos^\ell(\chi) \sum_{i=\max[0,(\ell-1)]}^{\min[p,q]} \\
&\quad \times \sum_{k=\max[0,(\ell-1)]}^{\min[\ell,i]} \sum_{w=0}^{\min[(p-i),(q-i)]} 2^i M_1^i M_2^i M_2^{(p+q-2i-w)} \\
&\quad \times F^{(i-k)} \binom{p+q-2i-w}{p-i} \binom{p-i}{w} \\
&\quad \times \binom{i}{k} \frac{G^w}{(i)!} \sum_{\eta=0}^{p+q+1-2i-w} (g^2)^{(\eta+i)} \\
&\quad \times \frac{(-1)^\eta}{(\eta)!(p+q+1-2i-\eta-w)!} \frac{(i+\eta+1)!}{(2i+2\eta+2)!} \\
&\quad \times \frac{(2(p+q+2-i)-2w)!}{(p+q+2-i-w)!} \frac{4^\eta}{4^{(p+q+1-2i-w)}} \\
&\quad \times [M_1(p+q+1-2i-\eta-w)\delta_{k,\ell} - M_2\eta\delta_{k,(\ell-1)}].
\end{aligned} \tag{91}$$

As before, note that the full integration involves the difference $[H_1(0) - H_1(\chi)]$ which yields terms containing $[1 - \cos^\ell(\chi)]$. When $\ell = 0$, this quantity is identically zero and, hence, without loss of generality, one may again neglect the lowest term of the summation over ℓ and express the limits of the ℓ summation accordingly. Also as before, since $\ell \geq 1$, one has that $\max[0, (\ell - 1)] = (\ell - 1)$. Thus:

$$\begin{aligned}
& \left(\frac{ST}{st}\right)^{5/2} \pi^{-3/2} [H_1(0) - H_1(\chi)] \\
&= \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} [s^p t^q] \exp(-g^2) \sum_{\ell=1}^{(\min[p,q]+1)} [1 - \cos^\ell(\chi)] \\
&\quad \times \sum_{i=(\ell-1)}^{\min[p,q]} \sum_{w=0}^{\min[(p-i),(q-i)]} \sum_{\eta=0}^{p+q+1-2i-w} (g^2)^{(\eta+i)}
\end{aligned}$$

$$\begin{aligned}
& \times \sum_{k=(\ell-1)}^{\min[\ell,i]} 2^i M_1^i M_2^i M_2^{(p+q-2i-w)} F^{(i-k)} \\
& \times \left(\frac{(p+q-2i-w)}{(p-i)} \right) \left(\frac{(p-i)}{w} \right) \left(\frac{i}{k} \right) \frac{G^w}{(i)!} \\
& \times \frac{(-1)^\eta}{(\eta)!(p+q+1-2i-\eta-w)!} \frac{(i+\eta+1)!}{(2i+2\eta+2)!} \\
& \times \frac{(2(p+q+2-i)-2w)!}{(p+q+2-i-w)!} \frac{4^\eta}{4^{(p+q+1-2i-w)}} \\
& \times [M_1(p+q+1-2i-\eta-w)\delta_{k,\ell} - M_2\eta\delta_{k,(\ell-1)}]. \quad (92)
\end{aligned}$$

Lastly, one needs to extract the (g^2) summation. Shifting the η index yields:

$$\begin{aligned}
& \left(\frac{ST}{st} \right)^{5/2} \pi^{-3/2} [H_1(0) - H_1(\chi)] \\
& = \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} [s^p t^q] \exp(-g^2) \sum_{\ell=1}^{(\min[p,q]+1)} [1 - \cos^\ell(\chi)] \\
& \times \sum_{i=(\ell-1)}^{\min[p,q]} \sum_{w=0}^{\min[(p-i),(q-i)]} \sum_{\eta=i}^{(p+q+1-i-w)} (g^2)^\eta \\
& \times \sum_{k=(\ell-1)}^{\min[\ell,i]} 2^i M_1^i M_2^i M_2^{(p+q-2i-w)} F^{(i-k)} \\
& \times \left(\frac{(p+q-2i-w)}{(p-i)} \right) \left(\frac{(p-i)}{w} \right) \left(\frac{i}{k} \right) \frac{G^w}{(i)!} \\
& \times \frac{(-1)^{(\eta-i)}}{(\eta-i)!(p+q+1-i-\eta-w)!} \frac{(\eta+1)!}{(2\eta+2)!} \\
& \times \frac{(2(p+q+2-i)-2w)!}{(p+q+2-i-w)!} \frac{4^{(\eta+i)}}{4^{(p+q+1-w)}} \\
& \times [M_1(p+q+1-i-\eta-w)\delta_{k,\ell} - M_2(\eta-i)\delta_{k,(\ell-1)}]. \quad (93)
\end{aligned}$$

From Figs. 6 and 8, one has that:

$$\begin{aligned}
& \sum_{i=(\ell-1)}^{\min[p,q]} \sum_{w=0}^{\min[(p-i),(q-i)]} \sum_{\eta=i}^{(p+q+1-i-w)} = \sum_{\eta=(\ell-1)}^{(p+q+2-\ell)} \\
& \times \sum_{i=(\ell-1)}^{\min[p,q,\eta,(p+q+1-\eta)]} \sum_{w=0}^{\min[(p-i),(q-i),(p+q+1-i-\eta)]}, \quad (94)
\end{aligned}$$

such that:

$$\begin{aligned}
& \left(\frac{ST}{st} \right)^{5/2} \pi^{-3/2} [H_1(0) - H_1(\chi)] \\
& = \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} [s^p t^q] \exp(-g^2) \sum_{\ell=1}^{(\min[p,q]+1)} [1 - \cos^\ell(\chi)] \\
& \times \sum_{\eta=(\ell-1)}^{(p+q+2-\ell)} (g^2)^\eta \sum_{i=(\ell-1)}^{\min[p,q,\eta,(p+q+1-\eta)]} \sum_{k=(\ell-1)}^{\min[\ell,i]} \\
& \times \sum_{w=0}^{\min[(p-i),(q-i),(p+q+1-i-\eta)]} 2^i M_1^i M_2^i M_2^{(p+q-2i-w)} \\
& \times F^{(i-k)} \left(\frac{(p+q-2i-w)}{(p-i)} \right) \left(\frac{(p-i)}{w} \right) \left(\frac{i}{k} \right) \frac{G^w}{(i)!} \\
& \times \frac{(-1)^{(\eta-i)}}{(\eta-i)!(p+q+1-i-\eta-w)!} \frac{(\eta+1)!}{(2\eta+2)!}
\end{aligned}$$

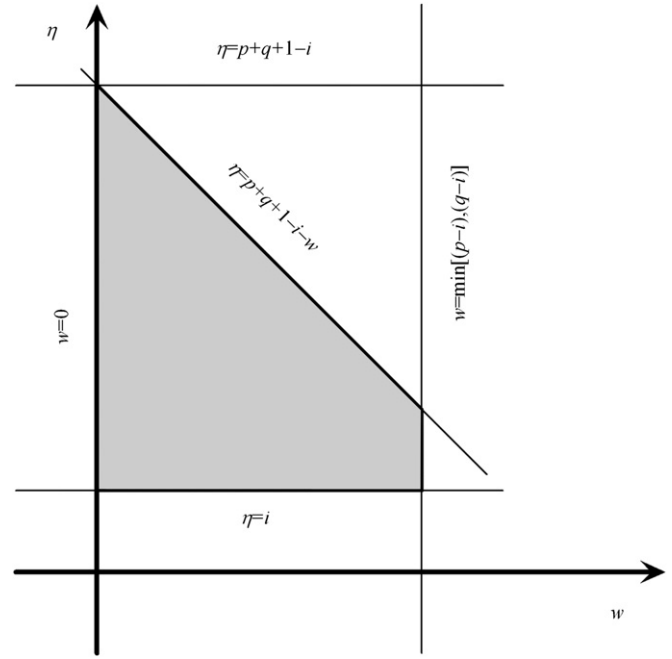


Fig. 8. The geometry of the summational transformation: $\sum_{w=0}^{\min[(p-i),(q-i)]} \sum_{\eta=i}^{(p+q+1-i-w)} = \sum_{\eta=i}^{(p+q+1-i)} \sum_{w=0}^{\min[(p-i),(q-i),(p+q+1-i-\eta)]}$.

$$\begin{aligned}
& \times \frac{(2(p+q+2-i)-2w)!}{(p+q+2-i-w)!} \frac{4^{(\eta+i)}}{4^{(p+q+1-w)}} \\
& \times [M_1(p+q+1-i-\eta-w)\delta_{k,\ell} - M_2(\eta-i)\delta_{k,(\ell-1)}], \quad (95)
\end{aligned}$$

and one need only let $\eta \rightarrow r$ to obtain the coefficient of $(g^2)^r$, i.e.:

$$\begin{aligned}
& \left(\frac{ST}{st} \right)^{5/2} \pi^{-3/2} [H_1(0) - H_1(\chi)] \\
& = \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} [s^p t^q] \exp(-g^2) \sum_{\ell=1}^{(\min[p,q]+1)} [1 - \cos^\ell(\chi)] \\
& \times \sum_{r=\ell}^{(p+q+2-\ell)} (g^2)^r \sum_{i=(\ell-1)}^{\min[p,q,r,(p+q+1-r)]} \sum_{k=(\ell-1)}^{\min[\ell,i]} \\
& \times \sum_{w=0}^{\min[(p-i),(q-i),(p+q+1-i-r)]} 2^i M_1^i M_2^i M_2^{(p+q-2i-w)} \\
& \times F^{(i-k)} \left(\frac{(p+q-2i-w)}{(p-i)} \right) \left(\frac{(p-i)}{w} \right) \left(\frac{i}{k} \right) \frac{G^w}{(i)!} \\
& \times \frac{(-1)^{(r-i)}}{(r-i)!(p+q+1-i-r-w)!} \frac{(r+1)!}{(2r+2)!} \\
& \times \frac{(2(p+q+2-i)-2w)!}{(p+q+2-i-w)!} \frac{4^{(r+i)}}{4^{(p+q+1-w)}} \\
& \times [M_1(p+q+1-i-r-w)\delta_{k,\ell} - M_2(r-i)\delta_{k,(\ell-1)}], \quad (96)
\end{aligned}$$

where, as before, $r=(\ell-1)$ implies that $i=k=r$ such that the coefficient is identically zero allowing the lowest term of the r summation to be omitted.

Now, after integration of the coefficient of $[s^p t^q]$ over ε and the directions of g , one has:

$$\left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_1^2) \mathcal{C}_1 \right]_{12} = 8 \sum_{\ell=1}^{(\min[p,q]+1)} \sum_{r=\ell}^{(p+q+2-\ell)} A'_{pqr\ell} \mathcal{Q}_{12}^{(\ell)}(r), \quad (97)$$

where:

$$\begin{aligned}
 A'_{pqre} = & \sum_{i=(\ell-1)}^{\min[p,q,r,(p+q+1-r)]} \sum_{k=(\ell-1)}^{\min[\ell,i]} \\
 & \times \sum_{w=0}^{(\min[p,q,(p+q+1-r)]-i)} \frac{8^i(p+q-2i-w)!}{(p-i-w)!(q-i-w)!} \\
 & \times \frac{(-1)^{(r+i)}}{(r-i)!(p+q+1-i-r-w)!(2r+2)!} \\
 & \times \frac{(2(p+q+2-i)-2w)!}{(p+q+2-i-w)!} \frac{2^{2r}}{4^{(p+q+1)}} \frac{F(i-k)}{(k)!(i-k)!} \\
 & \times \frac{G^w}{(w)!} 2^{(2w-1)} M_1^i M_2^i M_2^{(p+q-2i-w)} \\
 & \times 2[M_1(p+q+1-i-r-w)\delta_{k,\ell} \\
 & - M_2(r-i)\delta_{k,(\ell-1)}]. \quad (98)
 \end{aligned}$$

Now, one may introduce Pochhammer's notation [22,23] which is defined as:

$$(z)_n \equiv \frac{\Gamma(z+n)}{\Gamma(z)} = \frac{(z+n-1)!}{(z-1)!}, \quad (99)$$

such that:

$$(z)! = \frac{(z+n)!}{(z+1)_n}. \quad (100)$$

Using this notation, one may write:

$$(z-w)! = \frac{(z)!}{(z-w+1)_w}, \quad (101)$$

and:

$$(2z-2w)! = \frac{(2z)!}{(2z-2w+1)_w(2z-w+1)_w}, \quad (102)$$

such that:

$$\begin{aligned}
 A'_{pqre} = & \sum_{i=(\ell-1)}^{\min[p,q,r,(p+q+1-r)]} \sum_{k=(\ell-1)}^{\min[\ell,i]} \\
 & \times \frac{8^i(p+q-2i)!}{(p-i)!(q-i)!(r-i)!(p+q+1-i-r)!} \\
 & \times \frac{(r+1)!}{(2r+2)!} \frac{(2(p+q+2-i))!}{(p+q+2-i)!} \frac{2^{2r}}{4^{(p+q+1)}} \\
 & \times \sum_{w=0}^{(\min[p,q,(p+q+1-r)]-i)} \frac{F(i-k)}{(k)!(i-k)!} \frac{G^w}{(w)!} \\
 & \times \frac{(p+q+2-i-r-w)_w}{(2(p+q+2-i)-2w+1)_w} (p+1-i-w)_w \\
 & \times \frac{(p+q+3-i-w)_w}{(2(p+q+2-i)-w+1)_w} (q+1-i-w)_w \\
 & \times 2^{(2w-1)} \frac{M_1^i M_2^i M_2^{(p+q-2i-w)}}{(p+q+1-2i-w)_w} \\
 & \times [2M_1(p+q+1-i-r-w)\delta_{k,\ell} \\
 & - 2M_2(r-i)\delta_{k,(\ell-1)}]. \quad (103)
 \end{aligned}$$

Here, except for a factor of $(-1)^k$ and the mass- and w -dependencies in the last term, the terms preceding the summation over w are the same as those obtained for A_{pqre} in Eq. (69) and the entire mass dependence of A'_{pqre} has been collected inside the summation over w .

Now one may consider some additional simplification of A_{pqre} and A'_{pqre} . In both cases the summations over k contain, at most, two terms corresponding to $k=\ell-1$ and $k=\ell$. In Eq. (69), upon expanding the k summation, one has that:

$$\begin{aligned}
 & \sum_{k=(\ell-1)}^{\min[\ell,i]} \frac{(-1)^k}{(k)!(i-k)!} \{ (p+q+1-i-r)\delta_{k,\ell} + (r-i)\delta_{k,(\ell-1)} \} \\
 & = \frac{(-1)^{(\ell-1)}}{(\ell-1)!(i-(\ell-1))!} \\
 & \times \{ (p+q+1-i-r)\delta_{(\ell-1),\ell} + (r-i)\delta_{(\ell-1),(\ell-1)} \} \\
 & + \frac{(-1)^\ell}{(\ell)!(\ell-1)!} (1-\delta_{i,(\ell-1)}) \\
 & \times \{ (p+q+1-i-r)\delta_{\ell,\ell} + (r-i)\delta_{\ell,(\ell-1)} \} \\
 & = \frac{(-1)^\ell}{(\ell)!(i+1-\ell)!} \\
 & \times \{ (i+1-\ell)(p+q+1-i-r) - \ell(r-i) \}, \quad (104)
 \end{aligned}$$

such that:

$$\begin{aligned}
 A_{pqre} = & \sum_{i=(\ell-1)}^{\min[p,q,r,(p+q+1-r)]} \frac{8^i(p+q-2i)!}{(p-i)!(q-i)!} \\
 & \times \frac{(-1)^\ell}{(\ell)!(i+1-\ell)!} \frac{(-1)^{(r+i)}}{(r-i)!(p+q+1-i-r)!} \\
 & \times \frac{(r+1)!}{(2r+2)!} \frac{(2(p+q+2-i))!}{(p+q+2-i)!} \frac{2^{2r}}{4^{(p+q+1)}} \{ (i+1-\ell) \\
 & \times (p+q+1-i-r) - \ell(r-i) \}. \quad (105)
 \end{aligned}$$

Here, as an aside, note that the mass dependencies of the H_{12} bracket integrals may be incorporated into the associated A_{pqre} coefficient such that the H_{12} bracket integrals may be expressed in a form consistent with that used for the H_1 bracket integrals. Historically, in Chapman and Cowling, these dependencies were removed so that an emphasis could be placed on the fact that A_{pqre} is a pure number devoid of mass dependencies. Since this apparently cannot similarly be done for the A'_{pqre} coefficients, there seems little point in persisting with the original formulation of A_{pqre} . Thus, one may write:

$$[S_{3/2}^{(p)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_2^2)\mathcal{C}_2]_{12} = 8 \sum_{\ell=1}^{(\min[p,q]+1)} \sum_{r=\ell}^{(p+q+2-\ell)} A''_{pqre} Q_{12}^{(\ell)}(r), \quad (106)$$

in which one now has that:

$$\begin{aligned}
 A''_{pqre} = & M_2^{(p+1/2)} M_1^{(q+1/2)} \\
 & \times \sum_{i=(\ell-1)}^{\min[p,q,r,(p+q+1-r)]} \frac{8^i(p+q-2i)!}{(p-i)!(q-i)!} \\
 & \times \frac{(-1)^\ell}{(\ell)!(i+1-\ell)!} \frac{(-1)^{(r+i)}}{(r-i)!(p+q+1-i-r)!} \\
 & \times \frac{(r+1)!}{(2r+2)!} \frac{(2(p+q+2-i))!}{(p+q+2-i)!} \frac{2^{2r}}{4^{(p+q+1)}} \\
 & \times \{ (i+1-\ell)(p+q+1-i-r) - \ell(r-i) \}. \quad (107)
 \end{aligned}$$

In Eq. (103), upon expanding the k summation, one has that:

$$\begin{aligned}
 & \sum_{k=(\ell-1)}^{\min[\ell,i]} \frac{F(i-k)}{(k)!(i-k)!} \\
 & \times 2[M_1(p+q+1-i-r-w)\delta_{k,\ell} - M_2(r-i)\delta_{k,(\ell-1)}]
 \end{aligned}$$

$$\begin{aligned}
&= \frac{F^{(i-(\ell-1))}}{(\ell-1)!(i-(\ell-1))!} \\
&\quad \times \left[2M_1(p+q+1-i-r-w)\delta_{(\ell-1),\ell} - 2M_2(r-i)\delta_{(\ell-1),(\ell-1)} \right] \\
&\quad + \frac{F^{(i-\ell)}}{(\ell)!(i-\ell)!} (1 - \delta_{i,(\ell-1)}) \\
&\quad \times \left[2M_1(p+q+1-i-r-w)\delta_{\ell,\ell} - 2M_2(r-i)\delta_{\ell,(\ell-1)} \right] \\
&= \frac{F^{(i+1-\ell)}}{(\ell)!(i+1-\ell)!} \left[2M_1 F^{-1}(i+1-\ell)(p+q+1-i-r-w) \right. \\
&\quad \left. - 2M_2 \ell(r-i) \right], \tag{108}
\end{aligned}$$

such that:

$$\begin{aligned}
A'_{pq\ell} &= \sum_{i=(\ell-1)}^{\min[p,q,r,(p+q+1-r)]} \frac{8^i(p+q-2i)!}{(p-i)!(q-i)!} \\
&\quad \times \frac{1}{(\ell)!(i+1-\ell)!} \frac{(-1)^{(r+i)}}{(r-i)!(p+q+1-i-r)!} \\
&\quad \times \frac{(r+1)!}{(2r+2)!} \frac{(2(p+q+2-i))!}{(p+q+2-i)!} \frac{2^{2r}}{4^{(p+q+1)}} \\
&\quad \times \sum_{w=0}^{(\min[p,q,(p+q+1-r)]-i)} F^{(i+1-\ell)} \frac{G^w}{(w)!} \\
&\quad \times \frac{(p+q+2-i-r-w)_w}{(2(p+q+2-i)-2w+1)_w} (p+1-i-w)_w \\
&\quad \times \frac{(p+q+3-i-w)_w}{(2(p+q+2-i)-w+1)_w} (q+1-i-w)_w \\
&\quad \times 2^{(2w-1)} \frac{M_1^i M_2^i M_2^{(p+q-2i-w)}}{(p+q+1-2i-w)_w} \\
&\quad \times [2M_1 F^{-1}(i+1-\ell)(p+q+1-i-r-w) \\
&\quad - 2M_2 \ell(r-i)]. \tag{109}
\end{aligned}$$

In this expression, the portion of $A'_{pq\ell}$ that precedes the w summation is mostly identical to the expression for $A_{pq\ell}$ in Eq. (105) except for an absent factor of $(-1)^\ell$ which is present in $A_{pq\ell}$ due to the additional factor of $(-1)^k$ noted previously (and the mass- and w -dependent last term of the summation over w). Here, one can see that the total power of M contained in the combined i and w summations (or total power of $1/2$ in the limit when $M_1 = M_2 = (1/2)$ where $w=0$) is simply $p+q+1$. The quantities F and G make no net contribution to this total power of M although they do adjust the specific powers of M_1 and M_2 that contribute to it such that the mass dependence of each term ends up being a polynomial in various products of $M_1^a M_2^b$ where $a+b=p+q+1$. This is the total power of M that one expects to see out of this derivation and is the same as the total power of M seen in the previous derivation of the H_{12} bracket integrals. Thus, both derivations are consistent with the combinatorial rule for generation of the simple gas bracket integral as described in Chapman and Cowling [1] and in our previous work [19,20]. The extra factor of $(-1)^\ell$ that was generated in $A_{pq\ell}$ during the process of expanding and consolidating the k summation and which is not present in the expression for $A'_{pq\ell}$ is, again, expected in light of the combinatorial rule for the simple gas bracket integral which is discussed next.

6. Derivation of a summational representation for the simple gas bracket integral

Lastly, the simple gas bracket integral is considered. Here, a combinatorial rule is used to generate an appropriate expression for the bracket integral from the H_{12} and H_1 bracket integrals derived above. The appropriate combinatorial rule from Chapman and Cowling is:

$$\begin{aligned}
&\left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_1^2) \mathcal{C}_1 \right]_1 \\
&= \left\{ \left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_2^2) \mathcal{C}_2 \right]_{12} \right. \\
&\quad \left. + \left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_1^2) \mathcal{C}_1 \right]_{12} \right\} \Big|_{\substack{M_1=M_2=1/2 \\ \sigma_1=\sigma_2}} \tag{110}
\end{aligned}$$

From this, it is apparent that the use of Eqs. (97) and (106) yields:

$$\begin{aligned}
\left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_1^2) \mathcal{C}_1 \right]_1 &= 8 \sum_{\ell=1}^{(\min[p,q]+1)} \sum_{r=\ell}^{(p+q+2-\ell)} \Omega_1^{(\ell)}(r) \\
&\quad \times \left\{ A''_{pq\ell} + A'_{pq\ell} \right\} \Big|_{M_1=M_2=1/2}, \tag{111}
\end{aligned}$$

where $\Omega_1^{(\ell)}(r)$ are the simple gas omega integrals which can be obtained directly from the definition of the omega integrals given in Eq. (66). Since $w=0$ in the limit of $M_1=M_2=1/2$, since $(M_1-M_2)^0 \rightarrow 1$, and since $(z)_0 = (z-1)!/(z-1)! = 1$, one has from Eqs. (107) and (109) that:

$$\begin{aligned}
&\left\{ A''_{pq\ell} + A'_{pq\ell} \right\} \Big|_{M_1=M_2=1/2} \\
&= \left(\frac{1}{2} \right)^{(p+q+1)} \sum_{i=(\ell-1)}^{\min[p,q,r,(p+q+1-r)]} \frac{8^i(p+q-2i)!}{(p-i)!(q-i)!} \\
&\quad \times \frac{[1+(-1)^\ell]}{(\ell)!(i+1-\ell)!} \frac{(-1)^{(r+i)}}{(r-i)!(p+q+1-i-r)!} \\
&\quad \times \frac{(r+1)!}{(2r+2)!} \frac{(2(p+q+2-i))!}{(p+q+2-i)!} \frac{2^{2r}}{4^{(p+q+1)}} \\
&\quad \times \{(i+1-\ell)(p+q+1-i-r) - \ell(r-i)\}. \tag{112}
\end{aligned}$$

Thus, for the simple gas bracket integrals overall, one may write:

$$\left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_1^2) \mathcal{C}_1 \right]_1 = 8 \sum_{\ell=2}^{(\min[p,q]+1)} \sum_{r=\ell}^{(p+q+2-\ell)} A'''_{pq\ell} \Omega_1^{(\ell)}(r), \tag{113}$$

where:

$$\begin{aligned}
A'''_{pq\ell} &= \left\{ A''_{pq\ell} + A'_{pq\ell} \right\} \Big|_{M_1=M_2=1/2} \\
&= \left(\frac{1}{2} \right)^{(p+q+1)} \sum_{i=(\ell-1)}^{\min[p,q,r,(p+q+1-r)]} \frac{8^i(p+q-2i)!}{(p-i)!(q-i)!} \\
&\quad \times \frac{[1+(-1)^\ell]}{(\ell)!(i+1-\ell)!} \frac{(-1)^{(r+i)}}{(r-i)!(p+q+1-i-r)!} \\
&\quad \times \frac{(r+1)!}{(2r+2)!} \frac{(2(p+q+2-i))!}{(p+q+2-i)!} \frac{2^{2r}}{4^{(p+q+1)}} \\
&\quad \times \{(i+1-\ell)(p+q+1-i-r) - \ell(r-i)\}. \tag{114}
\end{aligned}$$

Here, as expected, a factor of $[1+(-1)^\ell]$ occurs which results in the elimination of all of the terms associated with odd values of ℓ and generates an additional factor of 2 in all of the terms associated with even values of ℓ . Thus, technically, for the simple gas bracket integrals only, one may also adjust the lower limit of

the ℓ summation from $\ell = 1$ to $\ell = 2$ as we have done above in Eq. (113).

7. Summary of the general bracket integral expressions

Summarizing the results of the above derivations for the convenience of the reader, one has the following general expressions for the diffusion- and thermal conductivity-related bracket integrals. First, the H_{12} bracket integrals are:

$$\left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_2^2) \mathcal{C}_2 \right]_{12} = 8 \sum_{\ell=1}^{(\min[p,q]+1)} \sum_{r=\ell}^{(p+q+2-\ell)} A''_{pqr\ell} \Omega_{12}^{(\ell)}(r), \quad (115)$$

where:

$$\begin{aligned} A''_{pqr\ell} &= M_2^{(p+1/2)} M_1^{(q+1/2)} \\ &\times \sum_{i=(\ell-1)}^{\min[p,q,r,(p+q+1-r)]} \frac{8^i (p+q-2i)!}{(p-i)!(q-i)!} \\ &\times \frac{(-1)^\ell}{(\ell)!(i+1-\ell)!} \frac{(-1)^{(r+i)}}{(r-i)!(p+q+1-i-r)!} \\ &\times \frac{(r+1)! (2(p+q+2-i))!}{(2r+2)! (p+q+2-i)!} \frac{2^{2r}}{4^{(p+q+1)}} \\ &\times \{(i+1-\ell)(p+q+1-i-r) - \ell(r-i)\}. \end{aligned} \quad (116)$$

Second, the H_1 bracket integrals are:

$$\left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_1^2) \mathcal{C}_1 \right]_{12} = 8 \sum_{\ell=1}^{(\min[p,q]+1)} \sum_{r=\ell}^{(p+q+2-\ell)} A'_{pqr\ell} \Omega_{12}^{(\ell)}(r), \quad (117)$$

where:

$$\begin{aligned} A'_{pqr\ell} &= \sum_{i=(\ell-1)}^{\min[p,q,r,(p+q+1-r)]} \frac{8^i (p+q-2i)!}{(p-i)!(q-i)!} \\ &\times \frac{1}{(\ell)!(i+1-\ell)!} \frac{(-1)^{(r+i)}}{(r-i)!(p+q+1-i-r)!} \\ &\times \frac{(r+1)! (2(p+q+2-i))!}{(2r+2)! (p+q+2-i)!} \frac{2^{2r}}{4^{(p+q+1)}} \\ &\times \sum_{w=0}^{(\min[p,q,(p+q+1-r)]-i)} F^{(i+1-\ell)} \frac{G^w}{(w)!} \\ &\times \frac{(p+q+2-i-r-w)_w}{(2(p+q+2-i)-2w+1)_w} (p+1-i-w)_w \\ &\times \frac{(p+q+3-i-w)_w}{(2(p+q+2-i)-w+1)_w} (q+1-i-w)_w \\ &\times 2^{(2w-1)} \frac{M_1^i M_2^i M_2^{(p+q-2i-w)}}{(p+q+1-2i-w)_w} \\ &\times \left[2M_1 F^{-1}(i+1-\ell)(p+q+1-i-r-w) \right. \\ &\left. - 2M_2 \ell(r-i) \right], \end{aligned} \quad (118)$$

and in which $F = (M_1^2 + M_2^2)/2M_1M_2$ and $G = (M_1 - M_2)/M_2$. Third, the simple gas bracket integrals are:

$$\left[S_{3/2}^{(p)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_1^2) \mathcal{C}_1 \right]_1 = 8 \sum_{\ell=2}^{(\min[p,q]+1)} \sum_{r=\ell}^{(p+q+2-\ell)} A'''_{pqr\ell} \Omega_1^{(\ell)}(r), \quad (119)$$

where:

$$\begin{aligned} A'''_{pqr\ell} &= \left(\frac{1}{2} \right)^{(p+q+1)} \sum_{i=(\ell-1)}^{\min[p,q,r,(p+q+1-r)]} \frac{8^i (p+q-2i)!}{(p-i)!(q-i)!} \\ &\times \frac{[1 + (-1)^\ell]}{(\ell)!(i+1-\ell)!} \frac{(-1)^{(r+i)}}{(r-i)!(p+q+1-i-r)!} \\ &\times \frac{(r+1)! (2(p+q+2-i))!}{(2r+2)! (p+q+2-i)!} \frac{2^{2r}}{4^{(p+q+1)}} \\ &\times \{(i+1-\ell)(p+q+1-i-r) - \ell(r-i)\}. \end{aligned} \quad (120)$$

In these results, the omega integrals are defined as:

$$\Omega_{12}^{(\ell)}(r) = \frac{1}{2} \sigma_{12}^2 \left(\frac{2\pi kT}{m_0 M_1 M_2} \right)^{1/2} W_{12}^{(\ell)}(r), \quad (121)$$

where:

$$\begin{aligned} W_{12}^{(\ell)}(r) &= 2 \int_0^\infty \exp(-g^2) g^{(2r+3)} \\ &\times \int_0^\pi [1 - \cos^\ell(\chi)] (b/\sigma_{12}) d(b/\sigma_{12}) d\chi, \end{aligned} \quad (122)$$

with $\sigma_{12} = \frac{1}{2}(\sigma_1 + \sigma_2)$ and $m_0 = m_1 + m_2$, for collisions between unlike molecules, and as:

$$\Omega_1^{(\ell)}(r) = \sigma_1^2 \left(\frac{\pi kT}{m_1} \right)^{1/2} W_1^{(\ell)}(r), \quad (123)$$

for collisions between like molecules where:

$$\begin{aligned} W_1^{(\ell)}(r) &= 2 \int_0^\infty \exp(-g^2) g^{(2r+3)} \\ &\times \int_0^\pi [1 - \cos^\ell(\chi)] (b/\sigma_1) d(b/\sigma_1) d\chi, \end{aligned} \quad (124)$$

$m_1 = m_2$, and $\sigma_1 = \sigma_2$ (the simple gas omega integrals).

8. Explicit expressions for the diffusion and thermal conductivity bracket integrals up to order 5

In most of the computer codes implemented to date that utilize bracket integrals in their calculations, the emphasis has been on the use of explicit bracket integral expressions up to orders 1, 2, or at most, 3. The reason for this is that the complexity of the explicit expressions has made them difficult to derive reliably by hand. This complexity increases so rapidly, in fact, that we have found that it is largely impractical to report explicit bracket integral expressions in the open literature beyond the lowest orders even when they are organized into compact form as we have done in what follows. However, insofar as such explicit expressions can be reasonably reported in the literature, they are valuable from the point of view of having them available for general use in the existing computer codes. Further, having such explicit expressions reported in the literature, even to limited order, has a certain archival value in the field where work continues with a variety of different intermolecular potentials. Thus, in this section, we report a set of completely general and explicit expressions for the bracket integrals necessary to complete the Chapman–Enskog diffusion and thermal

conductivity solutions up to order 5. Additionally, we note some basic relationships that occur between the various bracket integrals that make them more tractable to generate and manipulate in the context of the Chapman–Enskog solutions.

Of the three needed bracket integrals, the H_1 bracket integrals of Eq. (21) have the most complicated dependence upon the molecular masses of the constituent gases. Thus, while having general expressions for these bracket integrals would have proven most useful in terms of deriving general expressions for the remaining two bracket integrals, we actually began above with the derivation

of the H_{12} bracket integrals of Eq. (20) where the mass dependence is rather simple. Thus, in this section on explicit bracket integral expressions we follow the pattern established above and report explicit expressions for the H_{12} bracket integrals first. We then follow these with explicit expressions for the H_1 bracket integrals and the simple gas bracket integrals in that order. Note that the expressions with either $p=0$ or $q=0$ are needed only for the diffusion problems. For the H_{12} bracket integrals up to order 5, one has:

$$\left[S_{3/2}^{(0)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(0)}(\mathcal{C}_2^2) \mathcal{C}_2 \right]_{12} \left(M_1^{1/2} M_2^{1/2} \right)^{-1} = -8\Omega_{12}^{(1)}(1), \quad (125)$$

$$\left[S_{3/2}^{(0)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(1)}(\mathcal{C}_2^2) \mathcal{C}_2 \right]_{12} \left(M_1^{3/2} M_2^{1/2} \right)^{-1} = -20\Omega_{12}^{(1)}(1) + 8\Omega_{12}^{(2)}(2), \quad (126)$$

$$\left[S_{3/2}^{(0)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(2)}(\mathcal{C}_2^2) \mathcal{C}_2 \right]_{12} \left(M_1^{5/2} M_2^{1/2} \right)^{-1} = -35\Omega_{12}^{(1)}(1) + 28\Omega_{12}^{(1)}(2) - 4\Omega_{12}^{(1)}(3), \quad (127)$$

$$\left[S_{3/2}^{(0)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(3)}(\mathcal{C}_2^2) \mathcal{C}_2 \right]_{12} \left(M_1^{7/2} M_2^{1/2} \right)^{-1} = -\frac{105}{2} \Omega_{12}^{(1)}(1) + 63\Omega_{12}^{(1)}(2) - 18\Omega_{12}^{(1)}(3) + \frac{4}{3} \Omega_{12}^{(1)}(4), \quad (128)$$

$$\left[S_{3/2}^{(0)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(4)}(\mathcal{C}_2^2) \mathcal{C}_2 \right]_{12} \left(M_1^{9/2} M_2^{1/2} \right)^{-1} = -\frac{1155}{16} \Omega_{12}^{(1)}(1) + \frac{231}{2} \Omega_{12}^{(1)}(2) - \frac{99}{2} \Omega_{12}^{(1)}(3) + \frac{22}{3} \Omega_{12}^{(1)}(4) - \frac{1}{3} \Omega_{12}^{(1)}(5), \quad (129)$$

$$\left[S_{3/2}^{(0)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(5)}(\mathcal{C}_2^2) \mathcal{C}_2 \right]_{12} \left(M_1^{11/2} M_2^{1/2} \right)^{-1} = -\frac{3003}{32} \Omega_{12}^{(1)}(1) + \frac{3003}{16} \Omega_{12}^{(1)}(2) - \frac{429}{4} \Omega_{12}^{(1)}(3) + \frac{143}{6} \Omega_{12}^{(1)}(4) - \frac{13}{6} \Omega_{12}^{(1)}(5) + \frac{1}{15} \Omega_{12}^{(1)}(6), \quad (130)$$

$$\left[S_{3/2}^{(1)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(1)}(\mathcal{C}_2^2) \mathcal{C}_2 \right]_{12} \left(M_1^{3/2} M_2^{3/2} \right)^{-1} = -110\Omega_{12}^{(1)}(1) + 40\Omega_{12}^{(1)}(2) - 8\Omega_{12}^{(1)}(3) + 16\Omega_{12}^{(2)}(2), \quad (131)$$

$$\left[S_{3/2}^{(1)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(2)}(\mathcal{C}_2^2) \mathcal{C}_2 \right]_{12} \left(M_1^{5/2} M_2^{3/2} \right)^{-1} = -\frac{595}{2} \Omega_{12}^{(1)}(1) + 189\Omega_{12}^{(1)}(2) - 38\Omega_{12}^{(1)}(3) + 4\Omega_{12}^{(1)}(4) + 56\Omega_{12}^{(2)}(2) - 16\Omega_{12}^{(2)}(3), \quad (132)$$

$$\left[S_{3/2}^{(1)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(3)}(\mathcal{C}_2^2) \mathcal{C}_2 \right]_{12} \left(M_1^{7/2} M_2^{3/2} \right)^{-1} = -\frac{2415}{4} \Omega_{12}^{(1)}(1) + 588\Omega_{12}^{(1)}(2) - 162\Omega_{12}^{(1)}(3) + \frac{64}{3} \Omega_{12}^{(1)}(4) - \frac{4}{3} \Omega_{12}^{(1)}(5) + 126\Omega_{12}^{(2)}(2) - 72\Omega_{12}^{(2)}(3) + 8\Omega_{12}^{(2)}(4), \quad (133)$$

$$\left[S_{3/2}^{(1)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(4)}(\mathcal{C}_2^2) \mathcal{C}_2 \right]_{12} \left(M_1^{9/2} M_2^{3/2} \right)^{-1} = -\frac{33495}{32} \Omega_{12}^{(1)}(1) + \frac{22407}{16} \Omega_{12}^{(1)}(2) - \frac{2145}{4} \Omega_{12}^{(1)}(3) + \frac{539}{6} \Omega_{12}^{(1)}(4) - \frac{49}{6} \Omega_{12}^{(1)}(5) + \frac{1}{3} \Omega_{12}^{(1)}(6) + 231\Omega_{12}^{(2)}(2) - 198\Omega_{12}^{(2)}(3) + 44\Omega_{12}^{(2)}(4) - \frac{8}{3} \Omega_{12}^{(2)}(5), \quad (134)$$

$$\left[S_{3/2}^{(1)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(5)}(\mathcal{C}_2^2) \mathcal{C}_2 \right]_{12} \left(M_1^{11/2} M_2^{3/2} \right)^{-1} = -\frac{105105}{64} \Omega_{12}^{(1)}(1) + \frac{45045}{16} \Omega_{12}^{(1)}(2) - \frac{22737}{16} \Omega_{12}^{(1)}(3) + \frac{1859}{6} \Omega_{12}^{(1)}(4) - \frac{143}{4} \Omega_{12}^{(1)}(5) + \frac{7}{3} \Omega_{12}^{(1)}(6) - \frac{1}{15} \Omega_{12}^{(1)}(7) + \frac{3003}{8} \Omega_{12}^{(2)}(2) - 429\Omega_{12}^{(2)}(3) + 143\Omega_{12}^{(2)}(4) - \frac{52}{3} \Omega_{12}^{(2)}(5) + \frac{2}{3} \Omega_{12}^{(2)}(6), \quad (135)$$

$$\left[S_{3/2}^{(2)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(2)}(\mathcal{C}_2^2) \mathcal{C}_2 \right]_{12} \left(M_1^{5/2} M_2^{5/2} \right)^{-1} = -\frac{8505}{8} \Omega_{12}^{(1)}(1) + 833\Omega_{12}^{(1)}(2) - 241\Omega_{12}^{(1)}(3) + 28\Omega_{12}^{(1)}(4) - 2\Omega_{12}^{(1)}(5) + 308\Omega_{12}^{(2)}(2) - 112\Omega_{12}^{(2)}(3) + 16\Omega_{12}^{(2)}(4) - 16\Omega_{12}^{(3)}(3), \quad (136)$$

$$\left[S_{3/2}^{(2)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(3)}(\mathcal{C}_2^2) \mathcal{C}_2 \right]_{12} \left(M_1^{7/2} M_2^{5/2} \right)^{-1} = -\frac{42735}{16} \Omega_{12}^{(1)}(1) + \frac{22071}{8} \Omega_{12}^{(1)}(2) - \frac{2001}{2} \Omega_{12}^{(1)}(3) + \frac{499}{3} \Omega_{12}^{(1)}(4) - \frac{41}{3} \Omega_{12}^{(1)}(5) + \frac{2}{3} \Omega_{12}^{(1)}(6) + 945\Omega_{12}^{(2)}(2) - 522\Omega_{12}^{(2)}(3) + 100\Omega_{12}^{(2)}(4) - 8\Omega_{12}^{(2)}(5) - 72\Omega_{12}^{(3)}(3) + 16\Omega_{12}^{(3)}(4), \quad (137)$$

$$\begin{aligned}
\left[S_{3/2}^{(2)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(4)}(\mathcal{C}_2^2)\mathcal{C}_2\right]_{12} \left(M_1^{9/2}M_2^{5/2}\right)^{-1} = & -\frac{705705}{128}Q_{12}^{(1)}(1) + \frac{234927}{32}Q_{12}^{(1)}(2) - \frac{104973}{32}Q_{12}^{(1)}(3) + \frac{8437}{12}Q_{12}^{(1)}(4) - \frac{623}{8}Q_{12}^{(1)}(5) \\
& + \frac{29}{6}Q_{12}^{(1)}(6) - \frac{1}{6}Q_{12}^{(1)}(7) + \frac{4389}{2}Q_{12}^{(2)}(2) - 1716Q_{12}^{(2)}(3) + 440Q_{12}^{(2)}(4) - \frac{160}{3}Q_{12}^{(2)}(5) \\
& + \frac{8}{3}Q_{12}^{(2)}(6) - 198Q_{12}^{(3)}(3) + 88Q_{12}^{(3)}(4) - 8Q_{12}^{(3)}(5),
\end{aligned} \quad (138)$$

$$\begin{aligned}
\left[S_{3/2}^{(2)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(5)}(\mathcal{C}_2^2)\mathcal{C}_2\right]_{12} \left(M_1^{11/2}M_2^{5/2}\right)^{-1} = & -\frac{2567565}{256}Q_{12}^{(1)}(1) + \frac{2129127}{128}Q_{12}^{(1)}(2) - \frac{579579}{64}Q_{12}^{(1)}(3) + \frac{75933}{32}Q_{12}^{(1)}(4) \\
& - \frac{16237}{48}Q_{12}^{(1)}(5) + \frac{655}{24}Q_{12}^{(1)}(6) - \frac{79}{60}Q_{12}^{(1)}(7) + \frac{1}{30}Q_{12}^{(1)}(8) + \frac{69069}{16}Q_{12}^{(2)}(2) - \frac{35607}{8}Q_{12}^{(2)}(3) \\
& + \frac{3003}{2}Q_{12}^{(2)}(4) - \frac{715}{3}Q_{12}^{(2)}(5) + \frac{59}{3}Q_{12}^{(2)}(6) - \frac{2}{3}Q_{12}^{(2)}(7) \\
& - 429Q_{12}^{(3)}(3) + 286Q_{12}^{(3)}(4) - 52Q_{12}^{(3)}(5) + \frac{8}{3}Q_{12}^{(3)}(6),
\end{aligned} \quad (139)$$

$$\begin{aligned}
\left[S_{3/2}^{(3)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(3)}(\mathcal{C}_2^2)\mathcal{C}_2\right]_{12} \left(M_1^{7/2}M_2^{7/2}\right)^{-1} = & -\frac{255255}{32}Q_{12}^{(1)}(1) + \frac{76923}{8}Q_{12}^{(1)}(2) - \frac{34119}{8}Q_{12}^{(1)}(3) + 895Q_{12}^{(1)}(4) - \frac{201}{2}Q_{12}^{(1)}(5) \\
& + 6Q_{12}^{(1)}(6) - \frac{2}{9}Q_{12}^{(1)}(7) + \frac{14553}{4}Q_{12}^{(2)}(2) - 2430Q_{12}^{(2)}(3) + 626Q_{12}^{(2)}(4) - 72Q_{12}^{(2)}(5) \\
& + 4Q_{12}^{(2)}(6) - 444Q_{12}^{(3)}(3) + 144Q_{12}^{(3)}(4) - 16Q_{12}^{(3)}(5) + \frac{32}{3}Q_{12}^{(4)}(4),
\end{aligned} \quad (140)$$

$$\begin{aligned}
\left[S_{3/2}^{(3)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(4)}(\mathcal{C}_2^2)\mathcal{C}_2\right]_{12} \left(M_1^{9/2}M_2^{7/2}\right)^{-1} = & -\frac{4879875}{256}Q_{12}^{(1)}(1) + \frac{3516513}{128}Q_{12}^{(1)}(2) - \frac{919413}{64}Q_{12}^{(1)}(3) + \frac{118107}{32}Q_{12}^{(1)}(4) \\
& - \frac{8353}{16}Q_{12}^{(1)}(5) + \frac{339}{8}Q_{12}^{(1)}(6) - \frac{71}{36}Q_{12}^{(1)}(7) + \frac{1}{18}Q_{12}^{(1)}(8) + \frac{81081}{8}Q_{12}^{(2)}(2) - \frac{34155}{4}Q_{12}^{(2)}(3) \\
& + 2717Q_{12}^{(2)}(4) - 422Q_{12}^{(2)}(5) + 34Q_{12}^{(2)}(6) - \frac{4}{3}Q_{12}^{(2)}(7) - 1551Q_{12}^{(3)}(3) + \frac{2222}{3}Q_{12}^{(3)}(4) \\
& - 124Q_{12}^{(3)}(5) + 8Q_{12}^{(3)}(6) + \frac{176}{3}Q_{12}^{(4)}(4) - \frac{32}{3}Q_{12}^{(4)}(5),
\end{aligned} \quad (141)$$

$$\begin{aligned}
\left[S_{3/2}^{(3)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(5)}(\mathcal{C}_2^2)\mathcal{C}_2\right]_{12} \left(M_1^{11/2}M_2^{7/2}\right)^{-1} = & -\frac{20165145}{512}Q_{12}^{(1)}(1) + \frac{4327323}{64}Q_{12}^{(1)}(2) - \frac{329043}{8}Q_{12}^{(1)}(3) + \frac{200057}{16}Q_{12}^{(1)}(4) \\
& - \frac{34333}{16}Q_{12}^{(1)}(5) + \frac{881}{4}Q_{12}^{(1)}(6) - \frac{613}{45}Q_{12}^{(1)}(7) + \frac{23}{45}Q_{12}^{(1)}(8) - \frac{1}{90}Q_{12}^{(1)}(9) + \frac{1486485}{64}Q_{12}^{(2)}(2) \\
& - \frac{389961}{16}Q_{12}^{(2)}(3) + \frac{150293}{16}Q_{12}^{(2)}(4) - \frac{3653}{2}Q_{12}^{(2)}(5) + \frac{779}{4}Q_{12}^{(2)}(6) - \frac{35}{3}Q_{12}^{(2)}(7) + \frac{1}{3}Q_{12}^{(2)}(8) \\
& - \frac{8151}{2}Q_{12}^{(3)}(3) + \frac{8008}{3}Q_{12}^{(3)}(4) - \frac{1820}{3}Q_{12}^{(3)}(5) + 64Q_{12}^{(3)}(6) - \frac{8}{3}Q_{12}^{(3)}(7) + \frac{572}{3}Q_{12}^{(4)}(4) \\
& - \frac{208}{3}Q_{12}^{(4)}(5) + \frac{16}{3}Q_{12}^{(4)}(6),
\end{aligned} \quad (142)$$

$$\begin{aligned}
\left[S_{3/2}^{(4)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(4)}(\mathcal{C}_2^2)\mathcal{C}_2\right]_{12} \left(M_1^{9/2}M_2^{9/2}\right)^{-1} = & -\frac{105930825}{2048}Q_{12}^{(1)}(1) + \frac{10735725}{128}Q_{12}^{(1)}(2) - \frac{6435429}{128}Q_{12}^{(1)}(3) + \frac{483637}{32}Q_{12}^{(1)}(4) \\
& - \frac{165827}{64}Q_{12}^{(1)}(5) + \frac{2123}{8}Q_{12}^{(1)}(6) - \frac{1189}{72}Q_{12}^{(1)}(7) + \frac{11}{18}Q_{12}^{(1)}(8) - \frac{1}{72}Q_{12}^{(1)}(9) \\
& + \frac{525525}{16}Q_{12}^{(2)}(2) - \frac{127413}{4}Q_{12}^{(2)}(3) + \frac{48323}{4}Q_{12}^{(2)}(4) - 2310Q_{12}^{(2)}(5) + 247Q_{12}^{(2)}(6) \\
& - \frac{44}{3}Q_{12}^{(2)}(7) + \frac{4}{9}Q_{12}^{(2)}(8) - \frac{26169}{4}Q_{12}^{(3)}(3) + \frac{11374}{3}Q_{12}^{(3)}(4) - \frac{2566}{3}Q_{12}^{(3)}(5) + 88Q_{12}^{(3)}(6) \\
& - 4Q_{12}^{(3)}(7) + \frac{1232}{3}Q_{12}^{(4)}(4) - \frac{352}{3}Q_{12}^{(4)}(5) + \frac{32}{3}Q_{12}^{(4)}(6) - \frac{16}{3}Q_{12}^{(5)}(5),
\end{aligned} \quad (143)$$

$$\begin{aligned}
\left[S_{3/2}^{(4)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(5)}(\mathcal{C}_2^2)\mathcal{C}_2\right]_{12} \left(M_1^{11/2}M_2^{9/2}\right)^{-1} = & -\frac{489834345}{4096}Q_{12}^{(1)}(1) + \frac{452873421}{2048}Q_{12}^{(1)}(2) - \frac{38424243}{256}Q_{12}^{(1)}(3) + \frac{6633055}{128}Q_{12}^{(1)}(4) \\
& -\frac{1330927}{128}Q_{12}^{(1)}(5) + \frac{82491}{64}Q_{12}^{(1)}(6) - \frac{72643}{720}Q_{12}^{(1)}(7) + \frac{199}{40}Q_{12}^{(1)}(8) - \frac{109}{720}Q_{12}^{(1)}(9) \\
& + \frac{1}{360}Q_{12}^{(1)}(10) + \frac{10975965}{128}Q_{12}^{(2)}(2) - \frac{6239805}{64}Q_{12}^{(2)}(3) + \frac{1378663}{32}Q_{12}^{(2)}(4) \\
& -\frac{157651}{16}Q_{12}^{(2)}(5) + \frac{10391}{8}Q_{12}^{(2)}(6) - \frac{1229}{12}Q_{12}^{(2)}(7) + \frac{85}{18}Q_{12}^{(2)}(8) - \frac{1}{9}Q_{12}^{(2)}(9) \\
& -\frac{160875}{8}Q_{12}^{(3)}(3) + \frac{173173}{12}Q_{12}^{(3)}(4) - \frac{12103}{3}Q_{12}^{(3)}(5) + 562Q_{12}^{(3)}(6) - \frac{122}{3}Q_{12}^{(3)}(7) \\
& + \frac{4}{3}Q_{12}^{(3)}(8) + \frac{4862}{3}Q_{12}^{(4)}(4) - 676Q_{12}^{(4)}(5) + \frac{296}{3}Q_{12}^{(4)}(6) - \frac{16}{3}Q_{12}^{(4)}(7) - \frac{104}{3}Q_{12}^{(5)}(5) \\
& + \frac{16}{3}Q_{12}^{(5)}(6), \tag{144}
\end{aligned}$$

$$\begin{aligned}
\left[S_{3/2}^{(5)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(5)}(\mathcal{C}_2^2)\mathcal{C}_2\right]_{12} \left(M_1^{11/2}M_2^{11/2}\right)^{-1} = & -\frac{2505429927}{8192}Q_{12}^{(1)}(1) + \frac{1273569297}{2048}Q_{12}^{(1)}(2) - \frac{958832589}{2048}Q_{12}^{(1)}(3) \\
& + \frac{23205897}{128}Q_{12}^{(1)}(4) - \frac{10626655}{256}Q_{12}^{(1)}(5) + \frac{1923623}{320}Q_{12}^{(1)}(6) - \frac{181901}{320}Q_{12}^{(1)}(7) \\
& + \frac{12701}{360}Q_{12}^{(1)}(8) - \frac{2047}{1440}Q_{12}^{(1)}(9) + \frac{13}{360}Q_{12}^{(1)}(10) - \frac{1}{1800}Q_{12}^{(1)}(11) + \frac{257041785}{1024}Q_{12}^{(2)}(2) \\
& -\frac{20383935}{64}Q_{12}^{(2)}(3) + \frac{10212345}{64}Q_{12}^{(2)}(4) - \frac{673803}{16}Q_{12}^{(2)}(5) + \frac{210763}{32}Q_{12}^{(2)}(6) \\
& -\frac{2561}{4}Q_{12}^{(2)}(7) + \frac{1409}{36}Q_{12}^{(2)}(8) - \frac{13}{9}Q_{12}^{(2)}(9) + \frac{1}{36}Q_{12}^{(2)}(10) - \frac{1130415}{16}Q_{12}^{(3)}(3) \\
& + \frac{232375}{4}Q_{12}^{(3)}(4) - \frac{230789}{12}Q_{12}^{(3)}(5) + 3302Q_{12}^{(3)}(6) - 321Q_{12}^{(3)}(7) + \frac{52}{3}Q_{12}^{(3)}(8) \\
& -\frac{4}{9}Q_{12}^{(3)}(9) + \frac{15015}{2}Q_{12}^{(4)}(4) - \frac{11492}{3}Q_{12}^{(4)}(5) + \frac{2284}{3}Q_{12}^{(4)}(6) - \frac{208}{3}Q_{12}^{(4)}(7) + \frac{8}{3}Q_{12}^{(4)}(8) \\
& -\frac{4108}{15}Q_{12}^{(5)}(5) + \frac{208}{3}Q_{12}^{(5)}(6) - \frac{16}{3}Q_{12}^{(5)}(7) + \frac{32}{15}Q_{12}^{(6)}(6). \tag{145}
\end{aligned}$$

Next, we consider the H_1 bracket integrals of Eq. (21). For each (p, q) , these may be used to generate the corresponding H_{12} expression in Eqs. (125)–(145) above. In general, the expressions for the H_1 bracket integrals consist of a series of terms each of which is associated with a specific omega integral. Each of these omega integral terms also contains a sign, a constant factor, and some function of M_1 and M_2 . The conversion process from the H_1 expressions to the H_{12} expressions is quite straightforward as the magnitude of the numerical coefficients associated with each omega integral term are the same from the H_1 expressions to the H_{12} expressions. The differences are in the distributions of the constituent masses and the signs of the terms. Since the same omega integrals must occur in both the H_1 expressions and the H_{12} expressions, the total number of omega integral terms must be the same in each and there is, in effect, a one-to-one correspondence between terms. The sign difference between corresponding terms is dependent only upon ℓ and the appropriate sign transformation is to multiply each term in the H_1 expressions that follow by a factor of $(-1)^\ell$. The distribution of constituent masses is much simpler in the H_{12} expressions than in the H_1 expressions. In the H_{12} expressions, the distribution of the constituent masses is exactly the same in every omega integral term for a given (p, q) and amounts to nothing more than a common factor of $(M_1^{q+1/2}M_2^{p+1/2})$ in each expression. Thus, overall, the appropriate transformation from the H_1 expressions that follow to the H_{12} expressions in Eqs. (125)–(145) above is to first set $M_1 = M_2 = 1$ in each term in the H_1 expressions, second to multiply each expression

with the appropriate common factor of $(M_1^{q+1/2}M_2^{p+1/2})$, and third to multiply each term by a factor of $(-1)^\ell$. When the above prescription is followed, the expressions below yield the corresponding H_{12} bracket integrals reported in Eqs. (125)–(145). The explicit expressions for the H_1 bracket integrals up to order 5 are:

$$\left[S_{3/2}^{(0)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(0)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_{12} = 8M_2Q_{12}^{(1)}(1), \tag{146}$$

$$\left[S_{3/2}^{(0)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(1)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_{12} = 20M_2^2Q_{12}^{(1)}(1) - 8M_2^2Q_{12}^{(1)}(2), \tag{147}$$

$$\begin{aligned} \left[S_{3/2}^{(0)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(2)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_{12} = & 35M_2^3Q_{12}^{(1)}(1) - 28M_2^3Q_{12}^{(1)}(2) \\ & + 4M_2^3Q_{12}^{(1)}(3), \end{aligned} \tag{148}$$

$$\begin{aligned} \left[S_{3/2}^{(0)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(3)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_{12} = & \frac{105}{2}M_2^4Q_{12}^{(1)}(1) - 63M_2^4Q_{12}^{(1)}(2) \\ & + 18M_2^4Q_{12}^{(1)}(3) - \frac{4}{3}M_2^4Q_{12}^{(1)}(4), \end{aligned} \tag{149}$$

$$\begin{aligned} \left[S_{3/2}^{(0)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(4)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_{12} = & \frac{1155}{16}M_2^5Q_{12}^{(1)}(1) - \frac{231}{2}M_2^5Q_{12}^{(1)}(2) \\ & + \frac{99}{2}M_2^5Q_{12}^{(1)}(3) - \frac{22}{3}M_2^5Q_{12}^{(1)}(4) \\ & + \frac{1}{3}M_2^5Q_{12}^{(1)}(5), \end{aligned} \tag{150}$$

$$\left[S_{3/2}^{(0)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(5)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_{12} = \frac{3003}{32}M_2^6\mathcal{Q}_{12}^{(1)}(1) - \frac{3003}{16}M_2^6\mathcal{Q}_{12}^{(1)}(2) + \frac{429}{4}M_2^6\mathcal{Q}_{12}^{(1)}(3) - \frac{143}{6}M_2^6\mathcal{Q}_{12}^{(1)}(4) + \frac{13}{6}M_2^6\mathcal{Q}_{12}^{(1)}(5) - \frac{1}{15}M_2^6\mathcal{Q}_{12}^{(1)}(6), \quad (151)$$

$$\left[S_{3/2}^{(1)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(1)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_{12} = 110\left(\frac{6}{11}M_1^2M_2 + \frac{5}{11}M_2^3\right)\mathcal{Q}_{12}^{(1)}(1) - 40M_2^3\mathcal{Q}_{12}^{(1)}(2) + 8M_2^3\mathcal{Q}_{12}^{(1)}(3) + 16M_1M_2^2\mathcal{Q}_{12}^{(2)}(2), \quad (152)$$

$$\begin{aligned} \left[S_{3/2}^{(1)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(2)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_{12} = & \frac{595}{2}\left(\frac{12}{17}M_1^2M_2^2 + \frac{5}{17}M_2^4\right)\mathcal{Q}_{12}^{(1)}(1) - 189\left(\frac{4}{9}M_1^2M_2^2 + \frac{5}{9}M_2^4\right)\mathcal{Q}_{12}^{(1)}(2) + 38M_2^4\mathcal{Q}_{12}^{(1)}(3) - 4M_2^4\mathcal{Q}_{12}^{(1)}(4) \\ & + 56M_1M_2^3\mathcal{Q}_{12}^{(2)}(2) - 16M_1M_2^3\mathcal{Q}_{12}^{(2)}(3), \end{aligned} \quad (153)$$

$$\begin{aligned} \left[S_{3/2}^{(1)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(3)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_{12} = & \frac{2415}{4}\left(\frac{18}{23}M_1^2M_2^3 + \frac{5}{23}M_2^5\right)\mathcal{Q}_{12}^{(1)}(1) - 588\left(\frac{9}{14}M_1^2M_2^3 + \frac{5}{14}M_2^5\right)\mathcal{Q}_{12}^{(1)}(2) + 162\left(\frac{1}{3}M_1^2M_2^3 + \frac{2}{3}M_2^5\right)\mathcal{Q}_{12}^{(1)}(3) \\ & - \frac{64}{3}M_2^5\mathcal{Q}_{12}^{(1)}(4) + \frac{4}{3}M_2^5\mathcal{Q}_{12}^{(1)}(5) + 126M_1M_2^4\mathcal{Q}_{12}^{(2)}(2) - 72M_1M_2^4\mathcal{Q}_{12}^{(2)}(3) + 8M_1M_2^4\mathcal{Q}_{12}^{(2)}(4), \end{aligned} \quad (154)$$

$$\begin{aligned} \left[S_{3/2}^{(1)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(4)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_{12} = & \frac{33495}{32}\left(\frac{24}{29}M_1^2M_2^4 + \frac{5}{29}M_2^6\right)\mathcal{Q}_{12}^{(1)}(1) - \frac{22407}{16}\left(\frac{72}{97}M_1^2M_2^4 + \frac{25}{97}M_2^6\right)\mathcal{Q}_{12}^{(1)}(2) + \frac{2145}{4}\left(\frac{36}{65}M_1^2M_2^4\right. \\ & + \frac{29}{65}M_2^6\left.)\mathcal{Q}_{12}^{(1)}(3) - \frac{539}{6}\left(\frac{12}{49}M_1^2M_2^4 + \frac{37}{49}M_2^6\right)\mathcal{Q}_{12}^{(1)}(4) + \frac{49}{6}M_2^6\mathcal{Q}_{12}^{(1)}(5) - \frac{1}{3}M_2^6\mathcal{Q}_{12}^{(1)}(6) + 231M_1M_2^5\mathcal{Q}_{12}^{(2)}(2) \right. \\ & \left. - 198M_1M_2^5\mathcal{Q}_{12}^{(2)}(3) + 44M_1M_2^5\mathcal{Q}_{12}^{(2)}(4) - \frac{8}{3}M_1M_2^5\mathcal{Q}_{12}^{(2)}(5), \end{aligned} \quad (155)$$

$$\begin{aligned} \left[S_{3/2}^{(1)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(5)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_{12} = & \frac{105105}{64}\left(\frac{6}{7}M_1^2M_2^5 + \frac{1}{7}M_2^7\right)\mathcal{Q}_{12}^{(1)}(1) - \frac{45045}{16}\left(\frac{4}{5}M_1^2M_2^5 + \frac{1}{5}M_2^7\right)\mathcal{Q}_{12}^{(1)}(2) \\ & + \frac{22737}{16}\left(\frac{36}{53}M_1^2M_2^5 + \frac{17}{53}M_2^7\right)\mathcal{Q}_{12}^{(1)}(3) - \frac{1859}{6}\left(\frac{6}{13}M_1^2M_2^5 + \frac{7}{13}M_2^7\right)\mathcal{Q}_{12}^{(1)}(4) \\ & + \frac{143}{4}\left(\frac{2}{11}M_1^2M_2^5 + \frac{9}{11}M_2^7\right)\mathcal{Q}_{12}^{(1)}(5) - \frac{7}{3}M_2^7\mathcal{Q}_{12}^{(1)}(6) + \frac{1}{15}M_2^7\mathcal{Q}_{12}^{(1)}(7) + \frac{3003}{8}M_1M_2^6\mathcal{Q}_{12}^{(2)}(2) \\ & - 429M_1M_2^6\mathcal{Q}_{12}^{(2)}(3) + 143M_1M_2^6\mathcal{Q}_{12}^{(2)}(4) - \frac{52}{3}M_1M_2^6\mathcal{Q}_{12}^{(2)}(5) + \frac{2}{3}M_1M_2^6\mathcal{Q}_{12}^{(2)}(6), \end{aligned} \quad (156)$$

$$\begin{aligned} \left[S_{3/2}^{(2)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(2)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_{12} = & \frac{8505}{8}\left(\frac{40}{243}M_1^4M_2 + \frac{168}{243}M_1^2M_2^3 + \frac{35}{243}M_2^5\right)\mathcal{Q}_{12}^{(1)}(1) - 833\left(\frac{12}{17}M_1^2M_2^3 + \frac{5}{17}M_2^5\right)\mathcal{Q}_{12}^{(1)}(2) \\ & + 241\left(\frac{108}{241}M_1^2M_2^3 + \frac{133}{241}M_2^5\right)\mathcal{Q}_{12}^{(1)}(3) - 28M_2^5\mathcal{Q}_{12}^{(1)}(4) + 2M_2^5\mathcal{Q}_{12}^{(1)}(5) \\ & + 308\left(\frac{4}{11}M_1^3M_2^2 + \frac{7}{11}M_1M_2^4\right)\mathcal{Q}_{12}^{(2)}(2) - 112M_1M_2^4\mathcal{Q}_{12}^{(2)}(3) + 16M_1M_2^4\mathcal{Q}_{12}^{(2)}(4) + 16M_1^2M_2^3\mathcal{Q}_{12}^{(3)}(3), \end{aligned} \quad (157)$$

$$\begin{aligned} \left[S_{3/2}^{(2)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(3)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_{12} = & \frac{42735}{16}\left(\frac{120}{407}M_1^4M_2^2 + \frac{252}{407}M_1^2M_2^4 + \frac{35}{407}M_2^6\right)\mathcal{Q}_{12}^{(1)}(1) - \frac{22071}{8}\left(\frac{120}{1051}M_1^4M_2^2 + \frac{756}{1051}M_1^2M_2^4 + \frac{175}{1051}M_2^6\right) \\ & \times \mathcal{Q}_{12}^{(1)}(2) + \frac{2001}{2}\left(\frac{450}{667}M_1^2M_2^4 + \frac{217}{667}M_2^6\right)\mathcal{Q}_{12}^{(1)}(3) - \frac{499}{3}\left(\frac{198}{499}M_1^2M_2^4 + \frac{301}{499}M_2^6\right)\mathcal{Q}_{12}^{(1)}(4) \\ & + \frac{41}{3}M_2^6\mathcal{Q}_{12}^{(1)}(5) - \frac{2}{3}M_2^6\mathcal{Q}_{12}^{(1)}(6) + 945\left(\frac{8}{15}M_1^3M_2^3 + \frac{7}{15}M_1M_2^5\right)\mathcal{Q}_{12}^{(2)}(2) - 522\left(\frac{8}{29}M_1^3M_2^3 + \frac{21}{29}M_1M_2^5\right) \\ & \times \mathcal{Q}_{12}^{(2)}(3) + 100M_1M_2^5\mathcal{Q}_{12}^{(2)}(4) - 8M_1M_2^5\mathcal{Q}_{12}^{(2)}(5) + 72M_1^2M_2^4\mathcal{Q}_{12}^{(3)}(3) - 16M_1^2M_2^4\mathcal{Q}_{12}^{(3)}(4), \end{aligned} \quad (158)$$

$$\begin{aligned}
\left[S_{3/2}^{(2)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(4)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_{12} = & \frac{705705}{128} \left(\frac{240}{611} M_1^4 M_2^3 + \frac{336}{611} M_1^2 M_2^5 + \frac{35}{611} M_2^7 \right) \mathcal{Q}_{12}^{(1)}(1) \\
& - \frac{234927}{32} \left(\frac{80}{339} M_1^4 M_2^3 + \frac{224}{339} M_1^2 M_2^5 + \frac{35}{339} M_2^7 \right) \mathcal{Q}_{12}^{(1)}(2) + \frac{104973}{32} \left(\frac{240}{3181} M_1^4 M_2^3 + \frac{2304}{3181} M_1^2 M_2^5 \right. \\
& \left. + \frac{637}{3181} M_2^7 \right) \mathcal{Q}_{12}^{(1)}(3) - \frac{8437}{12} \left(\frac{480}{767} M_1^2 M_2^5 + \frac{287}{767} M_2^7 \right) \mathcal{Q}_{12}^{(1)}(4) + \frac{623}{8} \left(\frac{208}{623} M_1^2 M_2^5 + \frac{415}{623} M_2^7 \right) \mathcal{Q}_{12}^{(1)}(5) \\
& - \frac{29}{6} M_2^7 \mathcal{Q}_{12}^{(1)}(6) + \frac{1}{6} M_2^7 \mathcal{Q}_{12}^{(1)}(7) + \frac{4389}{2} \left(\frac{12}{19} M_1^3 M_2^4 + \frac{7}{19} M_1 M_2^6 \right) \mathcal{Q}_{12}^{(2)}(2) - 1716 \left(\frac{6}{13} M_1^3 M_2^4 \right. \\
& \left. + \frac{7}{13} M_1 M_2^6 \right) \mathcal{Q}_{12}^{(2)}(3) + 440 \left(\frac{1}{5} M_1^3 M_2^4 + \frac{4}{5} M_1 M_2^6 \right) \mathcal{Q}_{12}^{(2)}(4) - \frac{160}{3} M_1 M_2^6 \mathcal{Q}_{12}^{(2)}(5) + \frac{8}{3} M_1 M_2^6 \mathcal{Q}_{12}^{(2)}(6) \\
& + 198 M_1^2 M_2^5 \mathcal{Q}_{12}^{(3)}(3) - 88 M_1^2 M_2^5 \mathcal{Q}_{12}^{(3)}(4) + 8 M_1^2 M_2^5 \mathcal{Q}_{12}^{(3)}(5), \quad (159)
\end{aligned}$$

$$\begin{aligned}
\left[S_{3/2}^{(2)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(5)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_{12} = & \frac{2567565}{256} \left(\frac{80}{171} M_1^4 M_2^4 + \frac{84}{171} M_1^2 M_2^6 + \frac{7}{171} M_2^8 \right) \mathcal{Q}_{12}^{(1)}(1) \\
& - \frac{2129127}{128} \left(\frac{240}{709} M_1^4 M_2^4 + \frac{420}{709} M_1^2 M_2^6 + \frac{49}{709} M_2^8 \right) \mathcal{Q}_{12}^{(1)}(2) + \frac{579579}{64} \left(\frac{240}{1351} M_1^4 M_2^4 + \frac{936}{1351} M_1^2 M_2^6 \right. \\
& \left. + \frac{175}{1351} M_2^8 \right) \mathcal{Q}_{12}^{(1)}(3) - \frac{75933}{32} \left(\frac{80}{1593} M_1^4 M_2^4 + \frac{1128}{1593} M_1^2 M_2^6 + \frac{385}{1593} M_2^8 \right) \mathcal{Q}_{12}^{(1)}(4) + \frac{16237}{48} \left(\frac{708}{1249} M_1^2 M_2^6 \right. \\
& \left. + \frac{541}{1249} M_2^8 \right) \mathcal{Q}_{12}^{(1)}(5) - \frac{655}{24} \left(\frac{36}{131} M_1^2 M_2^6 + \frac{95}{131} M_2^8 \right) \mathcal{Q}_{12}^{(1)}(6) + \frac{79}{60} M_2^8 \mathcal{Q}_{12}^{(1)}(7) - \frac{1}{30} M_2^8 \mathcal{Q}_{12}^{(1)}(8) \\
& + \frac{69069}{16} \left(\frac{16}{23} M_1^3 M_2^5 + \frac{7}{23} M_1 M_2^7 \right) \mathcal{Q}_{12}^{(2)}(2) - \frac{35607}{8} \left(\frac{48}{83} M_1^3 M_2^5 + \frac{35}{83} M_1 M_2^7 \right) \mathcal{Q}_{12}^{(2)}(3) + \frac{3003}{2} \left(\frac{8}{21} M_1^3 M_2^5 \right. \\
& \left. + \frac{13}{21} M_1 M_2^7 \right) \mathcal{Q}_{12}^{(2)}(4) - \frac{715}{3} \left(\frac{8}{55} M_1^3 M_2^5 + \frac{47}{55} M_1 M_2^7 \right) \mathcal{Q}_{12}^{(2)}(5) + \frac{59}{3} M_1 M_2^7 \mathcal{Q}_{12}^{(2)}(6) - \frac{2}{3} M_1 M_2^7 \mathcal{Q}_{12}^{(2)}(7) \\
& + 429 M_1^2 M_2^6 \mathcal{Q}_{12}^{(3)}(3) - 286 M_1^2 M_2^6 \mathcal{Q}_{12}^{(3)}(4) + 52 M_1^2 M_2^6 \mathcal{Q}_{12}^{(3)}(5) - \frac{8}{3} M_1^2 M_2^6 \mathcal{Q}_{12}^{(3)}(6), \quad (160)
\end{aligned}$$

$$\begin{aligned}
\left[S_{3/2}^{(3)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(3)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_{12} = & \frac{255255}{32} \left(\frac{112}{2431} M_1^6 M_2 + \frac{1080}{2431} M_1^4 M_2^3 + \frac{1134}{2431} M_1^2 M_2^5 + \frac{105}{2431} M_2^7 \right) \mathcal{Q}_{12}^{(1)}(1) \\
& - \frac{76923}{8} \left(\frac{120}{407} M_1^4 M_2^3 + \frac{252}{407} M_1^2 M_2^5 + \frac{35}{407} M_2^7 \right) \mathcal{Q}_{12}^{(1)}(2) + \frac{34119}{8} \left(\frac{440}{3791} M_1^4 M_2^3 + \frac{2700}{3791} M_1^2 M_2^5 \right. \\
& \left. + \frac{651}{3791} M_2^7 \right) \mathcal{Q}_{12}^{(1)}(3) - 895 \left(\frac{594}{895} M_1^2 M_2^5 + \frac{301}{895} M_2^7 \right) \mathcal{Q}_{12}^{(1)}(4) + \frac{201}{2} \left(\frac{26}{67} M_1^2 M_2^5 + \frac{41}{67} M_2^7 \right) \mathcal{Q}_{12}^{(1)}(5) \\
& - 6 M_2^7 \mathcal{Q}_{12}^{(1)}(6) + \frac{2}{9} M_2^7 \mathcal{Q}_{12}^{(1)}(7) + \frac{14553}{4} \left(\frac{8}{77} M_1^5 M_2^2 + \frac{48}{77} M_1^3 M_2^4 + \frac{21}{77} M_1 M_2^6 \right) \mathcal{Q}_{12}^{(2)}(2) - 2430 \left(\frac{8}{15} M_1^3 M_2^4 \right. \\
& \left. + \frac{7}{15} M_1 M_2^6 \right) \mathcal{Q}_{12}^{(2)}(3) + 626 \left(\frac{176}{626} M_1^3 M_2^4 + \frac{450}{626} M_1 M_2^6 \right) \mathcal{Q}_{12}^{(2)}(4) - 72 M_1 M_2^6 \mathcal{Q}_{12}^{(2)}(5) + 4 M_1 M_2^6 \mathcal{Q}_{12}^{(2)}(6) \\
& + 444 \left(\frac{120}{444} M_1^4 M_2^3 + \frac{324}{444} M_1^2 M_2^5 \right) \mathcal{Q}_{12}^{(3)}(3) - 144 M_1^2 M_2^5 \mathcal{Q}_{12}^{(3)}(4) + 16 M_1^2 M_2^5 \mathcal{Q}_{12}^{(3)}(5) + \frac{32}{3} M_1^3 M_2^4 \mathcal{Q}_{12}^{(4)}(4), \quad (161)
\end{aligned}$$

$$\begin{aligned}
\left[S_{3/2}^{(3)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(4)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_{12} = & \frac{4879875}{256} \left(\frac{448}{4225} M_1^6 M_2^2 + \frac{2160}{4225} M_1^4 M_2^4 + \frac{1512}{4225} M_1^2 M_2^6 + \frac{105}{4225} M_2^8 \right) \mathcal{Q}_{12}^{(1)}(1) \\
& - \frac{3516513}{128} \left(\frac{448}{15223} M_1^6 M_2^2 + \frac{6480}{15223} M_1^4 M_2^4 + \frac{7560}{15223} M_1^2 M_2^6 + \frac{735}{15223} M_2^8 \right) \mathcal{Q}_{12}^{(1)}(2) + \frac{919413}{64} \left(\frac{2480}{9287} M_1^4 M_2^4 \right. \\
& + \frac{5904}{9287} M_1^2 M_2^6 + \frac{903}{9287} M_2^8 \left. \right) \mathcal{Q}_{12}^{(1)}(3) - \frac{118107}{32} \left(\frac{1040}{10737} M_1^4 M_2^4 + \frac{7632}{10737} M_1^2 M_2^6 + \frac{2065}{10737} M_2^8 \right) \mathcal{Q}_{12}^{(1)}(4) \\
& + \frac{8353}{16} \left(\frac{5304}{8353} M_1^2 M_2^6 + \frac{3049}{8353} M_2^8 \right) \mathcal{Q}_{12}^{(1)}(5) - \frac{339}{8} \left(\frac{40}{113} M_1^2 M_2^6 + \frac{73}{113} M_2^8 \right) \mathcal{Q}_{12}^{(1)}(6) + \frac{71}{36} M_2^8 \mathcal{Q}_{12}^{(1)}(7) \\
& - \frac{1}{18} M_2^8 \mathcal{Q}_{12}^{(1)}(8) + \frac{81081}{8} \left(\frac{8}{39} M_1^5 M_2^3 + \frac{24}{39} M_1^3 M_2^5 + \frac{7}{39} M_1 M_2^7 \right) \mathcal{Q}_{12}^{(2)}(2) - \frac{34155}{4} \left(\frac{8}{115} M_1^5 M_2^3 + \frac{72}{115} M_1^3 M_2^5 \right. \\
& + \frac{35}{115} M_1 M_2^7 \left. \right) \mathcal{Q}_{12}^{(2)}(3) + 2717 \left(\frac{1364}{2717} M_1^3 M_2^5 + \frac{1353}{2717} M_1 M_2^7 \right) \mathcal{Q}_{12}^{(2)}(4) - 422 \left(\frac{52}{211} M_1^3 M_2^5 \right. \\
& + \frac{159}{211} M_1 M_2^7 \left. \right) \mathcal{Q}_{12}^{(2)}(5) + 34 M_1 M_2^7 \mathcal{Q}_{12}^{(2)}(6) - \frac{4}{3} M_1 M_2^7 \mathcal{Q}_{12}^{(2)}(7) + 1551 \left(\frac{660}{1551} M_1^4 M_2^4 + \frac{891}{1551} M_1^2 M_2^6 \right) \mathcal{Q}_{12}^{(3)}(3) \\
& - \frac{2222}{3} \left(\frac{20}{101} M_1^4 M_2^4 + \frac{81}{101} M_1^2 M_2^6 \right) \mathcal{Q}_{12}^{(3)}(4) + 124 M_1^2 M_2^6 \mathcal{Q}_{12}^{(3)}(5) - 8 M_1^2 M_2^6 \mathcal{Q}_{12}^{(3)}(6) + \frac{176}{3} M_1^3 M_2^5 \mathcal{Q}_{12}^{(4)}(4) \\
& - \frac{32}{3} M_1^3 M_2^5 \mathcal{Q}_{12}^{(4)}(5), \tag{162}
\end{aligned}$$

$$\begin{aligned}
\left[S_{3/2}^{(3)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(5)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_{12} = & \frac{20165145}{512} \left(\frac{224}{1343} M_1^6 M_2^3 + \frac{720}{1343} M_1^4 M_2^5 + \frac{378}{1343} M_1^2 M_2^7 + \frac{21}{1343} M_2^9 \right) \mathcal{Q}_{12}^{(1)}(1) \\
& - \frac{4327323}{64} \left(\frac{112}{1441} M_1^6 M_2^3 + \frac{720}{1441} M_1^4 M_2^5 + \frac{567}{1441} M_1^2 M_2^7 + \frac{42}{1441} M_2^9 \right) \mathcal{Q}_{12}^{(1)}(2) + \frac{329043}{8} \left(\frac{112}{6136} M_1^6 M_2^3 \right. \\
& + \frac{2400}{6136} M_1^4 M_2^5 + \frac{3267}{6136} M_1^2 M_2^7 + \frac{357}{6136} M_2^9 \left. \right) \mathcal{Q}_{12}^{(1)}(3) - \frac{200057}{16} \left(\frac{320}{1399} M_1^4 M_2^5 + \frac{918}{1399} M_1^2 M_2^7 \right. \\
& + \frac{161}{1399} M_2^9 \left. \right) \mathcal{Q}_{12}^{(1)}(4) + \frac{34333}{16} \left(\frac{200}{2641} M_1^4 M_2^5 + \frac{1857}{2641} M_1^2 M_2^7 + \frac{584}{2641} M_2^9 \right) \mathcal{Q}_{12}^{(1)}(5) - \frac{881}{4} \left(\frac{525}{881} M_1^2 M_2^7 \right. \\
& + \frac{356}{881} M_2^9 \left. \right) \mathcal{Q}_{12}^{(1)}(6) + \frac{613}{45} \left(\frac{765}{2452} M_1^2 M_2^7 + \frac{1687}{2452} M_2^9 \right) \mathcal{Q}_{12}^{(1)}(7) - \frac{23}{45} M_2^9 \mathcal{Q}_{12}^{(1)}(8) + \frac{1}{90} M_2^9 \mathcal{Q}_{12}^{(1)}(9) \\
& + \frac{1486485}{64} \left(\frac{16}{55} M_1^5 M_2^4 + \frac{32}{55} M_1^3 M_2^6 + \frac{7}{55} M_1 M_2^8 \right) \mathcal{Q}_{12}^{(2)}(2) - \frac{389961}{16} \left(\frac{16}{101} M_1^5 M_2^4 + \frac{64}{101} M_1^3 M_2^6 \right. \\
& + \frac{21}{101} M_1 M_2^8 \left. \right) \mathcal{Q}_{12}^{(2)}(3) + \frac{150293}{16} \left(\frac{48}{1051} M_1^5 M_2^4 + \frac{640}{1051} M_1^3 M_2^6 + \frac{363}{1051} M_1 M_2^8 \right) \mathcal{Q}_{12}^{(2)}(4) - \frac{3653}{2} \left(\frac{128}{281} M_1^3 M_2^6 \right. \\
& + \frac{153}{281} M_1 M_2^8 \left. \right) \mathcal{Q}_{12}^{(2)}(5) + \frac{779}{4} \left(\frac{160}{779} M_1^3 M_2^6 + \frac{619}{779} M_1 M_2^8 \right) \mathcal{Q}_{12}^{(2)}(6) - \frac{35}{3} M_1 M_2^8 \mathcal{Q}_{12}^{(2)}(7) + \frac{1}{3} M_1 M_2^8 \mathcal{Q}_{12}^{(2)}(8) \\
& + \frac{8151}{2} \left(\frac{10}{19} M_1^4 M_2^5 + \frac{9}{19} M_1^2 M_2^7 \right) \mathcal{Q}_{12}^{(3)}(3) - \frac{8008}{3} \left(\frac{5}{14} M_1^4 M_2^5 + \frac{9}{14} M_1^2 M_2^7 \right) \mathcal{Q}_{12}^{(3)}(4) + \frac{1820}{3} \left(\frac{1}{7} M_1^4 M_2^5 \right. \\
& + \frac{6}{7} M_1^2 M_2^7 \left. \right) \mathcal{Q}_{12}^{(3)}(5) - 64 M_1^2 M_2^7 \mathcal{Q}_{12}^{(3)}(6) + \frac{8}{3} M_1^2 M_2^7 \mathcal{Q}_{12}^{(3)}(7) + \frac{572}{3} M_1^3 M_2^6 \mathcal{Q}_{12}^{(4)}(4) - \frac{208}{3} M_1^3 M_2^6 \mathcal{Q}_{12}^{(4)}(5) \\
& + \frac{16}{3} M_1^3 M_2^6 \mathcal{Q}_{12}^{(4)}(6), \tag{163}
\end{aligned}$$

$$\begin{aligned}
\left[S_{3/2}^{(4)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(4)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_{12} = & \frac{105930825}{2048} \left(\frac{1152}{91715} M_1^8 M_2 + \frac{19712}{91715} M_1^6 M_2^3 + \frac{47520}{91715} M_1^4 M_2^5 + \frac{22176}{91715} M_1^2 M_2^7 + \frac{1155}{91715} M_2^9 \right) \mathcal{Q}_{12}^{(1)}(1) \\
& - \frac{10735725}{128} \left(\frac{448}{4225} M_1^6 M_2^3 + \frac{2160}{4225} M_1^4 M_2^5 + \frac{1512}{4225} M_1^2 M_2^7 + \frac{105}{4225} M_2^9 \right) \mathcal{Q}_{12}^{(1)}(2) + \frac{6435429}{128} \left(\frac{5824}{195013} M_1^6 M_2^3 \right. \\
& + \frac{81840}{195013} M_1^4 M_2^5 + \frac{97416}{195013} M_1^2 M_2^7 + \frac{9933}{195013} M_2^9 \left. \right) \mathcal{Q}_{12}^{(1)}(3) - \frac{483637}{32} \left(\frac{1040}{3997} M_1^4 M_2^5 + \frac{2544}{3997} M_1^2 M_2^7 \right. \\
& + \frac{413}{3997} M_2^9 \left. \right) \mathcal{Q}_{12}^{(1)}(4) + \frac{165827}{64} \left(\frac{15600}{165827} M_1^4 M_2^5 + \frac{116688}{165827} M_1^2 M_2^7 + \frac{33539}{165827} M_2^9 \right) \mathcal{Q}_{12}^{(1)}(5) \\
& - \frac{2123}{8} \left(\frac{120}{193} M_1^2 M_2^7 + \frac{73}{193} M_2^9 \right) \mathcal{Q}_{12}^{(1)}(6) + \frac{1189}{72} \left(\frac{408}{1189} M_1^2 M_2^7 + \frac{781}{1189} M_2^9 \right) \mathcal{Q}_{12}^{(1)}(7) - \frac{11}{18} M_2^9 \mathcal{Q}_{12}^{(1)}(8) \\
& + \frac{1}{72} M_2^9 \mathcal{Q}_{12}^{(1)}(9) + \frac{525525}{16} \left(\frac{64}{2275} M_1^7 M_2^2 + \frac{792}{2275} M_1^5 M_2^4 + \frac{1188}{2275} M_1^3 M_2^6 + \frac{231}{2275} M_1 M_2^8 \right) \mathcal{Q}_{12}^{(2)}(2) \\
& - \frac{127413}{4} \left(\frac{8}{39} M_1^5 M_2^4 + \frac{24}{39} M_1^3 M_2^6 + \frac{7}{39} M_1 M_2^8 \right) \mathcal{Q}_{12}^{(2)}(3) + \frac{48323}{4} \left(\frac{312}{4393} M_1^5 M_2^4 + \frac{2728}{4393} M_1^3 M_2^6 \right. \\
& + \frac{1353}{4393} M_1 M_2^8 \left. \right) \mathcal{Q}_{12}^{(2)}(4) - 2310 \left(\frac{52}{105} M_1^3 M_2^6 + \frac{53}{105} M_1 M_2^8 \right) \mathcal{Q}_{12}^{(2)}(5) + 247 \left(\frac{60}{247} M_1^3 M_2^6 \right. \\
& + \frac{187}{247} M_1 M_2^8 \left. \right) \mathcal{Q}_{12}^{(2)}(6) - \frac{44}{3} M_1 M_2^8 \mathcal{Q}_{12}^{(2)}(7) + \frac{4}{9} M_1 M_2^8 \mathcal{Q}_{12}^{(2)}(8) + \frac{26169}{4} \left(\frac{56}{793} M_1^6 M_2^3 + \frac{440}{793} M_1^4 M_2^5 \right. \\
& + \frac{297}{793} M_1^2 M_2^7 \left. \right) \mathcal{Q}_{12}^{(3)}(3) - \frac{11374}{3} \left(\frac{20}{47} M_1^4 M_2^5 + \frac{27}{47} M_1^2 M_2^7 \right) \mathcal{Q}_{12}^{(3)}(4) + \frac{2566}{3} \left(\frac{260}{1283} M_1^4 M_2^5 \right. \\
& + \frac{1023}{1283} M_1^2 M_2^7 \left. \right) \mathcal{Q}_{12}^{(3)}(5) - 88 M_1^2 M_2^7 \mathcal{Q}_{12}^{(3)}(6) + 4 M_1^2 M_2^7 \mathcal{Q}_{12}^{(3)}(7) + \frac{1232}{3} \left(\frac{3}{14} M_1^5 M_2^4 + \frac{11}{14} M_1^3 M_2^6 \right) \mathcal{Q}_{12}^{(4)}(4) \\
& - \frac{352}{3} M_1^3 M_2^6 \mathcal{Q}_{12}^{(4)}(5) + \frac{32}{3} M_1^3 M_2^6 \mathcal{Q}_{12}^{(4)}(6) + \frac{16}{3} M_1^4 M_2^5 \mathcal{Q}_{12}^{(5)}(5), \tag{164}
\end{aligned}$$

$$\begin{aligned}
\left[S_{3/2}^{(4)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(5)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_{12} = & \frac{489834345}{4096} \left(\frac{1152}{32623} M_1^8 M_2^2 + \frac{9856}{32623} M_1^6 M_2^4 + \frac{15840}{32623} M_1^4 M_2^6 + \frac{5544}{32623} M_1^2 M_2^8 + \frac{231}{32623} M_2^{10} \right) \mathcal{Q}_{12}^{(1)}(1) \\
& - \frac{452873421}{2048} \left(\frac{384}{50269} M_1^8 M_2^2 + \frac{9856}{50269} M_1^6 M_2^4 + \frac{26400}{50269} M_1^4 M_2^6 + \frac{12936}{50269} M_1^2 M_2^8 + \frac{693}{50269} M_2^{10} \right) \mathcal{Q}_{12}^{(1)}(2) \\
& + \frac{38424243}{256} \left(\frac{8288}{89567} M_1^6 M_2^4 + \frac{44880}{89567} M_1^4 M_2^6 + \frac{33858}{89567} M_1^2 M_2^8 + \frac{2541}{89567} M_2^{10} \right) \mathcal{Q}_{12}^{(1)}(3) \\
& - \frac{6633055}{128} \left(\frac{224}{9277} M_1^6 M_2^4 + \frac{3696}{9277} M_1^4 M_2^6 + \frac{4818}{9277} M_1^2 M_2^8 + \frac{539}{9277} M_2^{10} \right) \mathcal{Q}_{12}^{(1)}(4) + \frac{1330927}{128} \left(\frac{24400}{102379} M_1^4 M_2^6 \right. \\
& + \frac{66132}{102379} M_1^2 M_2^8 + \frac{11847}{102379} M_2^{10} \left. \right) \mathcal{Q}_{12}^{(1)}(5) - \frac{82491}{64} \left(\frac{6800}{82491} M_1^4 M_2^6 + \frac{57420}{82491} M_1^2 M_2^8 + \frac{18271}{82491} M_2^{10} \right) \mathcal{Q}_{12}^{(1)}(6) \\
& + \frac{72643}{720} \left(\frac{43350}{72643} M_1^2 M_2^8 + \frac{29293}{72643} M_2^{10} \right) \mathcal{Q}_{12}^{(1)}(7) - \frac{199}{40} \left(\frac{190}{597} M_1^2 M_2^8 + \frac{407}{597} M_2^{10} \right) \mathcal{Q}_{12}^{(1)}(8) + \frac{109}{720} M_2^{10} \mathcal{Q}_{12}^{(1)}(9) \\
& - \frac{1}{360} M_2^{10} \mathcal{Q}_{12}^{(1)}(10) + \frac{10975965}{128} \left(\frac{256}{3655} M_1^7 M_2^3 + \frac{1584}{3655} M_1^5 M_2^5 + \frac{1584}{3655} M_1^3 M_2^7 + \frac{231}{3655} M_1 M_2^9 \right) \mathcal{Q}_{12}^{(2)}(2) \\
& - \frac{6239805}{64} \left(\frac{256}{14545} M_1^7 M_2^3 + \frac{4752}{14545} M_1^5 M_2^5 + \frac{7920}{14545} M_1^3 M_2^7 + \frac{1617}{14545} M_1 M_2^9 \right) \mathcal{Q}_{12}^{(2)}(3) \\
& + \frac{1378663}{32} \left(\frac{1776}{9641} M_1^5 M_2^5 + \frac{5984}{9641} M_1^3 M_2^7 + \frac{1881}{9641} M_1 M_2^9 \right) \mathcal{Q}_{12}^{(2)}(4) - \frac{157651}{16} \left(\frac{720}{12127} M_1^5 M_2^5 + \frac{7392}{12127} M_1^3 M_2^7 \right. \\
& + \frac{4015}{12127} M_1 M_2^9 \left. \right) \mathcal{Q}_{12}^{(2)}(5) + \frac{10391}{8} \left(\frac{4880}{10391} M_1^3 M_2^7 + \frac{5511}{10391} M_1 M_2^9 \right) \mathcal{Q}_{12}^{(2)}(6) - \frac{1229}{12} \left(\frac{272}{1229} M_1^3 M_2^7 \right. \\
& + \frac{957}{1229} M_1 M_2^9 \left. \right) \mathcal{Q}_{12}^{(2)}(7) + \frac{85}{18} M_1 M_2^9 \mathcal{Q}_{12}^{(2)}(8) - \frac{1}{9} M_1 M_2^9 \mathcal{Q}_{12}^{(2)}(9) + \frac{160875}{8} \left(\frac{56}{375} M_1^6 M_2^4 + \frac{220}{375} M_1^4 M_2^6 \right. \\
& + \frac{99}{375} M_1^2 M_2^8 \left. \right) \mathcal{Q}_{12}^{(3)}(3) - \frac{173173}{12} \left(\frac{56}{1211} M_1^6 M_2^4 + \frac{660}{1211} M_1^4 M_2^6 + \frac{495}{1211} M_1^2 M_2^8 \right) \mathcal{Q}_{12}^{(3)}(4) \\
& + \frac{12103}{3} \left(\frac{370}{931} M_1^4 M_2^6 + \frac{561}{931} M_1^2 M_2^8 \right) \mathcal{Q}_{12}^{(3)}(5) - 562 \left(\frac{50}{281} M_1^4 M_2^6 + \frac{231}{281} M_1^2 M_2^8 \right) \mathcal{Q}_{12}^{(3)}(6) + \frac{122}{3} M_1^2 M_2^8 \mathcal{Q}_{12}^{(3)}(7) \\
& - \frac{4}{3} M_1^2 M_2^8 \mathcal{Q}_{12}^{(3)}(8) + \frac{4862}{3} \left(\frac{6}{17} M_1^5 M_2^5 + \frac{11}{17} M_1^3 M_2^7 \right) \mathcal{Q}_{12}^{(4)}(4) - 676 \left(\frac{2}{13} M_1^5 M_2^5 + \frac{11}{13} M_1^3 M_2^7 \right) \mathcal{Q}_{12}^{(4)}(5) \\
& + \frac{296}{3} M_1^3 M_2^7 \mathcal{Q}_{12}^{(4)}(6) - \frac{16}{3} M_1^3 M_2^7 \mathcal{Q}_{12}^{(4)}(7) + \frac{104}{3} M_1^4 M_2^6 \mathcal{Q}_{12}^{(5)}(5) - \frac{16}{3} M_1^4 M_2^6 \mathcal{Q}_{12}^{(5)}(6), \tag{165}
\end{aligned}$$

$$\begin{aligned}
\left[S_{3/2}^{(5)}(\mathcal{C}_1^2) \mathcal{C}_1, S_{3/2}^{(5)}(\mathcal{C}_1^2) \mathcal{C}_1 \right]_{12} = & \frac{2505429927}{8192} \left(\frac{2816}{834309} M_1^{10} M_2 + \frac{74880}{834309} M_1^8 M_2^3 + \frac{320320}{834309} M_1^6 M_2^5 + \frac{343200}{834309} M_1^4 M_2^7 + \frac{90090}{834309} M_1^2 M_2^9 \right. \\
& + \frac{3003}{834309} M_2^{11} \Big) \Omega_{12}^{(1)}(1) - \frac{1273569297}{2048} \left(\frac{1152}{32623} M_1^8 M_2^3 + \frac{9856}{32623} M_1^6 M_2^5 + \frac{15840}{32623} M_1^4 M_2^7 + \frac{5544}{32623} M_1^2 M_2^9 \right. \\
& + \frac{231}{32623} M_2^{11} \Big) \Omega_{12}^{(1)}(2) + \frac{958832589}{2048} \left(\frac{17280}{2235041} M_1^8 M_2^3 + \frac{430976}{2235041} M_1^6 M_2^5 + \frac{1166880}{2235041} M_1^4 M_2^7 \right. \\
& + \frac{586872}{2235041} M_1^2 M_2^9 + \frac{33033}{2235041} M_2^{11} \Big) \Omega_{12}^{(1)}(3) - \frac{23205897}{128} \left(\frac{1120}{12483} M_1^6 M_2^5 + \frac{6160}{12483} M_1^4 M_2^7 + \frac{4818}{12483} M_1^2 M_2^9 \right. \\
& + \frac{385}{12483} M_2^{11} \Big) \Omega_{12}^{(1)}(4) + \frac{10626655}{256} \left(\frac{19040}{817435} M_1^6 M_2^5 + \frac{317200}{817435} M_1^4 M_2^7 + \frac{429858}{817435} M_1^2 M_2^9 + \frac{51337}{817435} M_2^{11} \right) \\
& \times \Omega_{12}^{(1)}(5) - \frac{1923623}{320} \left(\frac{34000}{147971} M_1^4 M_2^7 + \frac{95700}{147971} M_1^2 M_2^9 + \frac{18271}{147971} M_2^{11} \right) \Omega_{12}^{(1)}(6) \\
& + \frac{181901}{320} \left(\frac{129200}{1637109} M_1^4 M_2^7 + \frac{1127100}{1637109} M_1^2 M_2^9 + \frac{380809}{1637109} M_2^{11} \right) \Omega_{12}^{(1)}(7) - \frac{12701}{360} \left(\frac{570}{977} M_1^2 M_2^9 \right. \\
& + \frac{407}{977} M_2^{11} \Big) \Omega_{12}^{(1)}(8) + \frac{2047}{1440} \left(\frac{630}{2047} M_1^2 M_2^9 + \frac{1417}{2047} M_2^{11} \right) \Omega_{12}^{(1)}(9) - \frac{13}{360} M_2^{11} \Omega_{12}^{(1)}(10) + \frac{1}{1800} M_2^{11} \Omega_{12}^{(1)}(11) \\
& + \frac{257041785}{1024} \left(\frac{640}{85595} M_1^9 M_2^2 + \frac{13312}{85595} M_1^7 M_2^4 + \frac{41184}{85595} M_1^5 M_2^6 + \frac{27456}{85595} M_1^3 M_2^8 + \frac{3003}{85595} M_1 M_2^{10} \right) \Omega_{12}^{(2)}(2) \\
& - \frac{20383935}{64} \left(\frac{256}{3655} M_1^7 M_2^4 + \frac{1584}{3655} M_1^5 M_2^6 + \frac{1584}{3655} M_1^3 M_2^8 + \frac{231}{3655} M_1 M_2^{10} \right) \Omega_{12}^{(2)}(3) \\
& + \frac{10212345}{64} \left(\frac{1280}{71415} M_1^7 M_2^4 + \frac{23088}{71415} M_1^5 M_2^6 + \frac{38896}{71415} M_1^3 M_2^8 + \frac{8151}{71415} M_1 M_2^{10} \right) \Omega_{12}^{(2)}(4) \\
& - \frac{673803}{16} \left(\frac{720}{3987} M_1^5 M_2^6 + \frac{2464}{3987} M_1^3 M_2^8 + \frac{803}{3987} M_1 M_2^{10} \right) \Omega_{12}^{(2)}(5) + \frac{210763}{32} \left(\frac{12240}{210763} M_1^5 M_2^6 + \frac{126880}{210763} M_1^3 M_2^8 \right. \\
& + \frac{71643}{210763} M_1 M_2^{10} \Big) \Omega_{12}^{(2)}(6) - \frac{2561}{4} \left(\frac{272}{591} M_1^3 M_2^8 + \frac{319}{591} M_1 M_2^{10} \right) \Omega_{12}^{(2)}(7) \\
& + \frac{1409}{36} \left(\frac{304}{1409} M_1^3 M_2^8 + \frac{1105}{1409} M_1 M_2^{10} \right) \Omega_{12}^{(2)}(8) - \frac{13}{9} M_1 M_2^{10} \Omega_{12}^{(2)}(9) + \frac{1}{36} M_1 M_2^{10} \Omega_{12}^{(2)}(10) \\
& + \frac{1130415}{16} \left(\frac{48}{2635} M_1^8 M_2^3 + \frac{728}{2635} M_1^6 M_2^5 + \frac{1430}{2635} M_1^4 M_2^7 + \frac{429}{2635} M_1^2 M_2^9 \right) \Omega_{12}^{(3)}(3) - \frac{232375}{4} \left(\frac{56}{375} M_1^6 M_2^5 \right. \\
& + \frac{220}{375} M_1^4 M_2^7 + \frac{99}{375} M_1^2 M_2^9 \Big) \Omega_{12}^{(3)}(4) + \frac{230789}{12} \left(\frac{840}{17753} M_1^6 M_2^5 + \frac{9620}{17753} M_1^4 M_2^7 + \frac{7293}{17753} M_1^2 M_2^9 \right) \Omega_{12}^{(3)}(5) \\
& - 3302 \left(\frac{50}{127} M_1^4 M_2^7 + \frac{77}{127} M_1^2 M_2^9 \right) \Omega_{12}^{(3)}(6) + 321 \left(\frac{170}{963} M_1^4 M_2^7 + \frac{793}{963} M_1^2 M_2^9 \right) \Omega_{12}^{(3)}(7) - \frac{52}{3} M_1^2 M_2^9 \Omega_{12}^{(3)}(8) \\
& + \frac{4}{9} M_1^2 M_2^9 \Omega_{12}^{(3)}(9) + \frac{15015}{2} \left(\frac{16}{315} M_1^7 M_2^4 + \frac{156}{315} M_1^5 M_2^6 + \frac{143}{315} M_1^3 M_2^8 \right) \Omega_{12}^{(4)}(4) - \frac{11492}{3} \left(\frac{6}{17} M_1^5 M_2^6 \right. \\
& + \frac{11}{17} M_1^3 M_2^8 \Big) \Omega_{12}^{(4)}(5) + \frac{2284}{3} \left(\frac{90}{571} M_1^5 M_2^6 + \frac{481}{571} M_1^3 M_2^8 \right) \Omega_{12}^{(4)}(6) - \frac{208}{3} M_1^3 M_2^8 \Omega_{12}^{(4)}(7) + \frac{8}{3} M_1^3 M_2^8 \Omega_{12}^{(4)}(8) \\
& + \frac{4108}{15} \left(\frac{14}{79} M_1^6 M_2^5 + \frac{65}{79} M_1^4 M_2^7 \right) \Omega_{12}^{(5)}(5) - \frac{208}{3} M_1^4 M_2^7 \Omega_{12}^{(5)}(6) + \frac{16}{3} M_1^4 M_2^7 \Omega_{12}^{(5)}(7) + \frac{32}{15} M_1^5 M_2^6 \Omega_{12}^{(6)}(6). \quad (166)
\end{aligned}$$

Now that the H_1 and H_{12} bracket integrals up to order 5 have been explicitly expressed, they can be used to generate explicit expressions for the simple gas bracket integrals up to order 5 via the rule of Eq. (110) exactly as was done for the general simple gas bracket integral expression of Eqs. (113) and (114). Under the rule of Eq. (110), one has that $M_1 = M_2 = 1/2$ and the simple gas bracket integrals are then mass independent except for the presence of a single m_1 in the simple gas omega integrals. Since, for any given (p, q) all of the terms in the pairs of corresponding H_1 and H_{12} bracket integral expressions have the same total

power of the constituent masses, substitution of $M_1 = M_2 = 1/2$ simply yields an additional constant factor for the corresponding pairs of expressions of $(1/2)^{p+q+1}$. The difference in the signs of the terms in the corresponding expressions due to the factor of $(-1)^\ell$ has the effect that all terms involving omega integrals with odd values of ℓ cancel exactly and all terms involving omega integrals with even values of ℓ add identically to produce an additional factor of 2 in each surviving term. Since $p, q = 0 \Rightarrow \ell = 1$, and since all terms with odd values of ℓ cancel, it follows that:

$$\left[S_{3/2}^{(p)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(q)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_1 = 0; \quad p, q = 0, \quad (167)$$

For the rest of the simple gas bracket integrals up to order 5 one then has:

$$\left[S_{3/2}^{(1)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(1)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_1 = 4Q_1^{(2)}(2), \quad (168)$$

$$\left[S_{3/2}^{(1)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(2)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_1 = 7Q_1^{(2)}(2) - 2Q_1^{(2)}(3), \quad (169)$$

$$\left[S_{3/2}^{(1)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(3)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_1 = \frac{63}{8}Q_1^{(2)}(2) - \frac{9}{2}Q_1^{(2)}(3) + \frac{1}{2}Q_1^{(2)}(4), \quad (170)$$

$$\left[S_{3/2}^{(1)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(4)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_1 = \frac{231}{32}Q_1^{(2)}(2) - \frac{99}{16}Q_1^{(2)}(3) + \frac{11}{8}Q_1^{(2)}(4) - \frac{1}{12}Q_1^{(2)}(5), \quad (171)$$

$$\left[S_{3/2}^{(1)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(5)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_1 = \frac{3003}{512}Q_1^{(2)}(2) - \frac{429}{64}Q_1^{(2)}(3) + \frac{143}{64}Q_1^{(2)}(4) - \frac{13}{48}Q_1^{(2)}(5) + \frac{1}{96}Q_1^{(2)}(6), \quad (172)$$

$$\left[S_{3/2}^{(2)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(2)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_1 = \frac{77}{4}Q_1^{(2)}(2) - 7Q_1^{(2)}(3) + Q_1^{(2)}(4), \quad (173)$$

$$\left[S_{3/2}^{(2)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(3)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_1 = \frac{945}{32}Q_1^{(2)}(2) - \frac{261}{16}Q_1^{(2)}(3) + \frac{25}{8}Q_1^{(2)}(4) - \frac{1}{4}Q_1^{(2)}(5), \quad (174)$$

$$\left[S_{3/2}^{(2)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(4)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_1 = \frac{4389}{128}Q_1^{(2)}(2) - \frac{429}{16}Q_1^{(2)}(3) + \frac{55}{8}Q_1^{(2)}(4) - \frac{5}{6}Q_1^{(2)}(5) + \frac{1}{24}Q_1^{(2)}(6), \quad (175)$$

$$\left[S_{3/2}^{(2)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(5)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_1 = \frac{69069}{2048}Q_1^{(2)}(2) - \frac{35607}{1024}Q_1^{(2)}(3) + \frac{3003}{256}Q_1^{(2)}(4) - \frac{715}{384}Q_1^{(2)}(5) + \frac{59}{384}Q_1^{(2)}(6) - \frac{1}{192}Q_1^{(2)}(7), \quad (176)$$

$$\left[S_{3/2}^{(3)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(3)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_1 = \frac{14553}{256}Q_1^{(2)}(2) - \frac{1215}{32}Q_1^{(2)}(3) + \frac{313}{32}Q_1^{(2)}(4) - \frac{9}{8}Q_1^{(2)}(5) + \frac{1}{16}Q_1^{(2)}(6) + \frac{1}{6}Q_1^{(4)}(4), \quad (177)$$

$$\left[S_{3/2}^{(3)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(4)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_1 = \frac{81081}{1024}Q_1^{(2)}(2) - \frac{34155}{512}Q_1^{(2)}(3) + \frac{2717}{128}Q_1^{(2)}(4) - \frac{211}{64}Q_1^{(2)}(5) + \frac{17}{64}Q_1^{(2)}(6) - \frac{1}{96}Q_1^{(2)}(7) + \frac{11}{24}Q_1^{(4)}(4) - \frac{1}{12}Q_1^{(4)}(5), \quad (178)$$

$$\left[S_{3/2}^{(3)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(5)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_1 = \frac{1486485}{16384}Q_1^{(2)}(2) - \frac{389961}{4096}Q_1^{(2)}(3) + \frac{150293}{4096}Q_1^{(2)}(4) - \frac{3653}{512}Q_1^{(2)}(5) + \frac{779}{1024}Q_1^{(2)}(6) - \frac{35}{768}Q_1^{(2)}(7) + \frac{1}{768}Q_1^{(2)}(8) + \frac{143}{192}Q_1^{(4)}(4) - \frac{13}{48}Q_1^{(4)}(5) + \frac{1}{48}Q_1^{(4)}(6), \quad (179)$$

$$\left[S_{3/2}^{(4)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(4)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_1 = \frac{525525}{4096}Q_1^{(2)}(2) - \frac{127413}{1024}Q_1^{(2)}(3) + \frac{48323}{1024}Q_1^{(2)}(4) - \frac{1155}{128}Q_1^{(2)}(5) + \frac{247}{256}Q_1^{(2)}(6) - \frac{11}{192}Q_1^{(2)}(7) + \frac{1}{576}Q_1^{(2)}(8) + \frac{77}{48}Q_1^{(4)}(4) - \frac{11}{24}Q_1^{(4)}(5) + \frac{1}{24}Q_1^{(4)}(6), \quad (180)$$

$$\left[S_{3/2}^{(4)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(5)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_1 = \frac{10975965}{65536}Q_1^{(2)}(2) - \frac{6239805}{32768}Q_1^{(2)}(3) + \frac{1378663}{16384}Q_1^{(2)}(4) - \frac{157651}{8192}Q_1^{(2)}(5) + \frac{10391}{4096}Q_1^{(2)}(6) - \frac{1229}{6144}Q_1^{(2)}(7) + \frac{85}{9216}Q_1^{(2)}(8) - \frac{1}{4608}Q_1^{(2)}(9) + \frac{2431}{768}Q_1^{(4)}(4) - \frac{169}{128}Q_1^{(4)}(5) + \frac{37}{192}Q_1^{(4)}(6) - \frac{1}{96}Q_1^{(4)}(7), \quad (181)$$

$$\left[S_{3/2}^{(5)}(\mathcal{C}_1^2)\mathcal{C}_1, S_{3/2}^{(5)}(\mathcal{C}_1^2)\mathcal{C}_1\right]_1 = \frac{257041785}{1048576}Q_1^{(2)}(2) - \frac{20383935}{65536}Q_1^{(2)}(3) + \frac{10212345}{65536}Q_1^{(2)}(4) - \frac{673803}{16384}Q_1^{(2)}(5) + \frac{210763}{32768}Q_1^{(2)}(6) - \frac{2561}{4096}Q_1^{(2)}(7) + \frac{1409}{36864}Q_1^{(2)}(8) - \frac{13}{9216}Q_1^{(2)}(9) + \frac{1}{36864}Q_1^{(2)}(10) + \frac{15015}{2048}Q_1^{(4)}(4) - \frac{2873}{768}Q_1^{(4)}(5) + \frac{571}{768}Q_1^{(4)}(6) - \frac{13}{192}Q_1^{(4)}(7) + \frac{1}{384}Q_1^{(4)}(8) + \frac{1}{480}Q_1^{(6)}(6). \quad (182)$$

9. Discussion and conclusions

Our purpose in this series of papers has been to explore the use of Sonine polynomial expansions to high order results for the transport coefficients and the related Chapman–Enskog functions for simple gases and gas mixtures that are free of numerical error. In the current work we have presented summational expressions for the bracket integrals needed to compute the diffusion- and thermal conductivity-related Chapman–Enskog solutions to any arbitrary order of expansion in terms of Sonine polynomials. The summational nature of the expressions derived in this work will yield greatly improved computational efficiencies in determinations of the diffusion- and thermal conductivity-related matrix elements associated with our current *Mathematica*®-based programs and will undoubtedly prove substantially more conducive to use in computations that do not involve the use of *Mathematica*® but which, rather, employ the Fortran, C++, or other programming environments directly. In addition, the derived expressions which we have reported here clearly show exactly which omega integrals are needed in each (p, q) element of the coefficient matrix for a given order of the Sonine polynomial expansion approximation, m , which improves ease of understanding and utilization of the solution technique. The formulation of such summational representations for the bracket integrals constitutes a significant departure from the method that was used in our previous work [18–20] which followed the recommendation of Chapman and Cowling [1]. We will provide similarly derived expressions for the viscosity-related, bracket integrals in the near future.

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