Approximation of the Boltzmann Collision Operator Based on Hermite Spectral Method

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Abstract

Based on the Hermite expansion of the distribution function, we introduce a Galerkin spectral method for the spatially homogeneous Boltzmann equation with the realistic inverse-power-law models. A practical algorithm is proposed to evaluate the coefficients in the spectral method with high accuracy, and these coefficients are also used to construct new computationally affordable collision models. Numerical experiments show that our method captures the low-order moments very efficiently.

Keywords: Boltzmann equation, Hermite spectral method, inverse power law

1 Introduction

Over a century ago, Boltzmann devised a profound equation describing the statistical behavior of gas molecules. A number of interesting theoretical and practical problems emerged due to the birth of this equation, among which the numerical simulation for this six-dimensional Boltzmann equation is one significant topic after the invention of computers. The difficulty comes partly from its high dimensionality, and partly from its complicated integral operator modeling the binary collision of gas molecules. People have been using the Monte Carlo method [3] to overcome the difficulty caused by high dimensionality, but nowadays, a six-dimensional simulation using a deterministic solver is no longer unaffordable due to the fast growth of computer flops. Fully six-dimensional computations are carried out in [19, 10] for the simplified BGK-type collision terms. However, numerical simulation of the original Boltzmann equation with the binary collision operator still requires a large amount of computational resources [11].

Currently, the deterministic discretization of the binary collision operator can be categorized into three types: the discrete velocity method [15, 25], the Fourier spectral method [26, 12], and the Hermite spectral method [17, 13]. The discrete velocity method is hardly used in the numerical simulation due to its low order of convergence [25], whereas the Fourier spectral method is more popular because of its fast convergence rate and high numerical efficiency. Compared with the Fourier spectral method which requires periodization of the distribution function, the Hermite spectral method looks more natural since the basis functions with orthogonality in \( \mathbb{R}^3 \) are employed. In fact, the Hermite spectral method has a longer history and has been known as the moment method since Grad’s work [16]. Grad proposed in [16] a general method to find the expansion of the binary collision term with Hermite basis functions. Later, a similar way

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to expand the binary collision term using Sonine polynomials (also known as spherical Hermite polynomials) was proposed in [24]. The techniques used in formulating the expansion are also introduced in the book [30].

Despite these works, the Hermite spectral method is used in the numerical simulation only until recently [17, 13]. There are two major difficulties in applying this method: one is the evaluation of the coefficients in the expansion of the collision operator; the other is the huge computational cost due to its quadratic form. Although the general procedure to obtain the coefficients is given in [16, 30], following such a procedure involves expansion of a large number of huge polynomials, which is quite expensive even for a modern computer algebraic system; Kumar [24] provided a formula in his expansion using Sonine polynomials, while the formula involves evaluation of a large number of Talmi coefficients, which is not tractable either. As for the computational cost, the computational time of one evaluation of the collision operator is proportional to the cube of the number of degrees of freedom, while in the Fourier spectral method, the time complexity for a direct Galerkin discretization is only the square of the number of modes.

This work is devoted to both of the aforementioned issues. On one hand, by using a number of properties for relevant polynomials, we provide explicit formulas for all the coefficients appearing in the expansion of the collision operator with the Hermite spectral method. These formulas are immediately applicable in the sense of coding, and the computational cost is affordable for a moderate number of degrees of freedom. On the other hand, we combine the modeling strategy and the numerical technique to form a new way to discretize the collision term, where only a portion in the truncated series expansion is treated “quadratically”, and the remaining part just decays exponentially as in the BGK model. Thus the computational cost is greatly reduced and we can still capture the evolution of low-order moments accurately.

The rest of this paper is organized as follows. In Section 2, we briefly review the Boltzmann equation and the Hermite expansion of the distribution function. In Section 3, we first give an explicit expression for the series expansion of the quadratic collision operator, and then construct approximate collision models based on such an expansion. Some numerical experiments verifying our method are carried out in Section 4 and some concluding remarks are made in Section 5. Detailed derivation of the expansion is given in the Appendix.

2 Boltzmann equation and Hermite expansion of the distribution function

This section is devoted to the introduction of existing works needed by our further derivation. We will first give a brief review of the Boltzmann equation and the IPL (Inverse-Power-Law) model, and then introduce the expansion of the distribution function used in the Hermite spectral method.

2.1 Boltzmann equation

The Boltzmann equation describes the fluid state using a distribution function $f(t, x, v)$, where $t$ is the time, $x$ is the spatial coordinates, and $v$ stands for the velocity of gas molecules. The governing equation of $f$ is

$$\frac{\partial f}{\partial t} + \nabla_x \cdot (vf) = Q[f], \quad t \in \mathbb{R}^+, \quad x \in \mathbb{R}^3, \quad v \in \mathbb{R}^3,$$  \hspace{1cm} (2.1)
where $Q[f]$ is the collision operator which has a quadratic form

$$Q[f](t, x, v) = \int_{\mathbb{R}^3} \int_{n \perp g} \int_{0}^{\pi} [f(t, x, v_1') f(t, x, v') - f(t, x, v_1) f(t, x, v)] B(|g|, \chi) \, d\chi \, dn \, dv_1,$$

(2.2)

where $g = v - v_1$ and $n$ is a unit vector. Hence $\int_{n \perp g} \cdots \, dn$ is a one-dimensional integration over the unit circle perpendicular to $g$. The post-collisional velocities $v'$ and $v_1'$ are

$$v' = \cos^2(\chi/2) v + \sin^2(\chi/2) v_1 - |g| \cos(\chi/2) n,$$
$$v_1' = \cos^2(\chi/2) v_1 + \sin^2(\chi/2) v + |g| \cos(\chi/2) n,$$

(2.3)

and from the conservation of momentum and energy, it holds that

$$v + v_1 = v' + v_1', \quad |v|^2 + |v_1|^2 = |v'|^2 + |v_1'|^2.$$  

(2.4)

The collision kernel $B(|g|, \chi)$ is a non-negative function determined by the force between gas molecules.

In this paper, we are mainly concerned with the IPL model, for which the force between two molecules is always repulsive and proportional to a negative power of their distance. In this case, the kernel $B(|g|, \chi)$ in (2.2) has the form

$$B(|g|, \chi) := |g|^{\eta-5} W_0 \left| \frac{dW_0}{d\chi} \right|, \quad \eta > 3,$$

(2.5)

where $-\eta$ is the index in the power of distance. The case $\eta > 5$ corresponds to the “hard potential”, and the case $3 < \eta < 5$ corresponds to the “soft potential”. When $\eta = 5$, the collision kernel $B(|g|, \chi)$ is independent of $|g|$, and in this model the gas molecules are called “Maxwell molecules”. The dimensionless impact parameter $W_0$ is related to the angle $\chi$ by

$$\chi = \pi - 2 \int_{0}^{W_1} \left[ 1 - W^2 - \frac{2}{\eta - 1} \left( \frac{W}{W_0} \right)^{\eta-1} \right]^{-1/2} \, dW,$$

(2.6)

and $W_1$ is a positive real number satisfying

$$1 - W_1^2 - \frac{2}{\eta - 1} \left( \frac{W_1}{W_0} \right)^{\eta-1} = 0.$$  

(2.7)

It can be easily shown that the above equation of $W_1$ admits a unique positive solution when $\eta > 3$ and $W_0 > 0$.

Apparently, the quadratic collision term is the most complicated part in the Boltzmann equation. In this paper, we will focus on the numerical approximation of $Q[f]$. For simplicity, we assume that the gas is homogeneous in space, and thus we can remove the variable $x$ in the distribution function to get the spatially homogeneous Boltzmann equation

$$\frac{\partial f}{\partial t} = Q[f], \quad t \in \mathbb{R}^+, \quad v \in \mathbb{R}^3.$$  

(2.8)

It is well known that the steady state of this equation takes the form of the Maxwellian:

$$f(\infty, v) = M_{\rho, u, \theta}(v) := \frac{\rho}{(2\pi\theta)^{3/2}} \exp \left( - \frac{|v - u|^2}{2\theta} \right),$$

(2.9)
where the density $\rho$, velocity $u$ and temperature $\theta$ can be obtained by

$$
\rho = \int_{\mathbb{R}^3} f(t, v) \, dv, \quad u = \frac{1}{\rho} \int_{\mathbb{R}^3} v f(t, v) \, dv, \quad \theta = \frac{1}{3\rho} \int_{\mathbb{R}^3} |v - u|^2 f(t, v) \, dv.
$$

(2.10)

These quantities are invariant during the evolution, and therefore (2.10) holds for any $t$. By selecting proper frame of reference and applying appropriate non-dimensionalization, we can obtain

$$
\rho = 1, \quad u = 0, \quad \theta = 1,
$$

(2.11)

and thus the Maxwellian (2.9) is reduced to

$$
\mathcal{M}(v) := \frac{1}{(2\pi)^{3/2}} \exp\left(-\frac{|v|^2}{2}\right).
$$

(2.12)

Hereafter, the normalization (2.11) will always be assumed.

In the literature, people have been trying to avoid the complicated form of the collision operator $Q[f]$ by introducing simpler approximations to it. For example, the BGK collision model

$$
Q^{BGK}[f] = \frac{1}{\tau} (M - f)
$$

(2.13)

was proposed in [2]. Here $\tau$ is the mean relaxation time, which is usually obtained from the first approximation of the Chapman-Enskog theory [8]. When (2.13) is used to approximate the IPL model,

$$
\tau = \frac{5}{2^{3n+1} \sqrt{\pi} A_2(\eta) \Gamma(4 - 2/(\eta - 1))},
$$

(2.14)

where $A_2(\eta) = \int_0^{+\infty} W_0 \sin^2 \chi \, dW_0$. With $Q[f]$ replaced by $Q^{BGK}[f]$ in (2.8), the collision process becomes an exponential convergence to the Maxwellian. Such a simple approximation provides incorrect Prandtl number 1. Hence some other models such as the Shakhov model [28] and ES-BGK model [18] are later proposed to fix the Prandtl number by changing the Maxwellian in (2.13) to a non-equilibrium distribution function. We will call these models “BGK-type models” hereafter.

Numerical evaluations on these BGK-type models can be found in [14, 9], where one can find that these approximations are not accurate enough when the non-equilibrium is strong. Hence the study on efficient numerical methods for the original Boltzmann equation with the quadratic collision operator is still necessary.

### 2.2 Series expansion of the distribution function

Our numerical discretization will be based on the following series expansion of the distribution function in the weighted $L^2$ space $\mathcal{F} = L^2(\mathbb{R}^3; \mathcal{M}^{-1} \, dv)$:

$$
f(t, v) = \sum_{k_1 k_2 k_3} f_{k_1 k_2 k_3} (t) H^{k_1 k_2 k_3}(v) \mathcal{M}(v),
$$

(2.15)

where $\mathcal{M}(v)$ is the Maxwellian, and we have used the abbreviation

$$
\sum_{k_1 k_2 k_3} := \sum_{k_1=0}^{+\infty} \sum_{k_2=0}^{+\infty} \sum_{k_3=0}^{+\infty}.
$$

(2.16)

In (2.15), $H^{k_1 k_2 k_3}(v)$ are the Hermite polynomials defined as follows:
Definition 1 (Hermite polynomials). For $k_1, k_2, k_3 \in \mathbb{N}$, the Hermite polynomial $H^{k_1k_2k_3}(v)$ is defined as

$$H^{k_1k_2k_3}(v) = \frac{(-1)^n}{\mathcal{M}(v)} \frac{\partial^{k_1+k_2+k_3}}{\partial v_1^{k_1} \partial v_2^{k_2} \partial v_3^{k_3}} \mathcal{M}(v), \quad (2.17)$$

where $\mathcal{M}(v)$ is given in (2.12).

The expansion (2.2) was proposed by Grad in [16], where such an expansion was used to derive moment methods. The relation between the coefficients $f_{k_1k_2k_3}$ and the moments can be seen from the orthogonality of Hermite polynomials

$$\int_{\mathbb{R}^3} H^{k_1k_2k_3}(v) H^{l_1l_2l_3}(v) \mathcal{M}(v) \, dv = \delta_{k_1l_1} \delta_{k_2l_2} \delta_{k_3l_3} k_1!k_2!k_3!. \quad (2.18)$$

For example, by the above orthogonality, we can insert the expansion (2.15) into the definition of $\rho$ in (2.10) to get $f_{000} = \rho$. In our case, the normalization (2.11) gives us $f_{000} = 1$. Similarly, it can be deduced from the other two equations in (2.10) and (2.11) that

$$f_{100} = f_{010} = f_{001} = 0, \quad f_{200} + f_{020} + f_{002} = 0. \quad (2.19)$$

Other interesting moments include the heat flux $q_i$ and the stress tensor $\sigma_{ij}$, which are defined as

$$q_i = \frac{1}{2} \int_{\mathbb{R}^3} |v - u|^2 (v_i - u_i) f \, dv = \frac{1}{2} \int_{\mathbb{R}^3} |v|^2 v_i f \, dv, \quad i = 1, 2, 3,$$

$$\sigma_{ij} = \int_{\mathbb{R}^3} ((v_i - u_i)(v_j - u_j) - \frac{1}{3} \delta_{ij} |v - u|^2) f \, dv = \int_{\mathbb{R}^3} \left( v_i v_j - \frac{1}{3} \delta_{ij} |v|^2 \right) f \, dv, \quad i, j = 1, 2, 3.$$

They are related to the coefficients by

$$q_1 = 3f_{300} + f_{110} + f_{102}, \quad q_2 = 3f_{030} + f_{210} + f_{012}, \quad q_3 = 3f_{003} + f_{201} + f_{021},$$

and

$$\sigma_{11} = 2f_{200}, \quad \sigma_{12} = f_{110}, \quad \sigma_{13} = f_{101},$$
$$\sigma_{22} = 2f_{020}, \quad \sigma_{23} = f_{011}, \quad \sigma_{33} = 2f_{002}.$$

3 Approximation of the collision term

To get the evolution of the coefficients $f_{k_1k_2k_3}$ in the expansion (2.15), we need to expand the collision term using the same basis functions. The expansions of the BGK-type collision operators are usually quite straightforward. For instance, the series expansion of the BGK collision term (2.13) is given in [6] as

$$Q^{BGK}[f] = \sum_{k_1k_2k_3} Q^{BGK}_{k_1k_2k_3} H^{k_1k_2k_3}(v) \mathcal{M}(v), \quad (3.1)$$

where

$$Q^{BGK}_{k_1k_2k_3} = \begin{cases} 0, & k_1 = k_2 = k_3 = 0, \\ -\frac{1}{\tau} f_{k_1k_2k_3}, & \text{otherwise}. \end{cases}$$

The expansions for the ES-BGK and Shakhov operators can be found in [5, 4]. In this section, we will first discuss the series expansion of the quadratic collision term $Q[f]$ defined in (2.2), and then mimic the BGK-type collision operators to construct collision models with better accuracy.
3.1 Series expansions of general collision terms

Suppose the binary collision term $Q[f]$ can be expanded as

$$Q[f](v) = \sum_{k_1k_2k_3} Q_{k_1k_2k_3} H^{k_1k_2k_3}(v) \mathcal{M}(v). \quad (3.2)$$

By the orthogonality of Hermite polynomials, we get

$$Q_{k_1k_2k_3} = \frac{1}{k_1!k_2!k_3!} \int H^{k_1k_2k_3}(v) Q[f](v) \, dv = \sum_{i_1i_2i_3j_1j_2j_3} A^{i_1i_2i_3;j_1j_2j_3}_{k_1k_2k_3} f_{i_1i_2i_3} f_{j_1j_2j_3}, \quad (3.3)$$

where the second equality can be obtained by inserting (2.15) into (2.2), and

$$A^{i_1i_2i_3;j_1j_2j_3}_{k_1k_2k_3} = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{n \cdot g} \int_0^\pi B(|g|, \chi) \left[ H^{i_1i_2i_3}(v') H^{j_1j_2j_3}(v_1) \right] \, dv_1 \, \exp\left( -\frac{|v|^2 + |v_1|^2}{2} \right) \, d\chi \, dn_1 \, dv_1 \, dv. \quad (3.4)$$

It can be seen from (3.4) that the evaluation of every coefficient requires integration of an eight-dimensional function. In principle, this can be done by numerical quadrature; however, the computational cost for obtaining all these coefficients would be huge. Actually, in [16, 30], a strategy to simplify the above integral has been introduced, and for small indices, the values are given in the literature. However, when the indices are large, no explicit formulae are provided in [16, 30], and the procedure therein is not easy to follow. Inspired by these works, we give in this paper explicit equations of the coefficients $A^{i_1i_2i_3;j_1j_2j_3}_{k_1k_2k_3}$ for any collision kernel, except for an integral with respect the two parameters in the kernel function $B(\cdot, \cdot)$. The main results are summarized in the following two theorems:

**Theorem 1.** The expansion coefficients of the collision operator $Q[f](v)$ defined in (3.3) have the form below:

$$A^{i_1i_2i_3;j_1j_2j_3}_{k_1k_2k_3} = \sum_{i_1'=0}^{\min(i_1+j_1,k_1)} \sum_{i_2'=0}^{\min(i_1+j_2,k_2)} \sum_{i_3'=0}^{\min(i_1+j_3,k_3)} \frac{2^{-k/2}}{2^3\pi^{3/2} \sqrt{1!_i 2!_{i'} 3!_{i''}}} \gamma^{i_1i_2i_3;j_1j_2j_3}_{i'i''} \left( \frac{|g|}{\sqrt{2}} \right)^{i'i''} \left( \frac{|g|}{\sqrt{2}} \right)^{i'i''} \prod_{s=\max(0,i'-j)}^{\min(i',i)} \frac{(-1)^{i'-s}}{s!(i-s)! (i'-s)! (j'-i+s)!}, \quad (3.5)$$

where

$$j'_a = i_a + j_a - i'_a, \quad i'_a = k_a - i'_a, \quad s = 1, 2, 3. \quad (3.6)$$

The coefficients $a_{i'j'}^{ij}$ and $\gamma^{i_1i_2i_3;j_1j_2j_3}_{i'i''}$ are defined by

$$a_{i'j'}^{ij} = 2^{-(i'+j')/2} i! \sum_{s=\max(0,i'-j)}^{\min(i',i)} \frac{(-1)^{i'-s}}{s!(i-s)! (i'-s)! (j'-i+s)!}, \quad (3.7)$$

and

$$\gamma^{i_1i_2i_3;j_1j_2j_3}_{i'i''} := \int_{\mathbb{R}^3} \int_{n \cdot g} \int_0^\pi \left[ H^{j_1j_2j_3} \left( \frac{g'}{\sqrt{2}} \right) - H^{j_1j_2j_3} \left( \frac{g}{\sqrt{2}} \right) \right] H^{i_1i_2i_3} \left( \frac{g}{\sqrt{2}} \right) B(|g|, \chi) \exp\left( -\frac{|g|^2}{4} \right) \, d\chi \, dn \, dg, \quad (3.8)$$

where $g' = g \cos \chi - |g| n \sin \chi$ is the post-collisional relative velocity, and $B(|g|, \chi)$ is the collision kernel in (2.2).
Theorem 2. For any $k_1, k_2, k_3, l_1, l_2, l_3 \in \mathbb{N}$, let $k = k_1 + k_2 + k_3$ and $l = l_1 + l_2 + l_3$. Then the coefficients $\gamma_{l_1l_2l_3}^{k_1k_2k_3}$ defined in (3.8) satisfies

$$
\gamma_{l_1l_2l_3}^{k_1k_2k_3} = \sum_{m_1=0}^{\lfloor k_1/2 \rfloor} \sum_{m_2=0}^{\lfloor k_2/2 \rfloor} \sum_{m_3=0}^{\lfloor k_3/2 \rfloor} \sum_{n_1=0}^{\lfloor l_1/2 \rfloor} \sum_{n_2=0}^{\lfloor l_2/2 \rfloor} \sum_{n_3=0}^{\lfloor l_3/2 \rfloor} (2k-4m+1)C_{m_1,n_1} C_{m_2,n_2} C_{m_3,n_3} S_{l_1-2m_1,l_2-2n_2,l_3-2n_3} R_{m_1}^{k_1} R_{m_2}^{k_2} R_{m_3}^{k_3},
$$

(3.9)

where $m = m_1 + m_2 + m_3$, $n = n_1 + n_2 + n_3$, and

$$
C_{m_1,m_2,m_3}^{k_1,k_2,k_3} = \frac{(-1)^m 4\pi m!}{(2k-m+1)!!} \frac{k_1!k_2!k_3!}{m_1!m_2!m_3!}.
$$

(3.10)

In (3.9), $S_{l_1l_2l_3}^{k_1k_2k_3}$ is the coefficient of $v_1^{k_1}v_2^{k_2}v_3^{k_3}w_1^{l_1}w_2^{l_2}w_3^{l_3}$ in the polynomial

$$
S_k(v, w) := (|v||w|)^k P_k \left( \frac{v}{|w|}, \frac{w}{|w|} \right),
$$

(3.11)

and

$$
K_{mn}^{kl} = \int_0^{\infty} \int_0^{\pi} I_m^{k-2m+1/2} \left( \frac{g^2}{4} \right) I_n^{l-2n+1/2} \left( \frac{g^2}{4} \right) \times \left( \frac{g}{\sqrt{2}} \right)^{k+l+2-2(m+n)} \exp \left( -\frac{g^2}{4} \right) B(g, \chi) \left[ P_{k-2m} (\cos \chi - 1) \right] \exp \left( -\frac{g^2}{4} \right) \, dg \, d\chi.
$$

(3.12)

Here $L_n^{(\alpha)}(x)$ are the Laguerre polynomials and $P_k(x)$ are the Legendre polynomials, which are defined below.

Definition 2 (Legendre functions). For $\ell \in \mathbb{N}$, the Legendre polynomial $P_\ell(x)$ is defined as

$$
P_\ell(x) = \frac{1}{2^\ell \ell!} \frac{d^\ell}{dx^\ell} \left[ (x^2 - 1)^\ell \right].
$$

Definition 3 (Laguerre polynomials). For $\alpha > -1$, let $w^\alpha(x) = x^{n+\alpha} \exp(-x)$. For $n \in \mathbb{N}$, define the Laguerre polynomial as

$$
L_n^{(\alpha)}(x) = \frac{x^n}{n! w^\alpha(x)} \frac{d^n}{dx^n} w^\alpha(x).
$$

Through these two theorems, the eight-dimensional integration in (3.4) has been reduced into a series of summations and a two-dimensional integration. Among all the coefficients introduced in these theorems, $a_{ij}^{kl}$ and $C_{m_1,m_2,m_3}^{k_1,k_2,k_3}$ can be computed directly. As for $S_{l_1l_2l_3}^{k_1k_2k_3}$, we need to expand polynomial $S_k(v, w)$, which can be done recursively using the following recursion formula:

$$
S_0(v, w) = 1, \quad S_1(v, w) = v \cdot w,
$$

$$
S_{k+1}(v, w) = \frac{2k+1}{k+1} (v \cdot w) S_k(v, w) - \frac{k}{k+1} (|v||w|)^2 S_{k-1}(v, w).
$$

(3.13)

This recursion formula can be derived from the recursion relation of Legendre polynomials, and it also shows that for every monomial in the expansion of $S_k(v, w)$, the degree of $v$ equals the degree of $w$. Therefore $S_{l_1l_2l_3}^{k_1k_2k_3}$ is nonzero only when $k_1 + k_2 + k_3 = l_1 + l_2 + l_3$. This means in (3.9), the summand is nonzero only when

$$
k_1 + k_2 + k_3 = 2(m_1 + m_2 + m_3) = l_1 + l_2 + l_3 - 2(n_1 + n_2 + n_3).
$$

(3.14)

Consequently, when evaluating $K_{mn}^{kl}$ defined in (3.12), we only need to take into account the case $k - 2m = l - 2n$. Generally, $K_{mn}^{kl}$ can be computed by numerical quadrature; for the IPL model, the integral with respect to $g$ can be written explicitly, which will be elaborated in the following section.
3.2 Series expansion of collision operators for IPL models

The formulae given in the previous section are almost ready to be coded, except that specific collision models are needed to calculate the integral $K_{mn}^{kl}$ defined in (3.12). This section is devoted to further simplifying this integral for IPL models, which completes the algorithm for computing the coefficients $A_{k_1k_2k_3j_1j_2j_3}^{i_1i_2i_3j_1j_2j_3}$.

For the IPL model (2.5), we first consider the integral with respect to $\chi$ in (3.12). To this aim, we extract all the terms related to $\chi$ from (3.12), and define $\tilde{B}_k^{\eta}(\cdot)$ as

$$
\tilde{B}_k^{\eta}(g) := \int_0^{\pi} B(g, \chi) \left[ P_k(\cos \chi) - 1 \right] d\chi = g^{\frac{\eta-5}{2}} \int_0^{\pi} W_0 \left| \frac{dW_0}{d\chi} \right| \left[ P_k(\cos \chi) - 1 \right] d\chi, \quad \eta > 3, \quad g > 0.
$$

To evaluate the above integral, we follow the method introduced in [7] and apply the change of variable

$$
\chi = \pi - 2 \int_0^1 \left[ 1 - x^2(1 - y) - x^{\eta-1}y \right]^{-1/2} \sqrt{1 - y} dx,
$$

to get

$$
\tilde{B}_k^{\eta}(g) = 2^{-\frac{\eta-3}{2}} g^{\frac{\eta-5}{2}} \int_0^1 \left[ P_k(\cos \chi) - 1 \right][2(1 - y) + (\eta - 1)y][5\eta - 1]^{-\frac{\eta+1}{2}} dy, \quad (3.15)
$$

Below we write the above equation as

$$
\tilde{B}_k^{\eta}(g) = 2^{-\frac{\eta-3}{2}} g^{\frac{\eta-5}{2}} \mathcal{I}(k, \eta), \quad (3.16)
$$

where $\mathcal{I}(k, \eta)$ denotes the integral in (3.15). In general, we need to evaluate $\mathcal{I}(k, \eta)$ by numerical quadrature. In our implementation, the adaptive integrator introduced in [27, Section 3.3.7] is used to compute this integral.

Now we consider the integral with respect to $g$. Using the result (3.16), we can rewrite (3.12) as

$$
K_{mn}^{kl} = 2^{c(\eta)} \mathcal{I}(k - 2m, \eta) \int_0^{+\infty} L_m^{(k-2m+1/2)}(s)L_n^{(k-2m+1/2)}(s)c(\eta) \exp(-s) ds, \quad (3.17)
$$

where $c(\eta) = \frac{\eta-3}{2} + k - 2m$, and we have applied the change of variable $s = g^2/4$, and taken into account the relation $k - 2m = l - 2n$. In general, we can adopt the formula

$$
\int_0^{+\infty} L_m^{(\alpha)}(s)L_n^{(\alpha)}(s)s^\mu \exp(-s) ds = (-1)^{m+n}\Gamma(\mu + 1) \sum_{i=0}^{\min(m,n)} \binom{\mu - \alpha}{m - i} \binom{\mu - \alpha}{n - i} \left( i + \mu \right) \quad (3.18)
$$

introduced in [29, eq. (10)] to calculate (3.17). Specially, when $\eta = 5$, which corresponds to the model of Maxwell molecules, we can use the orthogonality of Laguerre polynomials to get

$$
K_{mn}^{kl} = 2^{k-2m+1/2} \mathcal{I}(k - 2m, 5) \binom{k - m + 1/2}{m} \Gamma(k - 2m + 3/2) \delta_{mn}, \quad (3.19)
$$

and thus the computational cost can be further reduced. In fact, Grad has already pointed out in [16] that for Maxwell molecules, $A_{k_1k_2k_3j_1j_2j_3}^{i_1i_2i_3j_1j_2j_3}$ is nonzero only when

$$
i_1 + i_2 + i_3 + j_1 + j_2 + j_3 = k_1 + k_2 + k_3. \quad (3.20)$$
This can also be seen from our calculation: from (3.19), we can find that only when \( k_1 + k_2 + k_3 = l_1 + l_2 + l_3 \), the coefficient \( \gamma_{l_1 l_2 l_3}^{k_1 k_2 k_3} \) given in (3.9) is nonzero; therefore in (3.5), if the summand is nonzero, the sum of \( j_1', j_2' \) and \( j_3' \) must equal the sum of \( l_1', l_2' \) and \( l_3' \), which is equivalent to (3.20) due to (3.6).

The above analysis shows that for the IPL model, we only need to apply the numerical quadrature to the one-dimensional integrals \( I(k, \eta) \), which makes it easier to obtain the coefficients \( A_{k_1 k_2 k_3}^{j_1 j_2 j_3} \) with high accuracy.

### 3.3 Approximation of the collision term

Until now, we already have a complete algorithm to calculate the coefficients \( A_{k_1 k_2 k_3}^{j_1 j_2 j_3} \). These coefficients can be used either to discretize the collision term or to construct new collision models. We will discuss both topics in this section.

#### 3.3.1 Discretization of the homogeneous Boltzmann equation

Based on the expansion of the distribution function (2.15), the most natural discretization of the homogeneous Boltzmann equation is to use the Galerkin spectral method. From this point of view, for any positive integer \( M \), we define the space of the numerical solution

\[
\mathcal{F}_M = \text{span}\{H^{k_1 k_2 k_3}(v)\mathcal{M}(v) \mid (k_1, k_2, k_3) \in I_M\} \subset \mathcal{F} = L^2(\mathbb{R}^3; \mathcal{M}^{-1} \, dv),
\]

where \( I_M \) is the index set

\[
I_M = \{(k_1, k_2, k_3) \mid 0 \leq k_1 + k_2 + k_3 \leq M, \, k_i \in \mathbb{N}, \, i = 1, 2, 3\}.
\]

Then the semi-discrete distribution function \( f_M(t, \cdot) \in \mathcal{F}_M \) satisfies

\[
\int_{\mathbb{R}^3} \frac{\partial f_M}{\partial t} \varphi \mathcal{M}^{-1} \, dv = \int_{\mathbb{R}^3} Q(f_M, f_M) \varphi \mathcal{M}^{-1} \, dv, \quad \forall \varphi \in \mathcal{F}_M.
\]

Suppose

\[
f_M(t, v) = \sum_{(k_1, k_2, k_3) \in I_M} f_{k_1 k_2 k_3}(t) H^{k_1 k_2 k_3}(v) \mathcal{M}(v) \in \mathcal{F}_M.
\]

The equations (3.2) and (3.3) show that the variational form (3.22) is equivalent to the following ODE system:

\[
\frac{df_{k_1 k_2 k_3}}{dt} = \sum_{(i_1, i_2, i_3) \in I_M} \sum_{(j_1, j_2, j_3) \in I_M} A^{i_1 i_2 i_3, j_1 j_2 j_3}_{k_1 k_2 k_3} f_{i_1 i_2 i_3} f_{j_1 j_2 j_3}, \quad (k_1, k_2, k_3) \in I_M.
\]

It is easy to see that the time complexity for the computation of all the right hand sides is \( O(N_M^3) \), where \( N_M \) is the number of elements in \( I_M \):

\[
N_M = \frac{(M + 1)(M + 2)(M + 3)}{6} \sim O(M^3).
\]

To fully formulate the ODE system (3.24), we need the coefficients \( A^{i_1 i_2 i_3, j_1 j_2 j_3}_{k_1 k_2 k_3} \) for all \((i_1, i_2, i_3), (j_1, j_2, j_3), (k_1, k_2, k_3) \in I_M\). When the collision kernel is chosen and \( M \) is fixed, we only need to compute these coefficients once, and then they can be used repeatedly. For a given \( M \), the algorithm for computing these coefficients is summarized in Table 1. The general procedure is to sequentially compute the coefficients in the first column, with indices described
in the third column, and the equations to follow are given in the second column. For IPL models, we can use (3.17) and (3.18) instead to obtain the values of $K_{mn}^{kl}$. In the third column of Table 1 it is worth mentioning that some indices are in the index set $I_{2M}$ instead of $I_M$, as is due to the equation (3.6), which shows that

$$ (j_1, j_2, j_3) \in I_{2M}, \quad \text{if } (i_1, i_2, i_3) \in I_M \text{ and } (j_1, j_2, j_3) \in I_M. $$

Therefore the corresponding indices for $\gamma$ and $C$ must lie in $I_{2M}$. Similar arguments hold for the coefficients $K$.

The last column in Table 1 shows an estimation of the computational cost for each coefficient, from which one can see that the total cost for getting $A_{k_1k_2k_3}^{i_1j_1j_2j_3}$ is $O(M^{12})$. Now we compare this with the numerical cost by applying numerical integration directly to (3.4). We assume the number of quadrature points on $\mathbb{R}^3$ is $O(M_\nu^3)$, and the number of quadrature points on the unit sphere (domain for $n$ and $\chi$) is $O(M_\gamma^2)$. Thus using numerical integration to evaluate all the coefficients $A_{k_1k_2k_3}^{i_1j_1j_2j_3}$ has time complexity $O(M\nu M^6_\nu M_\gamma^2)$. In most cases, we will choose $M_\nu > M$ to get accurate results. Hence our method listed in Table 1 is significantly faster.

| Coefficients | Formula | Constraints for the indices | Computational cost |
|--------------|---------|----------------------------|--------------------|
| $C_{m_1m_2m_3}^{k_1k_2k_3}$ | (3.10) | $(k_1, k_2, k_3) \in I_M$, $(m_1, m_2, m_3) \in I_M$ | $O(M^6)$ |
| $S_{l_1l_2l_3}^{k_1k_2k_3}$ | (3.11) | $(k_1, k_2, k_3) \in I_M$, $(l_1, l_2, l_3) \in I_M$, $k_1 + k_2 + k_3 = l_1 + l_2 + l_3$ | $O(M^5)$ |
| $K_{mn}^{kl}$ | (3.12) | $k \leq 2M$, $l \leq M$, $m \leq [k/2]$, $n \leq [l/2]$, $k - 2m = l - 2n$ | $O(M^4)$ |
| $\gamma_{l_1l_2l_3}^{k_1k_2k_3}$ | (3.8) | $(l_1, l_2, l_3) \in I_M$, $(k_1, k_2, k_3) \in I_{2M}$ | $O(M^{11})$ |
| $a_{ij}^{i_1j_1j_2j_3}$ | (3.7) | $i \leq M$, $j \leq M$, $i' \leq 2M$, $j' \leq 2M$, $i + j = i' + j'$ | $O(M^4)$ |
| $A_{k_1k_2k_3}^{i_1j_1j_2j_3}$ | (3.5) | $(k_1, k_2, k_3) \in I_M$, $(i_1, i_2, i_3) \in I_M$, $(j_1, j_2, j_3) \in I_M$ | $O(M^{12})$ |

Table 1: A summary for computation of all the coefficients.

### 3.3.2 Approximation of the collision operator

In the previous section, a complete numerical method has been given to solve the spatially homogeneous Boltzmann equation. However, due to the rapid growth of the number of coefficients as $M$ increases, the storage requirement of this algorithm is quite strong. Table 2 shows the memory required to store the coefficients $A_{k_1k_2k_3}^{i_1j_1j_2j_3}$, where we assume that the coefficients are represented in the double-precision floating-point format, whose typical size is 8 bytes per number. It can be seen that the case $M = 20$ has already exceeded the memory caps of most current desktops. Although the data given in Table 2 can be reduced by taking the symmetry of the coefficients into consideration, it can still easily hit our memory limit by increasing $M$ slightly. Even if the memory cost is acceptable for large $M$, the computational cost $O(M^9)$ becomes an issue especially when solving the spatially non-homogeneous problems.

To overcome this difficulty, we will only compute and store the coefficients $A_{k_1k_2k_3}^{i_1j_1j_2j_3}$ for a small number $M$ such that the computational cost for solving (3.24) is acceptable. When $(k_1, k_2, k_3) \notin I_M$, we apply the idea of the BGK-type models and let these coefficients decay to zero exponentially with a constant rate:

$$ \frac{df_{k_1k_2k_3}}{dt} = -\nu_M f_{k_1k_2k_3}, \quad (k_1, k_2, k_3) \notin I_M, \quad (3.26) $$
Table 2: Memory required to store $A_{k_1k_2k_3}^{ij1i2j1j2j3}$.

| $M$ | Memory (Gigabytes) | $M$ | Memory (Gigabytes) |
|-----|---------------------|-----|---------------------|
| 5   | $1.308 \times 10^{-3}$ | 25  | $2.620 \times 10^2$ |
| 10  | 0.1743              | 30  | $1.210 \times 10^3$ |
| 15  | 4.048               | 35  | $4.473 \times 10^3$ |
| 20  | 41.38               | 40  | $1.400 \times 10^4$ |

where $\nu_M$ is a constant independent of $k_1$, $k_2$ and $k_3$. Combining (3.24) and (3.26), we actually get a new collision operator

$$Q_M[f] = P_M Q[P_M f] - \nu_M (I - P_M) f, \quad \forall f \in F,$$

(3.27)

where $P_M$ is the orthogonal projection from $F$ onto $F_M$. Applying spectral method to this collision operator is quite straightforward, and it remains only to select the constant $\nu_M$.

In [7], the authors used a similar idea to approximate the linearized collision operator, where the evolution of the coefficients for high-degree basis functions is also approximated by an exponential decay. Here we choose the decay rate in the same way as in [7]: considering the discrete linearized collision operator $L_M : F_M \rightarrow F_M$ defined as

$$L_M[f] = \sum_{(k_1,k_2,k_3) \in I_M} \sum_{(j_1,j_2,j_3) \in I_M} (A_{k_1k_2k_3}^{000,j_1j_2j3} + A_{k_1k_2k_3}^{j_1j_2j3,000}) f_{j_1j_2j3} H^{k_1k_2k_3}(v) M(v),$$

(3.28)

we let $\nu_M$ be the spectral radius of this operator. Thus, the linearization of $Q_M[f]$ about the Maxwellian $M$ coincides with the approximation of the linearized collision operator proposed in [7].

By now, we have obtained a series of new collision models (3.27). It can be expected that these models are better approximations of the original quadratic operator than the simple BGK-type models, especially when the non-equilibrium is strong and the non-linearity takes effect. This will be observed in the numerical examples.

4 Numerical examples

In this section, we will show some results of our numerical simulation. In all the numerical experiments, we adopt the newly proposed collision operator (3.27), and solve the equation

$$\frac{\partial f}{\partial t} = Q_{M_0}[f]$$

umerically for some positive integer $M_0$. This equation is solved by the Galerkin spectral method with solution defined in the space $F_M$, and $M$ is always chosen to be greater than $M_0$. For the time discretization, we use the classical 4th-order Runge-Kutta method in all the examples, and the time step is chosen as $\Delta t = 0.01$.

4.1 BKW solution

For the Maxwell gas $\eta = 5$, the original spatially homogeneous Boltzmann equation (2.8) admits an exact solution with explicit expression:

$$f(t, v) = (2\pi \tau(t))^{-3/2} \exp \left( -\frac{|v|^2}{2\tau(t)} \right) \left[ 1 + \frac{1 - \tau(t)}{\tau(t)} \left( \frac{|v|^2}{2\tau(t)} - \frac{3}{2} \right) \right],$$

11
where $\tau(t) = 1 - \exp\left(\frac{\pi}{3} \tilde{B}_2^n(t + t_0)\right)$. In order that $f(v) \geq 0$ for all $t \in \mathbb{R}_+$ and $v \in \mathbb{R}^3$, the parameter $t_0$ must satisfy

$$-\frac{\pi}{3} \tilde{B}_2^n t_0 \geq \log\left(\frac{5}{2}\right) \approx 0.916291.$$  

(4.1)

Here we choose $t_0$ such that the left hand side of (4.1) equals to 0.92. To ensure a good approximation of the initial distribution function, we use $M_0 = 20$ (1771 degrees of freedom) in our simulation. For visualization purpose, we define the marginal distribution functions (MDFs)

$$g(t, v_1) = \int_{\mathbb{R}} f(t, v) \, dv_2 \, dv_3, \quad h(t, v_1, v_2) = \int_{\mathbb{R}} f(t, v) \, dv_3.$$ 

The initial MDFs are plotted in Figure 1, in which the lines for exact functions and their numerical approximation are hardly distinguishable.

![Figure 1](image1.png)

Figure 1: Initial marginal distribution functions. In (a) and (b), the blue solid lines correspond to the exact solution, and the red dashed lines correspond to the numerical approximation. Figure (c) shows only the numerical approximation.

Numerical results for $t = 0.2$, 0.4 and 0.6 are given in Figures 2 and 3 respectively for $M_0 = 5$ and $M_0 = 10$. For $M_0 = 5$, the numerical solution provides a reasonable approximation, but still with noticeable deviations, while for $M_0 = 10$, the two solutions match perfectly in all cases. To study the computational time, we run the simulation for $M_0 = 3, \ldots, 12$ until $t = 5$. The relation between the computational time and the value of $M_0$ is plotted in Figure 4. It can be seen that when $M_0$ is large, the computational time is roughly proportional to the cube of the number of degrees of freedom. Note that the computational time also includes the time for processing the coefficients of basis functions with degree between $M_0 + 1$ and $M$. Although the time complexity is only linear, when $M_0$ is small, the number of such coefficients is quite large, and they have a significant contribution to the total computational time. This explains why the curve in Figure 4 decreases fast for the first few points.

Now we consider the time evolution of the moments. By expanding the exact solution into Hermite series, we get the exact solution for the coefficients:

$$f_{k_1k_2k_3}(t) = \begin{cases} 
-\frac{1}{2} \exp\left(\frac{\pi}{3} \tilde{B}_2^n(t + t_0)\right) \frac{1 - (k_1 + k_2 + k_3)/2}{(k_1/2)!(k_2/2)!(k_3/2)!}, & \text{if } k_1, k_2, k_3 \text{ are even}, \\
0, & \text{otherwise}.
\end{cases}$$

Due to the symmetry of the distribution function, the coefficients $f_{k_1k_2k_3}$ are zero for any $t$ if $1 \leq k_1 + k_2 + k_3 \leq 3$. Hence we will focus on the coefficients $f_{400}$ and $f_{220}$, which are the fourth
moments of the distribution function. For Maxwell molecules, the discrete kernel $A_{k_1 k_2 k_3}^{l_1 l_2 l_3}$
Figure 4: The horizontal axis is the value of $M_0$, and the vertical axis is the value of $T_{M_0}/N_{M_0}^3$, where $T_{M_0}$ is the computational time (in milliseconds) for given $M_0$ and $N_{M_0}$ is defined in (3.25).

is nonzero when $k_1 + k_2 + k_3 = l_1 + l_2 + l_3 + m_1 + m_2 + m_3$. Therefore, for any $M \geq M_0 \geq 4$, the numerical results for these two coefficients $f_{400}$ and $f_{220}$ are exactly the same (regardless of round-off errors). Figure 5 gives the comparison between the numerical solution and the exact solution for these two coefficients. In both plots, the two lines almost coincide with each other.

Figure 5: The evolution of the coefficients. The blue lines correspond to the reference solution, and the red lines correspond to the numerical solution.

4.2 Bi-Gaussian initial data

In this example, we perform the numerical test for hard potential $\eta = 10$. The initial distribution function is

$$f(0, v) = \frac{1}{2\pi^{3/2}} \left[ \exp \left( -v_1 + \sqrt{3/2} + v_2^2 + v_3^2 \right) + \exp \left( -v_1 - \sqrt{3/2} + v_2^2 + v_3^2 \right) \right].$$

Again, in all our numerical tests, we use $M = 20$ which gives a good approximation of the initial distribution function (see Figure 6).

For this example, we consider the three cases $M_0 = 5, 10, 15$, and the corresponding one-dimensional marginal distribution functions at $t = 0.3, 0.6$ and 0.9 are given in Figure 7. In all the results, the lines for $M_0 = 10$ and $M_0 = 15$ are very close to each other. Due to the fast convergence of the spectral method, it is believable that $M_0 = 10$ can already provide a very good approximation. To get a clearer picture, similar comparison of two-dimensional results are also provided in Figure 8 and 9.

Now we consider the evolution of the moments. In this example, we always have $\sigma_{11} = -2\sigma_{22} = -2\sigma_{33}$ and $q_1 = q_2 = q_3 = 0$. Therefore we focus only on the evolution of $\sigma_{11}$, which
Figure 6: Initial marginal distribution functions. In (a) and (b), the blue solid lines correspond to the exact solution, and the red dashed lines correspond to the numerical approximation. Figure (c) shows only the numerical approximation.

Figure 7: Marginal distribution functions at different times.

Figure 8: Comparison of numerical results using $M_0 = 5$ and $M_0 = 15$. The blue contours and the red dashed contours are respectively the results for $M_0 = 5$ and $M_0 = 15$. It can be seen that three tests give almost identical results. Even for $M_0 = 5$, while the distribution function is not approximated very well, the evolution of the stress tensor is almost exact.
Figure 9: Comparison of numerical results using $M_0 = 10$ and $M_0 = 15$. The blue contours and the red dashed contours are respectively the results for $M_0 = 10$ and $M_0 = 15$.

Figure 10: Evolution of $\sigma_{11}(t)$. Three lines are on top of each other.

4.3 Discontinuous initial data

Here we consider the problem with a discontinuous initial condition:

$$f(0, v) = \begin{cases} 
\frac{\sqrt{2}(2 - \sqrt{2})}{\pi^{3/2}} \exp \left( \frac{-|v|^2}{\sqrt{2}} \right), & \text{if } v_1 > 0, \\
\frac{\sqrt{2}(2 - \sqrt{2})}{4\pi^{3/2}} \exp \left( \frac{-|v|^2}{2\sqrt{2}} \right), & \text{if } v_1 < 0.
\end{cases}$$

We refer the readers to [7] for the graphical profile of this initial value. As a spectral method, the truncated expansion (3.23) is difficult to capture an accurate profile of a discontinuous function. Therefore, we focus only on the evolution of the moments. The left column of Figure [11] shows the numerical results for $\eta = 10$ with different choices of $M_0$ and $M$. All the numerical tests show that the magnitude of the stress components $\sigma_{11}$ and $\sigma_{22}$, which are initially zero, increases to a certain number before decreasing again. Such phenomenon cannot be captured by the simple BGK-type models. The lines corresponding to the results of $M_0 = 10$, $M = 40$ and $M_0 = 15$, $M = 60$ are very close to each other, which indicates that they might be very close to the exact solution. For the case $M_0 = 5$, $M = 20$, although an obvious error can be observed, the trends of the evolution are qualitatively correct, and thus the corresponding collision model $Q_5[f]$ may also be used as a better alternative to the BGK-type models. For the heat flux $q_1$, the three results are hardly distinguishable.

The right column of Figure [11] gives the same moments for the soft potential $\eta = 3.1$. For
Figure 11: Evolution of the stress and the heat flux. The left column shows the results for $\eta = 10$, and the right column shows the results for $\eta = 3.1$. In the right column, the horizontal axes are the scaled time (see (4.2) and the context for details).

By such scaling, the two models $\eta = 10$ and $\eta = 3.1$ have the same mean relaxation time near equilibrium. The two columns in Figure 11 show quite different behavior for different collision models, while both numerical results indicate the high efficiency of this method in capturing the behavior of the moments.
5 Conclusion

This work aims at an affordable way to model and simulate the binary collision between gas molecules. Our new attempt is an intermediate approach between a direct discretization of the quadratic Boltzmann collision operator and simple modelling methods like BGK-type operators. In detail, we first focus on the relatively important physical quantities, which are essentially the first few coefficients in the Hermite expansion, and use an intricate and accurate way to describe their evolution. The strategy comes from the discretization of the quadratic collision operator. For the less important quantities, we borrow the idea of the BGK-type operators and let them converge to the equilibrium at a constant rate. Although the first part is computationally expensive, we can restrict the number of degrees of freedom such that the computational cost is acceptable. The accuracy of such a model depends apparently on the size of the accurately modelled part.

Our numerical examples show that this method can efficiently capture the evolution of lower-order moments in the spatially homogeneous Boltzmann equation. The method should be further validated in the numerical tests for the full Boltzmann equation with spatial variables, which will be one of the future works. Besides, we are also working on the reduction of the computational cost for the quadratic part.

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A Proof of Theorem 1

In order to prove Theorem 1, we first introduce the lemma below:

Lemma 3. Let \( v = h + g/2 \) and \( w = h - g/2 \). It holds that

\[
H^{k_1 k_2 k_3} (v) H^{l_1 l_2 l_3} (w) = \sum_{k_1' + l_1' = k_1 + l_1} \sum_{k_2' + l_2' = k_2 + l_2} \sum_{k_3' + l_3' = k_3 + l_3} a_{k_1' l_1'} a_{k_2' l_2'} a_{k_3' l_3'} H^{k_1' k_2' k_3'} (\sqrt{2}h) H^{l_1' l_2' l_3'} \left( \frac{g}{\sqrt{2}} \right),
\]

where the coefficients \( a_{k_s l_s} \), \( s = 1, 2, 3 \) are defined in (3.7).

Proof of Lemma 3. First, it is easy to verify that \( \exp \left( -\frac{1}{2} |v|^2 + \frac{|w|^2}{2} \right) = \exp \left( - \left( |h|^2 + \frac{|g|^2}{4} \right) \right) \) and \( dv \, dw = dg \, dh \). Based on the orthogonality of the Hermite polynomials (2.18), we just need to prove

\[
\zeta_{k_1 k_2 k_3 l_1 l_2 l_3} = \begin{cases} 
  k_1' l_1' k_2' l_2' k_3' l_3', & \text{if } k_s + l_s = k'_s + l'_s, \quad \forall s = 1, 2, 3, \\
  0, & \text{otherwise,}
\end{cases}
\]

(A.1)
From the orthogonality of Hermite polynomials and the differentiation relation

By the general Leibniz rule, we have the following relation for the derivatives of with respect to $v, w$ and $g, h$:

Then, following the definition of Hermite polynomials (2.17) and (A.3), and using integration by parts, we arrive at

From the orthogonality of Hermite polynomials and the differentiation relation

it holds that (A.4) is nonzero only when $i_s + j_s = k'_s$, $i'_s + j'_s = l'_s$, $s = 1, 2, 3$, which means

When (A.6) holds, we can apply (A.5) to (A.4) and get

Thus (A.1) is shown, which completes the proof of the lemma. □

**Corollary 1.** Let $v = h + g/2$. We have

**Proof of Corollary**

**Proof of Theorem** Let $w = v'$, $w_1 = v'_1$, $s = w - w_1$ and define the unit vector $\tilde{n}$ as $\tilde{n} = -(g \sin \chi / |g| + n \cos \chi)$. It holds that

|a| = |g|, \quad s \cdot n_w = 0,

\begin{align*}
|v|^2 + |v_1|^2 &= |w|^2 + |w_1|^2, \\
\mathrm{d}v \, \mathrm{d}v_1 &= \mathrm{d}w \, \mathrm{d}w_1, \\
|s| &= |g|, \\
\mathbf{w}' &= \cos^2(\chi/2)\mathbf{w} + \sin^2(\chi/2)\mathbf{w}_1 - |s|\cos(\chi/2)\sin(\chi/2)n_w = \mathbf{v},
\end{align*}

(A.8)
Combining Lemma 3, Corollary 1 and (A.12), we can rewrite (A.10) as an integral with respect to $\gamma$

$$\int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{n \perp \mathbf{g}} \int_0^\pi B(|\mathbf{g}|, \chi) H^{i_1 i_2 i_3}(\nu') H^{j_1 j_2 j_3}(\nu') H^{k_1 k_2 k_3}(\nu) \exp \left(-\frac{|\nu|^2 + |\nu_1|^2}{2}\right) d\chi d\nu_1 d\nu d\nu_1 d\nu.$$

Further simplification of (A.10) follows the method in [16], where the velocity of the mass center is defined as $h = (v + v_1)/2 = (v' + v_1)/2$. Hence,

$$v = h + \frac{1}{2} g, \quad v_1 = h - \frac{1}{2} g, \quad v' = h + \frac{1}{2} g', \quad v_1' = h - \frac{1}{2} g', \quad |v|^2 + |v_1|^2 = \frac{1}{2} |g|^2 + 2|h|^2, \quad dv dv_1 = dg dh. \quad (A.11)$$

Combining Lemma 3, Corollary 1 and (A.12), we can rewrite (A.10) as an integral with respect to $\mathbf{g}$ and $h$:

$$A_{111213,111213}^{i_1 i_2 i_3, j_1 j_1 j_3} = \sum_{l_1+j_1} \sum_{l_2+j_2} \delta_{i_1 l_1} \delta_{i_2 l_2} \delta_{i_3 l_3} \eta_{l_1 l_2 l_3}^{k_1 k_2 k_3} \frac{1}{(2\pi)^3 k_1 k_2 k_3} \int_{\mathbb{R}^3} B(|\mathbf{g}/\sqrt{2h}|, \chi) \left[H^{k_1 k_2 k_3}(\mathbf{v}) - H^{k_1 k_2 k_3}(\mathbf{v}_1)\right] \exp \left(-\frac{|\mathbf{g}^2 + |\mathbf{v}_1|^2}{2}\right) d\chi d\nu_1 d\nu d\nu_1 d\nu. \quad (A.13)$$

where the coefficients $\gamma_{l_1 l_2 l_3}^{k_1 k_2 k_3}$ defined in (A.8) are integrals with respect to $\mathbf{g}$, and $\eta_{l_1 l_2 l_3}^{k_1 k_2 k_3}$ are integrals with respect to $h$ defined by

$$\eta_{l_1 l_2 l_3}^{k_1 k_2 k_3} = \int_{\mathbb{R}^3} H^{l_1 l_2 l_3}(\sqrt{2h}) H^{k_1 k_2 k_3}(\sqrt{2h}) \exp(-|h|^2) dh = \pi^{3/2} k_1 k_2 k_3 \delta_{l_1 l_1} \delta_{l_2 l_2} \delta_{l_3 l_3}. \quad (A.14)$$

Thus the theorem is proven by substituting (A.14) into (A.13). \(\Box\)

**B Proof of Theorem 2**

We will first prove Theorem 2 based on several lemmas, and then prove these lemmas.

**B.1 Proof of Theorem 2**

In order to prove Theorem 2, we will introduce the definition of Ikenberry polynomials [20] and several lemmas.
Lemma 5. The Hermite polynomial

\[ Y(v) = 1, \quad Y_i(v) = v_i, \]
\[ Y_{i_1 \cdots i_n}(v) = v_{i_1} \cdots v_{i_n} + |v|^2 S_{n-2}^{i_1 \cdots i_n}(v) + |v|^4 S_{n-4}^{i_1 \cdots i_n}(v) + \cdots + |v|^{2(n/2)} S_{n-2n/2}^{i_1 \cdots i_n}(v), \]

where \( S_j^{i_1 \cdots i_n} \) is a homogeneous harmonic polynomial of degree \( j \) defined in [20], which can be determined by
\[ \Delta_v Y_1 \cdots i_n = \Delta_v^2 Y_1 \cdots i_n = \Delta_v^{[n/2]} Y_1 \cdots i_n = 0. \]

For \( k_1, k_2, k_3 \in \mathbb{N} \), define \( Y^{k_1 k_2 k_3}(v) \) as the polynomial \( Y_{i_1 \cdots i_n}(v) \) with
\[ n = k_1 + k_2 + k_3, \quad i_1 = \cdots = i_{k_1} = 1, \]
\[ i_{k_1+1} = \cdots = i_{k_1+k_2} = 2, \quad i_{k_1+k_2+1} = \cdots = i_n = 3. \]

Lemma 4. The integral
\[ \int_{\mathbb{S}^2} Y^{k_1 k_2 k_3}(n) Y^{i_1 i_2 i_3}(n) \, dn \]
is the coefficient of \( v_1^{k_1} v_2^{k_2} v_3^{k_3} w_1^{i_1} w_2^{i_2} w_3^{i_3} \) in the polynomial
\[ \frac{4\pi}{2k + 1} \frac{k_1! k_2! k_3! i_1! i_2! i_3!}{[(2k - 1)!!]^2} (|v||w|)^k P_k \left( \frac{v}{|v|}, \frac{w}{|w|} \right), \quad k = k_1 + k_2 + k_3. \]

Lemma 5. The Hermite polynomial \( H^{k_1 k_2 k_3}(v) \) can be represented as
\[ H^{k_1 k_2 k_3}(v) = \sum_{m_1=0}^{[k_1/2]} \sum_{m_2=0}^{[k_2/2]} \sum_{m_3=0}^{[k_3/2]} \frac{(-1)^m m! (2k - 4m + 1)!!}{(2k - m)!! (2k - m + 1)!!} \left( \prod_{i=1}^{3} \frac{k_i!}{m_i! (k_i - 2m_i)!} \right) \]
\[ L_m^{(k-2m+1/2)} \left( \frac{|v|^2}{2} \right) Y^{k_1-2m_1, k_2-2m_2, k_3-2m_3}(v), \]
where \( k = k_1 + k_2 + k_3 \) and \( m = m_1 + m_2 + m_3 \).

Lemma 6. Given a vector \( g \) and \( \chi \in [0, \pi] \), let \( g'(n) = g \cos \chi - |g| n \sin \chi \), where \( n \) is a unit vector. It holds that
\[ \int_{n \perp g} Y^{k_1 k_2 k_3}(g'/|g|) \, dn = 2\pi Y^{k_1 k_2 k_3}(g'/|g|) P_k(\cos \chi), \]
where \( k = k_1 + k_2 + k_3 \) and \( P_k \) is Legendre polynomial.

In above lemmas, Lemma 4 and Lemma 5 will be proved in Appendix B.2 and B.3 respectively. Lemma 6 is proved in [23]. By Lemma 5 and Lemma 6, we can derive the corollary below

Corollary 2. Given a vector \( g \) and \( \chi \in [0, \pi] \), define \( g'(n) \) the same as in Theorem 6. We have
\[ \int_{n \perp g} H^{k_1 k_2 k_3}(g') \, dn = 2\pi \sum_{m_1=0}^{[k_1/2]} \sum_{m_2=0}^{[k_2/2]} \sum_{m_3=0}^{[k_3/2]} \frac{(-1)^m m! (2k - 4m + 1)!!}{(2k - m)!! (2k - m + 1)!!} \times \]
\[ \left( \prod_{i=1}^{3} \frac{k_i!}{m_i! (k_i - 2m_i)!} \right) L_m^{(k-2m+1/2)} \left( \frac{|g|^2}{2} \right) Y^{k_1-2m_1, k_2-2m_2, k_3-2m_3}(g) P_{k-2m}(\cos \chi), \]
where \( k = k_1 + k_2 + k_3, m = m_1 + m_2 + m_3 \).
functions are defined as
\[ Y_l^m(\theta, \phi) \]
Definition 6
\[ P_l^m(x) = \frac{(-1)^m}{2^l l!} (1 - x^2)^{m/2} \frac{d^{l+m}}{dx^{l+m}} (x^2 - 1)^l. \]

Definition 5 (Associated Legendre functions). For \( m = -l, \ldots, l \), the associated Legendre functions are defined as
\[ P_l^m(x) = \frac{(-1)^m}{2^l l!} (1 - x^2)^{m/2} \frac{d^{l+m}}{dx^{l+m}} (x^2 - 1)^l. \]

Definition 6 (Spherical harmonics). For \( l \in \mathbb{N} \) and \( m = -l, \ldots, l \), the spherical harmonic \( Y_l^m(\theta, \varphi) \) is defined as
\[ Y_l^m(n) = Y_l^m(\theta, \varphi) = \sqrt{\frac{2l + 1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos \theta) \exp(im\varphi), \quad n \in \mathbb{S}^2, \]
where \((\theta, \varphi)\) is the spherical coordinates of \( n \).

Lemma 7 (Addition theorem). For any \( l \in \mathbb{N} \), it holds that
\[ P_l(n_1 \cdot n_2) = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_l^m(n_1) \overline{Y_l^m(n_2)}, \]
where \( P_l \) is Legendre polynomial.

Lemma 8. For any \( l \in \mathbb{N} \), it holds that
\[ (|v||w|)^l P_l \left( \frac{v}{|v|} \cdot \frac{w}{|w|} \right) = \frac{(2l)!}{2^{2l} l!!} \sum_{i_1=1}^{3} \cdots \sum_{i_l=1}^{3} w_{i_1} \cdots w_{i_l} Y_{i_1 \ldots i_l}(v). \]

In the above lemmas, Lemma 7 and Lemma 8 are well-known and their proofs can be found in [11] and [21] respectively. Based on these two lemmas, the following corollary holds.

Corollary 3. The harmonic polynomial \( Y_{k_1 k_2 k_3}(w) \) is the coefficient of the monomial \( w_1^{k_1} w_2^{k_2} w_3^{k_3} \) in the following polynomial of \( w \):
\[ \frac{k_1! k_2! k_3!}{(2k-1)!} (|v||w|)^k P_k \left( \frac{v}{|v|} \cdot \frac{w}{|w|} \right), \quad k = k_1 + k_2 + k_3. \]
Proof of Corollary 3. Since
\[
\sum_{i_1=1}^{3} \cdots \sum_{i_k=1}^{3} w_{i_1} \cdots w_{i_k} Y_{i_1, \ldots, i_k}(v) = \frac{k!}{k_1!k_2!k_3!} \sum_{k_1+k_2+k_3=k} w_{i_1}^k w_{i_2}^k w_{i_3}^k Y_{k_1,k_2,k_3}(v),
\]
and matching the term of \( w_{i_1}^k w_{i_2}^k w_{i_3}^k \) in Lemma 8, we complete this proof. 

Proof of Lemma 4. From Corollary 3, we can derive that \( \int_{S^2} Y_{k_1,k_2,k_3}(n) Y_{l_1,l_2,l_3}(n) \, dn \) is the coefficient of \( v_{i_1}^k v_{i_2}^k v_{i_3}^k w_{i_1}^l w_{i_2}^l w_{i_3}^l \) in the polynomial
\[
\int_{S^2} \left[ \beta_{k_1,k_2,k_3} (|n||v|)^k P_k \left( n \cdot \frac{v}{|v|} \right) \right] \left[ \beta_{l_1,l_2,l_3} (|n||w|)^l P_l \left( n \cdot \frac{w}{|w|} \right) \right] \, dn,
\]
where \( k = k_1 + k_2 + k_3, l = l_1 + l_2 + l_3 \) and \( \beta_{k_1,k_2,k_3} = \frac{k_1!k_2!k_3!}{(2k-1)!} \). Following Theorem 7, it holds
\[
\int_{S^2} \left[ (|n||v|)^k P_k \left( n \cdot \frac{v}{|v|} \right) \right] \left[ (|n||w|)^l P_l \left( n \cdot \frac{w}{|w|} \right) \right] \, dn
\]
\[
= (|v||w|)^{k+l} \frac{(4\pi)^2}{(2k+1)(2l+1)} \sum_{m=-k}^{k} \sum_{n=-l}^{l} Y_k^m(v) Y_l^n(w) \delta_{kk} \delta_{nn}
\]
\[
= \frac{4\pi \delta_{kl}}{2k+1} (|v||w|)^k P_k \left( \frac{v}{|v|} \cdot \frac{w}{|w|} \right).
\]
Thus if \( k = l \), this corollary is proved. If \( k \neq l \), we can deduce that \( \int_{S^2} Y_{k_1,k_2,k_3}(n) Y_{l_1,l_2,l_3}(n) \, dn = 0 \). In this case, the coefficient of \( v_{i_1}^k v_{i_2}^k v_{i_3}^k w_{i_1}^l w_{i_2}^l w_{i_3}^l \) in the polynomial \((|v||w|)^k P_k \left( \frac{v}{|v|} \cdot \frac{w}{|w|} \right)\) is also zero, and this completes the proof. 

B.3 Proof of Lemma 5

We will prove Lemma 5 in this section.

Proof of Lemma 5. Define the homogeneous spherical harmonic \( Z_{i_1, \ldots, i_k}^{(k,m)} \) of degree \( k - 2m \) as
\[
Z_{i_1, \ldots, i_k}^{(k,m)} = \frac{1}{k!} \sum_{\sigma \in S_k} Y_{i_{\sigma(1)}, i_{\sigma(2)}, \ldots, i_{\sigma(k)}} \delta_{i_{\sigma(1)}, i_{\sigma(2)}, \ldots, i_{\sigma(k)}, i_k}, \tag{B.2}
\]
where \( r = k - 2m \) and the sum is taken over all permutations of the set \( \{1, 2, \ldots, k\} \), i.e.
\[
S_k = \{ \sigma \mid \sigma : \{1, 2, \ldots, k\} \to \{1, 2, \ldots, k\} \text{ is a bijection} \}.
\]

It has been proven in \[22\], eqs. (3)(8)(9)(31) that \[1\]
\[
H_{k_1,k_2,k_3}^{(k,m)}(v) = \sum_{m=0}^{(k/2)} \frac{(-1)^m k!(2k - 4m + 1)!!}{(k - 2m)!(2k - 2m + 1)!!} \int_{S^2} |v|^2 \, Z_{i_1, \ldots, i_k}^{(k,m)}(v), \tag{B.3}
\]
where the indices \( i_1, \ldots, i_k \) satisfy:
\[
i_1 = \cdots = i_{k_1} = 1, \quad i_{k_1 + 1} = \cdots = i_{k_1 + k_2} = 2, \quad i_{k_1 + k_2 + 1} = \cdots = i_k = 3.
\]

\[1\]In \[22\], the definition of the Laguerre polynomial differs from Definition 3 by a constant, which makes the coefficient in our paper slightly different from the one in \[22\].
To prove Lemma 5, we just need to provide a more explicit expression for (B.2). In order that the summand in (B.2) is nonzero, the two indices of every Kronecker symbol must be the same. When all the Kronecker symbols take 2m₁ ones, 2m₂ twos and 2m₃ threes as their indices, the summand will actually be $Y^{k₁−2m₁,k₂−2m₂,k₃−2m₃}(v)$ according to Definition 4. Apparently $(m₁,m₂,m₃)$ must be indices from the following set:

$$\mathcal{M}_{k₁k₂k₃}^m = \{(m₁,m₂,m₃) \mid m₁ + m₂ + m₃ = m, 2m₁ \leq k₁, 2m₂ \leq k₂, 2m₃ \leq k₃\}.$$ 

Next, we are going to count how many times $Y^{k₁−2m₁,k₂−2m₂,k₃−2m₃}(v)$ appears in the sum in (B.2). This can be observed by noting that

1. The $m$ Kronecker symbols choosing from $m₁$ pairs of ones, $m₂$ pairs of twos and $m₃$ pairs of threes gives a factor $m!/(m₁!m₂!m₃!)$;

2. The $k − 2m$ indices of $Y$ choosing from $k₁ − 2m₁$ ones, $k₂ − 2m₂$ twos and $k₃ − 2m₃$ threes gives a factor $(k − 2m)!/((k₁ − 2m₁)!(k₂ − 2m₂)!(k₃ − 2m₃)!)$.

3. Permutations of $k₁$ ones, $k₂$ twos and $k₃$ threes give respectively factors $k₁!, k₂!$ and $k₃!$.

Summarizing all these results, we get

$$Z_{i₁i₂⋯iₖ}^{(k,m)} = \frac{1}{k!} \sum_{(m₁,m₂,m₃)\in\mathcal{M}_{k₁k₂k₃}^m} \frac{(k − 2m)!m!}{3 \prod_{i=1}^{3} k_i!} \prod_{i=1}^{3} (k_i − 2m_i)!m_i! Y^{k₁−2m₁,k₂−2m₂,k₃−2m₃}(v). \quad (B.4)$$

By (B.3) and (B.4), the proof is completed. □

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