A multiple-relaxation-time collision model by Hermite expansion

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Abstract

The Bhatnagar-Gross-Krook (BGK) single-relaxation-time collision model for the Boltzmann equation serves as the foundation of the lattice BGK (LBGK) method developed in recent years. The description of the collision as a uniform relaxation process of the distribution function towards its equilibrium is, in many scenarios, simplistic. Based on a previous series of papers, we present a collision model formulated as independent relaxations of the irreducible components of the Hermit coefficients in the reference frame moving with the fluid. These components, corresponding to the irreducible representation of the rotation group, are the minimum tensor components that can be separately relaxed without violating rotation symmetry. For the 2nd, 3rd and 4th moments respectively, two, two and three independent relaxation rates can exist, giving rise to the shear and bulk viscosity, thermal diffusivity and some high-order relaxation process not explicitly manifested in the Navier-Stokes-Fourier equations. Using the binomial transform, the Hermite coefficients are evaluated in the absolute frame to avoid the numerical dissipation introduced by interpolation. Extensive numerical verification is also provided.

I. INTRODUCTION

A well-known artifact of the Bhatnagar-Gross-Krook (BGK) collision model [1] is the uniform relaxation of the distribution function towards its equilibrium which bound all transport coefficients, e.g., the shear and bulk viscosity and thermal diffusivity, to a single relaxation time. The most noticeable manifestation is that the Prandtl number is unphysically fixed at unity. For kinetic theory in continuum, a couple of remedies [2, 3] were suggested by explicitly dialing the Prandtl number in the equilibrium distribution. In the context of the lattice BGK model [4], the multiple-relaxation-time (MRT) LB models [5] was proposed to independently relax the eigen-states of the discrete distribution corresponding to the hydrodynamic moments. The details of this decomposition of the discrete distribution is lattice-dependent. As the velocity sets used in this class of MRT models are insufficient for representing the third-order moments, the unity Prandtl number was not fixed although the original MRT model was widely used for its improved numerical stability.

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In a previous series of papers [6–9], an Hermite expansion based lattice-independent MRT collision model was developed. The basic idea is to expand the collision term in terms of Hermite polynomials [10, 11] and assign a separate relaxation time to each of the terms. As the viscous and thermal transports are given by the second and third moments separately, decoupling of the two were naturally achieved. Furthermore, using sufficiently accurate quadrature rules in the velocity space, the energy equation can be recovered. Although yielding an adjustable Prandtl number, the first version [6] relaxes the raw moments and results in a Mach-number-dependent thermal diffusivity similar to the well known “cubic error” [12] when the thermal diffusivity is different from the viscosity. The second version [7,8] relaxes the central moments and restored the Galilean invariance. Furthermore, by using the binomial transform, the relaxation of the central moments is carried out in the absolute reference frame without incurring the additional numerical dissipation due to interpolation. In a more recent work [9], the relaxation was applied at the even finer scope of the irreducible representation of the rotation group which is the minimal tensor space closed under spatial rotation. For the second moment, this yields independent shear and bulk viscosity.

The present work gives in detail a coherent presentation of the multi-relaxation model. In particular, the tensor decomposition beyond the second rank is given. For the third-rank tensor one of the two possible relaxation times is identified with the relaxation rate of the translational kinetic energy while the other, and all three of the fourth-rank tensor, are found to have no significant effect to the four linear hydrodynamic modes. Similar to the BGK operator, the first-order spac-time discretization is found to give second-order accuracy as long as the relaxation times are shifted by one half. The paper is organized as the following. In Sec. II we give the theoretical formulation of the model. Numerical verification of the transport coefficients using the linear hydrodynamic modes are presented in Sec. III. In Sec. IV further discussion are given. More mathematical details pertaining to the binomial transform between the moving and laboratory frames are given in the Appendix.
II. MODEL CONSTRUCTION

A. Velocity-space discretization by Hermite expansion

Starting from the Boltzmann-BGK equation:

\[
\frac{\partial f}{\partial t} + \xi \cdot \nabla f = \Omega(f) \equiv -\frac{1}{\tau} [f - f^{(0)}],
\]

where \( f(x, \xi, t) \) is the single-particle distribution function, \( \xi \) the microscopic velocity, \( x \) and \( t \) the space and time, and \( f^{(0)} \) the Maxwell-Boltzmann equilibrium distribution:

\[
f^{(0)} = \frac{\rho}{(2\pi\theta)^{D/2}} \exp \left[ -\frac{\xi - u}{2\theta} \right],
\]

where \( \rho, u \) and \( \theta \) are the fluid density, velocity and temperature respectively, all non-dimensionalized using the scheme given in Ref. \[11\].

The lattice-Boltzmann equation \[4\] can be formulated as a velocity discretization of Eq. (1) \[11\]. Expanding \( f \) in Hermite series and truncating at order \( N \):

\[
f^{(N)}(x, \xi, t) = \omega(\xi) \sum_{n=0}^{N} \frac{1}{n!} a^{(n)}(x, t) : \mathcal{H}^{(n)}(\xi),
\]

where \( \omega(\xi) \equiv (2\pi)^{-D/2} \exp(-\xi^2/2) \) is the weight function, \( \mathcal{H}^{(n)} \) the \( n \)-th Hermite polynomial, and \( a^{(n)} \) the expansion coefficients given by:

\[
a^{(n)} = \int f^{N}(\xi) \mathcal{H}^{(n)}(\xi) d\xi.
\]

Let \( \{(\xi_i, w_i), i = 1, \cdots, d\} \) be the set of abscissas and weights of a \( Q \)-th degree quadrature such that the identity:

\[
\int \omega(\xi)p(\xi)d\xi = \sum_{i=1}^{d} w_i p(\xi_i),
\]

holds for all \( Q \)-th degree polynomial, \( p(\xi) \). Since \( f^{N}(\xi)/\omega(\xi) \) is a polynomial of a degree \( \leq N \), defining

\[
f_i \equiv \frac{w_i f^{(N)}(\xi_i)}{\omega(\xi_i)},
\]

as long as \( Q \geq 2N \), the following isomorphism between the discrete distribution, \( f_i \), and the moment, \( a^{(n)} \) can be established using Eqs. (4) and (3):

\[
a^{(n)} = \sum_{i=1}^{d} f_i \mathcal{H}^{(n)}(\xi_i), \quad \text{and} \quad f_i = w_i \sum_{n=0}^{N} \frac{1}{n!} a^{(n)} : \mathcal{H}^{(n)}(\xi_i).
\]

On evaluating Eq. (1) at \( \xi_i, f_i \) obeys the following lattice BGK equation:

\[
\frac{\partial f_i}{\partial t} + \xi_i \cdot \nabla f_i = \Omega_i \equiv -\frac{1}{\tau} [f_i - f^{(0)}].
\]
B. Chapman-Enskog asymptotic expansion

To determine the minimum conditions for the collision term to yield correct hydrodynamic equations, we now briefly recap how the hydrodynamic equations are derived from Eqs. (1) \[13\]. As required by fundamental physics, the collision term conserves mass, momentum and kinetic energy. By taking the corresponding moments of Eqs. (1), we have the conservation equations:

\[
\frac{d\rho}{dt} + \rho \nabla \cdot \mathbf{u} = 0, \quad (9a) \\
\rho \frac{d\mathbf{u}}{dt} + \nabla \cdot \mathbf{P} = 0, \quad (9b) \\
\rho \frac{d\varepsilon}{dt} + \nabla \cdot \mathbf{u} : \mathbf{P} + \nabla \cdot \mathbf{q} = 0, \quad (9c)
\]

where \(\frac{d}{dt} \equiv \partial/\partial t + \mathbf{u} \cdot \nabla\) is the material derivative, and

\[
P \equiv \int f c c d\mathbf{c}, \quad \text{and} \quad q \equiv \frac{1}{2} \int f c^2 d\mathbf{c},
\]

are the pressure tensor and energy flux respectively. Eqs. (9) must be closed by expressing \(P\) and \(q\) in terms of \(\rho, u, \theta\). At the crudest level \(f\) in Eq. (10) is approximated by \(f^{(0)}\) to yield \(P^{(0)} = \rho \theta \delta\) and \(q^{(0)} = 0\), which lead to the Euler’s equations. More accurate hydrodynamic equations are obtained via the Chapman-Enskog asymptotic calculation \[13\] \[14\]. Let \(f \approx f^{(0)} + f^{(1)}\) where \(f^{(1)} \ll f^{(0)}\) is the first approximation of the non-equilibrium part of the distribution. On substituting into Eq. (1) and keeping only the leading terms on both sides, we have:

\[
\frac{\partial f^{(0)}}{\partial t} + \mathbf{\xi} \cdot \nabla f^{(0)} = \Omega = -\frac{f^{(1)}}{\tau}. \quad (11)
\]

The left-hand-side is then written in terms of \(\rho, u, \theta\) and their spatial derivatives with the help of Euler’s equations. By taking the moments in Eqs. (10) of both sides, \(P^{(1)}\) and \(q^{(1)}\) are expressed in terms of \(\rho, u, \theta\). When plugged into Eq. (9), we arrive at the Navier-Stokes equations.

As shown previously \[11\], this procedure survives the velocity-space discretization of Eqs. (7). Furthermore, it was realized \[8\] that the same \(P^{(1)}\) and \(q^{(1)}\) with independent proportional coefficients are obtained as long as the following conditions are met:

\[
\int \Omega c^n d\mathbf{c} = -\frac{1}{\tau_n} \int f^{(1)} c^n d\mathbf{c}, \quad \text{for} \quad n = 2, 3, \quad (12)
\]
where $\tau_n$ are separate relaxation times. Here both sides vanish for $n = 0$ and 1 due to conservation of mass and momentum. The BGK operator is a special case with $\tau_2 = \tau_3 = \tau$. A natural generalization is to require Eq. (12) to hold for all $n$ up to the order supported by the underlying quadrature so that each of the central moments is independently relaxed with relaxation time $\tau_n$.

We now formulate the collision operator in the spectral space of Hermite polynomials. Defining $v \equiv (\xi - u)/\sqrt{\theta}$ and the corresponding Hermite expansion:

$$f(v) = \omega(v) \sum_{n=0}^{\infty} \frac{1}{n!} d^{(n)}(x, t) : \mathcal{H}^{(n)}(v),$$

(13)

where $d^{(n)}$ is the $n$-th expansion coefficient. Note that the expansion above is in the moving reference frame and scaled by local temperature. It is exactly the same expansion used by Grad [10]. Denoting the expansion coefficients of $f^{(0)}$ and $f^{(1)}$ by $d_0^{(n)}$ and $d_1^{(n)}$ respectively, we have $d_0^{(0)} = \rho$, $d_0^{(n)} = 0$ for all $n > 0$, and:

$$f^{(1)} = \omega(v) \sum_{n=2}^{\infty} \frac{1}{n!} d_1^{(n)} : \mathcal{H}^{(n)}(v).$$

(14)

The collision operator is defined via its Hermite expansion coefficients as:

$$d_1^{(n)} = -\frac{1}{\tau_n} d_1^{(n)}, \text{ for } n = 2, \cdots, \infty.$$

(15)

It can be verified to satisfy Eq. (12).

C. Tensor decomposition

As $d_1^{(n)}$ and $d_1^{(n)}$ are tensors consisting of multiple components, a question arises as if the relaxation can be made at a finer scale. We note that the tensor space of a given rank can be decomposed into subspaces that furnish the irreducible representations of the rotation group SO(3) which are the minimal units closed under spatial rotation [15]. Particularly, a rank-$n$ fully symmetric tensor can be decomposed into irreducible components by repeatedly subtract from it its rank-$(n-2)$ traces [16]. Assuming Einstein summation convention, the explicit decomposition of the 2nd, 3rd and 4th rank symmetric tensors in $d$-dimensions
where $a'_{ij}$, $a'_{ijk}$ and $a'_{ijkl}$ are all traceless, meaning that the contractions with respect to any pair of indexes vanishes, and

$$a''_{ppij} = a_{ppij} - \frac{1}{d} a_{ppqq} \delta_{ij}$$

is a traceless second rank tensor. Denote the $k$-th irreducible components of $d^{(n)}_1$ and $d^{(n)}_\Omega$ by $d^{(n)}_{1,k}$ and $d^{(n)}_{\Omega,k}$, respectively in the orders of the terms on the right-hand-side of Eqs. (16).

The collision operator defined by Eq. (15) can be further refined as:

$$d^{(n)}_{\Omega,k} = -\frac{1}{\tau_{nk}} d^{(n)}_{1,k},$$

where $k \in \{1, 2\}$ for $n = 2, 3$, and $k \in \{1, 2, 3\}$ for $n = 4$. Thus, up to the 4th order, we can have up to seven independent relaxation times: $\tau_{21}$ and $\tau_{22}$ for $d^{(2)}_\Omega$, $\tau_{31}$ and $\tau_{32}$ for $d^{(3)}_\Omega$, and $\tau_{41}$, $\tau_{42}$, $\tau_{43}$ for $d^{(4)}_\Omega$. Among them, $\tau_{21}$, $\tau_{22}$ and $\tau_{32}$ dictate respectively the shear viscosity, bulk viscosity in a gas with internal degrees of freedom, and thermal diffusivity. The other four do not explicitly manifest in the Navier-Stokes-Fourier equations.

D. Binomial transform

Direct determination of $d^{(n)}_1$ and $d^{(n)}_\Omega$ from $f(v_i)$ by Eqs. (7) requires an interpolation scheme of some kind as $v_i$ depends on $u$ and $\theta$ and varies with space and time [18, 19]. To avoid the associated numerical dissipation, the binomial transform, Eq. (A25), between the Hermite expansion coefficients in the absolute and relative frame can be used to obtain $d^{(n)}_1$ from $a^{(n)}_1$ as:

$$\theta \frac{D + 2}{4} d^{(2)}_1 = a^{(2)}_1,$$

$$\theta \frac{D + 3}{4} d^{(3)}_1 = a^{(3)}_1 - 3u a^{(2)}_1,$$

$$\theta \frac{D + 4}{4} d^{(4)}_1 = a^{(4)}_1 - 4u a^{(3)}_1 + 6 [uu + (1 - \theta) \delta] a^{(2)}_1,$$
and from $d^{(n)}_\Omega$ to $a^{(n)}_\Omega$ as:

$$a^{(2)}_\Omega = \frac{\tau^2}{\theta^2} d^{(2)}_\Omega,$$

$$a^{(3)}_\Omega = \frac{\tau^3}{\theta^2} d^{(3)}_\Omega + 3u a^{(2)}_\Omega,$$

$$a^{(4)}_\Omega = \frac{\tau^4}{\theta^2} d^{(4)}_\Omega + 4u a^{(3)}_\Omega - 6[uu + (1 - \theta)\delta] a^{(2)}_\Omega. \tag{20c}$$

Here the fact that $a^{(n)}_\Omega = a^{(n)}_\Omega = 0$ for $n = 0, 1$ is used. On substituting Eqs. (19) into Eqs. (20), we have:

$$a^{(2)}_\Omega = -\omega_2 a^{(2)}_1,$$

$$a^{(3)}_\Omega = -\omega_3 a^{(3)}_1 + 3(\omega_3 - \omega_2) u a^{(2)}_1,$$

$$a^{(4)}_\Omega = -\omega_4 a^{(4)}_1 + 4(\omega_4 - \omega_3) u a^{(3)}_1$$

$$-6[(\omega_4 + \omega_2 - 2\omega_3)uu + (\omega_4 - \omega_2)(1 - \theta)\delta] a^{(2)}_1. \tag{21c}$$

The only difference with the previous model without temperature scaling \cite{7, 8} is the additional factor of $1 - \theta$ in Eq. (21c).

### E. Space-time discretization

To numerically solve Eq. (8), the time and spatial derivatives on the left-hand-side must be discretized. Integrating using the first-order forward-Euler scheme from $t = 0$ to 1, we have:

$$f_i(x + \xi_i, t + 1) - f_i(x, t) = \Omega(f_i). \tag{22}$$

It is well-known \cite{4} that the effect of the implicit second-order error can be absorbed into the dissipation term, effectively making the scheme second-order accurate with a viscosity proportional to $\tau + 1/2$ instead of $\tau$. Alternatively, a second-order implicit scheme can be obtained by integrating Eq. (8) using the trapezoidal rule \cite{20}:

$$f_i(x + \xi_i, t + 1) - f_i(x, t) = \frac{1}{2} \left[ \Omega(f_i(x + \xi_i, t + 1)) + \Omega(f_i(x, t)) \right]. \tag{23}$$

With the BGK operator, by introducing an auxiliary variable, it was shown that the dynamics of the distribution at the second order is equivalent to that at the first order with $\tau$ replaced by $\tau + 1/2$ \cite{20}. With the more complicated collision operator defined above, such a change-of-variable is not directly possible. Nevertheless the dynamics of the moments can be
analyzed in a similar fashion. Define the moment operator $M_{n,k}(f_i)$ as the $k$-th component of the $n$th order moment of $f_i$. Noting that:

$$M_{n,k}(\Omega(f_i)) = -\frac{1}{\tau_{nk}} \left[ M_{n,k}(f_i) - M_{n,k}(f_i^{(0)}) \right], \quad (24)$$

by taking moments of Eq. (23) and noting $f_i(x + \xi_i, t + 1)$ is the out-going distribution after collision, we write:

$$M_{n,k}^{\text{out}} - M_{n,k}^{\text{in}} = -\frac{1}{\tau_{nk}} \left[ \frac{1}{2} (M_{n,k}^{\text{out}} + M_{n,k}^{\text{in}}) - M_{n,k}^{\text{eq}} \right]. \quad (25)$$

where the superscripts $\text{out}$, $\text{in}$ and $\text{eq}$ denote respectively the out-going, in-coming and equilibrium moments. After some straightforward manipulations, we have:

$$M_{n,k}^{\text{out}} - M_{n,k}^{\text{in}} = -\frac{1}{\tau_{nk} + 1/2} \left[ M_{n,k}^{\text{in}} - M_{n,k}^{\text{eq}} \right]. \quad (26)$$

Evidently, at the second order of space-time discretization, the behavior of the moments, consequently the hydrodynamics, is the same as that at the first order but with $\tau_{nk}$ replaced by $\tau_{nk} + 1/2$. This correspondence is essentially a consequence of the orthogonal relaxation of the moments.

The actual implementation of the collision operator goes as the following. From the post-streaming $f_i$, we compute $f_i^{(0)}$ and then $f_i^{(1)}$. Using Eq. (7) we obtain $a_i^{(n)}$ and then $d_i^{(n)}$ using Eqs. (19). Decomposing $d_i^{(n)}$ according to Eqs. (16) if necessary, applying the relaxation factor according to Eqs. (18) and re-assembling, we obtain $d_i^{(n)}$ and then $a_i^{(n)}$ using Eqs. (20). Using the second part of Eq. (7) to calculate the bracket on the right-hand-side of Eq. (22) all together which effectively trims the part of the distribution function lying outside of the functional space spanned by the Hermite polynomials.

### III. NUMERICAL VERIFICATION

To verify the model, the transport coefficients are measured form the dynamics of the linear hydrodynamic modes and compared with their theoretical values. The case setup has been extensively discussed previously [6, 8, 21]. Here we briefly summarize the analytical results. Consider the monochromatic plane wave perturbation:

$$\begin{pmatrix} \rho \\ u \\ \theta \end{pmatrix} = \begin{pmatrix} \rho_0 \\ u_0 \\ \theta_0 \end{pmatrix} + \begin{pmatrix} \bar{\rho} \\ \bar{u} \\ \bar{\theta} \end{pmatrix} e^{i\omega t + ik \cdot (x - u_0 t)} \quad (27)$$
where the subscript 0 denotes the base flow and $\bar{\rho}$, $\bar{u}$ and $\bar{\theta}$ perturbation amplitudes. $k$ and $\omega$ respectively are the wave vector and angular frequency of the plane wave. Decomposing the velocity into components parallel and perpendicular to the wave vector and substituting into the Navier-Stokes-Fourier equation, we obtain an eigen-system in the linear space of $(\bar{\rho}, \bar{u}_\parallel, \bar{\theta}, \bar{u}_\perp)^T$ where $\bar{u}_\parallel$ and $\bar{u}_\perp$ are the amplitudes of velocity perturbation in the parallel and perpendicular directions. The dispersion relations of the four linear modes are:

$$\omega_v = -\nu k^2,$$

(28a)

$$\omega_t = -\kappa k^2 \left[ 1 + \frac{(\gamma - 1)\lambda}{Pe^2} \right] + O\left(\frac{1}{Pe^4}\right),$$

(28b)

$$\omega_\pm = -\alpha k^2 \left[ 1 - \frac{(\gamma - 1)\lambda}{(\gamma - \lambda)Pe^2} \right] \pm ic_s k \left[ 1 - \frac{(\gamma + \lambda)^2 - 4\lambda}{8Pe^2} \right] + O\left(\frac{1}{Pe^4}\right),$$

(28c)

where $\omega_v$, $\omega_t$, and $\omega_\pm$ are the angular frequencies of the viscous, thermal and two acoustic modes, $c_s \equiv \sqrt{\gamma \theta_0}$ is a characteristic speed of sound, $k \equiv |k|$ the wave number, $Re \equiv c_s / \nu k$, $Pe \equiv c_s / \kappa k$ and $Pr \equiv \nu / \kappa$ the acoustic Reynolds, Péclet and Prandtl numbers, and

$$\lambda \equiv 1 - \left(2 - \frac{2}{D} + \frac{\nu_b}{\nu}\right) Pr$$

(29)

a constant defined for brevity. $\alpha$ is the leading order sound attenuation rate which is a weighted sum of the shear viscosity, bulk viscosity and thermal diffusivity:

$$\alpha = \frac{\gamma - 1}{2} \frac{\kappa}{\nu} + \frac{D - 1}{D} \frac{\nu_b}{\nu} + \frac{1}{2} \nu_b.$$ 

(30)

All the transport coefficients above are given by the relaxation times and the internal degree of freedom, $S$, by:

$$\nu = \theta_0 \left(\tau_{21} - \frac{1}{2}\right), \quad \nu_b = \frac{2S\theta_0}{D(D + S)} \left(\tau_{22} - \frac{1}{2}\right), \quad \kappa = \theta_0 \left(\tau_{32} - \frac{1}{2}\right), \quad \gamma = 1 + \frac{2}{D + S}.$$ 

(31)

Some remarks are called for at this point. First, while the viscous mode is independent of the other three and its dispersion relation exact, the dispersion relations of the thermal and acoustic modes are coupled solutions of a cubic characteristic equation and only their asymptotic form at large-$Pe$ limit are given above. Second, the bulk viscosity has a leading-order effect on the sound attenuation but its effects everywhere else is second order. In the following tests we numerically measure $\omega_v$, $\omega_t$, and $\omega_\pm$ for ranges of the relaxation times and the internal degree of freedom $S$. Agreement between the numerical and theoretical values, measured by the relative error:

$$\omega^* \equiv \left|\frac{\omega_{\text{numerical}} - \omega_{\text{theoretical}}}{\omega_{\text{theoretical}}}\right|,$$

(32)
FIG. 1: The relative errors in the four eigen-frequencies of the hydrodynamic modes for a wide range of the three relaxation times $\tau_{21}$, $\tau_{22}$ and $\tau_{32}$.

sufficiently verifies the accuracy of the model.

Shown in Fig. 1 are the relative errors in $\omega_v$, $\omega_t$, and $\omega_{\pm}$ for ranges of the relaxation times and the internal degree of freedom $S$. The angular frequencies are extracted by fitting the time history of the amplitudes of the four modes. The numerical simulations were conducted in the same fashion reported previously [8, 21] on a lattice of $100 \times 100$. It can be seen that the relative error in the angular frequencies are generally less than 1%, verifying the correctness of Eqs. (31).

IV. CONCLUSIONS AND DISCUSSIONS

In the present work we present in detail a generic multiple relaxation collision model based on Hermite expansion and tensor decomposition. The collision operator is first expanded
in terms of the Hermite tensorial polynomials in the reference frame moving with the fluid. Each of the polynomials is further decomposed into traceless components corresponding to the irreducible representations of the rotation group and relaxed with independent relaxation rate which is the most generic form of relaxation without violating rotation symmetry. The number of the independent relaxation rates are given by the number of traceless tensors of each tensor rank and is 2, 2, and 3 for the 2nd, 3rd, and 4th rank tensors respectively. To avoid possible numerical dissipation due to interpolation, the expansion coefficients are transformed into laboratory frame for evaluation with fixed-velocity quadrature rules. In its crudest form the model reverts to the BGK model. The first few relaxation rates are shown to correspond to the shear and bulk viscosity and the thermal diffusivity of the translational and other forms of motion. Numerical measurements of the eigen-frequencies of the linear hydrodynamic modes agree well with theoretical predictions. Although the other relaxation times do not appear in the hydrodynamic equations and have negligible effect in continuum, their effects are presumably more explicit in situations such as rarefied gases where the distribution is away from the Maxwell-Boltzmann equilibrium. At least in the linear regime, the spectrum of the relaxation times dictates the behavior of the collision operator and could potentially serve as a set of definitive variables.

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Appendix A: Transforms between the central and raw moments

The \( n \)-th order Hermite polynomial in \( D \)-dimensions is defined by the Rodrigues’ formula:

\[
H^{(n)}(\xi) = \frac{(-1)^n}{\omega(\xi)} \nabla^n \omega(\xi),
\]

where \( \omega(\xi) \) is the weight function:

\[
\omega(\xi) = \frac{1}{(2\pi)^{D/2}} e^{-\xi^2/2},
\]

with \( \xi^2 = \xi \cdot \xi \). \( H^{(n)}(\xi) \) is a fully symmetric rank-\( n \) tensor and an \( n \)-th degree polynomial in \( \xi \). The explicit form of \( H^{(n)}(\xi) \) is:

\[
H^{(n)}(\xi) = \sum_{k=0}^{[n/2]} (-1)^k D^k_\xi \xi^{-2k} \delta^k,
\]

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where the floor function, \([x]\), stands for the largest integer not exceeding \(x\), and:

\[
D_n^k \equiv \frac{n!}{(n-2k)!2^k k!} = C_n^{2k} (2k-1)!! , \tag{A4}
\]

where \(C_n^k\) is the binomial coefficient. The leading values of \(D_n^k\) are listed in Tab. I for convenience.

| \(k\) | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|------|---|---|---|---|---|---|---|---|
| \(0\) | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| \(1\) | 1 | 3 | 6 | 10 | 15 | 21 |
| \(2\) | 3 | 15 | 45 | 105 |
| \(3\) | 15 | 105 |

TABLE I: Leading values of the coefficients \(D_n^k\).

Differentiating Eqs. (A1) and (A3) and noticing \(\nabla \omega^{-1} = \xi/\omega\), we have respectively:

\[
\nabla H^{(n)}(\xi) = (-1)^n \left( \frac{\nabla^{n+1} \omega}{\omega} + \frac{\xi \nabla^n \omega}{\omega} \right) = -H^{(n+1)}(\xi) + \xi H^{(n)}(\xi), \tag{A5}
\]

and:

\[
\nabla H^{(n)}(\xi) = \sum_{k=0}^{\lfloor n/2 \rfloor} (n-2k) D_n^k \xi^{n-2k} \delta \delta^k = n \delta H^{(n-1)}(\xi). \tag{A6}
\]

Combining the two equations above, we have the recurrence relation:

\[
\xi H^{(n)}(\xi) = H^{(n+1)}(\xi) + n \delta H^{(n-1)}(\xi). \tag{A7}
\]

We first establish by induction that the monomials can be expressed by Hermite polynomials as the following:

\[
\xi^n = \sum_{k=0}^{\lfloor n/2 \rfloor} D_n^k H^{(n-2k)}(\xi) \delta^k. \tag{A8}
\]

It is trivially true for \(n = 0\). Multiple the above by \(\xi\) and using Eq. (A7), we have:

\[
\xi^{n+1} = \sum_{k=0}^{\lfloor n/2 \rfloor} D_n^k [H^{(n+1-2k)}(\xi) + (n-2k) \delta H^{(n-1-2k)}(\xi)] \delta^k
\]

\[
= \sum_{k=0}^{\lfloor n/2 \rfloor} D_n^k H^{(n+1-2k)}(\xi) \delta^k + \sum_{k=0}^{\lfloor n/2 \rfloor} (n-2k) D_n^k H^{(n-1-2k)}(\xi) \delta^{k+1}. \tag{A9}
\]
Applying the change of variable $k + 1 \to k$ to the second term, we have:

$$\xi^{n+1} = \sum_{s=0}^{\lfloor (n+1)/2 \rfloor} \left[ 1 + \frac{2k}{(n + 1 - 2k)} \right] D_n^k \mathcal{H}^{(n+1-2k)}(\xi) \delta^k$$

$$= \sum_{k=0}^{\lfloor (n+1)/2 \rfloor} D_{n+1}^k \mathcal{H}^{(n+1-2k)}(\xi) \delta^k,$$  \hspace{1cm} (A10)

completing the induction.

We now establish the following relation by induction:

$$\mathcal{H}^{(n)}(\xi + u) = \sum_{k=0}^{n} C_n^k \mathcal{H}^{(k)}(\xi) u^{-k},$$  \hspace{1cm} (A11)

Again it is trivially true for $n = 0$. Using Eq. (A7) repeatedly, we have

$$\mathcal{H}^{(n+1)}(\xi + u) = (\xi + u) \mathcal{H}^{(n)}(\xi + u) - n\delta \mathcal{H}^{(n-1)}(\xi + u)$$

$$= (\xi + u) \sum_{k=0}^{n} C_n^k \mathcal{H}^{(k)}(\xi) u^{-k} - n\delta \sum_{k=0}^{n-1} C_n^{k-1} \mathcal{H}^{(k)}(\xi) u^{-k}$$

$$= \sum_{i=0}^{n} C_n^k \mathcal{H}^{(k+1)}(\xi) u^{-k} + \delta \sum_{k=0}^{n} k C_n^k \mathcal{H}^{(k-1)}(\xi) u^{-k}$$

$$+ \sum_{k=0}^{n} C_n^k \mathcal{H}^{(k)}(\xi) u^{-k} - n\delta \sum_{k=0}^{n-1} C_n^{k-1} \mathcal{H}^{(k)}(\xi) u^{-k}.$$  \hspace{1cm} (A12)

Noticing that $nC_n^{k-1} = (k + 1)C_n^{k+1}$, after a change of variable $k + 1 \to k$, the second term cancels the last term, and the first term becomes:

$$\sum_{k=1}^{n+1} C_n^{k-1} \mathcal{H}^{(k)}(\xi) u^{n+1-k}.$$  \hspace{1cm} (A13)

On combining with the third term and noting that if we define $C_n^{-1} \equiv C_n^{n+1} \equiv 0$,

$$C_n^{k-1} + C_n^k = C_n^{k+1}, \hspace{1cm} \text{for} \hspace{1cm} k = 0, \ldots, n,$$  \hspace{1cm} (A14)

we have:

$$\mathcal{H}^{(n+1)}(\xi + u) = \sum_{k=0}^{n+1} C_n^{k+1} \mathcal{H}^{(k)}(\xi) u^{n+1-k},$$  \hspace{1cm} (A15)

completing the induction.

Now consider the Hermite polynomials under coordinate scaling by a constant factor, $\alpha$. Using Eq. (A3), we have:

$$\mathcal{H}^{(n)}(\alpha \xi) = \sum_{k=0}^{[n/2]} (-1)^k \alpha^{n-2k} D_n^k \xi^{n-2k} \delta^k.$$  \hspace{1cm} (A16)
On substituting Eq. (A8) into the equation above, we have:

\[
\mathcal{H}^{(n)}(\alpha \xi) = \sum_{k=0}^{[n/2]} (-1)^k \alpha^{n-2k} D_n^k \delta^k \left[ \sum_{t=0}^{[n/2]-k} D_{n-2k}^t \mathcal{H}^{(n-2k-2t)}(\xi) \delta^t \right]
\]

\[
= \sum_{k=0}^{[n/2]} \sum_{t=0}^{[n/2]-k} \frac{(-1)^k \alpha^{n-2k}}{(n-2k-2t)!2^{k+t}k!t!} \mathcal{H}^{(n-2k-2t)}(\xi) \delta^{k+t}.
\]  

(A17)

Realizing that the double summation is over all combinations of \(k\) and \(t\) such that \(k + t \leq [n/2]\), we define \(m = k + t\) and re-arrange the summation to write:

\[
\mathcal{H}^{(n)}(\alpha \xi) = \alpha^n \sum_{m=0}^{[n/2]} \frac{n!}{(n-2m)!2^mm!} \left[ \sum_{k=0}^{m} \frac{m!(-\alpha^{-2})^k}{k!(m-k)!} \right] \mathcal{H}^{(n-2m)}(\xi) \delta^m
\]

\[
= \alpha^n \sum_{m=0}^{[n/2]} (1 - \alpha^{-2})^m D_n^m \mathcal{H}^{(n-2m)}(\xi) \delta^m.
\]  

(A18)

Combining Eqs. (A11) and (A18), we can express the Hermite polynomials in the moving reference frame scaled by temperature using the ones in the absolute frame. We write:

\[
\theta^\frac{n}{2} \mathcal{H}^{(n)} \left( \frac{\xi - u}{\sqrt{\theta}} \right) = \sum_{k=0}^{[n/2]} D_n^k (1 - \theta)^k \mathcal{H}^{(n-2k)}(\xi - u) \delta^k
\]

\[
= \sum_{k=0}^{[n/2]} D_n^k (1 - \theta)^k \left[ \sum_{m=0}^{n-2k} C_n^{m-2k} \mathcal{H}^{(m)}(\xi)(-u)^{n-2k-m} \right] \delta^k
\]

\[
= \sum_{k=0}^{[n/2]} \sum_{m=0}^{n-2k} \frac{(-1)^{n-m-2k} n! (1 - \theta)^k}{(n - m - 2k)!k!m!2^k} C_n^m D_{n-m}^k (1 - \theta)^k u^{n-m-2k} \delta^k.
\]

Again, realizing that the summation is over all \(k\) and \(m\) such that \(m + 2k \leq n\), the order of the two summations can be swapped:

\[
\sum_{k=0}^{[n/2]} \sum_{m=0}^{n-2k} = \sum_{m=0}^{[(n-m)/2]} \sum_{k=0}^{[n/2]}.
\]  

(A19)

Also notice that \((-1)^{n-m-2k} = (-1)^{n-m}\) and

\[
\frac{n!}{(n - m - 2k)!k!m!2^k} = \frac{n!(n-m)!}{(n-m)!m!(n-m-2k)!k!2^k} = C_n^m D_{n-m}^k,
\]  

(A20)

we have:

\[
\theta^\frac{n}{2} \mathcal{H}^{(n)} \left( \frac{\xi - u}{\sqrt{\theta}} \right) = \sum_{m=0}^{n} (-1)^{n-m} C_n^m \mathcal{H}^{(m)}(\xi) \sum_{k=0}^{[(n-m)/2]} D_{n-m}^k (1 - \theta)^k u^{n-m-2k} \delta^k.
\]  

(A21)
where the inner summation is a function of $u$ and $\theta$. Defining:

$$A_m(u, \theta) = \left\lfloor \frac{m}{2} \right\rfloor \sum_{k=0}^{m} D_m^k (1 - \theta)^k u^{m-2k} \delta^k,$$

with $A_0 = 1$, $A_1 = u$, \hspace{1cm} (A22)

we can finally write:

$$H_n\left(\frac{\xi - u}{\sqrt{\theta}}\right) = \theta^{-\frac{n}{2}} \sum_{k=0}^{n} (-1)^{n-k} e_n^{(k)}(\xi) A_{n-k}(u, \theta).$$ \hspace{1cm} (A23)

Note that if $\theta = 1$, $A_m = u^m$ and the above reverts to Eq. (A11).

Denoting $v = (\xi - u)/\sqrt{\theta}$, Hermite expansion can be shifted and/or scaled as:

$$f(v) = \omega(v) \sum_{n=0}^{\infty} \frac{1}{n!} d^{(n)} : H^{(n)}(v),$$

$$d^{(n)} = \int f(v) H^{(n)}(v) dv, \hspace{0.5cm} n = 0, \ldots, \infty,$$ \hspace{1cm} (A24a)

On substituting Eq. (A23) and $dv = \theta^{-D/2} d\xi$ into Eq. (A24b), we have:

$$d^{(n)} = \theta^{-\frac{D+n}{2}} \sum_{k=0}^{n} (-1)^{n-k} e_n^{(k)} A_{n-k}.$$ \hspace{1cm} (A25)

Noticing that the Maxwell-Boltzmann distribution function is:

$$f^{(0)} \equiv \frac{\rho}{(2\pi\theta)^{D/2}} \exp \left[ -\frac{(\xi - u)^2}{2\theta} \right] = \rho \theta^{-\frac{D}{2}} \omega(v),$$ \hspace{1cm} (A26)

its Hermite expansion coefficients in the absolute frame \cite{22,23} is:

$$a^{(n)} = \rho \theta^{-\frac{D}{2}} \int \omega(v) H^{(n)}(\xi) d\xi = \rho \int \omega(v) H^{(n)}(\sqrt{\theta}v + u) dv.$$ \hspace{1cm} (A27)

Using Eq. (A23) to expand $H^{(n)}(\sqrt{\theta}v + u)$ in terms of $H^{(n)}(v)$, owing to the orthogonal relation, only the zero-th order term survives the integration. We have:

$$a^{(n)} = \rho \theta^{-n/2} (-1)^n A_n \left(-\sqrt{\theta}v, \frac{1}{\sqrt{\theta}}\right) = \rho \sum_{k=0}^{\left\lfloor m/2 \right\rfloor} D_m^k (\theta - 1)^k u^{m-2k} \delta^k.$$ \hspace{1cm} (A28)

\hspace{1cm} 

\hspace{1cm} 

\hspace{1cm} 

\hspace{1cm} 

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