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Rotational symmetry of the multiple-relaxation-time collision model

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We point out that the minimal components of the tensorial moments of the distribution that can be independently relaxed in collision without violating rotational symmetry are its irreducible representation (irrep) of SO(3), and a generic multiple-relaxation-time collision model can be constructed by independently relaxing these components. As the simplest example the irreps of the second moment are the traceless deviatoric stress and an isotropic tensor which is conserved in monatomic gases. Applying the decomposition to the thermal lattice Boltzmann model for polyatomic gases [Phys. Rev. E **77**, 035701(R) (2008)], the shear and bulk viscosities are decoupled by two independent relaxation times. The hydrodynamic equation of the model is obtained *via* Chapman-Enskog calculation and verified by numerical simulation.

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I. INTRODUCTION

A well-known deficiency of the lattice Boltzmann-BGK (LBGK) approach [1] is its simplistic single-relaxation-time (SRT) collision operator [2] adopted from continuum kinetic theory. It relaxes all moments of the distribution function with a single rate, resulting in the unphysical artifact that the thermal diffusivity and viscosity are always the same. In continuum kinetic theory a couple of models were proposed [3,4] to decouple the thermal diffusivity from viscosity by modifying the equilibrium distribution. In the context of LBGK, a multiple-relaxation-time (MRT) model [5,6] was suggested to assign separate relaxation rates to the eigenvectors of the collision matrix in the space of discrete velocities. The eigenvectors represent the hydrodynamic moments that one is concerned with. Nevertheless, as the underlying lattices used therein are insufficient to accurately represent the third moments and beyond, the Fourier equation of heat transfer is beyond the reach, leaving an adjustable Prandtl number unattainable. However, the numerical stability was indeed drastically improved, essentially due to the trimming of the moments not fully supported by the underlying lattice [7].

The idea of MRT was later applied to the high-order LB which employs lattices accurate enough to recover the full Navier-Stokes-Fourier equations [8]. The collision term is expanded in terms of the tensorial Hermite polynomials [9] of which, each term is assigned an independent relaxation time. The thermal diffusivity is decoupled from the viscosity as they are dictated by the third and second moments, respectively. A remaining issue is that thermal diffusion is not Galilean invariant when the thermal diffusivity is set to be different from the viscosity. This abnormality was later removed by explicitly correcting the third-order moment [10], or more systematically, by carrying out the Hermite expansion in the reference frame moving with the fluid [11,12], or relaxing the *central moments* directly.

As each of the tensorial moments consists of multiple components, a question arises as what the minimum unit is that can be assigned a separate relaxation time. As a fundamental requirement, the physics of relaxation should be independent of the coordinate system and invariant under spatial rotation. Therefore, the tensor components that can be assigned independent relaxation times must form an *irreducible representation* of the rotation group SO(3) [13]. For instance, the irreducible components of the second moment consist of a traceless symmetric tensor and an isotropic tensor. The linear relaxation of the second moment can have at most two rates, in analog to the two coefficients in the constitutive relation that give rise to the shear and bulk viscosities [14].

Microscopically bulk viscosity [15,16] stems from either the finite energy-equilibrating time between the translational and the internal degrees of freedom of molecular motion, or from the dense gas effect. Here we are only concerned with the former mechanism which has been extensively discussed in classic kinetic theory [17–21]. Describing a monatomic gas, the original Boltzmann equation yields zero bulk viscosity. In the lattice Boltzmann community, the early a-thermal LBGK models with no energy conservation exhibits an *artificial* nonzero bulk viscosity which becomes absent once the correct energy conservation is recovered [22,23]. This artifact can also be eliminated by explicitly modifying the equilibrium distribution [24]. To reflect the effect of energy exchange between translational and other forms of molecular motion, a lattice BGK model [25] was proposed to model the evolution of the kinetic energy of internal motions by an additional distribution in the same way as the approach used to reduce the BGK equation to lower dimensions [26]. The same idea was adopted to the entropic lattice Boltzmann model [27], and in a recent model the internal energy is modeled by a scalar [28]. In these models, although an adjustable specific

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heat ratio is achieved, the bulk and shear viscosity are coupled together by the same relaxation time.

In the present paper, based on the mathematical fact on the minimum rotational invariant components that a tensor can be decomposed into, we construct a Hermite-expansion-based MRT collision model with maximum number of relaxation times. Particularly, the second moment in the polyatomic model [25] is decomposed into the two parts corresponding to shear and bulk viscosities to arrive at a model with adjustable bulk-to-shear viscosity ratio independent of the specific heat ratio γ. Instead of predicting experimental measurements, our goal is to derive a model that allows the bulk viscosity freely adjusted without violating fundamental principles. The rest of the paper is organized as the following. In Sec. II we give the theoretical derivation. After a brief review of of the background, we present the tensor decomposition in Sec. II A, followed by an introduction of the SRT polyatomic gas model in Sec. II B, and its extension to MRT in Sec. II C. The hydrodynamic equation of the model is derived *via* Chapman-Enskog calculation in Sec. II D. In Sec. III numerical verification is presented, and finally conclusions and some discussions are given in Sec. IV.

II. THEORETICAL DERIVATION

In a previous series of papers [8,11,12] we propose to define the collision process through its action on the nonequilibrium part of the distribution function. Specifically, we expand the distribution function in terms of Hermite polynomials [9] as

$$f(\boldsymbol{\xi},\boldsymbol{x},t)=\omega(\boldsymbol{\eta})\sum_{n=0}^{\infty}\frac{1}{n!}\boldsymbol{a}^{(n)}(\boldsymbol{x},t):\mathcal{H}^{(n)}(\boldsymbol{\eta}), \tag{1}$$

where $\boldsymbol{\eta}$ can be $\boldsymbol{\xi}$, $\boldsymbol{c}\equiv\boldsymbol{\xi}-\boldsymbol{u}$, or $\boldsymbol{v}\equiv\boldsymbol{c}/\sqrt{\theta}$, respectively, corresponding to expansions in the laboratory frame, frame moving with the fluid, and thermally scaled moving frame, respectively. Here, $\boldsymbol{c}$ is the *peculiar velocity*, θ is the temperature, and $\omega(\boldsymbol{\eta})\equiv(2\pi)^{-D/2}\exp(-\eta^2/2)$ is the weight function. The expansion coefficients$\boldsymbol{a}^{(n)}(\boldsymbol{x},t)$ are the moments of the distribution function or their combinations in the various frames. The whole set of $\boldsymbol{a}^{(n)}$ completely and uniquely specifies $f(\boldsymbol{\xi},\boldsymbol{x},t)$ and vice versa. In case $\boldsymbol{c}$ or $\boldsymbol{v}$ is used, the *binomial transform* and a further scaling can be used to transform $\boldsymbol{a}^{(n)}$ back to the laboratory frame where they can be exactly represented by a set of fixed discrete velocities [29].

Now consider the collision operator $\Omega(f)$ which represents the change to the distribution due to the local collision process. As apparently $\Omega(f^{(\mathrm{eq})})=0$ for convenience, we denote the nonequilibrium part of the distribution by $f^{(\mathrm{neq})}\equiv f-f^{(\mathrm{eq})}$ and redefine Ω as a functional of $f^{(\mathrm{neq})}$ such that $\Omega(0)=0$. For instance, the well-known BGK collision operator is simply $\Omega(f^{(\mathrm{neq})})=-\omega f^{(\mathrm{neq})}$ where $\omega\equiv1/\tau$ is the collision frequency and τ is the collision time. Let the expansion coefficients of $f^{(\mathrm{neq})}$ and $\Omega(f^{(\mathrm{neq})})$ in terms of $\mathcal{H}^{(n)}(\boldsymbol{v})$ be $\boldsymbol{d}_1^{(n)}$ and $\boldsymbol{d}_\Omega^{(n)}$, respectively. Note that if the construction of $f^{(\mathrm{eq})}$ guarantees the conservation of mass, momentum, and energy, we have $\boldsymbol{d}_1^{(0)}=0$, $\boldsymbol{d}_1^{(1)}=\boldsymbol{0}$, and $\boldsymbol{d}_1^{(2)}$ is traceless. The collision operator can be specified *via* the expansion coefficients. The previous MRT model is defined by [11]

$$\boldsymbol{d}_\Omega^{(n)}=-\omega_n\boldsymbol{d}_1^{(n)},\qquad n=2,3,\dots, \tag{2}$$

which gives each of the Hermite terms a separate relaxation frequency ω_n.

A. Rotational symmetry of a rank-2 tensor

A well-known conclusion of group theory [13] is that the nine-dimensional representation of the rotation group SO(3) furnished by a rank-2 tensor can be decomposed into a five-dimensional space of a traceless symmetric tensor, a three-dimensional space of an antisymmetric tensor, and a one-dimensional space of a unit tensor, commonly noted as $5\oplus3\oplus1$, each of which is closed under the transform of SO(3). Hence, the second tensorial moment, which is symmetric by definition, can be decomposed into the spaces of a traceless symmetric tensor and a unit tensor ($5\oplus1$), both can be relaxed separately without breaking rotational symmetry.

To further illustrate, let us define two operators $\bar{\boldsymbol{a}}$ and $\tilde{\boldsymbol{a}}$, respectively, which take the trace and traceless symmetric components of the rank-2 tensor $\boldsymbol{a}$. Assuming Einstein summation, in component form we define

$$\bar{a}\equiv a_{ii},\quad\text{and}\quad\tilde{a}_{ij}\equiv\frac{1}{2}(a_{ij}+a_{ji})-\frac{\bar{a}}{D}\delta_{ij}. \tag{3}$$

Any symmetric rank-2 tensor can be decomposed as

$$\boldsymbol{a}=\frac{\bar{a}}{D}\boldsymbol{\delta}+\tilde{\boldsymbol{a}}. \tag{4}$$

Particularly, the second-order term in a Hermite expansion can be decomposed into two parts that are orthogonal under spatial rotation,

$$\boldsymbol{a}:\mathcal{H}^{(2)}(\boldsymbol{v})=\tilde{\boldsymbol{a}}:\mathcal{H}^{(2)}(\boldsymbol{v})+\frac{\bar{a}}{D}\boldsymbol{\delta}:\mathcal{H}^{(2)}(\boldsymbol{v}). \tag{5}$$

The action of the most general rotationally symmetric linear relaxation operator on such a functional can be defined as

$$\Omega[\boldsymbol{a}:\mathcal{H}^{(2)}(\boldsymbol{v})]=-\left[\frac{1}{\tau_1}\tilde{\boldsymbol{a}}+\frac{1}{\tau_2}\frac{\bar{a}}{D}\boldsymbol{\delta}\right]:\mathcal{H}^{(2)}(\boldsymbol{v}), \tag{6}$$

with two independent relaxation times τ_1 and τ_2.

We note that for the two tensor contractions on the right-hand side of Eq. (5), only the traceless component and the trace of $\mathcal{H}^{(n)}(\boldsymbol{v})$ have contributions. Hence, the same term can take several equivalent forms, e.g.,

$$\boldsymbol{a}:\mathcal{H}^{(2)}(\boldsymbol{v})=\tilde{\boldsymbol{a}}:\boldsymbol{v}\boldsymbol{v}+\frac{\bar{a}}{D}(v^2-D). \tag{7}$$

B. BGK model with internal degrees of freedom

For a monatomic gas in which the translational kinetic energy is conserved, $\boldsymbol{d}_1^{(2)}$ is traceless so that $\overline{\boldsymbol{d}_1^{(2)}}=0$. Only a single relaxation time can exist. Previously, a lattice BGK model was proposed for gases with internal degrees of freedom [25]. The approach is essentially the same as the one developed to reduce spatial dimensionality [26]. In this approach, a polyatomic gas is described by a pair of distribution functions in the *reduced* phase space $(\boldsymbol{\xi}, \boldsymbol{x})$, obeying the following BGK equations:

$$\frac{\partial g}{\partial t} + \boldsymbol{\xi} \cdot \nabla g = \Omega_g \equiv -\frac{1}{\tau}[g - g^{(\mathrm{eq})}], \tag{8a}$$

$$\frac{\partial h}{\partial t} + \boldsymbol{\xi} \cdot \nabla h = \Omega_h \equiv -\frac{1}{\tau}[h - g^{(\mathrm{eq})}\theta], \tag{8b}$$

where Ω_g and Ω_h are the collision operators for g and h, and

$$g^{(\mathrm{eq})} = \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left(-\frac{c^2}{2\theta}\right) = \frac{\rho}{\theta^{D/2}}\omega(\boldsymbol{v}) \tag{9}$$

is the Maxwellian in the reduced phase space. Here ρ is the density, $c \equiv |\boldsymbol{c}|$, and θ is the temperature which is related to the *energy density* per mass ϵ by

$$\epsilon = \frac{1}{2}(D+S)\theta. \tag{10}$$

where S is the number of internal degrees of freedom. The specific heat ratio can be obtained as

$$\gamma \equiv \frac{c_p}{c_v} = \frac{D+S+2}{D+S}. \tag{11}$$

The variables ρ, $\boldsymbol{u}$, and ϵ, are moments of the two distributions,

$$\rho = \int g\, d\boldsymbol{\xi}, \tag{12a}$$

$$\rho\boldsymbol{u} = \int g\boldsymbol{\xi}\, d\boldsymbol{\xi}, \tag{12b}$$

$$\rho\epsilon = \frac{1}{2}\int gc^2 d\boldsymbol{\xi} + \frac{S}{2}\int h\, d\boldsymbol{\xi}. \tag{12c}$$

The above equations can then be discretized in velocity space using Gauss quadrature [29,30]. As the model involves energy transfer and, hence, the third moments, a Gauss quadrature of, at least, eighth degree is required to recover the hydrodynamic equation with full Galilean invariance [31]. Although originally a fourth-order 121-velocity quadrature was used [25], quadrature rules with fewer velocities are also available [23,32]. Once discretized in velocity space, the standard lattice Boltzmann computation can be carried out following the standard procedure outlined in Refs. [25,29].

Although Eq. (8a) appears to be identical to the BGK equation for monatomic gases, a critical difference lies in the calculation of $g^{(\mathrm{eq})}$ where θ is now given by Eqs. (10) and (12c) which couple g and h. This coupling reflects energy transfer between the translational and the internal degrees of freedom. As the translational energy is not conserved, $g^{(\mathrm{neq})} \equiv g - g^{(\mathrm{eq})}$ can have a nonvanishing trace. Nevertheless, the *total* energy is still conserved as from Eqs. (12c) and (10), we have

$$\int gc^2 d\boldsymbol{\xi} + S\int h\, d\boldsymbol{\xi} = (D+S)\rho\theta. \tag{13}$$

The definition of $g^{(\mathrm{eq})}$ of Eq. (9) gives

$$\int g^{(\mathrm{eq})}c^2 d\boldsymbol{\xi} = D\rho\theta, \quad \text{and} \quad \int g^{(\mathrm{eq})} d\boldsymbol{\xi} = \rho. \tag{14}$$

The above two equations lead to

$$\int g^{(\mathrm{neq})}c^2 d\boldsymbol{\xi} + S\int h^{(\mathrm{neq})} d\boldsymbol{\xi} = 0. \tag{15}$$

Together with the fact that the two relaxation times in Eqs. (8) are identical, it ensures that

$$\int (\Omega_g c^2 + S\Omega_h) d\boldsymbol{\xi} = 0, \tag{16}$$

namely, $\rho\epsilon$ as defined by Eq. (12c) is conserved by the collision operator. Obviously, mass and momentum are also conserved as

$$\int \Omega_g d\boldsymbol{\xi} = 0, \quad \text{and} \quad \int \Omega_g \boldsymbol{\xi}\, d\boldsymbol{\xi} = 0. \tag{17}$$

C. MRT extension

Now let $\boldsymbol{d}_g^{(n)}$ and $\boldsymbol{d}_h^{(n)}$, respectively, be the Hermite expansion coefficients of $g^{(\mathrm{neq})}$ and $h^{(\mathrm{neq})} \equiv h - g^{(\mathrm{eq})}\theta$, i.e.,

$$g^{(\mathrm{neq})} = \omega(\boldsymbol{v})\sum_{n=2}^{\infty}\frac{1}{n!}\boldsymbol{d}_g^{(n)}:\mathcal{H}^{(n)}(\boldsymbol{v}), \tag{18a}$$

$$h^{(\mathrm{neq})} = \omega(\boldsymbol{v})\sum_{n=0}^{\infty}\frac{1}{n!}\boldsymbol{d}_h^{(n)}:\mathcal{H}^{(n)}(\boldsymbol{v}). \tag{18b}$$

Due to the conservation of mass and momentum, $\boldsymbol{d}_g^{(0)}$ and $\boldsymbol{d}_g^{(1)}$ vanish. The leading coefficient of $g^{(\mathrm{neq})}$ is as follows:

$$\begin{aligned}\boldsymbol{d}_g^{(2)} &= \int [g - g^{(\mathrm{eq})}]\mathcal{H}^{(2)}(\boldsymbol{v})d\boldsymbol{v}\\ &= \int (\boldsymbol{v}\boldsymbol{v} - \boldsymbol{\delta})g\, d\boldsymbol{v}\\ &= \theta^{-[(D+2)/2]}\left[\int g\boldsymbol{c}\boldsymbol{c}\, d\boldsymbol{c} - \rho\theta\boldsymbol{\delta}\right],\end{aligned} \tag{19}$$

where the fact $\int g^{(\mathrm{eq})}\mathcal{H}^{(2)}(\boldsymbol{v})d\boldsymbol{v} = 0$ is used. The trace and traceless component of $\boldsymbol{d}_g^{(2)}$ can be computed as

$$\bar{d}_g^{(2)} = \theta^{-[(D+2)/2]}\left[\int gc^2 d\boldsymbol{c} - D\rho\theta\right], \tag{20a}$$

$$\tilde{\boldsymbol{d}}_g^{(2)} = \theta^{-[(D+2)/2]}\int g\left[\boldsymbol{c}\boldsymbol{c} - \frac{c^2}{D}\boldsymbol{\delta}\right]d\boldsymbol{c}. \tag{20b}$$

Similarly the leading coefficient of $h^{(\mathrm{neq})}$ is as follows:

$$d_h^{(0)} = \int \left[h - \frac{\rho\theta}{\theta^{D/2}}\omega(\boldsymbol{v})\right]d\boldsymbol{v} = \theta^{-(D/2)}\left[\int h\, d\boldsymbol{c} - \rho\theta\right]. \tag{21}$$

Using Eqs. (10) and (12c), $d_h^{(0)}$ is related to $\bar{d}_g^{(2)}$ by

$$\theta\bar{d}_g^{(2)} + Sd_h^{(0)} = 0. \tag{22}$$

Using Eq. (4), the leading term in Eq. (18a) can be decomposed to have

$$\frac{g^{(\mathrm{neq})}}{\omega(\boldsymbol{v})} = \frac{1}{2!}\left[\tilde{\boldsymbol{d}}_g^{(2)} + \frac{\bar{d}_g^{(2)}}{D}\boldsymbol{\delta}\right]:\mathcal{H}^{(2)} + \frac{\boldsymbol{d}_g^{(3)}:\mathcal{H}^{(3)}}{3!} + \cdots. \tag{23}$$

A corresponding MRT collision model can then be devised as

$$-\frac{\Omega_g}{\omega(\boldsymbol{v})} = \frac{1}{2}\left[\frac{\tilde{\boldsymbol{d}}_g^{(2)}}{\tau_{21}} + \frac{\bar{d}_g^{(2)}\boldsymbol{\delta}}{\tau_{22}D}\right]:\mathcal{H}^{(2)} + \frac{\boldsymbol{d}_g^{(3)}:\mathcal{H}^{(3)}}{3!\tau_3} + \cdots, \tag{24a}$$

$$-\frac{\Omega_h}{\omega(\boldsymbol{v})} = \frac{d_h^{(0)}}{\tau_0} + \frac{\boldsymbol{d}_h^{(1)}:\mathcal{H}^{(1)}}{\tau_1} + \cdots, \tag{24b}$$

where, τ_{21}, τ_{22}, τ_3, τ_0, and τ_1 are independent relaxation times. We now show that the energy conservation of Eq. (16) demands that $\tau_0 = \tau_{22}$. For translational energy we note that

$$\begin{aligned}\int \Omega_g c^2 d\boldsymbol{\xi} &= \theta^{(D+2)/2}\mathrm{Tr}\int \Omega_g \boldsymbol{v}\boldsymbol{v}\, d\boldsymbol{v}\\ &= \theta^{(D+2)/2}\mathrm{Tr}\int \Omega_g[\mathcal{H}^{(2)}(\boldsymbol{v}) + \boldsymbol{\delta}\mathcal{H}^{(0)}(\boldsymbol{v})]d\boldsymbol{v}. \quad (25)\end{aligned}$$

Using the orthogonal relations and the fact that $\mathrm{Tr}(\tilde{\boldsymbol{d}}_g^{(2)}) = 0$, we have

$$\int \Omega_g c^2 d\boldsymbol{\xi} = -\frac{\theta^{[(D+2)/2]}\bar{d}_g^{(2)}}{\tau_{22}} = -\frac{1}{\tau_{22}}\left[\int g c^2 d\boldsymbol{c} - D\rho\theta\right], \quad (26)$$

and similarly,

$$\int \Omega_h d\boldsymbol{\xi} = -\frac{\theta^{D/2} d_h^{(0)}}{\tau_0} = -\frac{1}{\tau_0}\left[\int h\, d\boldsymbol{c} - \rho\theta\right]. \quad (27)$$

Noting Eq. (13) in order for Eqs. (24) to satisfy Eq. (16), we must have $\tau_0 = \tau_{22}$.

D. Hydrodynamic equations

We now derive the hydrodynamic equations of Eqs. (8) and (24). By taking the moments in Eqs. (17) and (16) of Eqs. (8), we have the conservation equations,

$$\frac{d\rho}{dt} + \rho\nabla\cdot\boldsymbol{u} = 0, \quad (28a)$$

$$\rho\frac{d\boldsymbol{u}}{dt} + \nabla\cdot\boldsymbol{P} = 0, \quad (28b)$$

$$\rho\frac{d\epsilon}{dt} + \nabla\boldsymbol{u}{:}\boldsymbol{P} + \nabla\cdot\boldsymbol{q} = 0, \quad (28c)$$

where $d/dt \equiv \partial/\partial t + \boldsymbol{u}\cdot\nabla$ is the *material derivative*, and

$$\boldsymbol{P} \equiv \int g\boldsymbol{c}\boldsymbol{c}\, d\boldsymbol{c}, \quad \text{and} \quad \boldsymbol{q} \equiv \frac{1}{2}\int (gc^2 + Sh)\boldsymbol{c}\, d\boldsymbol{c} \quad (29)$$

are the *pressure tensor* and *energy flux*, respectively. Except for the last term in the definition of $\boldsymbol{q}$, all are the same as in a monatomic gas. The *hydrostatic pressure*,

$$p \equiv \frac{P_{ii}}{D} = \frac{1}{D}\int gc^2 d\boldsymbol{c} \quad (30)$$

is defined as the average of the normal components of $\boldsymbol{P}$ and the *deviatoric stress* $\boldsymbol{\sigma} \equiv -(\boldsymbol{P} - p\boldsymbol{\delta})$ is the negative of the traceless part of $\boldsymbol{P}$. In particular, if g and h are expanded in terms of Hermite polynomials $\mathcal{H}^{(n)}(\boldsymbol{v})$, we have

$$\begin{aligned}\boldsymbol{P} &= \theta^{[(D+2)/2]}\int g[\boldsymbol{\delta} + \mathcal{H}^{(2)}(\boldsymbol{v})]d\boldsymbol{v}\\ &= \theta^{[(D+2)/2]}[d^{(0)}\boldsymbol{\delta} + \boldsymbol{d}^{(2)}]. \quad (31)\end{aligned}$$

On decomposing $\boldsymbol{d}^{(2)}$ according to Eq. (4), we have

$$p = \theta^{[(D+2)/2]}\left[d^{(0)} + \frac{\bar{d}^{(2)}}{D}\right], \quad \text{and} \quad \boldsymbol{\sigma} = -\theta^{[(D+2)/2]}\tilde{\boldsymbol{d}}^{(2)}. \quad (32)$$

As the zeroth approximation, taking g and h as their equilibria, $g^{(\mathrm{eq})}$ and $g^{(\mathrm{eq})}\theta$, we have the ideal gas equation of state,

$$p = \rho\theta, \quad (33)$$

and

$$\boldsymbol{\sigma} = \boldsymbol{0}, \quad \text{and} \quad \boldsymbol{q} = \boldsymbol{0}, \quad (34)$$

which yield Euler's equations when plugged into Eqs. (28). The first Chapman-Enskog approximation [33] amounts to substituting $f = f^{(\mathrm{eq})} + f^{(1)} + \cdots$ into the Boltzmann-BGK equation and keeping the leading terms on both sides to yield

$$f^{(1)} \cong -\tau\left(\frac{\partial}{\partial t} + \boldsymbol{\xi}\cdot\nabla\right)f^{(\mathrm{eq})}. \quad (35)$$

Using Euler's equation to convert the time derivatives to spatial ones, $f^{(1)}$ can be written in terms of the hydrodynamic variables and their spatial derivatives. On substituting into Eq. (29), we obtain $\boldsymbol{P}^{(1)}$ and $\boldsymbol{q}^{(1)}$ and, in turn, the Navier-Stokes-Fourier equations when plugged into Eqs. (28).

It was noted [12] that in this procedure, $\boldsymbol{P}^{(1)}$ and $\boldsymbol{q}^{(1)}$ can be obtained by taking the corresponding moments of the BGK equation directly without computing $f^{(1)}$ explicitly. We now apply the same procedure to Eqs. (8) and (24). Define the differential operator for brevity,

$$\mathcal{D} \equiv \frac{\partial}{\partial t} + \boldsymbol{\xi}\cdot\nabla = \frac{d}{dt} + \boldsymbol{c}\cdot\nabla, \quad (36)$$

where d/dt is the material derivative, the first Chapman-Enskog approximation can be written as

$$\mathcal{D}g^{(\mathrm{eq})} = -\omega(\boldsymbol{v})\left[\frac{1}{2}\left(\frac{\tilde{\boldsymbol{d}}_g^{(2)}}{\tau_{21}} + \frac{\bar{d}_g^{(2)}\boldsymbol{\delta}}{\tau_{22}D}\right){:}\mathcal{H}^{(2)} + \frac{\boldsymbol{d}_g^{(3)}{:}\mathcal{H}^{(3)}}{3!\tau_3} + \cdots\right], \quad (37a)$$

$$\mathcal{D}(g^{(\mathrm{eq})}\theta) = -\omega(\boldsymbol{v})\left[\frac{d_h^{(0)}}{\tau_{22}} + \frac{\boldsymbol{d}_h^{(1)}{:}\mathcal{H}^{(1)}}{\tau_1} + \cdots\right]. \quad (37b)$$

For the left-hand side of Eqs. (37a) and (37b), using the chain rule by following the standard procedure [33], we have

$$\mathcal{D}g^{(\mathrm{eq})} = \left[\mathcal{D}\rho\frac{\partial}{\partial\rho} + \mathcal{D}u_i\frac{\partial}{\partial u_i} + \mathcal{D}\theta\frac{\partial}{\partial\theta}\right]. \quad (38)$$

The derivatives with respect to ρ, u_i, and θ can be conveniently carried out by differentiating the logarithm of Eq. (9),

$$\frac{1}{g^{(\mathrm{eq})}}\frac{\partial g^{(\mathrm{eq})}}{\partial \rho} = \frac{1}{\rho}, \tag{39a}$$

$$\frac{1}{g^{(\mathrm{eq})}}\frac{\partial g^{(\mathrm{eq})}}{\partial u_i} = \frac{c_i}{\theta}, \tag{39b}$$

$$\frac{1}{g^{(\mathrm{eq})}}\frac{\partial g^{(\mathrm{eq})}}{\partial \theta} = \left(\frac{c^2}{2\theta} - \frac{D}{2}\right)\frac{1}{\theta}. \tag{39c}$$

Ignore the high-order terms in Eq. (28), the Euler equations can be written as

$$\mathcal{D}\rho = -\rho\nabla\cdot\boldsymbol{u} + \boldsymbol{c}\cdot\nabla\rho, \tag{40a}$$

$$\mathcal{D}\boldsymbol{u} = -\nabla\theta - \frac{\theta}{\rho}\nabla\rho + \boldsymbol{c}\cdot\nabla\boldsymbol{u}, \tag{40b}$$

$$\mathcal{D}\theta = -\frac{2\theta}{D+S}\nabla\cdot\boldsymbol{u} + \boldsymbol{c}\cdot\nabla\theta. \tag{40c}$$

Combine the above, we have

$$\mathcal{D}g^{(\mathrm{eq})} = \frac{1}{\theta}\left[\left(\boldsymbol{cc} - \frac{c^2\boldsymbol{\delta}}{D}\right):\nabla\boldsymbol{u} + \left(\frac{c^2}{2\theta} - \frac{D+2}{2}\right)\boldsymbol{c}\cdot\nabla\theta + \frac{S}{D+S}\left(\frac{c^2}{D} - \theta\right)\nabla\cdot\boldsymbol{u}\right]g^{(\mathrm{eq})}, \tag{41a}$$

$$\mathcal{D}(g^{(\mathrm{eq})}\theta) = \left[\left(\boldsymbol{cc} - \frac{c^2\boldsymbol{\delta}}{D}\right):\nabla\boldsymbol{u} + \left(\frac{c^2}{2\theta} - \frac{D}{2}\right)\boldsymbol{c}\cdot\nabla\theta + \frac{S}{D+S}\left[\frac{c^2}{D} - \left(1 + \frac{2}{S}\right)\theta\right]\nabla\cdot\boldsymbol{u}\right]g^{(\mathrm{eq})}, \tag{41b}$$

where the first two terms in the brackets of the first equation are the same as in the monatomic case, whereas the third one is due to the internal degrees of freedom. Now taking the moment $\int\cdot\boldsymbol{cc}\,d\boldsymbol{c}$ of Eq. (37a), the moment equation for the pressure and stress tensor can be obtained

$$\begin{aligned} 2\rho\theta\left[\left(\boldsymbol{\Lambda} - \frac{\boldsymbol{\delta}\nabla\cdot\boldsymbol{u}}{D}\right) + \frac{S\boldsymbol{\delta}\nabla\cdot\boldsymbol{u}}{D(D+S)}\right] \\ = -\theta^{(D+2)/2}\left[\frac{\tilde{\boldsymbol{d}}_g^{(2)}}{\tau_{21}} + \frac{\bar{d}_g^{(2)}\boldsymbol{\delta}}{D\tau_{22}}\right], \end{aligned} \tag{42}$$

where $\boldsymbol{\Lambda} \equiv \frac{1}{2}[\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T]$ is the *strain rate*. Matching up the trace and traceless part on both sides, we have the correction to the hydrostatic pressure and deviatoric stress as

$$\begin{aligned} p^{(1)} &= \theta^{(D+2)/2}\frac{\bar{d}_g^{(2)}}{D} \\ &= -\frac{2S}{D(D+S)}\tau_{22}\rho\theta\nabla\cdot\boldsymbol{u}, \end{aligned} \tag{43a}$$

$$\begin{aligned} \boldsymbol{\sigma}^{(1)} &= -\theta^{(D+2)/2}\tilde{\boldsymbol{d}}_g^{(2)} \\ &= 2\tau_{21}\rho\theta\left(\boldsymbol{\Lambda} - \frac{\boldsymbol{\delta}\nabla\cdot\boldsymbol{u}}{D}\right) \end{aligned} \tag{43b}$$

corresponding to the kinematic shear viscosity ν and the kinematic bulk viscosity ν_b,

$$\nu = \tau_{21}\theta, \quad \text{and} \quad \nu_b = \frac{2S}{D(D+S)}\tau_{22}\theta. \tag{44}$$

Note that τ_{22} in the second equation makes the bulk viscosity independent to the shear viscosity, whereas in Ref. [25] they have a fixed ratio. Similarly taking the moments $\int c^2\boldsymbol{c}\,d\boldsymbol{c}$ and $\int \boldsymbol{c}\,d\boldsymbol{c}$ of Eqs. (37a) and (37b), respectively, the moment equations for the translational heat flux and internal heat flux can be obtained

$$\theta^{(D+3)/2}\boldsymbol{d}_g^{(3)} = -\tau_3(D+2)\rho\theta\nabla\theta, \tag{45a}$$

$$\theta^{(D+1)/2}\boldsymbol{d}_h^{(1)} = -\tau_1\rho\theta\nabla\theta. \tag{45b}$$

Take the summation, the first-order correction to the total heat flux is as follows:

$$\boldsymbol{q}^{(1)} = -\frac{(D+2)\tau_3 + S\tau_1}{2}\rho\theta\nabla\theta \tag{46}$$

corresponding to a *heat conductivity* of

$$\lambda = \frac{(D+2)\tau_3 + S\tau_1}{2}\rho\theta. \tag{47}$$

Noting that $c_p = (D+S+2)/2$, the kinematic *thermal diffusivity* is as follows:

$$\kappa \equiv \frac{\lambda}{\rho c_p} = \frac{(D+2)\tau_3 + S\tau_1}{D+S+2}\theta, \tag{48}$$

which reduces to $\tau\theta$ if $S = 0$ as for monatomic gases, or $\tau_1 = \tau_3 = \tau$ as for the single-relaxation-time polyatomic model [25]. The adjustable Prandtl number is

$$\Pr = \frac{\nu}{\kappa} = \frac{\tau_{21}(D+S+2)}{\tau_3(D+2) + \tau_1 S}, \tag{49}$$

which recovers the results in Refs. [8,12,34] if $\tau_3 = \tau_1$.

III. NUMERICAL VERIFICATION

To verify the model, the transport coefficients are measured from the dynamics of the linear hydrodynamic modes in a one-dimensional periodic setup and compared with their theoretical values. The case setup has been extensively discussed previously [8,12,34]. Here we briefly summarize the analytical results. Consider the monochromatic plane wave perturbation,

$$\begin{pmatrix}\rho \\ \boldsymbol{u} \\ \theta\end{pmatrix} = \begin{pmatrix}\rho_0 \\ \boldsymbol{u}_0 \\ \theta_0\end{pmatrix} + \begin{pmatrix}\bar{\rho} \\ \bar{\boldsymbol{u}} \\ \bar{\theta}\end{pmatrix}e^{\omega t + i\boldsymbol{k}\cdot(\boldsymbol{x} - \boldsymbol{u}_0 t)}, \tag{50}$$

where the subscript 0 denotes the base flow and $\bar{\rho}$, $\bar{\boldsymbol{u}}$, and $\bar{\theta}$ are the perturbation amplitudes. Both the base state and the perturbation amplitudes are homogeneous and constant. $\boldsymbol{k}$ and ω, 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 Eqs. (28), we obtain an eigensystem in the space of $(\bar{\rho}, \bar{u}_{\parallel}, \bar{\theta}, \bar{u}_{\perp})^T$ from which the dimensionless dispersion relations of four linear modes can be obtained

$$-\frac{\omega_v}{c_s k} = \frac{1}{\mathrm{Re}}, \tag{51a}$$

$$-\frac{\omega_t}{c_s k} = \frac{1}{\mathrm{Pe}} + \frac{(\gamma-1)\lambda}{\mathrm{Pe}^3} + O\left(\frac{1}{\mathrm{Pe}^5}\right), \tag{51b}$$

$$-\frac{\omega_\pm}{c_s k} = \frac{\gamma-\lambda}{2\,\mathrm{Pe}} - \frac{(\gamma-1)\lambda}{2\,\mathrm{Pe}^3} + O\left(\frac{1}{\mathrm{Pe}^5}\right) \pm i\left[1 - \frac{(\gamma+\lambda)^2-4\lambda}{8\,\mathrm{Pe}^2} + O\left(\frac{1}{\mathrm{Pe}^4}\right)\right], \tag{51c}$$

where ω_v, ω_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, $k \equiv |\boldsymbol{k}|$ is the *wave number*, $\mathrm{Re} \equiv c_s/\nu k$, $\mathrm{Pe} \equiv c_s/\kappa k$, and $\mathrm{Pr} \equiv \nu/\kappa$ are the *acoustic* Reynolds, Péclet, and Prandtl numbers, and

$$\lambda \equiv 1 - \left(2 - \frac{2}{D} + \frac{\nu_b}{\nu}\right)\mathrm{Pr} \tag{52}$$

is a constant defined for brevity which is the only place where bulk viscosity affects the dispersion relations. Although the viscous mode is independent from the other three, and its dispersion relation is exact, the dispersion relations of the thermal and acoustic modes are solutions of a cubic characteristic equation and only their asymptotic form at the large-Pe limit are given. Up to the order of $O(\mathrm{Pe}^{-2})$, the decay rates of the viscous and thermal modes are as follows:

$$\omega_v = -\nu k^2, \quad \text{and} \quad \omega_t \cong -\kappa k^2\left[1 + \frac{(\gamma-1)\lambda}{\mathrm{Pe}^2}\right]. \tag{53}$$

The *sound attenuation rate* is a weighted sum of the shear viscosity, bulk viscosity, and thermal diffusivity,

$$\alpha \cong -k^2\left[a\kappa + (1-a)\nu + \frac{\nu_b}{2}\right]\left[1 + \frac{(\gamma-1)\lambda}{(\gamma-\lambda)\mathrm{Pe}^2}\right], \tag{54}$$

where $a = (\gamma-1)/2$. The speed of sound is also corrected by the dissipation rates as

$$\sqrt{\gamma\theta_0}\left[1 - \frac{(\gamma+\lambda)^2-4\lambda}{8\,\mathrm{Pe}^2}\right]. \tag{55}$$

Although the effects of the bulk viscosity on sound speed and decay rate of the thermal mode is on the order of $O(\mathrm{Pe}^{-2})$, its effect on sound attenuation is on the leading order. As a verification of the bulk viscosity, we numerically measure the sound attenuation rate and compare with the theoretical value.

The simulation is performed on a $256 \times 5 \times 5$ periodic lattice using the minimal ninth-order $E^9_{3,103}$ quadrature [23] capable of representing the fourth moments exactly. As the acoustic modes are isentropic, we set $\rho = \rho_0 + \rho' \sin(\boldsymbol{k}\cdot\boldsymbol{x})$ and initialize θ using the *isentropic invariant* $\theta\rho^{1-\gamma} = \theta_0\rho_0^{1-\gamma}$. The sound attenuation rate α and the sound frequency ω are measured by fitting the pressure fluctuation with the model $a_s e^{-\alpha t}\sin(\omega t + \phi)$.

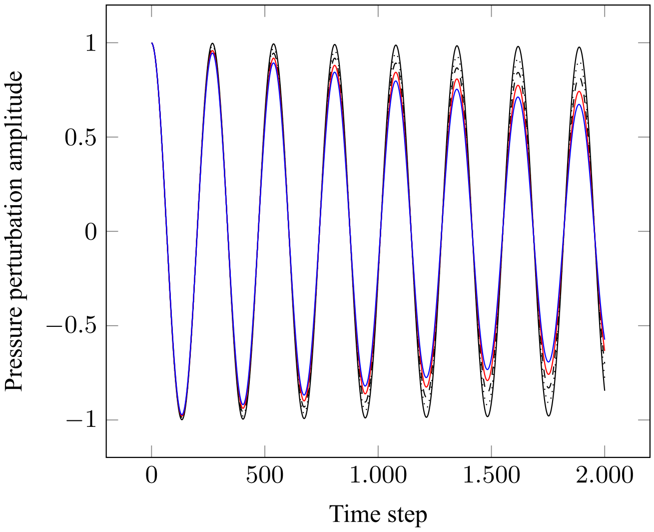

FIG. 1. Time history of the amplitude of pressure perturbation in acoustic waves with the varying ratio of bulk to shear viscosities. The solid black, dotted black, dashed black, solid red, and solid blue curves denote the cases with $\nu_b/\nu = 100, 500, 1000, 1500, 2000$, respectively. The other parameters are $\tau_{21} = 0.5005$, $\gamma = 1.3$, $\mathrm{Pr} = 2.1$, and $\tau_1 = \tau_3$.

Shown in Fig. 1 are the time histories of the pressure perturbation amplitude for various ratios of bulk to shear viscosities. The shear viscosity and all other parameters are fixed. Clearly the sound attenuation rate increases with the bulk viscosity. As shown in Fig. 2, the relative error of sound attenuation rate against its theoretical value is below 1% over a wide range of the viscosity ratio. As a relaxation time of $\tau_{21} \lesssim 0.5005$ with small bulk viscosity could cause stability problem, and $\tau_{22} \gtrsim 2$ corresponds to a finite Knudsen number, two different τ_{21}'s is used. Also worth noting is that, at least, in the continuum flow regime as long as the total thermal

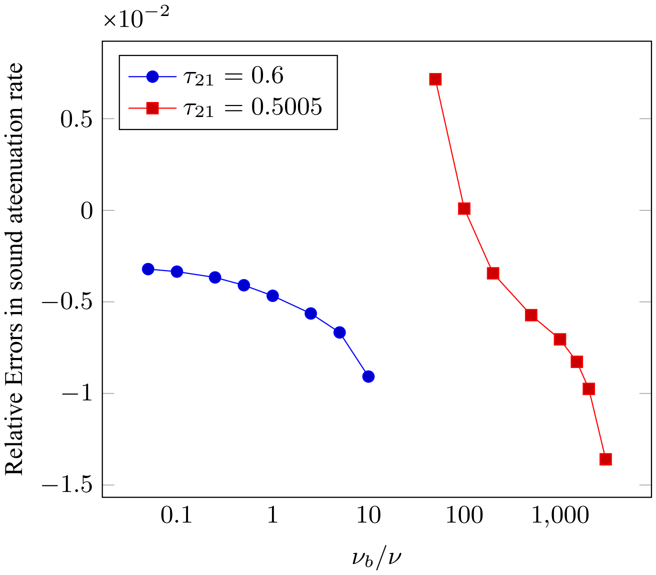

FIG. 2. Relative error of the decay rate with the varying ratio of bulk viscosity to shear viscosity. Two cases are tested: $\tau_{21} = 0.5005$ and $\tau_{21} = 0.6$. In both cases $\gamma = 1.3$, $\mathrm{Pr} = 2.1$, and $\tau_1 = \tau_3$. To be seen is that the relative error is generally below 1% over a large range of ν_b/ν.

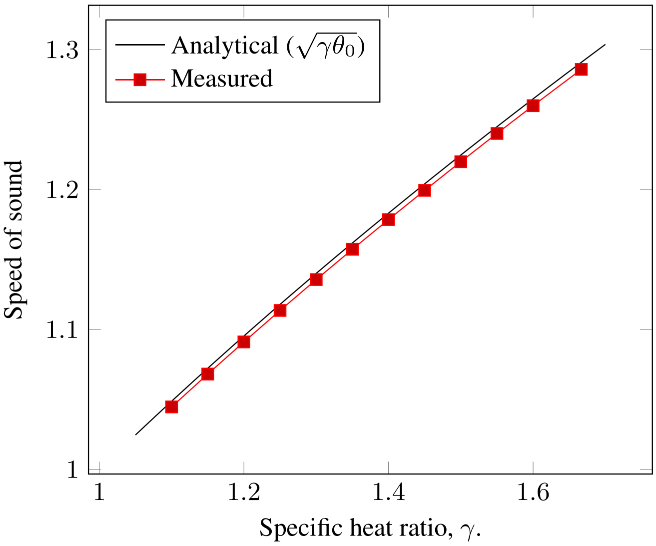

FIG. 3. Sound speed: analytical solution $c_s = \sqrt{\gamma\theta_0}$ versus numerical measurement with varying specific heat ratio. Parameters are $\mathrm{Pr} = 2.1$, $\tau_{21} = 0.501$, $\nu_b/\nu = 100$, and $\tau_1 = \tau_3$.

conductivity remain the same, τ_1 and τ_3 can be adjusted freely according the constraint Eq. (47) without causing any visible effect. The effect of τ_1 and τ_3 in rarefied gas flow regime remains to be investigated in a future work.

Shown in Fig. 3 are the sound speed measured through the angular frequency of the pressure perturbation. For the usual range of specific heat ratio, numerical measurements agree well with theoretical predictions.

IV. CONCLUSIONS AND DISCUSSION

To summarize, we point out that a collision operator can be defined as a spectral expansion where the eigenstates to which separate relaxation times can be assigned to correspond to the irreducible representations of SO(3) to preserve rotational symmetry. As the direct derivative at the second order, a LB model with arbitrarily adjustable bulk viscosity independent of the shear viscosity is constructed and numerically verified. Comparing with the similar model in Ref. [28], the present model employs a full distribution function to describe the additional energy transfer and a central-moment expansion which recovers the full Galilean invariance in the energy equation. More importantly the present model can be viewed as the first of a more comprehensive MRT model with a spectrum of relaxation times that can capture the details of the collision kernel and capable of simulating gases in a broader flow regime. An interesting future direction is that the same decomposition can be applied to the higher moments. For instance, the space of rank-3 tensors is 27 dimensional, which according to group theory, can be decomposed into seven lower-dimensional subspaces as commonly noted as $7 \oplus 5 \oplus 5 \oplus 3 \oplus 3 \oplus 3 \oplus 1$. Each of these spaces is closed under spatial rotation. Obviously many of these seven subspaces are not fully symmetric as the third moment should be. It would be interesting to know the maximum number of relaxation times a given order of moment can accommodate, and physical transport coefficients the relaxation times correspond to.

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