Alternative approach to the solution of the dispersion relation for a generalized lattice Boltzmann equation

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The simplest and most efficient lattice Boltzmann model that is able to recover the Navier-Stokes equations is based on a single-parameter scattering matrix, where the parameter is the first nonzero eigenvalue of the collision matrix. This simple model, based on a single relaxation time, has many shortcomings. Among these is the lack of freedom to extend the model to complex fluids whose stress tensors are characterized by more complicated constitutive relations. The lattice Boltzmann methodology may be generalized by considering the full collision matrix and tuning the matrix elements to obtain the desired macroscopic properties. The generalized hydrodynamics of a generalized lattice Boltzmann equation (LBE) was studied by Lallemand and Luo [Phys. Rev. E **61**, 6546 (2000)] by solving the dispersion equation of the linearized LBE. In this paper, an alternative approach to solving the dispersion equation based on a formal perturbation analysis is described. The methodology outlined is systematic, can be readily applied to other lattices, and does not require the reciprocals of the relaxation times to be small.

I. INTRODUCTION

The lattice Boltzmann equation (LBE) is a relatively new numerical technique based on kinetic theory for simulating fluid flow. The LBE evolved from the lattice gas cellular automata (LGCA) model of Frisch *et al.* [1], who showed that a simple automaton living on a triangular lattice could provide, in the limit of large-scale motion, a faithful representation of the dynamics of real fluids. The main advantages of the LGCA model are the absence of round-off error, regular data structures that are ideal for vector processing, local interactions that are ideal for parallel processing, and ease of implementation of highly irregular boundary conditions. However, there are some disadvantages, such as statistical noise, exponential complexity of the collision operator with increasing number of states per site, and restricted values of the transport coefficients. These disadvantages are due to the Boolean properties of the LGCA model. The issue of statistical noise is characteristic of all particle methods and substantial time and/or space averaging is required to extract reasonably smooth hydrodynamic signals from LGCA microdynamics. The issue of exponential complexity is also typical of finite-state algorithms. Each time a bit is added the collision rules roughly double in complexity. The LBE, as an alternative description of hydrodynamics, can be viewed as a direct extension of the LGCA model developed to overcome the LGCA shortcomings.

The LBE has a mesoscopic character and therefore lies between the classical macroscopic approach to the modeling of fluids based on the Navier-Stokes equations and the microscopic approach based on molecular dynamics. The essential idea behind the method is to model fluid flows by simplified kinetic equations which describe the time evolution of the distribution functions of particles having a discrete set of velocities and moving on a regular lattice. The LBE of McNamara and Zanetti [2] averages the microdynamics before the simulation rather than after it by solving the kinetic equation for the particle distribution instead of tracking the motion of each particle. Therefore, it is less susceptible to noise. Higuera *et al.* [3] realized that the one-to-one correspondence of the entries of the collision matrix to the underlying LGCA dynamics could be abandoned, and that the equilibria and entries of the collision matrix could be constructed independently to yield a self-standing mathematical tool for modeling the behavior of fluid motion. The problem of exponential complexity, which made the nonlinear LBE unviable for three-dimensional calculations, was solved by Higeuera and Jimenez [4] by considering perturbations of the local equilibrium function, resulting in a quasilinear LBE.

Lallemand and Luo [5] systematically studied the dispersion effects due to the presence of a lattice space by constructing a LBE model in moment space based on the generalized LBE due to d'Humières [6]. An analysis of the generalized hydrodynamics of the model characterized by dispersion, anisotropy, and lack of Galilean invariance, for example, facilitates the optimization of the properties of the model through the choice of free parameters associated with a given set of discrete velocities linked to the lattice. The analysis provides a mechanism by which comparisons with traditional methods for solving the Navier-Stokes equations can be made. A major advantage of this approach is that the Chapman-Enskog analysis, which is normally used to derive the macroscopic equations from the LBE, becomes redundant. Since the Chapman-Enskog analysis is applicable only when the Knudsen number, which is the ratio of the kinetic to hydrodynamic length scales, is small, the analysis based on the generalized hydrodynamics of the model is more generally valid. The so-called multiple-relaxation-time LBE developed by Lallemand and Luo [5] is simply a refined, and renamed, version of the quasilinear LBE of Higuera and Jimenez [4].

The motivation for this work is to study the small deviations from local equilibria, which are triggered by spontaneous fluctuations. In real fluids, these excitations extend over a range of wavelengths between the hydrodynamic and inter-

molecular scales (separated by expansions in the Knudsen number). There is no theory that provides a fully analytic link between kinetic and hydrodynamic theory. Asymptotic expansions of generalized LBEs provide a way of examining these fluctuations at different scales.

Apart from the work of Lallemand and Luo [5], Behrend *et al.* [7] have also studied the generalized hydrodynamics of LBE models. The method employed by Lallemand and Luo [5] for solving the dispersion equation of the linearized LBE involves eliminating the off-diagonal terms in the determinant corresponding to the interaction between the conserved and nonconserved moments and expanding in powers of the wave number. This reduces the dispersion equation to a 3 ×3 determinant for the conserved modes. The elements of the reduced determinant are then expanded in a series of reciprocals of the relaxation times and the wave number using an appropriate number of terms in order to compute the roots to the required accuracy. This approach requires that the reciprocals of the relaxation times are small in order to perform the expansion.

An alternative, more elegant and transparent approach to the difficult dispersion problem is described in the present paper based on a formal perturbation expansion of the dispersion relation. To our knowledge, the solution of the dispersion equation has only been accomplished, without resorting to numerics, using the approach of Lallemand and Luo [5]. Apart from lacking rigor, there are cases when this approach is unjustified, in particular when the Knudsen number is large. The range of applicability of LB methods, however, is not bounded by the domain of validity of the Chapman-Enskog method, as shown in the recent analysis of Sbragaglia and Succi [8], which is valid for finite Knudsen numbers. This analysis has validated numerical simulations that show, using appropriate boundary conditions, that LBE models can reproduce some of the important features beyond the hydrodynamic regime, such as the onset of slip [9]. The approach described in this paper is systematic and is readily applied to other lattices. Furthermore, it does not require the reciprocals of the relaxation times to be small in order to perform the analysis. Although it may be true that instabilities in the LBE are triggered more often by boundaries rather than at high Knudsen numbers, our approach shows that the derived transport coefficients (which are identical to those derived by Lallemand and Luo [5]) are valid for all Knudsen numbers.

II. THE D2Q9 LBE MODEL

The LBE is characterized by a lattice and some rule describing the manner in which distributions of particles move along lattice directions from one node to another. A simple yet sufficiently symmetric and multispeed lattice is the two-dimensional nine-velocity (D2Q9) lattice, shown in Fig. 1. It is a nine-velocity model (including a rest particle at the center) for which an equilibrium solution with all the properties needed to recover the macroscopic hydrodynamic equations can be derived. The nine discrete velocities are given by
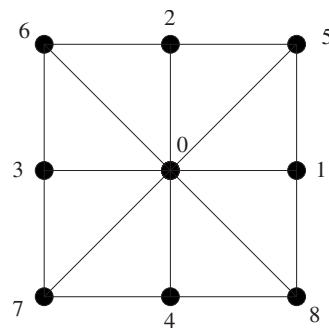

FIG. 1. The D2Q9 lattice.

$$
\mathbf{c}_i = \begin{cases} (0,0), & i = 0, \\ (\cos[(\alpha-1)\pi/2], \sin[(\alpha-1)\pi/2]), & i = 1, \ldots, 4, \\ \sqrt{2}(\cos[(2\alpha-9)\pi/4], \sin[(2\alpha-9)\pi/4]), & i = 5, \ldots, 8, \end{cases}
\tag{1}
$$

where we have assumed that the unit of velocity is unity.

At each time step, each particle jumps to a neighboring lattice node and collides with other particles. These advection and collision steps may be described by the equation

$$
N_i(\mathbf{x} + \mathbf{c}_i, t + 1) = N_i(\mathbf{x}, t) + \Omega_i(\mathbf{N}),
\tag{2}
$$

where $\mathbf{N} = [N_0, \ldots, N_8]^T$ and $N_i(\mathbf{x}, t)$, $i = 0, \ldots, 8$, is a distribution function corresponding to velocity $\mathbf{c}_i$ at the lattice point $\mathbf{x}$ at time t. This is the so-called lattice Boltzmann equation. The nine components of $\mathbf{N}$ describe the fluid at each node on the lattice. Once $\mathbf{N}$ is specified at a node on the lattice, the state of the fluid is fully prescribed at this point.

During these collisions the particles scatter but mass and momentum are conserved. In the lattice Boltzmann framework the macroscopic density and momentum are defined by the zeroth and first moments of the distribution function, respectively,

$$
\rho = \sum_i N_i,
\tag{3}
$$

$$
\rho \mathbf{u} = \sum_i N_i \mathbf{c}_i.
\tag{4}
$$

In the LBE approach, the collision operator can be linearized about a local equilibrium distribution function and the elements of the so-called collision matrix may be regarded as a set of free parameters that may be chosen, subject to the conservation constraints, to obtain the desired macroscopic quantities [2].

Higuera and Jimenez [4] conquered the exponential complexity limitation by considering perturbations about the local equilibrium function, i.e.,

$$
N_i = N_i^{(\mathrm{eq})} + \epsilon N_i^{(1)} + \epsilon^2 N_i^{(2)} + \cdots,
\tag{5}
$$

where $\epsilon \ll 1$ is the ratio of the microscopic scale to the smallest macroscopic scale. The equilibrium distribution function is required to satisfy the following constraints:

$$\sum_{i=0}^{8} N_i^{(eq)} = \rho, \tag{6}$$

$$\sum_{i=0}^{8} N_i^{(eq)} \mathbf{c}_i = \rho \mathbf{u}. \tag{7}$$

Now, inserting this form of N_i into the collision term and expanding in a Taylor series about $N_i^{(eq)}$ gives the quasilinear lattice Boltzmann equation of Higuera and Jimenez [4],

$$N_i(\mathbf{x} + \mathbf{c}_i, t + 1) - N_i(\mathbf{x}, t) = \sum_j M_{ij}(N_j - N_j^{(eq)}), \tag{8}$$

where

$$M_{ij} = \frac{\partial \Omega_i(\mathbf{N}^{(eq)})}{\partial N_j} \tag{9}$$

defines the collision matrix which determines the scattering rate between directions i and j. This matrix is isotropic and cyclic since the scattering depends only on the absolute value of the incoming populations. The importance of this procedure is that it reduces the collision term complexity from 2^b to b^2 and then, because of the symmetry of M_{ij}, to order b, thus making it computationally feasible to perform lattice Boltzmann simulations in three dimensions. A detailed analysis of matrix LBE methods, in terms of coupling of hydrodynamic to ghost modes, was first presented by Benzi *et al.* [10]. Ghost modes represent that part of the spectrum of the collision matrix that never makes the transition from the microscopic to the macroscopic level but which, nevertheless, are essential to the preservation of the essential symmetries of the system.

We note that the elements M_{ij} of the collision matrix $\mathbf{M}$ are parameters that can be chosen so that $\mathbf{M}$ satisfies the conservation laws and is compatible with the symmetry of the model. These elements are expressed in terms of the nonzero eigenvalues of $\mathbf{M}$, and the spectral analysis of the scattering matrix yields the mass and momentum quantities (associated with the null eigenvalues) and the momentum flux tensor (associated with the first nonzero eigenvalue) as well as faster-decaying kinetic modes. From this the exact expression for the fluid viscosity can be obtained. In view of the fact that the momentum flux, which is the slowest non-conserved quantity, needs only the leading nonzero eigenvalue of the collision matrix, the LBE model can be simplified yet further to obtain the so-called lattice Bhatnagar-Gross-Krook (LBGK) model:

$$N_i(\mathbf{x} + \mathbf{c}_i, t + 1) - N_i(\mathbf{x}, t) = \omega[N_i^{(e)}(\mathbf{x}, t) - N_i(\mathbf{x}, t)], \tag{10}$$

where ω, which is the first nonzero eigenvalue of $\mathbf{M}$, is a relaxation parameter. This is the simplest and most efficient lattice Boltzmann model that recovers the Navier-Stokes equations.

The equilibrium distribution for the D2Q9 LBGK model is usually taken to be

$$N_i^{(eq)} = \rho w_i \left(1 + 3\mathbf{c}_i \mathbf{u} - \frac{3}{2} u^2 + \frac{9}{2}(\mathbf{c}_i \cdot \mathbf{u})^2 \right), \tag{11}$$

where $w_0 = 4/9$, $w_i = 1/9$ ($i = 1, \ldots, 4$), and $w_i = 1/36$ ($i = 5, \ldots, 8$). Note that the pressure, defined by $P_0 = \rho/3$, satisfies an ideal equation of state. The factor $1/3$ is the square of the speed of sound, c_s^2.

The D2Q9 LBGK model is isotropic up to fourth order. A tensor is said to be isotropic if it is invariant under arbitrary rotations and reflections. Isotropic tensors associated with a lattice are constructed from the link vectors $\mathbf{c}_i$ by summing over all lattice directions i, weighted by a coefficient w_i. Fourth-order isotropy requires

$$\sum_i w_i = 1, \tag{12}$$

$$\sum_i w_i c_{i\alpha} = 0, \tag{13}$$

$$\sum_i w_i c_{i\alpha} c_{i\beta} = \lambda_1 \delta_{\alpha\beta}, \tag{14}$$

$$\sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} = 0, \tag{15}$$

$$\sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\delta} = \lambda_2 (\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}), \tag{16}$$

where λ_1 and λ_2 are constants, $\delta_{\alpha\beta}$ is the Kronecker delta function, and the greek indices refer to the Cartesian coordinates. For the D2Q9 lattice, we have $\lambda_1 = 1/3$ and $\lambda_2 = 1/9$.

The viscosity that appears in the Navier-Stokes equations obtained from this model is proportional to $1/\omega - 1/2$. To increase the Reynolds number by lowering the viscosity, one can "over-relax" the collision operator by using values of ω in the range $(1,2)$. The method is guaranteed to be numerically stable for $\omega \leq 1$. However, no such guarantees apply when $\omega \geq 1$, and the method can suffer from numerical instabilities, which can limit the highest Reynolds numbers attainable.

The generalized LBE, which is based on multiple relaxation times, leads to improved stability compared with single-relaxation-time LBGK models [11]. However, alternative approaches have been developed to overcome the stability issue. These include entropic lattice Boltzmann models [12–14], which have been shown to be nonlinearly numerical stable [15]. These models are motivated by the fact that the loss of numerical stability is due to the absence of an H theorem [14]. The idea behind these models is to specify an H function, rather than just the form of the equilibrium distribution. The methodology allows for arbitrarily low viscosity together with a rigorous discrete-time H theorem, and thus absolute stability. The upper limit to the Reynolds numbers attainable by the model is therefore determined by loss of resolution of the smallest eddies, rather than by loss of stability [14].

III. GENERALIZED LBE

Although simple and elegant, the LBGK Eq. (10) is not without its shortcomings. The single relaxation parameter ω implies that heat transfer takes place at the same rate as momentum transfer. Therefore, the Prandtl number, which is defined to be Pr$=\nu/\alpha$, where α is the thermal diffusivity, is always of unit value, making Eq. (10) appropriate for isothermal flows only. In addition, the ratio between the bulk and shear viscosities is fixed for LBGK models, causing difficulties in simulating flows at high Reynolds number, and there is scant freedom to extend the model to complex fluids, whose stress tensors are characterized by more complicated constitutive relations. These problems can be addressed by considering the full collision operator in Eq. (8) and tuning the matrix elements to obtain the desired properties. This task was systematically studied by Lallemand and Luo [5] and in this section we adopt their strategy.

Although we are using the D2Q9 lattice here, the application to other lattices follows a similar procedure. Equation (8) can be written in the following concise form:

$$|\delta N(\mathbf{x} + \mathbf{c}_i, t+1)\rangle = |\delta N(\mathbf{x},t)\rangle + \mathbf{M}|\delta N(\mathbf{x},t)\rangle, \quad (17)$$

where $|X\rangle = (X_0, X_1, \ldots, X_8)^\dagger$ with the superscript $\dagger$ denoting the matrix transpose, and $|\delta N\rangle$ is the fluctuating (nonequilibrium) part of the distribution function. Most D2Q9 models are constructed in a nine-dimensional vector space $\mathbf{R}^9$ spanned by $|N\rangle$, but the generalized LBE of Lallemand and Luo is instead based upon the moments $\{m_k | k = 0, \ldots, 8\}$ of N_i which are defined as

$$m_k = \langle \psi_k | N \rangle = \langle N | \psi_k \rangle, \quad \langle N | = (N_0, \ldots, N_8), \quad (18)$$

where $\{|\psi_k\rangle\}$ is an orthogonal dual basis set obtained by the Gram-Schmidt procedure from polynomials of the lattice vectors $c_{i\alpha}$. If the members of the basis $\{|\psi_k\rangle\}$ are also set to be the eigenvectors of the matrix $\mathbf{M}$, the linear relaxation in moment space naturally accomplishes the collision process [11]. To ensure that the correct expressions for density, momentum, and stress are obtained, the following vectors are used:

$$|\psi_0\rangle_i = |\mathbf{c}_i|^0 = 1, \quad (19)$$

$$|\psi_1\rangle_i = c_{ix}, \quad (20)$$

$$|\psi_2\rangle_i = c_{iy}, \quad (21)$$

$$|\psi_3\rangle_i = c_{ix}^2 - c_{iy}^2, \quad (22)$$

$$|\psi_4\rangle_i = c_{ix} c_{iy}. \quad (23)$$

The corresponding moments m_k, $k = 0, \ldots, 4$, give the density, x component of momentum, y component of momentum, and the diagonal and off-diagonal components of the stress tensor, respectively. The remaining moments can be chosen according to the meso- or macroscopic phenomena that are being modeled, such as multiphase effects [16] and viscoelastic effects [17], for example. Lallemand and Luo [5] find the following remaining (kinetic) moments:

$$|\psi_5\rangle_i = -4|\mathbf{c}_i|^0 + 3(c_{ix}^2 + c_{iy}^2), \quad (24)$$

$$|\psi_6\rangle_i = 4|\mathbf{c}_i|^0 - \frac{21}{2}(c_{ix}^2 + c_{iy}^2) + \frac{9}{2}(c_{ix}^2 + c_{iy}^2)^2, \quad (25)$$

$$|\psi_7\rangle_i = [-5|\mathbf{c}_i|^0 + 3(c_{ix}^2 + c_{iy}^2)]c_{ix}, \quad (26)$$

$$|\psi_8\rangle_i = [-5|\mathbf{c}_i|^0 + 3(c_{ix}^2 + c_{iy}^2)]c_{iy}, \quad (27)$$

corresponding to the physical quantities of energy, squared energy, and the x and y components of the energy flux, so that

$$|m\rangle = (\rho, j_x, j_y, P_{xx}, P_{yy}, e, \epsilon, q_x, q_y)^\dagger. \quad (28)$$

Note that, to simplify the algebra, the eigenvectors $|\psi_k\rangle$ have not been normalized. Each nonconserved moment has its own equilibrium state which is a function of the conserved moments. A possible choice for these states is [5]

$$\psi_3^{(e)} = \alpha_1 \frac{1}{\langle \psi_4 | \psi_4 \rangle}(\langle \psi_1 | \psi_1 \rangle j_x^2 - \langle \psi_2 | \psi_2 \rangle j_y^2) = \frac{3}{2}\alpha_1(j_x^2 - j_y^2),$$
$$(29)$$

$$\psi_4^{(e)} = \alpha_2 \frac{\sqrt{\langle \psi_1 | \psi_1 \rangle \langle \psi_2 | \psi_2 \rangle}}{\langle \psi_5 | \psi_5 \rangle}(j_x j_y) = \frac{3}{2}\alpha_2(j_x j_y), \quad (30)$$

$$\psi_5^{(e)} = \frac{1}{\langle \psi_6 | \psi_6 \rangle}[\beta_1 \langle \psi_0 | \psi_0 \rangle \rho + \alpha_3(\langle \psi_1 | \psi_1 \rangle j_x^2 + \langle \psi_2 | \psi_2 \rangle j_y^2)]$$
$$= \frac{1}{4}\beta_1 \rho + \frac{1}{6}\alpha_3(j_x^2 + j_y^2), \quad (31)$$

$$\psi_6^{(e)} = \frac{1}{\langle \psi_7 | \psi_7 \rangle}[\beta_2 \langle \psi_0 | \psi_0 \rangle \rho + \alpha_4(\langle \psi_1 | \psi_1 \rangle j_x^2 + \langle \psi_2 | \psi_2 \rangle j_y^2)]$$
$$= \frac{1}{4}\beta_2 \rho + \frac{1}{6}\alpha_4(j_x^2 + j_y^2), \quad (32)$$

$$\psi_7^{(e)} = \frac{\langle \psi_1 | \psi_1 \rangle}{\langle \psi_7 | \psi_7 \rangle}\gamma_1 j_x = \frac{1}{2}\gamma_1 j_x, \quad (33)$$

$$\psi_8^{(e)} = \frac{\langle \psi_2 | \psi_2 \rangle}{\langle \psi_8 | \psi_8 \rangle}\gamma_1 j_y = \frac{1}{2}\gamma_3 j_y, \quad (34)$$

where $\alpha_{1,2,3,4}$, $\beta_{1,2}$, and γ_1 are constants that will be determined in the next section. Based on the assumption that the nonconserved modes relax linearly toward their equilibrium state, the postcollision moments $\hat{m}_k$ are given by

$$\hat{P}_{xx} = P_{xx} - \tau_1(P_{xx} - P_{xx}^{(e)}), \quad (35)$$

$$\hat{P}_{xy} = P_{xy} - \tau_2(P_{xy} - P_{xy}^{(e)}), \quad (36)$$

$$\hat{e} = e - \tau_3(e - e^{(e)}), \quad (37)$$

$$\hat{\epsilon} = \epsilon - \tau_4(\epsilon - \epsilon^{(e)}), \quad (38)$$

$$\hat{q}_x = q_x - \tau_5(q_x - q_x^{(e)}), \qquad (39)$$

$$\hat{q}_y = q_y - \tau_6(q_y - q_y^{(e)}), \qquad (40)$$

where $\tau_1, \ldots, \tau_6$, are the relaxation parameters.

There exists a simple linear mapping $\mathbf{T}$ that relates the distribution functions $|N\rangle$ to the moments $|m\rangle$, $|m\rangle = \mathbf{T}|N\rangle$ and $|N\rangle = \mathbf{T}^{-1}|m\rangle$, and the linearized lattice Boltzmann equation (17) may be written as

$$|\delta N(\mathbf{x} + \mathbf{c}_i, t + 1)\rangle = |\delta N(\mathbf{x}, t)\rangle + \mathbf{T}^{-1}\mathbf{CT}|\delta N(\mathbf{x}, t)\rangle, \quad (41)$$

where

$$C_{ji} = \left. \frac{\langle m_j | m_j \rangle}{\langle m_i | m_i \rangle} \frac{\partial \hat{m}_i}{\partial m_j} \right|_{|m\rangle = |m^{(e)}\rangle} \qquad (42)$$

is the collision operator in moment space and is found to be

$$\mathbf{C} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3\tau_1\alpha_1 V_x & -3\tau_1\alpha_1 V_y & -\tau_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3\tau_2\alpha_2 V_y/2 & 3\tau_2\alpha_2 V_x/2 & 0 & -\tau_2 & 0 & 0 & 0 & 0 \\ \tau_3\beta_1/3 & \tau_3\alpha_3 V_x/3 & \tau_3\alpha_3 V_y/3 & 0 & 0 & -\tau_3 & 0 & 0 & 0 \\ \tau_4\beta_2/4 & \tau_4\alpha_4 V_x/3 & \tau_4\alpha_4 V_y/3 & 0 & 0 & 0 & -\tau_4 & 0 & 0 \\ 0 & \tau_5\gamma_1/2 & 0 & 0 & 0 & 0 & 0 & -\tau_5 & 0 \\ 0 & 0 & \tau_6\gamma_1/2 & 0 & 0 & 0 & 0 & 0 & -\tau_6 \end{pmatrix}. \qquad (43)$$

Clearly, $\mathbf{T} = (|\psi_0\rangle, \ldots, |\psi_8\rangle)^t$.

To examine how the transport coefficients depend on the wave vector $\mathbf{k}$ and to determine the LBE stability properties a Fourier transform is performed on Eq. (41), which yields

$$\mathbf{A}|\delta N(\mathbf{k} + \mathbf{c}_i, t + 1)\rangle = (\mathbf{I} + \mathbf{T}^{-1}\mathbf{CT})|\delta N(\mathbf{k}, t)\rangle, \qquad (44)$$

where $\mathbf{I}$ denotes the identity matrix,

$$A_{ij} = \exp(\iota \mathbf{c}_i \cdot \mathbf{k})\delta_{ij} \qquad (45)$$

is the streaming operator, and $\iota = \sqrt{-1}$. A more concise form of (44) is

$$|\delta N(\mathbf{k}, t + 1)\rangle = \mathbf{L}|\delta N(\mathbf{k}, t)\rangle, \qquad (46)$$

where

$$\mathbf{L} = \mathbf{A}^{-1}(\mathbf{I} + \mathbf{T}^{-1}\mathbf{CT}) \qquad (47)$$

is the linearized evolution operator.

The difference Eq. (46) has solutions of the form

$$|G(\mathbf{x}, t)\rangle = \lambda^t K_x^m K_y^n |X\rangle \qquad (48)$$

where t here denotes time and m and n are indices for space ($\mathbf{x} = m\overline{\mathbf{x}} + n\overline{\mathbf{y}}$ and $\overline{\mathbf{x}}$ and $\overline{\mathbf{y}}$ are unit vectors in Cartesian coordinates). $|X\rangle$ is the initial state. For a fully periodic system the above solution can be chosen as

$$|\delta N\rangle = \exp(\lambda t - \iota \mathbf{k} \cdot \mathbf{x})|G\rangle, \qquad (49)$$

which leads to the following eigenvalue problem [5]:

$$\lambda|X\rangle = \mathbf{L}|X\rangle, \qquad (50)$$

where λ satisfies the dispersion relation

$$\det(\mathbf{I} - \lambda\mathbf{L}) = 0. \qquad (51)$$

A. Perturbation expansion of the dispersion relation

The roots of the dispersion relation (51) determine the transport coefficients and their dependence on $\mathbf{k}$. The solution of the above equation also provides the solution of the initial value problem (46):

$$|\delta N(\mathbf{k}, t + 1)\rangle = \mathbf{L}^t|\delta N(\mathbf{k}, 0)\rangle = \sum_\mu \lambda_\mu^t |\phi_\mu\rangle\langle\phi_\mu'|\delta N(\mathbf{k}, 0)\rangle, \qquad (52)$$

where $|\phi_\mu\rangle$ is the right eigenvector of $\mathbf{L}$ corresponding to eigenvalue λ_μ and $\langle\phi_\mu'|$ is the left eigenvector. Note that, since the matrix $\mathbf{L}$ is nonsymmetric and non-Hermitian, the right and left eigenvectors are neither equal nor orthogonal, but they do form a complete biorthonormal set, i.e.,

$$\sum_\mu |\phi_\mu\rangle\langle\phi_\mu'| = \mathbf{I}, \qquad (53)$$

$$\langle\phi_\nu'|\phi_\mu\rangle = \delta_{\nu\mu}. \qquad (54)$$

The dispersion relation is complicated and one cannot get analytic expressions for the roots in z, except for some very special cases. The analysis in this paper is used to compute the eigenvalues of the dispersion equation in the (linearized) hydrodynamic regime (i.e., small k). This procedure yields three eigenvectors corresponding to one shear and two sound modes. Terms of $O(k^3)$ do not appear in the hydrodynamic spectrum.

When $k_x = k_y = 0$ Eq. (51) factorizes as

$$(1-\lambda)^3[\lambda - (1-\tau_1)][\lambda - (1-\tau_2)][\lambda - (1-\tau_3)]$$
$$\times [\lambda - (1-\tau_4)][\lambda - (1-\tau_5)][\lambda - (1-\tau_6)] = 0, \tag{55}$$

and since the hydrodynamic regime corresponds to long times and large spatial scales (i.e., when $k = |\mathbf{k}| \to 0$), the hydrodynamic eigenvalues are those with z close to 1. Luo and Lallemand [5] suggest solving Eq. (50) by expanding the evolution operator $\mathbf{L}$ in powers of k and applying Gaussian elimination to the matrix using $1/\tau_\alpha$ as small parameters for the nonconserved (kinetic) modes. Doing this successfully leads to a new 3×3 determinant for the conserved (hydrodynamic) modes. Due to the complexity of the dispersion matrix and the large number of unknowns, this procedure is rather cumbersome. Therefore, we choose to solve the dispersion equation by considering a perturbation expansion of Eq. (50) [18], i.e.,

$$\mathbf{L} = \mathbf{L}^{(0)} + \mathbf{L}^{(1)} + \mathbf{L}^{(2)} + \cdots, \tag{56}$$

$$\phi_\mu = \phi_\mu^{(0)} + \phi_\mu^{(1)} + \phi_\mu^{(2)} + \cdots, \tag{57}$$

$$z_\mu = \lambda_\mu^{(0)} + \lambda_\mu^{(1)} + \lambda_\mu^{(2)} + \cdots, \tag{58}$$

where the superscripts refer to the order of $k \ll 1$ and

$$\mathbf{L}^{(n)} = \mathbf{K}^{(n)}(\mathbf{I} + \mathbf{M}^{-1}\mathbf{C}\mathbf{M}), \tag{59}$$

$$K_{ij}^n = \frac{1}{n!}(-\iota\mathbf{k} \cdot \mathbf{c}_i)^n \delta_{ij}. \tag{60}$$

The transport coefficients are related to the eigenvalues of $\mathbf{L}$ through the following [5]:

$$\nu(\mathbf{k}) = -\frac{1}{k^2}\text{Re}[\ln \lambda_T(\mathbf{k})], \tag{61}$$

$$g(\mathbf{k})V \cos \psi = -\frac{1}{k}\text{Im}[\ln \lambda_T(\mathbf{k})], \tag{62}$$

$$\frac{1}{2}\nu(\mathbf{k}) + \zeta(\mathbf{k}) = -\frac{1}{k^2}\text{Re}[\ln \lambda_\pm(\mathbf{k})], \tag{63}$$

$$c_s(\mathbf{k}) \pm g(\mathbf{k})V \cos \psi = \mp \frac{1}{k}\text{Im}[\ln \lambda_\pm(\mathbf{k})], \tag{64}$$

where ν is the kinematic viscosity, ζ is the bulk viscosity, g is a Galilean invariant factor ($g=1$ implies Galilean invariance), ψ is the angle between $\mathbf{V}$ and $\mathbf{k}$, and λ_T and $\lambda_\pm$ are the eigenvalues corresponding to the transverse and longitudinal hydrodynamic modes of the system. The transport coefficients are to be obtained through a perturbation analysis so the following series expansion is used:

$$\nu(\mathbf{k}) = \nu^{(0)} + \nu^{(1)}k^2 + \cdots + \nu^{(n)}k^{2n} + \cdots, \tag{65}$$

$$\zeta(\mathbf{k}) = \zeta^{(0)} + \zeta^{(1)}k^2 + \cdots + \zeta^{(n)}k^{2n} + \cdots, \tag{66}$$

$$C(\mathbf{k}) = C^{(0)} + C^{(1)}k^2 + \cdots + C^{(n)}k^{2n} + \cdots, \tag{67}$$

$$g(\mathbf{k}) = g^{(0)} + g^{(1)}k^2 + \cdots + g^{(n)}k^{2n} + \cdots. \tag{68}$$

Examining the resulting dispersion equation at different orders of k gives the transport coefficients and the bounds on the free parameters.

B. The eigenvalues and transport coefficients

Substituting the expansions (56)–(58) into the dispersion Eq. (50) yields the set of equations

$$\mathbf{L}^{(0)}|\phi_\mu^{(0)}\rangle = \lambda_\mu^{(0)}|\phi_\mu^{(0)}\rangle, \tag{69}$$

$$(\mathbf{L}^{(0)} - \lambda_\mu^{(0)}\mathbf{I})|\phi_\mu^{(1)}\rangle = -(\mathbf{L}^{(1)} - \lambda_\mu^{(1)}\mathbf{I})|\phi_\mu^{(0)}\rangle, \tag{70}$$

$$(\mathbf{L}^{(0)} - \lambda_\mu^{(0)}\mathbf{I})|\phi_\mu^{(2)}\rangle = -(\mathbf{L}^{(2)} - \lambda_\mu^{(2)}\mathbf{I})|\phi_\mu^{(0)}\rangle$$
$$- (\mathbf{L}^{(1)} - \lambda_\mu^{(1)}\mathbf{I})|\phi_\mu^{(1)}\rangle. \tag{71}$$

We first consider the simpler case in which the streaming velocity $\mathbf{V} = \mathbf{0}$. Equation (69) is easily solved and an eigenvalue $\lambda_\mu^{(0)} = 1$ with a threefold degeneracy is found. These eigenvalues correspond to three hydrodynamic (conserved) modes. Due to the degeneracy of $\lambda_\mu^{(0)}$, the corresponding $O(1)$ eigenvectors, $|z_n\rangle$, are linearly dependent and the general solution to Eq. (69) is a linear combination of these vectors:

$$|\phi_\mu^{(0)}\rangle = \sum_n B_{\mu,n}|z_n\rangle, \tag{72}$$

where the $B_{\mu,n}$'s are coefficients to be determined.

To solve the order-k equation we multiply (70) to the left with $\langle z_m'|$:

$$\langle z_m'|\mathbf{L} - \lambda_\mu^{(1)}\mathbf{I}|\phi_\mu^{(0)}\rangle = \sum_n \langle z_m'|\mathbf{L} - \lambda_\mu^{(1)}\mathbf{I}|z_n\rangle B_{\mu,n} = 0,$$

where the left vectors, $\langle z_m'|$, are found by solving the transpose of Eq. (69). For future reference we define the general solution to the "left" equation to be

$$\langle \phi_v'^{(0)}| = \sum_m B_{v,m}'\langle z_m'|. \tag{73}$$

Equation (73) is an eigenvalue problem to order k in the subspace spanned by the hydrodynamic modes, i.e., $\det(\mathbf{L} - \lambda_\mu^{(1)}\mathbf{I}) = 0$. The characteristic polynomial is of degree 3 in $\lambda_\mu^{(1)}$ and can be solved to find

$$\lambda_T^{(1)} = 0, \tag{74}$$

$$\lambda_\pm^{(1)} = \pm \iota k c_s, \tag{75}$$

with the speed of sound squared given by

$$c_s^2 = \frac{1}{3}\left(2 + \frac{\beta_1}{8}\right). \tag{76}$$

To ensure positivity of the speed of sound we require $\beta_1 > -16$. The coefficients $B_{\mu,n}$, and hence the eigenvectors $|\phi_\mu^{(0)}\rangle$, are found by substituting $\lambda_\mu^{(1)}$ into Eq. (73) and solving the linear system. A similar procedure applied to the left equa-

tion yields the particular solution $\langle \phi'^{(0)}_\mu |$. The general solution to Eq. (70) is

$$|\phi^{(1)}_\mu\rangle = -(\mathbf{L}^{(0)} - \lambda^{(0)}_\mu \mathbf{I})^{-1}(\mathbf{L}^{(1)} - \lambda^{(1)}_\mu \mathbf{I})|\phi^{(0)}_\mu\rangle + \sum_n D_{\mu,n}|\phi^{(0)}_\mu\rangle, \tag{77}$$

where $D_{\mu,n}$ are constant coefficients. Since the matrix $\mathbf{L}^{(0)} - \lambda^{(0)}_\mu \mathbf{I}$ is singular, we find the first term on the right-hand side of Eq. (77), which we call $|\sigma^{(1)}_\mu\rangle$, by applying the method of Gaussian elimination and back substitution to the linear system (70).

To find the eigenvalues at order k^2 we multiply Eq. (71) to the left by $\langle \phi'^{(0)}_v |$ and rearrange to obtain

$$\lambda^{(2)}_\mu = \frac{1}{\langle \phi'^{(0)}_v | \phi^{(0)}_\mu \rangle}(\langle \phi'^{(0)}_v | \mathbf{L}^{(2)} | \phi^{(1)}_\mu \rangle + \langle \phi'^{(0)}_v | \mathbf{L}^{(1)} - \lambda^{(1)}_\mu \mathbf{I} | \sigma^{(1)}_\mu \rangle$$
$$+ \sum_n D_{\mu,n}\langle \phi'^{(0)}_v | \mathbf{L}^{(1)} - \lambda^{(1)}_\mu \mathbf{I} | \phi^{(0)}_\mu \rangle). \tag{78}$$

For $v = \mu$ the last term on the right-hand side of Eq. (78) vanishes and we find the following expressions for the eigenvalues:

$$\lambda^{(2)}_T = -k^2 \nu_0 = \frac{\langle \phi'^{(0)}_T | \mathbf{L}^{(2)} | \phi^{(1)}_T \rangle + \langle \phi'^{(0)}_T | \mathbf{L}^{(1)} | \sigma^{(1)}_T \rangle}{\langle \phi'^{(0)}_T | \phi^{(0)}_T \rangle}, \tag{79}$$

$$\lambda^{(2)}_\pm = -k^2(\nu_0 + \zeta_0)$$
$$= \frac{\langle \phi'^{(0)}_\pm | \mathbf{L}^{(2)} | \phi^{(1)}_\pm \rangle + \langle \phi'^{(0)}_\pm | \mathbf{L}^{(1)} \pm \imath k c_s \mathbf{I} | \sigma^{(1)}_\pm \rangle}{\langle \phi'^{(0)}_\pm | \phi^{(0)}_\pm \rangle}. \tag{80}$$

The above depend on the direction of the wave vector $\mathbf{k}$. To eliminate this effect and ensure isotropy we require the expressions to factorize in k^2. This is achieved if we set

$$\frac{1}{\tau_2} - \frac{1}{2} = 2\left(\frac{1}{\tau_1} - \frac{1}{2}\right)\frac{\gamma_1 + 4}{2 - \gamma_1}, \tag{81}$$

which leads to expressions for the kinematic and bulk viscosity in the long-wavelength limit ($\mathbf{k} \to \mathbf{0}$):

$$\nu_0 = \frac{2 - \gamma_1}{12}\left(\frac{1}{\tau_1} - \frac{1}{2}\right), \tag{82}$$

$$\zeta_0 = \frac{\gamma_1 + 10 - 12c_s^2}{24}\left(\frac{1}{\tau_3} - \frac{1}{2}\right), \tag{83}$$

where $-4 < \gamma_1 < 2$ and $0 < \tau_1, \tau_2, \tau_3 < 2$ by the positivity of the transport coefficients.

To determine the other adjustable parameters and narrow the bounds of β_1 and γ_1, we now consider the dispersion equation with a constant streaming velocity $\mathbf{V}$. To satisfy Galilean invariance we must have $g_0 = 1$, which is obtained only when

$$\alpha_1 = \alpha_2 = \frac{2}{3}, \quad \alpha_3 = 18. \tag{84}$$

We proceed in the same way as in the case when $\mathbf{V} = \mathbf{0}$ by examining the dispersion equation to different orders in k.

After solving Eq. (69), Eq. (70) is solved to find the speed of sound, C_s:

$$C_s = \mathbf{V} \cdot \mathbf{k} \pm \sqrt{c_s^2 + (\mathbf{V} \cdot \mathbf{k})^2}. \tag{85}$$

The second-order eigenvalues are complicated expressions that depend on the direction of the wave vector $\mathbf{k}$. If we set $\gamma_1 = -2$, the shear and bulk viscosities are found to be

$$\nu_0 = \{\tau_3(2 - \tau_1)[c_s^2 + (1 - 3c_s^2)(\mathbf{V} \cdot \mathbf{k})^2] + 3[2(\tau_1 - \tau_3)$$
$$+ \tau_1(\tau_3 - 2)(\mathbf{V} \cdot \mathbf{k})^2/V]\}/\{6\tau_3\tau_1[(\mathbf{V} \cdot \mathbf{k})^2 + c_s^2]\}, \tag{86}$$

$$\zeta_0 = ((\mathbf{V} \cdot \mathbf{k})\sqrt{c_s^2 + (\mathbf{V} \cdot \mathbf{k})^2}\{12V^2[(\tau_3 - \tau_1) + \tau_3(\tau_1 - 2)$$
$$\times (\mathbf{V} \cdot \mathbf{k})^2/V^2](2\tau_3 - 3\tau_3\tau_1 + 4\tau_1)(1 - 3c_s^2)\}$$
$$+ 3(\mathbf{V} \cdot \mathbf{k})^2[(\mathbf{V} \cdot \mathbf{k})^2(2\tau_1 + 3\tau_1\tau_3 - 8\tau_1)6V^2(\tau_3 - \tau_1)]$$
$$+ 2(\mathbf{V} \cdot \mathbf{k})^2[6(2\tau_1\tau_3 - \tau_3 - \tau_1)c_s^2 + \tau_1(2 - \tau_3)]$$
$$+ c_s^2[6V^2(\tau_3 - \tau_1) + \tau_1(2 - \tau_3)$$
$$\times (2 - 3c_s^2)])/\{12\tau_1\tau_3[(\mathbf{V} \cdot \mathbf{k})^2 + c_s^2]\}. \tag{87}$$

The effect of V on the transport coefficients is clear. Setting $c_s^2 = 1/3$ (that is, $\beta_1 = -8$) eliminates the first-order effect of $\mathbf{V}$ on ζ_0 and the second-order effect on ν_0. Lallemand and Luo [5] argue that the second-order effects of $\mathbf{V}$ on C_s and ζ_0 can be removed by considering a more complicated 13-velocity lattice and allowing for compressibility effects in the equilibrium properties. Note that the model reduces to the LBGK equation (10) if we set all the relaxation parameters to be equal ($\tau_\alpha = \omega$) and choose $\beta_2 = 4$ and $\alpha_4 = -18$.

IV. CONCLUSIONS

The generalized hydrodynamics of a generalized LBE is studied using a transparent and formal perturbation analysis. The value of this approach is that it provides a means to analyze the generalized hydrodynamic behavior of the LBE, which can be compared to that of the Navier-Stokes equations. The perturbation analysis obviates the need to perform a Chapman-Enskog analysis, which is applicable only when the Knudsen number is small, to retrieve the macroscopic equations. If (to a certain value of $\mathbf{k}$) the modes of the LBE and Navier-Stokes equations behave in exactly the same way (as shown in [5]) then there is no distinction between the two sets of equations (to a given order of $\mathbf{k}$) and the Chapman-Enskog analysis [which can be rather cumbersome for models more complicated than the D2Q9 LBGK equation (10)] can be bypassed. Note, however, recent work by Sbragalia and Succi [8], who perform a nonperturbative analysis of the LBGK equation that overcomes the restrictions imposed by the standard Chapman-Enksog analysis and is valid for Knudsen numbers of the order of unity.

The approach described here provides an alternative treatment to generalized hydrodynamics to that presented by Lallemand and Luo [5], which is not restricted to situations where $1/\tau_i$, $i = 1, \dots, 6$, are small. Numerical results on shear flow with an initial discontinuous velocity profile with or without a constant streaming velocity are presented by Lallemand and Luo [5]. These demonstrate the dispersion

effects in the LBE model. The expressions obtained for the hydrodynamic transport coefficients agree with those in [5] and are optimal in the sense that they yield the desirable properties, and therefore numerical simulations are not presented here. The methodology described here is systematic and can be readily modified to study any lattice. The perturbation analysis of the dispersion equation for the D2Q9 LBE yields the desired transport coefficients.

The ability to study the LBE for a range of k (which the Chapman-Enskog analysis cannot do) reveals some shortcomings of the D2Q9 model, namely, the dependence of the transport coefficients on the mean velocity **V**. The generalized LBE separates different time scales within the model, allowing for the incorporation of sophisticated physics such as energy modes (important for defining nonisothermal LBEs that are consistent with thermodynamics) and non-

Newtonian constitutive relations for the stress tensor. It has been shown that having separate relaxation times for the kinetic modes can increase the stability of the model [5].

This approach also suggests a means for developing a LBE for viscoelastic fluids by extending the lattice domain (e.g., from D2Q9 to D2Q11) and coupling the eigenvectors associated with the viscous stress tensor to two new eigenvectors that are responsible for memory effects. The coupling is obtained by modifying the original viscous eigenvectors. Therefore, we have the modified eigenvalues of the collision and evolution operator together with two additional ones. To obtain viscoelastic effects it is also important that the different modes relax at different rates, which is achieved though the values of the eigenvalues. In other words, to develop a class of viscoelastic LBEs, the choice of collision matrix and eigenvectors is important.

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