



Galilean-invariant multi-speed entropic lattice Boltzmann models

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Abstract

In recent work [Phys. Rev. E 68 (2003) 025103], it was shown that the requirement of Galilean invariance determined the form of the H function used in entropic lattice Boltzmann models for the incompressible Navier–Stokes equations in D dimensions. The form obtained was that of the Burg entropy for $D = 2$, and the Tsallis entropy with $q = 1 - 2/D$ for $D \neq 2$. The conclusions obtained in that work were restricted to particles of a single-mass and speed on a Bravais lattice. In this work, we generalize the construction of such Galilean-invariant entropic lattice Boltzmann models by allowing for certain models with multiple masses and speeds. We show that the required H function for these models must be determined by solving a certain functional differential equation. Remarkably, the solutions to this equation also have the form of the Tsallis entropy, where q is determined by the solution to a certain transcendental equation, involving the dimension and symmetry properties of the lattice, as well as the masses and speeds of the particles.

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1. Introduction

Lattice Boltzmann models of fluids [2,3] evolve single-particle distribution functions in discrete-time steps on a regular spatial lattice. That is, velocity space is discrete, and is comprised of (possibly linear combinations of) the lattice vectors themselves. In spite of this very radical simplification of the Boltzmann equation, it has been shown that the incompressible Navier–Stokes equations emerge unscathed in the limit of small Mach and Knudsen numbers.

In the most general situation, the collection of velocities that is retained do not all have the same magnitude, and we denote them by $\mathbf{c}_{a,j}$, where the index a is associated with the magnitude, $c_a \equiv |\mathbf{c}_{a,j}|$, and j enumerates the velocity vectors with that speed; velocities with the same index a are said to be in the same *speed class*. The single-particle distribution corresponding to lattice vector $\mathbf{c}_{a,j}$ at lattice position \mathbf{x} and time step t is denoted by $N_{a,j}(\mathbf{x}, t)$. The simplest lattice Boltzmann models employ a collision operator of BGK form [4], so that their evolution equation is

$$N_{a,j}(\mathbf{x} + \mathbf{c}_{a,j}, t + \Delta t) = N_{a,j}(\mathbf{x}, t) + \frac{1}{\tau} [N_{a,j}^{(\text{eq})}(\mathbf{x}, t) - N_{a,j}(\mathbf{x}, t)] \quad (1)$$

for $j = 1, \dots, b_a$, for each speed a . Here b_a is the number of velocities with speed c_a , $N_{a,j}^{(\text{eq})}(\mathbf{x}, t)$ is a specified equilibrium distribution function that depends only on the values of the conserved quantities at a site, and τ is

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a characteristic collisional relaxation time. Using a discrete-velocity version of the Chapman–Enskog analysis [3], we shall show that the mass and momentum moments of the distribution function obey the incompressible Navier–Stokes equations for certain choices of equilibrium distribution.

The viscosity that appears in the Navier–Stokes equations obtained from these models is proportional to $\tau - 1/2$. To lower viscosity and thereby increase Reynolds number, practitioners often “over-relax” the collision operator by using values of τ in the range $(1/2, 1]$. Though the method is guaranteed to be numerically stable for $\tau \geq 1$, no such guarantees apply when $\tau < 1$, and the method is fraught with numerical instabilities, which limit the highest Reynolds numbers attainable.

In an effort to understand and thereby avoid these instabilities, there has been much recent interest in *entropic lattice Boltzmann models* [5–7]. These models are motivated by the fact that the loss of numerical stability is due to the absence of an H -theorem [7]. Numerical instabilities evolve in ways that would be precluded by the existence of a well-behaved Lyapunov function. The idea behind entropic lattice Boltzmann models is to specify an H function, rather than just the form of the equilibrium distribution; of course, the latter is that which extremizes the former. The evolution will be required never to decrease H , yielding a discrete-time H -theorem; this is to be distinguished from other discrete models of fluid dynamics for which an H -theorem may be demonstrated only in the limit of vanishing time step [8], or not at all.

To ensure that collisions never decrease H , the characteristic collision time τ is made a function of the incoming state by solving for the smallest value $\tau_{\min} < 1$ that does not increase H . The value then used is $\tau = \tau_{\min}/\kappa$, where $0 < \kappa < 1$. It has been shown that the expression for the viscosity obtained by the Chapman–Enskog analysis will approach zero as κ approaches unity [5–7]. Thus, the entropic lattice Boltzmann 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 [7,9–11].

In an earlier paper, we constructed entropic lattice Boltzmann models for the incompressible Navier–Stokes equations that are Galilean-invariant to second order in Mach number, and we showed that the requirement of Galilean invariance makes the choice of H function unique. More specifically, we showed that the required function has the form of the Burg entropy [12] in two dimensions, and the Tsallis entropy in higher dimensions. These conclusions were based on single-speed lattice Boltzmann models on Bravais lattices.

In this work, we generalize the construction of such Galilean-invariant entropic lattice Boltzmann models by allowing for the treatment of certain models with multiple particle masses and speeds. We show that the required H function for these more general models must be determined by solving a certain functional differential equation. Remarkably, the solutions to this equation also have the form of the Tsallis entropy, where q is determined by the solution to a certain transcendental equation. This equation involves the dimension and symmetry properties of the lattice, as well as the masses and speeds of the particles in the model.

In [Section 2](#), we describe the lattices used for our multispeed lattice Boltzmann models. In particular, we introduce notation for sums of outer products of velocity vectors, which play an important role in the Mach number expansion of the equilibrium distribution and the Chapman–Enskog analysis. To make the analysis tractable, we restrict our attention to multi-speed models for which each speed class separately satisfies the isotropy requirements. In [Section 3](#), we specify the form of the equilibrium distribution function, assuming only that the H function is of trace form, and we derive the Mach number expansion of this equilibrium. In [Appendix A](#) we construct a lattice BGK kinetic equation with this equilibrium distribution and apply the Chapman–Enskog analysis to it, solving it in the asymptotic limit of small Knudsen and Mach number. The resulting hydrodynamic equations are presented in [Section 4](#). These are of Navier–Stokes form, and the derivation yields the equation of state for the pressure, the viscosity, and the g factor that may multiply the convective derivative. In [Section 5](#), we examine the requirement that $g = 1$, needed to restore Galilean invariance in the context of four examples. The first is the single-speed model, in order to show that

our methodology is able to recover the previously known results; the second is a single-speed model augmented by the addition of rest particles of the same mass; the third allows the rest particles to have a different mass from the moving particles; and the fourth is the general case, subject to the above-described restriction on our lattice.

2. Description of lattice

As noted above, velocity vectors are grouped into “speed classes” based on their magnitudes. We may associate these magnitudes with speeds, since the unit of time is taken to be $\Delta t = 1$. We denote the velocity vectors by $\mathbf{c}_{a,j}$, and assume that these are (linear combinations of) lattice vectors. Here a is an index denoting a certain speed class, and j indexes the vectors within that class. All lattice vectors within a speed class have the same magnitude $|\mathbf{c}_{a,j}| = c_a$, and are associated with particles of the same mass, m_a .

Sums of outer products of the velocity vectors arise frequently in the analysis of lattice Boltzmann models. Within a speed class, these sums are denoted by

$$\mathbf{b}_{n,a} \equiv \sum_j^{b_a} \otimes^n \mathbf{c}_{a,j}, \tag{2}$$

so that, in particular, $\mathbf{b}_{0,a} = b_a$. We assume that these quantities vanish for odd n , and that they are isotropic tensors for even $n \leq 4$. That is, we assume that

$$\mathbf{b}_{2,a} = b_{2,a} \mathbf{1}, \tag{3}$$

$$\mathbf{b}_{4,a} = b_{4,a} \text{per}(\mathbf{1} \otimes \mathbf{1}), \tag{4}$$

where “per” denotes a sum over all symmetric permutations of tensor components.¹ A Bravais lattice [1,3] will have

$$b_{2,a} = \frac{b_a c_a^2}{D}, \tag{5}$$

$$b_{4,a} = \frac{b_a c_a^4}{D(D+2)}, \tag{6}$$

but we shall not specialize to this case in what follows. The assumption that the outer products of lattice vectors for even $n \leq 4$ be isotropic tensors, separately within each speed class, is restrictive. It eliminates from our consideration certain interesting models (such as the D2Q9, D3Q15 and D3Q19 models [3]) in which these tensors are not isotropic within each speed class, but are so when combined in weighted sums across speed classes. Nevertheless, it admits an important class of multi-speed models while simplifying the analysis considerably, so we restrict attention to that case in this paper.

3. Equilibrium distribution

The conserved quantities that we shall consider are the mass density, given by

$$\rho = \sum_a^n \sum_j^{b_a} m_a N_{a,j}, \tag{7}$$

¹ That is, if $A_{\alpha\beta\gamma}$ are the components of a rank-three tensor, then $\text{per}(A)_{\alpha\beta\gamma} = A_{\alpha\beta\gamma} + A_{\gamma\alpha\beta} + A_{\beta\gamma\alpha}$.

and the momentum density, given by

$$\rho \mathbf{u} = \sum_a^n \sum_j^{b_a} m_a \mathbf{c}_{a,j} N_{a,j}. \quad (8)$$

We do not consider a hydrodynamic equation for energy since, in the incompressible limit, that decouples from the evolution equations for mass and momentum. That is, the incompressibility condition and momentum equation may be solved for ρ and \mathbf{u} without need for the energy equation though, of course, the reverse is not true. In other words, the energy becomes a passive variable with respect to the dynamics in the incompressible limit, so we need not consider it here.

In keeping with earlier work [1], we assume that the H function is of trace form

$$H = \sum_a \sum_{i=1}^{b_a} h(N_i), \quad (9)$$

where $h'(x) \geq 0$ for $x > 0$. If we extremize this under the assumption that ρ and $\rho \mathbf{u}$ are conserved, we find the equilibrium distribution function

$$N_{a,j}^{(\text{eq})} = \phi(\mu m_a + \boldsymbol{\beta} \cdot m_a \mathbf{c}_{a,j}), \quad (10)$$

where μ and $\boldsymbol{\beta}$ are the Lagrange multipliers determined by the constraints, and ϕ the inverse function of h' .

We expand the equilibrium distribution to second order in Mach number formally, using $\boldsymbol{\beta}$ as an expansion parameter

$$N_{a,j}^{(\text{eq})} = \phi(\mu m_a) + m_a \phi'(\mu m_a) \boldsymbol{\beta} \cdot \mathbf{c}_{a,j} + \frac{1}{2} m_a^2 \phi''(\mu m_a) \boldsymbol{\beta} \boldsymbol{\beta} : \mathbf{c}_{a,j} \mathbf{c}_{a,j}. \quad (11)$$

Eqs. (7) and (8) are then used to derive the constraints

$$\rho = \sum_{a,j} m_a N_{a,j}^{(\text{eq})} = \sum_a m_a \phi(\mu m_a) \mathbf{b}_{0,a} + \frac{1}{2} \boldsymbol{\beta} \boldsymbol{\beta} : \sum_a m_a^3 \phi''(\mu m_a) \mathbf{b}_{2,a}, \quad (12)$$

$$\rho \mathbf{u} = \sum_{a,j} m_a \mathbf{c}_{a,j} N_{a,j}^{(\text{eq})} = \boldsymbol{\beta} \cdot \sum_a m_a^2 \phi'(\mu m_a) \mathbf{b}_{2,a}. \quad (13)$$

Under the assumption that $\mathbf{b}_{\ell,a} = b_{\ell,a} \mathbf{1}_\ell$ for $\ell \leq 4$, the above equations become

$$\rho = \sum_a m_a b_{0,a} \phi(\mu m_a) + \frac{\beta^2}{2} \sum_a m_a^3 b_{2,a} \phi''(\mu m_a), \quad (14)$$

$$\rho \mathbf{u} = \boldsymbol{\beta} \sum_a m_a^2 b_{2,a} \phi'(\mu m_a). \quad (15)$$

The second of these yields

$$\boldsymbol{\beta} = \frac{\rho \mathbf{u}}{\sum_a m_a^2 b_{2,a} \phi'(\mu m_a)}, \quad (16)$$

and the first then yields

$$\rho = \sum_a m_a b_{0,a} \phi(\mu m_a) + \frac{\rho^2 u^2}{2} \frac{\sum_a m_a^3 b_{2,a} \phi''(\mu m_a)}{[\sum_a m_a^2 b_{2,a} \phi'(\mu m_a)]^2}. \quad (17)$$

To proceed, we define the functions

$$\Phi_n(z) \equiv \sum_a m_a b_{n,a} \phi(zm_a). \tag{18}$$

Note that the ℓ th derivative of these is given by

$$\Phi_n^{(\ell)}(z) \equiv \sum_a m_a^{\ell+1} b_{n,a} \phi^{(\ell)}(zm_a). \tag{19}$$

In terms of these, ρ may be written

$$\begin{aligned} \rho &= \Phi_0(\mu) + \frac{\rho^2 u^2}{2} \frac{\Phi_2''(\mu)}{[\Phi_2'(\mu)]^2} = \Phi_0(\mu) + \Phi_0'(\mu) \frac{\rho^2 u^2}{2} \frac{\Phi_2''(\mu)}{\Phi_0'(\mu)[\Phi_2'(\mu)]^2} \\ &= \Phi_0 \left(\mu + \frac{\rho^2 u^2}{2} \frac{\Phi_2''(\mu)}{\Phi_0'(\mu)[\Phi_2'(\mu)]^2} \right). \end{aligned} \tag{20}$$

The Lagrange multiplier μ is then obtained by first writing

$$\mu = \Phi_0^{-1}(\rho) - \frac{\rho^2 u^2}{2} \frac{\Phi_2''(\mu)}{\Phi_0'(\mu)[\Phi_2'(\mu)]^2}, \tag{21}$$

and applying this equation to itself iteratively, until the right-hand side no longer contains μ explicitly. We find

$$\mu = \Phi_0^{-1}(\rho) - \frac{\rho^2 u^2}{2} \frac{\Phi_2''(\Phi_0^{-1}(\rho))}{\Phi_0'(\Phi_0^{-1}(\rho))[\Phi_2'(\Phi_0^{-1}(\rho))]^2}. \tag{22}$$

It follows that the first term on the right in Eq. (11) may be written

$$\phi(\mu m_a) = \phi(\Phi_0^{-1}(\rho) m_a) - \frac{\rho^2 u^2}{2} \frac{\Phi_2''(\Phi_0^{-1}(\rho)) m_a \phi'(\Phi_0^{-1}(\rho) m_a)}{\Phi_0'(\Phi_0^{-1}(\rho))[\Phi_2'(\Phi_0^{-1}(\rho))]^2}. \tag{23}$$

Finally, the Lagrange multiplier β is given by

$$\beta = \frac{\rho \mathbf{u}}{\Phi_2'(\mu)} = \frac{\rho \mathbf{u}}{\Phi_2'(\Phi_0^{-1}(\rho))}, \tag{24}$$

and we are ready to write down the complete Mach-expanded equilibrium distribution function, expressed in terms of the conserved quantities ρ and $\rho \mathbf{u}$

$$\begin{aligned} N_{a,j}^{(\text{eq})} &= \phi(\Phi_0^{-1}(\rho) m_a) + \frac{m_a \phi'(\Phi_0^{-1}(\rho) m_a)}{\Phi_2'(\Phi_0^{-1}(\rho))} \rho \mathbf{u} \cdot \mathbf{c}_{a,j} \\ &+ \frac{\rho^2 \mathbf{u} \mathbf{u}}{2[\Phi_2'(\Phi_0^{-1}(\rho))]^2} : \left\{ m_a^2 \phi''(\Phi_0^{-1}(\rho) m_a) \mathbf{c}_{a,j} \mathbf{c}_{a,j} - m_a \phi'(\Phi_0^{-1}(\rho) m_a) \frac{\Phi_2''(\Phi_0^{-1}(\rho))}{\Phi_0'(\Phi_0^{-1}(\rho))} \mathbf{1} \right\}. \end{aligned} \tag{25}$$

4. Hydrodynamic equations

We now insert the form of the equilibrium distribution derived in Section 3 into the BGK kinetic equation, Eq. (1), and perform the Chapman–Enskog asymptotic analysis for small Knudsen number. In fact, we take the Knudsen and Mach numbers to be of the same order, as is appropriate for the incompressible Navier–Stokes equations. The

details of this analysis are presented in [Appendix A](#). The resulting hydrodynamic equations are $\nabla \cdot \mathbf{u} = 0$ and the incompressible Navier–Stokes equation

$$\frac{\partial \mathbf{u}}{\partial t} + g \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla P + \nu \nabla^2 \mathbf{u}, \quad (26)$$

where we have defined the scalar pressure

$$P = \Phi_2 + \left[\frac{\Phi_0 \Phi_4''}{(\Phi_2')^2} - \frac{\Phi_0 \Phi_2''}{\Phi_0' \Phi_2'} \right] \frac{\rho u^2}{2}, \quad (27)$$

the kinematic viscosity

$$\nu = \left(\tau - \frac{1}{2} \right) \frac{\Phi_4'}{\Phi_2'}, \quad (28)$$

and the factor multiplying the convective derivative

$$g = \frac{\Phi_0 \Phi_4''}{(\Phi_2')^2}. \quad (29)$$

Here, all of the functions Φ_n are understood to be evaluated at $\Phi_0^{-1}(\rho)$. We note that the correct form of the convective derivative, and therefore Galilean invariance, is recovered when $g = 1$.

It should be noted that the expression for ν above is specific to the choice of a BGK collision operator with constant τ , but the results for g and P are more general than that. Once we determine the form for the function h that will make $g = 1$, we could use it to construct a variable- τ entropic lattice Boltzmann collision operator, with relaxation parameter κ as described above, and perform a Chapman–Enskog analysis of that. The important result that $g = 1$ would be unaltered, as would the equation of state, but the expression for the viscosity would be different, approaching zero as κ approaches unity. We shall not provide the details of this entropic collision operator in this paper, but rather focus solely on the determination of h .

5. Examples

The requirement of Galilean invariance is then $g = 1$, or

$$\frac{\Phi_0 \Phi_4''}{(\Phi_2')^2} = 1. \quad (30)$$

In this section, we solve this equation for four different example lattice models. The first is the single-speed lattice Boltzmann equation with a Bravais lattice; here we make contact with previous results. In our second example, we generalize this to include a zero-velocity component to the distribution—the case of so-called “rest particles”—with the same mass as the moving particles. Here we show that the solution for h still has power-law form, and present an analytic form for it that generalizes the result for a Bravais lattice. In our third example, we allow the rest particle to have a different mass from the moving particles. Remarkably, we can show that a power-law solution for h is still obtained, that the power required satisfies a certain transcendental equation, and that this equation is guaranteed to have a solution for that power. Finally, we treat the general case, subject to the restrictions on our choice of lattice that were described above. We show that the power-law form again holds, and that the power required again satisfies a certain transcendental equation; in this general case, however, we are unable to demonstrate the existence of a solution for that power.

5.1. Single-speed models

In the case of a single-speed model, the index a takes on only one value, which we may suppress. We have

$$\Phi_0(z) = mb_0\phi(zm), \tag{31}$$

$$\Phi_2(z) = mb_2\phi(zm) = \frac{b_2}{b_0}\Phi_0(z), \tag{32}$$

$$\Phi_4(z) = mb_4\phi(zm) = \frac{b_4}{b_0}\Phi_0(z), \tag{33}$$

so Eq. (30) yields

$$\phi(x)\phi''(x) = \lambda^2[\phi'(x)]^2, \tag{34}$$

where we have defined the new independent variable $x = zm$, and the coefficient

$$\lambda \equiv \frac{b_2}{\sqrt{b_0b_4}}. \tag{35}$$

Eq. (34) is a generalization of the differential equation derived in [1]. This equation has solution

$$\phi(x) = A(x - B)^{1/(1-\lambda^2)}, \tag{36}$$

where A and B are arbitrary constants. The inverse function of this must then be

$$h'(z) = B + \left(\frac{z}{A}\right)^{1-\lambda^2}, \tag{37}$$

which integrates to yield

$$h(z) = \begin{cases} h_0 + Bz + A \ln z & \text{if } \lambda = \sqrt{2}, \\ h_0 + Bz - \left(\frac{\lambda^2 - 1}{\lambda^2 - 2}\right) A^{\lambda^2-1} \left(\frac{z^2-\lambda^2 - z}{\lambda^2 - 1}\right) & \text{otherwise.} \end{cases} \tag{38}$$

The leading linear function of z is unimportant, as it results in nothing more than a constant addition to the H function; likewise, the multiplicative constant in front of the remaining piece is unimportant and may be set to unity. What remains has the form of a Tsallis entropy with $q = 2 - \lambda^2$ for $\lambda \neq \sqrt{2}$, and a Burg entropy otherwise. For a Bravais lattice, we have $\lambda = \sqrt{1 + 2/D}$, so that $q = 1 - 2/D$, as reported in earlier work [1].

5.2. Models with rest particles of the same mass

To understand the complications that arise when more than one speed is used in entropic lattice Boltzmann models, we next consider the addition of b_r “rest particles” to the b_m single-speed model described above. Here we have introduced the speed labels $a = r$ for the rest particles, and $a = m$ for the moving particles. We note that $b_{0,r} = b_r$, but that $b_{2,r} = b_{4,r} = 0$ since the rest particles have zero speed. It follows that

$$\Phi_0(z) = m_m b_{0,m} \phi(zm_m) + m_r b_{0,r} \phi(zm_r), \tag{39}$$

$$\Phi_2(z) = m_m b_{2,m} \phi(zm_m), \tag{40}$$

$$\Phi_4(z) = m_m b_{4,m} \phi(zm_m), \tag{41}$$

so Eq. (30) yields

$$[\phi(x) + \gamma\phi(\mu x)]\phi''(x) = \lambda^2[\phi'(x)]^2, \quad (42)$$

where we have defined the new independent variable $x = zm$, and the coefficients

$$\lambda \equiv \frac{b_{2,m}}{\sqrt{b_{0,m}b_{4,m}}}, \quad (43)$$

$$\mu \equiv \frac{m_r}{m_m}, \quad (44)$$

$$\gamma \equiv \frac{m_r}{m_m} \frac{b_{0,r}}{b_{0,m}}. \quad (45)$$

If the rest particles have the same mass as the moving particles, then $\mu = 1$, and Eq. (42) reduces to

$$\phi(x)\phi''(x) = \frac{\lambda^2}{1 + \gamma}[\phi'(x)]^2. \quad (46)$$

This is of the same form as the equation obtained with no rest particles, except with the substitution $\lambda^2 \rightarrow \lambda^2/(1 + \gamma)$. It follows that the required H function again has the form of the Tsallis entropy with

$$q = 2 - \frac{\lambda^2}{1 + \gamma} \quad (47)$$

with the Burg entropy recovered in the special case that $\lambda^2 = 2(1 + \gamma)$.

For a Bravais lattice, the expression for q reduces to

$$q = 2 - \frac{1 + 2/D}{1 + b_{0,r}/b_{0,m}}. \quad (48)$$

When the number of rest particles, $b_{0,r}$ goes to zero, this reduces to the single-speed result.

5.3. Models with rest particles of a different mass

If the moving particle mass and rest particle mass differ, then $\mu \neq 1$, and Eq. (42) is an example of a *functional differential equation* [13]. Such equations relate the dependent variable and its derivatives at more than one value of the independent variable.² In this case, the value of the dependent variable ϕ and those of its derivatives at x are related to its value at μx . Such equations are difficult to solve, even when they are linear and the relevant values of the independent variable are related by additive shifts; our equation is nonlinear, and the relevant values of the independent variable are related by a multiplicative shift. Remarkably, in spite of all this, our equation admits an analytic solution, namely the power-law

$$\phi(x) = Ax^\beta, \quad (49)$$

where A is an arbitrary constant, and β solves the transcendental equation

$$\frac{1 + \gamma\mu^\beta}{\lambda^2} = \frac{\beta}{\beta - 1}. \quad (50)$$

² Here we are using the term *functional differential equation* in a sense most often used by mathematicians [13]. Physicists often use the term to refer to differential equations that involve what they call *functional derivatives*, which are what mathematicians call *Frechet derivatives*. Let there be any confusion, that is most emphatically *not* what we are talking about here.

The inverse function of ϕ is

$$h'(z) = \left(\frac{z}{A}\right)^{1/\beta}, \tag{51}$$

and this integrates to give

$$h(z) = h_0 + \frac{A\beta}{1 + \beta} \left(\frac{z}{A}\right)^{1+1/\beta}. \tag{52}$$

The contribution to H from a given site is then

$$\sum_a^n \sum_j^{b_a} h(N_{a,j}) = h_0 \left(\sum_a^n \sum_j^{b_a} 1 \right) + \frac{1}{A^{1/\beta}} \left(\frac{\beta}{1 + \beta} \right) \sum_a^n \sum_j^{b_a} N_{a,j}^{1+1/\beta}. \tag{53}$$

Since A and h_0 are arbitrary, it is clear that this can be brought into correspondence with the Tsallis entropic form, which is a linear function of the sum over $N_{a,j}^q$. We thus identify $q = 1 + 1/\beta$, where β must be found by solving the transcendental equation, Eq. (50).

Since we would like the distribution function ϕ to decrease with increasing argument, we are interested in solutions with $\beta < 0$. If $\lambda > 1$ and $\mu > 1$, such a solution will always exist. To see this, note that the function $\lambda^2\beta/(\beta - 1)$ is zero when $\beta = 0$ and approaches $\lambda^2 > 1$ as $\beta \rightarrow -\infty$; then note that the function $1 + \gamma\mu^\beta$ is $1 + \gamma > 1$ when $\beta = 0$ and approaches 1 as $\beta \rightarrow -\infty$. Since both curves are continuous, they must cross for some $\beta < 0$.

5.4. The general case

Encouraged by the last example, we may check to see if a power-law solution always exists for ϕ . If we assume $\phi(x) = Ax^\beta$, then

$$\Phi_n(z) = \sum_a m_a b_{n,a} A (zm_a)^\beta = Az^\beta \sum_a m_a^{1+\beta} b_{n,a}. \tag{54}$$

Inserting this into Eq. (30), we quickly find that β must satisfy the transcendental equation

$$\frac{\left(\sum_a m_a^{1+\beta} b_{0,a}\right) \left(\sum_a m_a^{1+\beta} b_{4,a}\right)}{\left(\sum_a m_a^{1+\beta} b_{2,a}\right)^2} = \frac{\beta}{\beta - 1}. \tag{55}$$

The existence of power-law solutions for ϕ then hinges on the existence of solutions to this transcendental equation with $\beta < 0$. Though we saw that such solutions exist for single-speed models and models with a single-speed plus rest particles, it seems difficult to draw conclusions about the existence of more general solutions to this transcendental equation, and we leave the matter to future inquiry.

6. Conclusions

Previous work [1] has established that the requirement of Galilean invariance determines the form of the H function for single-speed, single-mass entropic lattice Boltzmann models on a Bravais lattice. This function was found to have the form of a Tsallis entropy, with $q = 1 - 2/D$, where D is the spatial dimension. In this study, we have extended the validity of this result to models with multiple speeds, and particles of different masses. We carried out the full Boltzmann/Chapman–Enskog analysis for such models, and applied our results to four examples. The first was the single-speed model, to verify that we could reproduce the earlier result. The second was the same

model with the addition of rest particles of the same mass; here we showed that the only effect was to change the value of q . Our third and fourth examples involved particles of more than one mass; here we showed that h must satisfy a certain functional differential equation, that this equation has a solution in power-law form, and that the power is determined by a transcendental equation. Thus, we have shown that the power-law form for h is extremely robust.

We note that our choice of the form of H differs from that of Karlin et al. [6], which is of the form $H = \sum_i^b N_i \ln(N_i/W_i)$, where the W_i are speed-dependent weights. These weights are equal to the global equilibrium at zero flow; thus, when $N_i = W_i$ they have $H = 0$. Thus, by allowing weighted contributions to H , they found solutions for which h has the form of a (relative) Boltzmann entropy; by contrast, the present work assumes uniform contributions to H , and finds solutions for which h is not a Boltzmann entropy. Both approaches are capable of yielding Galilean-invariant hydrodynamics. A more general form for H that will subsume both approaches as special cases, remains an interesting theoretical challenge.

Another outstanding problem involves the restriction that we imposed on the choice of lattice. Though the requirement that the second-rank and fourth-rank tensors formed from sums of outer products of the velocities be isotropic within each speed class *separately* allowed for a simplified analysis, it seems unnecessary. There are known lattice Boltzmann models for which this is not true, but which nevertheless yield the isotropic Navier–Stokes equations in the hydrodynamic limit; this is because the union of velocity vectors across all speed classes does satisfy the isotropy requirements. For example, the very popular D2Q9, D3Q15 and D3Q19 models fall into this category [3].

The analysis of the transcendental equation for β , Eq. (55), to see under what circumstance there exist solutions with $\beta < 0$, remains yet another outstanding problem.

Finally, in addition to these technical challenges, it would be useful and enlightening to have some physical reason for the appearance of the Tsallis entropic form in this context. This form has often been reported as arising from a lack of ergodicity, or a fractal spatiotemporal structure. There is no clear reason to believe that either of these ingredients are present in the current context; yet the Tsallis entropic form appeared quite naturally from our mathematical development. Thus, a clear and illuminating physical interpretation of our result remains perhaps the most important outstanding challenge that we leave for future work.

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Appendix A. Lattice Boltzmann equation and Chapman–Enskog analysis

Using the equilibrium distribution function derived in Section 3, the kinetic equation, Eq. (1), may be rewritten as

$$N_{a,j}(\mathbf{x}, t) + \tau[N_{a,j}(\mathbf{x} + \mathbf{c}_{a,j}, t + \Delta t) - N_{a,j}(\mathbf{x}, t)] = N_{a,j}^{(\text{eq})}(\mathbf{x}, t) \quad (\text{A.1})$$

or

$$\left\{ 1 + \tau \left[\exp(\mathbf{c}_{a,j} \cdot \nabla) \exp \left(\Delta t \frac{\partial}{\partial t} \right) - 1 \right] \right\} N_{a,j}(\mathbf{x}, t) = N_{a,j}^{(\text{eq})}(\mathbf{x}, t), \quad (\text{A.2})$$

which has the formal solution

$$N_{a,j}(\mathbf{x}, t) = \left\{ 1 + \tau \left[\exp(\mathbf{c}_{a,j} \cdot \nabla) \exp \left(\Delta t \frac{\partial}{\partial t} \right) - 1 \right] \right\}^{-1} N_{a,j}^{(\text{eq})}(\mathbf{x}, t). \quad (\text{A.3})$$

We introduce the order parameter ϵ by the following prescription, appropriate for viscous incompressible flow (Mach and Knudsen numbers of order ϵ)

$$\mathbf{c}_{a,j} \rightarrow \epsilon \mathbf{c}_{a,j}, \quad (\text{A.4})$$

$$\Delta t \rightarrow \epsilon^2 \Delta t, \quad (\text{A.5})$$

and we allow for the equilibrium distribution to be ordered in Mach number

$$N_{a,j}^{(\text{eq})} = \sum_{\ell=0}^{\infty} \epsilon^{\ell} N_{a,j}^{(\text{eq},\ell)}. \quad (\text{A.6})$$

The result

$$N_{a,j} = \left\{ 1 + \tau \left[\exp(\epsilon \mathbf{c}_{a,j} \cdot \nabla) \exp \left(\epsilon^2 \Delta t \frac{\partial}{\partial t} \right) - 1 \right] \right\}^{-1} \left(\sum_{\ell=0}^{\infty} \epsilon^{\ell} N_{a,j}^{(\text{eq},\ell)} \right) \quad (\text{A.7})$$

may be solved perturbatively by ordering $N_{a,j}$ in the expansion parameter ϵ

$$N_{a,j} = \sum_{\ell=0}^{\infty} \epsilon^{\ell} N_{a,j}^{(\ell)}. \quad (\text{A.8})$$

At orders zero, one and two, we find

$$N_{a,j}^{(0)} = N_{a,j}^{(\text{eq},0)}, \quad (\text{A.9})$$

$$N_{a,j}^{(1)} = N_{a,j}^{(\text{eq},1)} - \tau \mathbf{c}_{a,j} \cdot \nabla N_{a,j}^{(\text{eq},0)}, \quad (\text{A.10})$$

$$N_{a,j}^{(2)} = N_{a,j}^{(\text{eq},2)} - \tau \mathbf{c}_{a,j} \cdot \nabla N_{a,j}^{(\text{eq},1)} - \tau \left[\Delta t \frac{\partial}{\partial t} - \left(\tau - \frac{1}{2} \right) \mathbf{c}_{a,j} \mathbf{c}_{a,j} : \nabla \nabla \right] N_{a,j}^{(\text{eq},0)}. \quad (\text{A.11})$$

We shall use these to derive the leading gradient corrections to the distribution function, and insert these into the conservation equations to arrive at the hydrodynamical equations for the system.

We now proceed to the Chapman–Enskog analysis. The ordering of our local equilibrium distribution function is

$$N_{a,j}^{(\text{eq},0)} = \phi(\Phi_0^{-1}(\rho) m_a), \quad (\text{A.12})$$

$$N_{a,j}^{(\text{eq},1)} = \frac{m_a \phi'(\Phi_0^{-1}(\rho) m_a)}{\Phi_2'(\Phi_0^{-1}(\rho))} \rho \mathbf{u} \cdot \mathbf{c}_{a,j}, \quad (\text{A.13})$$

$$N_{a,j}^{(\text{eq},2)} = \frac{m_a \rho^2 \mathbf{u} \mathbf{u}}{2[\Phi_2'(\Phi_0^{-1}(\rho))]^2} : \left\{ m_a \phi''(\Phi_0^{-1}(\rho) m_a) \mathbf{c}_{a,j} \mathbf{c}_{a,j} - \phi'(\Phi_0^{-1}(\rho) m_a) \frac{\Phi_2''(\Phi_0^{-1}(\rho))}{\Phi_0'(\Phi_0^{-1}(\rho))} \mathbf{1} \right\}. \quad (\text{A.14})$$

Inserting Eqs. (A.12)–(A.14) into Eqs. (A.9)–(A.11), we get

$$N_{a,j}^{(0)} = \phi(\Phi_0^{-1}(\rho)m_a), \quad (\text{A.15})$$

$$N_{a,j}^{(1)} = \frac{m_a \phi'(\Phi_0^{-1}(\rho)m_a)}{\Phi_2'(\Phi_0^{-1}(\rho))} \rho \mathbf{u} \cdot \mathbf{c}_{a,j}, \quad (\text{A.16})$$

$$N_{a,j}^{(2)} = \frac{\rho^2 \mathbf{u} \mathbf{u}}{2[\Phi_2'(\Phi_0^{-1}(\rho))]^2} : \left\{ m_a^2 \phi''(\Phi_0^{-1}(\rho)m_a) \mathbf{c}_{a,j} \mathbf{c}_{a,j} - m_a \phi'(\Phi_0^{-1}(\rho)m_a) \frac{\Phi_2''(\Phi_0^{-1}(\rho))}{\Phi_0'(\Phi_0^{-1}(\rho))} \mathbf{1} \right\} \\ - \frac{\tau m_a \phi'(\Phi_0^{-1}(\rho)m_a)}{\Phi_2'(\Phi_0^{-1}(\rho))} \rho \mathbf{c}_{a,j} \mathbf{c}_{a,j} : (\nabla \mathbf{u}). \quad (\text{A.17})$$

The solution to the kinetic equation to second order is then the sum of these

$$N_{a,j} = N_{a,j}^{(0)} + \epsilon N_{a,j}^{(1)} + \epsilon^2 N_{a,j}^{(2)} + \mathcal{O}(\epsilon^3), \quad (\text{A.18})$$

and the conservation equations are obtained by taking moments of the Taylor-expanded kinetic equation to second order

$$\Delta t \frac{\partial N_{a,j}}{\partial t} + \mathbf{c}_{a,j} \cdot \nabla N_{a,j} + \frac{1}{2} \mathbf{c}_{a,j} \mathbf{c}_{a,j} : \nabla \nabla N_{a,j} = \Omega_{a,j}, \quad (\text{A.19})$$

where $\Omega_{a,j}$ denotes the collision operator. The mass moment yields

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) + \frac{1}{2} \nabla \nabla : \left(\sum_a^n \sum_j^{b_a} m_a \mathbf{c}_{a,j} \mathbf{c}_{a,j} N_{a,j} \right) = 0, \quad (\text{A.20})$$

while the momentum moment yields

$$\frac{\partial}{\partial t} (\rho \mathbf{u}) + \nabla \cdot \left(\sum_a^n \sum_j^{b_a} m_a \mathbf{c}_{a,j} \mathbf{c}_{a,j} N_{a,j} \right) + \frac{1}{2} \nabla \nabla : \left(\sum_a^n \sum_j^{b_a} m_a \mathbf{c}_{a,j} \mathbf{c}_{a,j} \mathbf{c}_{a,j} N_{a,j} \right) = 0. \quad (\text{A.21})$$

We now evaluate the second and third moments which appear in these equations, order by order. For the second moments, we find

$$\sum_a^n \sum_j^{b_a} m_a \mathbf{c}_{a,j} \mathbf{c}_{a,j} N_{a,j}^{(0)} = \Phi_2, \quad (\text{A.22})$$

$$\sum_a^n \sum_j^{b_a} m_a \mathbf{c}_{a,j} \mathbf{c}_{a,j} N_{a,j}^{(1)} = \mathbf{0}, \quad (\text{A.23})$$

$$\sum_a^n \sum_j^{b_a} m_a \mathbf{c}_{a,j} \mathbf{c}_{a,j} N_{a,j}^{(2)} = \left[\frac{\Phi_0 \Phi_4''}{(\Phi_2')^2} - \frac{\Phi_0 \Phi_2''}{\Phi_0' \Phi_2'} \right] \frac{\rho u^2}{2} \mathbf{1} + \frac{\Phi_4''}{(\Phi_2')^2} \rho^2 \mathbf{u} \mathbf{u} - \tau \frac{\Phi_4'}{\Phi_2'} \rho [(\nabla \cdot \mathbf{u}) \mathbf{1} + \nabla \mathbf{u} + (\nabla \mathbf{u})^T], \quad (\text{A.24})$$

where the superscript T denotes “transpose”, and the arguments of all the Φ 's are understood to be $\Phi_0^{-1}(\rho)$. For the third moments, we find

$$\sum_a^n \sum_j^{b_a} m_a \mathbf{c}_{a,j} \mathbf{c}_{a,j} \mathbf{c}_{a,j} N_{a,j}^{(0)} = \mathbf{0}, \quad (\text{A.25})$$

$$\sum_a^n \sum_j^{b_a} m_a \mathbf{c}_{a,j} \mathbf{c}_{a,j} \mathbf{c}_{a,j} N_{a,j}^{(1)} = \frac{\Phi'_4}{\Phi'_2} \rho \text{per}(\mathbf{1} \otimes \mathbf{u}), \quad (\text{A.26})$$

$$\sum_a^n \sum_j^{b_a} m_a \mathbf{c}_{a,j} \mathbf{c}_{a,j} \mathbf{c}_{a,j} N_{a,j}^{(2)} = \mathbf{0}, \quad (\text{A.27})$$

where, as noted earlier, “per” denotes a sum over all symmetric permutations of tensor components.

We now insert the above results into Eqs. (A.20) and (A.21), and we adhere to the incompressible limit so that time and space derivatives of ρ are of higher order in ϵ and hence ignored. The hydrodynamic equations given in Section 4 follow immediately.

References

- [1] B.M. Boghosian, P.J. Love, P.V. Coveney, I.V. Karlin, S. Succi, J. Yepez, Galilean-invariant lattice-Boltzmann models with H -theorem, *Phys. Rev. E* 68 (2003) 025103.
- [2] R. Benzi, S. Succi, M. Vergassola, *Phys. Rep.* 222 (1992) 145.
- [3] S. Succi, *The Lattice Boltzmann Equation—For Fluid Dynamics and Beyond*, Oxford University Press, Oxford, 2001.
- [4] Y.-H. Qian, D. d’Humières, P. Lallemand, *Europhys. Lett.* 17 (1992) 479.
- [5] I.V. Karlin, A.N. Gorban, S. Succi, V. Boffi, *Phys. Rev. Lett.* 81 (1998) 6.
- [6] I.V. Karlin, A. Ferrante, H.C. Öttinger, *Europhys. Lett.* 47 (1999) 187.
- [7] B.M. Boghosian, J. Yepez, P.V. Coveney, A. Wagner, *Proc. Roy. Soc. Lond. A* 457 (2001) 717.
- [8] C. Marsh, P.V. Coveney, *J. Phys. A: Math. Gen.* 31 (1998) 6561.
- [9] S. Ansumali, I.V. Karlin, *Phys. Rev. E* 62 (2000) 7999.
- [10] S. Ansumali, I.V. Karlin, *Phys. Rev. E* 65 (2002) 056312.
- [11] S. Succi, I.V. Karlin, H. Chen, *Rev. Mod. Phys.* 74 (2002) 1203.
- [12] A.N. Gorban, I.V. Karlin, *Phys. Rev. E* 67 (2003) 016104.
- [13] J.K. Hale, S.M. Verduyn Lunel, *Introduction to Functional Differential Equations*, Springer-Verlag, Berlin, 1993.