Existence of the $H$ theorem for the athermal lattice Boltzmann models with nonpolynomial equilibria

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Abstract

The entropy function is found for the two-dimensional seven-velocity lattice Boltzmann method on a triangular lattice. Some issues pertinent to the stability and accuracy of the seven velocity lattice Boltzmann method are discussed.

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I. INTRODUCTION

The Lattice Boltzmann method (LBM) is a useful tool for simulations of the complex hydrodynamic phenomena such as turbulent flows, multiphase flows and suspensions. It is even believed that the subsequent development of the lattice Boltzmann method may provide a new paradigm in the kinetic modeling due to its mathematical simplicity and computational efficiency [1].

One important issue, which attracted considerable attention recently, is the enhancement of stability of the method [2]. We remind that the early predecessor of the LBM, the lattice gas method of Frisch, Hasslacher and Pomeau [3], was consistent with the $H$ theorem by the microscopic detailed balance and was supported by nonpolynomial equilibria (maximizers of the Fermi-Dirac entropy). The method was unconditionally stable, but in the course of the subsequent development of the LBM this feature of the unconditional stability, which otherwise would distinguish the lattice Boltzmann method among other methods of computational fluid dynamics, was gradually lost. The reason why this happened can be traced back to the earliest versions of the LBM, derived from the lattice gas model, where the true nonpolynomial equilibria were replaced by their low-order polynomial approximations. Of course, this was motivated by a search for computationally more effective schemes, beginning with the work of Higuera, Succi and Benzi [4], and which eventually culminated in the athermal single relaxation time lattice Bhatnagar-Gross-Krook model (LBGK) [5, 6] based on polynomial equilibria. Later studies aimed at restoring the $H$-theorem for the LBM are well documented (see, e. g. [2]). At present, the entropic LBGK models which combine computational efficiency of the standard LBGK with the unconditional stability pertinent to genuine kinetic models are constructed [7]. First results of simulation of high Reynolds number flows confirm the theoretically expected significant overall gain in performance of the LBM by using the entropic formulations [8].

The present study is motivated in part by a recent publication [9] entitled “Nonexistence of $H$ theorems for the athermal lattice Boltzmann models with polynomial equilibria”. Therein, the authors demonstrated that polynomial equilibria used in the lattice Boltzmann method on the two-dimensional triangular lattice (the D2Q7 model, see section III) do not minimize any convex function, at least when parameters of these local equilibria are in a certain range. Since the fact that polynomial equilibria are at odds with the maximum entropy
principle (and thus they are not local equilibria in a thermodynamic sense) was pointed out already for some time (see, for instance, [10]), and actually the experience gained from many studies of various discrete velocity models [11] does not indicate that polynomials are expected as local equilibria, it is therefore not surprising that the computation [9] failed to derive a suitable entropy function for the D2Q7 model.

In this paper, we revisit the problem of finding the $H$ function for the D2Q7 model. Our approach to derivation of the $H$ function follows the method suggested earlier in [12]. The straightforward computation presented in detail results in the unique Boltzmann-like entropy function for the D2Q7 setup, thereby enabling construction of the entropic lattice Boltzmann models for this lattice.

The structure of the paper is as follows: In section II, for the sake of completeness, we review briefly the athermal LBGK and the athermal entropic LBM, in particular, the entropic LBGK. This section contains no new results. In section III, we consider the 2DQ7 lattice, and find the appropriate $H$ function. In section IV, we find an approximate solution to the equilibrium distribution and discuss its accuracy. Finally, in section V we put the entropic lattice Boltzmann method into a perspective with other recent approaches to stabilization of the athermal lattice Boltzmann models.

II. LATTICE BOLTZMANN AND ENTROPIC LATTICE BOLTZMANN

In this section, for the sake of completeness, we briefly compare the entropic lattice Boltzmann method (ELBM) and the standard lattice Boltzmann method (LBM) of athermal hydrodynamics.

In both the LBM and ELBM methods, one considers populations $f_i$ of discrete velocities $C_i$, where $i = 1, \ldots, m$, at discrete time $t$. The discrete velocities form the links of a regular and sufficiently isotropic lattice, and it may also include a zero vector. It is convenient to introduce $m$-dimensional population vectors $f$. In the isothermal case, local hydrodynamic variables (density $\rho$ and momentum density $\rho u$) are defined at lattice sites $r$ as:

$$
\rho = \sum_{i=1}^{m} f_i(r, t),
\rho u = \sum_{i=1}^{m} C_i f_i(r, t).
$$

(1)
The ELBM begins with finding a convex function of populations, \( H \), which satisfies the following condition: If \( f_{eq}^i(\rho, \rho \mathbf{u}) \) minimizes \( H \) subject to the hydrodynamic constraints (1), then \( f_{eq} \) also verifies the Galilean invariance of the stress tensor:

\[
\sum_{i=1}^{m} C_{i\alpha} C_{i\beta} f_{eq}^i(\rho, \rho \mathbf{u}) = \rho c_s^2 \delta_{\alpha\beta} + \rho u_{\alpha} u_{\beta}.
\]  

Here \( c_s \) is sound speed.

The \( H \) function which satisfies this condition to the accuracy of \( u^4 \), and thus is valid to all purposes of incompressible simulations was derived in [12] for the the D1Q3 and the D2Q9 lattices. Later, this result was extended to the three-dimensional D3Q27 lattice in [13]. Recently, other \( H \) functions which verify equation (2) to the accuracy of \( u^4 \) were found for isotropic Bravais lattices in [17], in particular for the D2Q6 model. In order to illustrate this, we list here the results for the \( H \) functions and their minimizers for the DkQ3\(^k \) lattices [7, 12, 13, 15, 16, 19]. Let \( D \) be the spatial dimension. For \( D = 1 \), the three discrete velocities are \( \mathbf{C} = \{-1, 0, 1\} \). In higher dimensions, the discrete velocities are tensor products of the discrete velocities of these one-dimensional velocities. The \( H \) function is Boltzmann-like:

\[
H = \sum_{i=1}^{3^D} f_i \ln \left( \frac{f_i}{w_i} \right).
\]  

Here \( w_i \) is the weight associated with the \( i \)th discrete velocity \( \mathbf{C}_i \). For \( D = 1 \), the weights corresponding to the velocities \( \mathbf{C} = \{-1, 0, 1\} \) are \( w = \{ \frac{1}{6}, \frac{2}{3}, \frac{1}{6} \} \). For \( D > 1 \), the weights are constructed by multiplying the weights associated with each component direction.

The local equilibrium which minimizes (3) subject to the fixed density and momentum reads:

\[
f_{eq}^i = \rho w_i \prod_{\alpha=1}^{D} \left( 2 - \sqrt{1 + 3 u_{\alpha}^2} \right) \left( \frac{2 u_{\alpha} + \sqrt{1 + 3 u_{\alpha}^2}}{1 - u_{\alpha}} \right)^{C_{i\alpha}}.
\]  

The speed of sound, \( c_s \), in this model is \( 1/\sqrt{3} \).

Once the entropy function \( H \) is found, the basic equation of ELBM to be constructed and to be solved is

\[
f_i(\mathbf{r} + \mathbf{C}_i, t + 1) - f_i(\mathbf{r}, t) = -\beta \alpha [\mathbf{f}(\mathbf{r}, t)] \mathbf{\Delta}_i [\mathbf{f}(\mathbf{r}, t)],
\]  

where the right hand side represents the collision process. The \( m \)-dimensional vector function \( \mathbf{\Delta} \) (so-called bare collision integral), must satisfy the conditions:

\[
\sum_{i=1}^{m} \mathbf{\Delta}_i \{1, \mathbf{C}_i\} = 0 \text{ (local conservation laws),}
\]
\[
\sigma = \sum_{i=1}^{m} \Delta_i \frac{\partial H}{\partial f_i} \leq 0 \text{ (entropy production inequality)}.
\]

Moreover, the local equilibrium vector \( f^{eq} \) must be the only zero point of \( \Delta \), that is, \( \Delta(f^{eq}) = 0 \), and, finally, \( f^{eq} \) must be the only zero point of the local entropy production, \( \sigma(f^{eq}) = 0 \).

The conditions just listed are standard requirements taken directly from the well known theory of the continuous Boltzmann equation. The lattice specifics comes through the factor \( \beta \alpha[f(r,t)] \) in equation (5). Here \( \beta \) is a fixed parameter in the interval \([0,1]\), and is related to the viscosity (the limit \( \beta \to 1 \) is the zero viscosity limit). The scalar function \( \alpha \) is the nontrivial root of the nonlinear equation \([12,14,18]\):

\[
H(f) = H(f + \alpha\Delta[f]).
\]

(6)

It is the function \( \alpha \) which ensures the discrete-time \( H \)-theorem, unlike in the continuous-time case where it essentially suffices to ensure only the entropy production inequality. Function \( \alpha \) has to be computed numerically on each lattice site at each time step. In the fully resolved hydrodynamic limit, when \( f \to f^{eq} \), the solution \( \alpha(f) \) tends to its limiting value \( \alpha = 2 \).

In practice, construction of the bare collision integral \( \Delta \) is guided by simplicity. For the \( H \) functions (3), the local equilibria are given by explicit formula (4), and thus the BGK form, \( \Delta = f - f^{eq} \) becomes available for efficient numerical realizations. We further refer to this model as the entropic lattice BGK (ELBGK). A gradient single-relaxation time models circumventing the BGK form, and which are readily constructed once just the \( H \)-function is known, were developed in \([13,15,19]\) (see also their discussion in the context of reaction kinetics, \([22]\)).

The standard (nonentropic, second-order polynomial) LBM can be considered as a truncation of the ELBM’s just discussed. This truncation is done in three steps. First, the local equilibria are replaced by their second-order in \( u \) polynomials. For example, for \( D = 2 \), if we expand the local equilibrium (4) to second order in \( u/c_s \), we derive the polynomial equilibrium of the standard D2Q9 model \([6]\). In order to distinguish between the local equilibria when they are minimizers of appropriate entropy functions and the \( k \)th order polynomial approximations to them, we denote the latter as \( \tilde{f}^{(k)} \). Second, instead of nonlinear bare collision integrals one considers linearized forms, \( \Delta_i = \sum_{j=1}^{m} A_{ij}(f_j - \tilde{f}^{(2)}_i) \). The simplest option is the BGK form which becomes always available, \( \Delta_i = f_j - \tilde{f}^{(2)}_i \). Third, when the
latter expression is substituted into the right hand side of equation (5), the root of the equation (6) is replaced by \( \alpha = 2 \). Obviously, these operations do not leave the \( H \)-theorem intact, and it is maybe not surprising that a polynomial cannot be itself a minimizer of any entropy function anymore, as was demonstrated for the D2Q7 lattice in [9]. In the subsequent section we find the \( H \) function for this lattice without assuming a polynomial ansatz for the equilibrium.

III. \( H \) FUNCTION FOR THE 2DQ7 MODEL

The discrete velocities of the D2Q7 model at each site of a planar triangular lattice consist of a zero vector \( \mathbf{C}_0 = 0 \), and of six vectors of equal length, \( \mathbf{C}_i \), where \( i = 1, \ldots, 6 \), \( \mathbf{C}_i = (\cos((i-1)\pi/3), \sin((i-1)\pi/3)) \). The explicit form of the seven-dimensional vectors corresponding to the \( x \) and \( y \) components of velocities are as follows:

\[
\mathbf{C}_x = \{0, 1, 1/2, -1/2, -1, -1/2, 1/2\},
\]

\[
\mathbf{C}_y = \frac{\sqrt{3}}{2} \{0, 0, 1, 1, 0, -1, -1\}.
\]

Accordingly, the population vector \( \mathbf{f} \) is,

\[
\mathbf{f} = \{f_0, f_1, f_2, f_3, f_4, f_5, f_6\}.
\]

By symmetry arguments, it is sufficient to seek the \( H \) function of the form,

\[
H(\mathbf{f}) = h_0(f_0) + \sum_{i=1}^{6} h(f_i),
\]

where \( h_0(x) \) and \( h(x) \) are two convex functions of one variable to be determined. [We could equally begin with a more general form, \( H = \sum_{i=0}^{6} h_i(f_i) \), assuming a separate unknown function for each population. However, the result would be the same.]

The local equilibrium \( \mathbf{f}^{eq} \) is the minimizer of the function \( H \) (10) subject to the con-
\begin{align}
\rho &= \sum_{i=0}^{6} f_{i}^{eq}, \\
\rho u_{x} &= \sum_{i=0}^{6} f_{i}^{eq} C_{ix} = f_{1}^{eq} - f_{4}^{eq} + \frac{1}{2} (f_{2}^{eq} + f_{6}^{eq} - f_{3}^{eq} - f_{5}^{eq}), \\
\rho u_{y} &= \sum_{i=0}^{6} f_{i}^{eq} C_{iy} = \sqrt{3} \left( \frac{1}{2} f_{2}^{eq} - f_{3}^{eq} - f_{5}^{eq} + f_{6}^{eq} \right). 
\end{align} 
(11)

Let us denote the inverse of the derivative of \( h_0 \) and \( h \) as \( \mu_0 = [h_0']^{-1} \) and \( \mu = [h']^{-1} \). Then, the formal solution to the minimization problem reads,

\begin{align}
f_{0}^{eq} &= \mu_0 (\chi), \\
f_{1}^{eq} &= \mu (\chi + \zeta), \\
f_{2}^{eq} &= \mu (\chi + \frac{1}{2} \zeta) , \\
f_{3}^{eq} &= \mu (\chi - \frac{1}{2} \zeta), \\
f_{4}^{eq} &= \mu (\chi - \zeta), \\
f_{5}^{eq} &= \mu (\chi - \frac{1}{2} \zeta), \\
f_{6}^{eq} &= \mu (\chi + \frac{1}{2} \zeta). 
\end{align} 
(12)

Here \( \chi, \zeta_x \) and \( \zeta_y \) are Lagrange multipliers associated with the constraints.

By choosing various pairs of functions for \( \mu_0 \) and \( \mu \) constitutive relations for the stress tensors \( \mathbb{2} \) is satisfied with varying degrees of accuracy, and the goal is to find such functions \( \mu_0 \) and \( \mu \) for which the error reduces to higher orders in the powers of velocity \( \mathbb{u} \). We rewrite the constitutive relation \( \mathbb{2} \) in the form of a discrepancy of the components of the stress tensor as:

\begin{align}
T_{xx} &= \rho c_{s}^2 + \left( \frac{\rho u_{x}}{\rho} \right)^2 - \sum_{i=0}^{6} f_{i}^{eq} C_{ix} C_{ix}, \\
T_{yy} &= \rho c_{s}^2 + \left( \frac{\rho u_{y}}{\rho} \right)^2 - \sum_{i=0}^{6} f_{i}^{eq} C_{iy} C_{iy}, \\
T_{xy} &= \left( \frac{\rho u_{x}}{\rho} \right) \left( \frac{\rho u_{y}}{\rho} \right) - \sum_{i=0}^{6} f_{i}^{eq} C_{ix} C_{iy}. 
\end{align} 
(13)
Note that the sound speed is not yet defined in these expressions. In fact, as we will see soon, the choice of the sound speed is a solvability condition in our procedure.

The next step is crucial [12]: We are going to find such functions \( \mu_0 \) and \( \mu \) which contain no discrepancy up to the orders \( c_s^2, \zeta_x^2, \zeta_y \), and \( \zeta_x \zeta_y \). In order to do this, we expand the terms in equations (13) to relevant orders around the point \( \zeta_x = \zeta_y = 0 \):

\[
\rho(\chi, \zeta) = \mu_0(\chi) + 6\mu(\chi) + \frac{3}{2}\mu''(\chi)\zeta_x^2 + 2\mu''(\chi)\zeta_y^2 + O(|\zeta|^2),
\]

\[
\rho u_x(\chi, \zeta) = 3\mu'(\chi)\zeta_x + O(|\zeta|^2),
\]

\[
\rho u_y(\chi, \zeta) = 2\sqrt{3}\mu'(\chi)\zeta_y + O(|\zeta|),
\]

\[
\sum_{i=0}^{6} f_i^{(\xi)}(\chi, \zeta) C_{ix}C_{ix} = 3\mu(\chi) + \frac{1}{4}\mu''(\chi) \left( \frac{9}{2}\zeta_x^2 + 2\zeta_y^2 \right) + O(|\zeta|^2),
\]

\[
\sum_{i=0}^{6} f_i^{(\xi)}(\chi, \zeta) C_{iy}C_{iy} = 3\mu(\chi) + \frac{3}{4}\mu''(\chi) \left( \frac{1}{2}\zeta_x^2 + 2\zeta_y^2 \right) + O(|\zeta|^2),
\]

\[
\sum_{i=0}^{6} f_i^{(\xi)}(\chi, \zeta) C_{ix}C_{iy} = \frac{\sqrt{3}}{2}\mu''(\chi)\zeta_x\zeta_y + O(|\zeta|^2).
\]

Here primes denote corresponding derivatives.

Substituting expansions (14) in equations (13), we require that discrepancy (13) vanishes to second order in \( \zeta \).

At zero order we have two identical equations:

\[
T_{xx}^{(0)} = c_s^2(\mu_0(\chi) + 6\mu(\chi)) - 3\mu(\chi) = 0,
\]

\[
T_{yy}^{(0)} = c_s^2(\mu_0(\chi) + 6\mu(\chi)) - 3\mu(\chi) = 0.
\]

whereupon,

\[
c_s^2 = \frac{3\mu(\chi)}{\mu_0(\chi) + 6\mu(\chi)}.
\]

There are no terms linear in \( \zeta \) in the expansion of \( T_{\alpha\beta} \). At second order we get the following equations:

\[
T_{xx}^{(2)} = \left\{ \left( \frac{3}{2}c_s^2 - \frac{9}{8} \right) \mu''(\chi) + \frac{9\mu'(\chi)^2}{\mu_0(\chi) + 6\mu(\chi)} \right\} \zeta_x^2 + \left( 2c_s^2 - \frac{1}{2} \right) \mu''(\chi)\zeta_y^2,
\]

\[
T_{yy}^{(2)} = \left( \frac{3}{2}c_s^2 - \frac{3}{8} \right) \mu''(\chi)\zeta_x^2 + \left( \left( 2c_s^2 - \frac{3}{2} \right) \mu''(\chi) + \frac{12\mu'(\chi)^2}{\mu_0(\chi) + 6\mu(\chi)} \right) \zeta_y^2,
\]

\[
T_{xy}^{(2)} = \frac{\sqrt{3}}{2} \left\{ \frac{12\mu'(\chi)^2}{\mu_0(\chi) + 6\mu(\chi)} - \mu''(\chi) \right\} \zeta_x\zeta_y.
\]
We now require $T^{(2)}_{\alpha\beta} = 0$ independently of the values of $\zeta$. Thus, setting to zero each term in front of each combination $\zeta^\alpha \zeta^\beta$ in equations (17), (18), and (19), we obtain five equations:

\[
\left( \frac{3}{2}c_s^2 - \frac{9}{8} \right) \mu''(\chi) + \frac{9[\mu'(\chi)]^2}{\mu_0(\chi) + 6\mu(\chi)} = 0, \tag{20}
\]

\[
\left( 2c_s^2 - \frac{1}{2} \right) \mu''(\chi) = 0, \tag{21}
\]

\[
\left( \frac{3}{2}c_s^2 - \frac{3}{8} \right) \mu''(\chi) = 0, \tag{22}
\]

\[
\left( 2c_s^2 - \frac{3}{2} \right) \mu''(\chi) + \frac{12[\mu'(\chi)]^2}{\mu_0(\chi) + 6\mu(\chi)} = 0, \tag{23}
\]

\[
\frac{12[\mu'(\chi)]^2}{\mu_0(\chi) + 6\mu(\chi)} - \mu''(\chi) = 0. \tag{24}
\]

Equations (21) and (22) are identical. Assuming $\mu'' \neq 0$, equations (21) and (22) fix the value of sound speed:

\[
c_s = \frac{1}{2}. \tag{25}
\]

It is straightforward to demonstrate that with the value of sound speed (25) the remaining three equations are resolvable. Indeed, substituting (25) into the zero-order relation (16), we obtain,

\[
\mu_0(\chi) = 6\mu(\chi). \tag{26}
\]

Substituting equations (25) and (26) into equations (20), (23), and (24), we find out that each of the latter three equations reduce to the same ordinary differential equation:

\[
\frac{[\mu'(\chi)]^2}{\mu(\chi)} - \mu''(\chi) = 0. \tag{27}
\]

The general solution to this equation is

\[
\mu(\chi) = A \exp(\chi) + B. \tag{28}
\]

Now, from the requirement that $\mu'' \neq 0$ we get $A \neq 0$, and furthermore $A > 0$ by required concavity of $H$. Substituting the general solution (28) into the equation (27), we find $B = 0$. From equation (26) we then have $\mu_0(\chi) = 6A \exp(\chi)$. Therefore, $h'(x) = \mu^{-1}(x) = \ln(x/A)$, so that $h(x) = x(\ln(x/A) - 1) + k_1$, and similarly, $h_0(x) = x(\ln(x/(6A)) - 1) + k_2$, where $k_1$ and $k_2$ are arbitrary constants. Thus, we obtain the family of Boltzmann-like $H$ function of the 2DQ7 model:

\[
H = f_0 \left( \ln \left( \frac{f_0}{6A} \right) - 1 \right) + \sum_{i=1}^{6} f_i \left( \ln \left( \frac{f_i}{A} \right) - 1 \right) + C. \tag{29}
\]
As is well known, adding a linear combination of the locally conserved quantities to the entropy function is immaterial, so we can fix $A = 1/e$, where $e$ is the base of natural logarithm, and $C = 0$:

$$H = f_0 \ln \left( \frac{f_0}{6} \right) + \sum_{i=1}^{6} f_i \ln (f_i).$$

(30)

In the next section, we shall study the equilibria corresponding to the entropy function (30).

IV. EQUILIBRIUM POPULATIONS

By construction, the expansion of the minimizers of $H$ (30) around the point $u = 0$ to the order $u^2$ satisfy all the usual requirements needed to derive the athermal Navier-Stokes equations (cf. Ref. 12, see also below for the present case). The exact minimizers are nonpolynomial, and are not always available in a closed form. Nevertheless, a glimpse of the full solution is possible since the explicit solution can be computed for a few special cases. For example, when $u_x = \sqrt{3} u_y$, we find the exact minimizer of the $H$ function (30),

$$f_0^\text{eq} = \rho \left[ 1 - \frac{1}{6} \sqrt{(9 + 48u_x^2)} \right],$$

$$f_4^\text{eq} = f_5^\text{eq} = f_6^\text{eq} = \frac{\rho}{36} \left[ 2 \sqrt{(9 + 48u_x^2)} - 3 - 12u_x \right],$$

$$f_3^\text{eq} = f_6^\text{eq} = \frac{f_0^\text{eq}}{6},$$

$$f_1^\text{eq} = f_2^\text{eq} = \frac{2 \rho u_x}{3} + f_4^\text{eq}. $$

(31)

The exact solution (31) will be used below to test the accuracy of various approximations to the equilibrium populations.

For practical realizations, we describe a systematic procedure to obtain the equilibrium in a series representation. The procedure relies on the fact that at zero velocity equilibrium is known exactly,

$$f_i^\text{eq}(\rho, 0) = f_i^{(0)} = \rho w_i, \ w_0 = 1/2, \ w_j = 1/12, \ j = 1, \ldots, 6.$$

(32)

Once the exact solution for zero velocity is known, extension to $u \neq 0$ is found by perturbation. Specifically, the Lagrange multipliers are expanded as

$$\chi = \sum_{n=0}^{\infty} \epsilon^n \chi^{(n)}; \quad \zeta = \sum_{n=0}^{\infty} \epsilon^n \zeta^{(n)},$$

(33)
where we have introduced a bookkeeping parameter $\epsilon$, such that $u_\alpha \rightarrow \epsilon u_\alpha$, and $\epsilon$ is set to one in the end of computation. This series representation of Lagrange multipliers, when substituted into equations for the constraints, induces polynomial approximations $\tilde{f}_i^{(k)}$ of increasingly higher order,

$$\tilde{f}_i^{(k)} = \sum_{n=0}^{k} \epsilon^n \tilde{f}_i^{(n)}.$$  

Further, we seek the expansion parameters consistent with the conservation constraints at all orders. This translates into a set of linear equation solved recursively:

$$\sum_{i=0}^{m} \tilde{f}_i^{(k)} = \rho, \quad \sum_{i=0}^{m} C_{\alpha i} \tilde{f}_i^{(k)} = \epsilon \rho u_\alpha, \quad k \geq 2.$$  

For example, at first order of this expansion

$$\sum_{i=1}^{6} f_i^{(0)} \left[ \chi^{(1)} + \zeta_x^{(1)} C_{ix} + \zeta_y^{(1)} C_{iy} \right] = 0,$$

$$\sum_{i=1}^{6} f_i^{(0)} C_{ix} \left[ \chi^{(1)} + \zeta_x^{(1)} C_{ix} + \zeta_y^{(1)} C_{iy} \right] = \rho u_x,$$

$$\sum_{i=1}^{6} f_i^{(0)} C_{iy} \left[ \chi^{(1)} + \zeta_x^{(1)} C_{ix} + \zeta_y^{(1)} C_{iy} \right] = \rho u_y.$$  

By solving this linear system of three equations we get,

$$\chi^{(1)} = 0, \quad \zeta_x^{(1)} = 4 u_x, \quad \zeta_y^{(1)} = 4 u_y.$$  

Similarly, at second order:

$$\sum_{i=1}^{6} f_i^{(0)} \left[ \frac{2 \chi^{(2)} + 2 \left( \zeta_\alpha^{(2)} C_{i \alpha} \right) + \left( \zeta_\alpha^{(1)} C_{i \alpha} \right)^2}{2} \right] = 0,$$

$$\sum_{i=1}^{6} f_i^{(0)} C_{ix} \left[ \frac{2 \chi^{(2)} + 2 \left( \zeta_\alpha^{(2)} C_{i \alpha} \right) + \left( \zeta_\alpha^{(1)} C_{i \alpha} \right)^2}{2} \right] = 0,$$

$$\sum_{i=1}^{6} f_i^{(0)} C_{iy} \left[ \frac{2 \chi^{(2)} + 2 \left( \zeta_\alpha^{(2)} C_{i \alpha} \right) + \left( \zeta_\alpha^{(1)} C_{i \alpha} \right)^2}{2} \right] = 0,$$

which gives:
\[ \chi^{(2)} = -2 \left( u_x^2 + u_y^2 \right), \quad \zeta_x^{(2)} = 0, \quad \zeta_y^{(2)} = 0. \quad (39) \]

Solutions at higher orders are easily found using symbolic computation facilities. In Table I we present terms of the expansion of the Lagrange multipliers up to 8th order in \( u \).

| \( k \) | \( \chi^{(k)} \) | \( \zeta_x^{(k)} \) | \( \zeta_y^{(k)} \) |
|-------|----------------|----------------|----------------|
| 1     | 0              | \( 4 u_x \)     | \( 4 u_y \)     |
| 2     | \(-2 \left( u_x^2 + u_y^2 \right)\) | 0              | 0              |
| 3     | 0              | 0              | 0              |
| 4     | 0              | 0              | 0              |
| 5     | 0              | \( \frac{32}{15} u_x^3 \left( u_x^2 + 5 u_y^2 \right) \) | \( \frac{16}{15} u_y \left( 5 u_x^4 + 3 u_y^4 \right) \) |
| 6     | \(-\frac{8}{9} \left( 2 u_x^6 + 15 u_x^4 u_y^2 + 3 u_y^6 \right)\) | 0              | 0              |
| 7     | 0              | \(-\frac{32}{15} u_y \left( 14 u_x^6 + 21 u_x^4 u_y^2 + 9 u_y^6 \right)\) | \(-\frac{32}{15} \left( 5 u_x^7 + 42 u_x^5 u_y^2 + 21 u_y^7 \right)\) |
| 8     | \( \frac{4}{3} \left( 5 u_x^8 + 56 u_x^6 u_y^2 + 42 u_x^4 u_y^4 + 9 u_y^8 \right)\) | 0              | 0              |

This simple procedure gives the equilibrium distribution at eventually any desired order of accuracy. For example, the \( O(u^6) \) accurate approximation of the equilibrium is,

\[
\tilde{f}_i^{(5)} = \rho w_i \left[ 1 + \zeta_x^{(1)} C_{i\alpha} + \frac{2 \chi^{(2)} + \left( \zeta_x^{(1)} C_{i\alpha} \right)^2}{2} + \frac{6 \chi^{(2)} + \left( \zeta_x^{(1)} C_{i\alpha} \right)^2}{6} \zeta_x^{(1)} C_{i\alpha} 
+ 12 \chi^{(2)} \left( \chi^{(2)} + \left( \zeta_x^{(1)} C_{i\alpha} \right)^2 \right) + \left( \zeta_x^{(1)} C_{i\alpha} \right)^4 \right.
+ \frac{24}{120} \chi^{(2)} \left( \zeta_x^{(1)} C_{i\alpha} \right) \left( 3 \chi^{(2)} + \left( \zeta_x^{(1)} C_{i\alpha} \right)^2 \right) + \left( \zeta_x^{(1)} C_{i\alpha} \right)^5 + \left. \left( \zeta_x^{(5)} C_{i\alpha} \right)^5 \right].
\] (40)

We note in passing that, by construction, each approximate equilibrium population, \( \tilde{f}_i^{(k)}(\rho, u) \), satisfies exactly the consistency relations, \( \rho(\tilde{f}_i^{(k)}(\rho, u)) = \rho \), and \( \rho u(\tilde{f}_i^{(k)}(\rho, u)) = \rho u \), at each order \( k \).

With the above results, we proceed now to evaluate the higher order moments of the local equilibrium pertinent to establishing the hydrodynamic limit of the model. The components
of the equilibrium pressure tensor are:

\[
\begin{align*}
P_{xx}^{\text{eq}} &= \rho \left( c_s^2 + u_x^2 \right) - \rho \left[ \frac{u_x^2}{3} \left( \frac{2}{3} u_x^2 + 3 u_y^2 \right) \right] + O(u^6), \\
P_{yy}^{\text{eq}} &= \rho \left( c_s^2 + u_y^2 \right) - \rho \left[ \frac{u_y^2}{3} \left( \frac{2}{3} u_x^4 + 3 u_y^4 \right) \right] + O(u^6), \\
P_{xy}^{\text{eq}} &= \rho u_x u_y - \frac{4}{3} \rho u_x^3 u_y + O(u^6), \\
P_{yx}^{\text{eq}} &= \rho u_y u_x - \frac{4}{3} \rho u_x^3 u_y + O(u^6).
\end{align*}
\] (41)

Here the leading in \( u \) terms are responsible for Galilean invariance of the momentum equation, whereas the under-braced term give the leading-order deviations. All these deviations are of order \( O(u^4) \), as expected by construction of the \( H \) function (30). We note in passing that in the D2Q7 case under consideration, the accuracy of the equilibrium stress tensor, as compared with the entropic 2DQ9 model (4), is reduced on two counts: First, since \( c_s^2 \) is smaller, the effect of deviations is larger, and secondly, the off-diagonal part in equation (41) is \( O(u^4) \) accurate whereas it is \( O(u^6) \) accurate in the entropic 2DQ9 model (4). Similarly, the contracted third order moment, \( Q_{\alpha\beta\beta}^{\text{eq}} = \sum_{i=0}^{6} c_i c_i^2 f_i^{\text{eq}} \), related to the equilibrium energy flux, is

\[
Q_{\alpha\beta\beta}^{\text{eq}} = (\rho c_s^2(D + 2) + \rho u^2)u_\alpha - \rho u_\alpha u^2.
\] (42)

Again, the first term in the latter equation correspond to the well-known result of the continuous kinetic theory, whereas the under-braced term is the deviation. Due to the lattice symmetry, the moment \( Q_{\alpha\beta\beta}^{\text{eq}} \) is the same for any equilibrium on the D2Q7 lattice, and it is only accurate to the linear order. As we will see it below, it is the accuracy of \( Q_{\alpha\beta\beta}^{eq} \) which dictates the working window of the method.

With the expansion method described above, one can develop the D2Q7 ELBGK model. The bare collision integral (cf. section [11]) is assumed in the form, \( \Delta_i = -(f_i - f_i^{(k)}) \), where it should be decided that up to which order \( k \) is appropriate. Three condition guide the choice of the order \( k \):

- Approximation of the populations should be good enough to enable solving for the entropy estimate (43);
• Deviations in the stress tensor and in the energy flux should be small. Since the deviations in the stress tensor are one order higher as compared to the energy flow, the latter will be most crucial;

• The velocity window should not be too close to zero in order to avoid large computational time, and also in order to avoid computations with too small numbers.

In order to establish the working window and the required order of accuracy of the approximation \( \tilde{f}^{(k)} \), we test the results of the expansion against the exact solution (31). In Fig. 1, zero velocity component \( \tilde{f}_0^{(k)} \) is compared with the exact solution for various \( k \). It is clear that the usual second-order approximation \( \tilde{f}_0^{(2)} \) is good enough only for \( u \leq 0.001 \). However, for a larger velocity window, \( u \leq 0.1 \), a much better choice is to use the 4th or 6th order approximation in actual simulations. Still higher order approximations do not gain much because they improve the values of the functions only at velocity too close to the sound speed.

Deviations of the stress tensor and of the energy flow are demonstrated in Fig. 2. This figure shows that for \( u \sim 0.075 \), the gain in exactness of the equilibrium populations greatly outweighs the minor deviations in the pressure tensor. On the other hand, Fig. 2 also shows that the dominant deviation is in the energy flow. This error is exactly the same for all quadratic approximations employed in the standard LBGK simulations, and it can be compensated by lowering the viscosity.

An alternative to the ELBGK model just described, is a straightforward realization of the gradient single relaxation time model [15], using the \( H \) function (30) derived here. In the present context, construction of the corresponding bare collision integral requires only the inversion of a \( 4 \times 4 \) matrix with populations-dependent entries which can be done analytically. This realization does not require any approximation on the equilibrium populations.

V. DISCUSSION

In this paper, we derived the \( H \) function for the D2Q7 lattice. This makes it possible to derive and implement the entropic lattice Boltzmann scheme for the triangular lattice, in addition to already established models on square lattices.

The goal of the entropic schemes is to achieve nonlinear unconditional stability in lattice
FIG. 1: Deviations of the approximate equilibrium population $\tilde{f}_0^{(k)}$ from the exact solution (see Eq. (31) for $f_0^{eq}$). Function $\varepsilon = 10^5 \times (f_0^{eq} - \tilde{f}_0^{(k)})/\rho$ is plotted for three different values of $k$. Notice that for $k = 2$, which correspond to the standard second-order polynomial equilibrium used in the LBM simulations, the error starts to increase rapidly already at $\nu \sim 0.001$. All the quantities are given in dimensionless units.

Boltzmann simulations through creation of valid kinetic models. We recall that the notion of the kinetic model of the Boltzmann equation includes the $H$ theorem as one of the important properties [20, 21]. In the construction of entropic lattice Boltzmann models, the second-order polynomial approximations to the generically non-polynomial equilibria of the pertinent $H$ functions do appear in the derivations in the same sense as they appeared in the lattice gas model, that is, to establish theoretically the hydrodynamic limit to an appreciable degree of accuracy in terms of the Mach number. However, these low-order polynomial approximations do not show up explicitly in the numerical simulation. Of course, this analogy should not be misinterpreted, the entropic lattice Boltzmann equations [15] are mesoscopic kinetic equations rather than a lattice gas. As to the numerical efficiency, for the already existing ELBGK model, with all the additional burden to solve for the discrete-time entropy estimate, the serial processor realization requires only 5 to 10 percent more CPU time as compared to the usual polynomial LBGK on the 2DQ9 lattice.
FIG. 2: Deviations of equilibrium higher order moments $M$. Functions $\varepsilon = 10^5 \times (\Delta M^{\text{ELBM}})/\rho$ are shown, where, the deviation from the continuous case is denoted by $\Delta M^{\text{ELBM}}$ and are the same as the under-braced term in Eq. (41) and Eq. (42). All the quantities are given in dimensionless units.

Our final comment concerns the so-called multiple relaxation times models [23]. The idea behind this approach is as follows: If one uses a second-order polynomial approximation to the equilibrium, then not all of the linearized collision integrals of the form $\Delta_i = \sum_{j=1}^{m} A_{ij} (f_j - \tilde{f}_{i}^{(2)})$ have the same spectral properties, and one can make use of this to enhance linear stability by choosing an appropriate matrix $A_{ij}$. This is done upon considering spectra of space-dependent problems (in particular, in a periodic domain [23]). Although the choice depends on the boundary conditions in the specific spectral problem used to determine $A_{ij}$, it might perform better than the standard LBGK also in other flow situations.

To conclude, it is possible to obtain the $H$ function, and a good approximation to the correct equilibria for hydrodynamics on the D2Q7 lattice. It was shown, that the quadratic polynomial form of the equilibria used in the lattice Boltzmann method is a good approximation to the correct equilibria for velocity $u \sim 0.001$. It is possible to obtain a good approximation to the equilibria for velocity up to $u \sim 0.1$ by taking 6th order approximation to the correct equilibria. Further, lattice Boltzmann simulations on D2Q7 lattice
should avoid using average velocity larger than $u \sim 0.075$ due to the dominant errors in the heat flux. Finally, quadratic polynomials are just a good approximation to the equilibria for $u \sim 0.001$ and should not be confused with the correct equilibria.

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