Nonexistence of H theorems for the athermal lattice Boltzmann models with polynomial equilibria

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We prove that no H theorem exists for the athermal lattice Boltzmann equation with polynomial equilibria satisfying the conservation laws exactly and explicitly. The proof is demonstrated by using the seven-velocity model in a triangular lattice in two dimensions, and can be readily extended to other lattice Boltzmann models in two and three dimensions. Some issues pertinent to the numerical instabilities of the lattice Boltzmann method are disscussed.

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The lattice Boltzmann method [1–11] has been proven to be a viable simulation tool for turbulent flows [12,13], multiphase [8], and multicomponent [9] flows, and particulate suspensions [13–16]. Although historically the lattice Boltzmann equation (LBE) was developed from the lattice gas cellular automata [17], it is now well understood that the LBE models are a special finite-difference form of the continuous Boltzmann equations with linearized collision operators [7–11]. As an effective simulation tool for computational fluid dynamics (CFD), the LBE method has several attractive features: (a) linear advection term; (b) exact conservation laws with the necessary symmetries; and (c) broad applications. The lattice Boltzmann method differs from all conventional Navier-Stokes solvers because of its kinetic origin. The kinetic origin of the lattice Boltzmann method would allow it, with suitable modifications, to be applicable to situations where the continuum theory breaks down [18].

Because of its close tie to kinetic theory, one important question is whether the lattice Boltzmann equation possesses an H theorem. This question has indeed attracted much attention [19–32], because it is not only of theoretical importance, but also of practical significance, for it is closely related to the stability of the LBE method. Because it is believed that an H theorem does not exist for the lattice Boltzmann equation with polynomial equilibria [19,20], much emphasis has been focused on analytic construction of equilibria which admit H theorems [21–31], or on numerical entropic schemes [32].

In this paper, we shall rigorously prove that an H theorem does not exist for the lattice Boltzmann equation with polynomial equilibria. We shall also place our work in perspective, and discuss issues pertinent to the numerical stability of the LBE method, in general.

Our proof consists of two steps. First, we prove that the local entropy function H must be a sum of strictly convex functions $\{h_i(f_i)\}$, of which each depends only on the discrete distribution function $f_i := f(\boldsymbol{x},\boldsymbol{c}_i,t)$, where $\{\boldsymbol{c}_i | i = 0,1,\ldots,N\}$ is the discrete velocity set, and $\boldsymbol{c}_0$ always denotes the zero velocity. We then show that the required strictly convex function $h_i(f_i)$ does not exist.

In general, the lattice Boltzmann equation is

$$f_i(\boldsymbol{x}+\mathbf{c}_i\delta_t, t+\delta_t) - f_i(\boldsymbol{x},t) = J_i(\{f_i(\boldsymbol{x},t)\}), \tag{1}$$

where $\boldsymbol{x}$ is a point in a D-dimensional lattice space with a lattice constant δ_x, i.e., $\boldsymbol{x}\in\delta_x\mathbb{Z}^D$, and t is the discrete time with a time step δ_t, i.e., $t\in\delta_t\mathbb{N}$. The discrete velocity set $\{\boldsymbol{c}_i\}$ of a lattice Boltzmann model is so constructed that for any $\boldsymbol{x}\in\delta_x\mathbb{Z}^D$ and $\boldsymbol{c}_i$, $\boldsymbol{x}+\boldsymbol{c}_i\delta_t\in\delta_x\mathbb{Z}^D$. The evolution of an LBE model defined by Eq. (1) is usually decomposed into two elementary steps: (1) collision prescribed by the collision operator J_i and (2) advection of f_i from one lattice point to another according to $\boldsymbol{c}_i$. This can be expressed as the following:

$$\text{collision:} \qquad \tilde{\mathbf{f}}(\boldsymbol{x},t) = \mathbf{f}(\boldsymbol{x},t) + \mathbf{J}(\mathbf{f}), \tag{2a}$$

$$\text{advection:} \qquad \mathbf{f}(\boldsymbol{x}+\boldsymbol{c}_i\delta_t, t+\delta_t) = \tilde{\mathbf{f}}(\boldsymbol{x},t), \tag{2b}$$

where the following notation is used to denote column vectors in space $\mathbb{R}^{N+1}$,

$$\mathbf{f}(\boldsymbol{x},t) := (f_0, f_1, \ldots, f_N)^{\mathsf{T}}, \quad \mathbf{J}(\mathbf{f}) := (J_0, J_1, \ldots, J_N)^{\mathsf{T}},$$

$$\mathbf{f}(\boldsymbol{x}+\boldsymbol{c}\delta_t, t+\delta_t) := [f_0(\boldsymbol{x}, t+\delta_t),$$

$$f_1(\boldsymbol{x}+\boldsymbol{c}_1\delta_t, t+\delta_t), \ldots, f_N(\boldsymbol{x}+\boldsymbol{c}_N\delta_t, t+\delta_t)]^{\mathsf{T}},$$

and T denotes the transpose operator.

Consider a *finite* and *periodic* lattice space with total number of lattice points L. The H theorem for the system of Eq. (1) on a finite lattice space with periodic boundary conditions states that there exists a strictly convex function (entropy) $H = H(\mathbf{f})$ such that (i) the total entropy of the system remains intact under advection and (ii) $\mathbf{J}(\mathbf{f}^{(\mathrm{eq})}) = \mathbf{0}$ if and only if $\mathbf{f}^{(\mathrm{eq})}$ minimizes the entropy $H(\mathbf{f})$ with some given constraints. According to (i), we have

$$\sum_{\boldsymbol{x}} H(\mathbf{f}(\boldsymbol{x}, t+\delta_t)) = \sum_{\boldsymbol{x}} H(\tilde{\mathbf{f}}(\boldsymbol{x},t)). \tag{3}$$

Now consider the following initial conditions. Initialize

$$\tilde{\mathbf{f}}(\boldsymbol{x}_0, t=0) = \mathbf{A} \in \mathbb{R}^{N+1}$$

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at an arbitrary point $\boldsymbol{x}_0$ in the finite lattice system, and

$$\tilde{\mathbf{f}}(\boldsymbol{x},t=0)=\mathbf{B}\in\mathbb{R}^{N+1}\qquad\forall\boldsymbol{x}\neq\boldsymbol{x}_0.$$

Then the sum in the right hand side of Eq. (3) is

$$H(\mathbf{A})+(L-1)H(\mathbf{B}).$$

Since $\boldsymbol{c}_i$'s are distinct, the sum in the left hand side of Eq. (3) is

$$[L-(N+1)]H(\mathbf{B})+\sum_i H(\hat{\mathbf{B}}_i),$$

where $\hat{\mathbf{B}}_i$ is $\mathbf{B}$ with its ith component B_i replaced by A_i, the ith component of $\mathbf{A}$. Thus, Eq. (3) becomes

$$\sum_i H(\hat{\mathbf{B}}_i)=H(\mathbf{A})+N\,H(\mathbf{B}).\tag{4}$$

For a smooth function H, Eq. (4) implies that

$$H_{f_if_j}:=\frac{\partial^2 H}{\partial f_i\partial f_j}\equiv 0\quad\forall\ i\neq j.\tag{5}$$

To show this, we choose two arbitrary unequal indices i and j, i.e., $i\neq j$, $i,j\in\{0,1,\ldots,N\}$, such that $A_k=B_k$ for all $k\notin\{i,j\}$. With this particular choice of $\mathbf{A}$ and $\mathbf{B}$, Eq. (4) reduces to

$$H(A_i,B_j)+H(B_i,A_j)=H(A_i,A_j)+H(B_i,B_j)\quad\forall\ i\neq j,$$

where all other $(N-1)$ equal arguments of H are omitted for conciseness. Equivalently,

$$\int_0^1\int_0^1 H_{f_if_j}[A_i+\phi(B_i-A_i),A_j+\varphi(B_j-A_j)]\,d\phi\, d\varphi=0.$$

In the limit of $(B_i,B_j)\to(A_i,A_j)$, it is obvious that $H_{f_if_j}(\mathbf{A})=0$. Consequently, $H(\mathbf{f})$ must be of the form

$$H(\mathbf{f})=\sum_{i=0}^{N} h_i(f_i),\tag{6}$$

where $h_i(f_i)$ is strictly convex. We note that although Eq. (6) has been motivated by plausible arguments [20], for the most part, generally it has simply been taken as a key assumption [21–31].

Athermal LBE models satisfy only mass and momentum conservation. Thus, the equilibrium $\mathbf{f}^{(\mathrm{eq})}$ minimizes $H(\mathbf{f})$ with the mass and momentum constraints:

$$H(\mathbf{f}^{(\mathrm{eq})})=\min_{\mathbf{f}}\left\{H(\mathbf{f}):\sum_i f_i=\rho,\sum_i \boldsymbol{c}_i f_i=\rho\boldsymbol{u}\right\}.$$

Equivalently, the equilibrium distribution $\mathbf{f}^{(\mathrm{eq})}$ is the solution of the following minimization problem:

$$\mathcal{H}(\mathbf{f})=\sum_i h_i(f_i)-a\left(\sum_i f_i-\rho\right)-\boldsymbol{b}\cdot\left(\sum_i \boldsymbol{c}_i f_i-\rho\boldsymbol{u}\right),$$

where a and $\boldsymbol{b}$ are Lagrangian multipliers due to the conservation constraints

$$\rho=\sum_i f_i^{(\mathrm{eq})},\qquad \rho\boldsymbol{u}=\sum_i \boldsymbol{c}_i f_i^{(\mathrm{eq})}.\tag{7}$$

The variation of $\mathcal{H}=\mathcal{H}(\mathbf{f})$

$$(\delta\mathcal{H})(\mathbf{f})=\sum_i(\delta f_i)[h_i'(f_i)-a-\boldsymbol{b}\cdot\boldsymbol{c}_i]$$

vanishes at equilibrium $\mathbf{f}=\mathbf{f}^{(\mathrm{eq})}$ that must satisfy

$$h_i'(f_i^{(\mathrm{eq})})=a+\boldsymbol{b}\cdot\boldsymbol{c}_i\quad\forall\ i,\tag{8}$$

where $a=a(\rho,\boldsymbol{u})$ and $\boldsymbol{b}=\boldsymbol{b}(\rho,\boldsymbol{u})$ are determined by the conservation constraints of Eqs. (7).

The discrete velocity set $\{\boldsymbol{c}_i\}$ for a lattice Boltzmann model usually has the symmetry that the nonzero velocities always come in pair with opposite directions, i.e., if $\boldsymbol{c}_i\in\{\boldsymbol{c}_i\}$ and $\boldsymbol{c}_i\neq\mathbf{0}$, then $\boldsymbol{c}_{\bar{\imath}}\in\{\boldsymbol{c}_i\}$, where $\boldsymbol{c}_{\bar{\imath}}:=-\boldsymbol{c}_i$. By exploiting this symmetry of $\{\boldsymbol{c}_i\}$, from Eq. (8), we have

$$h_i'(f_i^{(\mathrm{eq})})+h_{\bar{\imath}}'(f_{\bar{\imath}}^{(\mathrm{eq})})=2a=h_j'(f_j^{(\mathrm{eq})})+h_{\bar{\jmath}}'(f_{\bar{\jmath}}^{(\mathrm{eq})}),\tag{9}$$

for any i and j. In particular, if $\boldsymbol{c}_0=\mathbf{0}\in\{\boldsymbol{c}_i\}$, we have

$$2h_0'(f_0^{(\mathrm{eq})})=h_i'(f_i^{(\mathrm{eq})})+h_{\bar{\imath}}'(f_{\bar{\imath}}^{(\mathrm{eq})}).\tag{10}$$

Note that up to now we have not used any properties specific to a lattice Boltzmann model.

We proceed to prove that the strictly convex function $h_i(f_i)$ does not exist. The proof requires some knowledge of the equilibrium $f_i^{(\mathrm{eq})}$. We shall only consider the equilibria that are polynomials of the conserved quantities (ρ and $\boldsymbol{u}$ for athermal models). The reason is that only the polynomial-type equilibria can enforce the conservation constraints *exactly* and *elicitly*. This point is crucial for the lattice Boltzmann method to be computationally efficient and competitive. In what follows the seven-velocity model on a two-dimensional triangular lattice (D2Q7 model) is used as an example for the sake of concreteness yet without losing generality. The discrete velocity set $\{\boldsymbol{c}_i|i=0,1,\ldots,6\}$ of the model is

$$\boldsymbol{c}_i=\begin{cases}(0,0), & i=0\\ [\cos(i-1)\pi/3,\sin(i-1)\pi/3], & i\neq 0,\end{cases}\tag{11}$$

and the equilibria are usually written as

$$f_0^{(\mathrm{eq})}=\rho[(1-\alpha)-\boldsymbol{u}^2],\tag{12a}$$

$$f_i^{(\mathrm{eq})}=\frac{1}{6}\rho[\alpha+2\boldsymbol{c}_i\cdot\boldsymbol{u}+4(\boldsymbol{c}_i\cdot\boldsymbol{u})^2-\boldsymbol{u}^2],\tag{12b}$$

where $i\neq 0$, and the lattice units of $\delta_x=1$ and $\delta_t=1$ have been used. The parameter α, $0<\alpha<1$, is the fractional density of moving particles, which in turn determines the sound speed of the model ($c_s^2=\alpha$).

For this model, when $(\rho,\boldsymbol{u})=(1,\mathbf{0})$, Eq. (10) becomes

$$2h_0'(1-\alpha)=h_i'(\alpha/6)+h_{\bar{\imath}}'(\alpha/6) \quad \text{for } i\neq 0. \tag{13}$$

Suppose that there exists one other state $(\rho,\boldsymbol{u})\neq(1,\mathbf{0})$ such that $\rho\boldsymbol{c}_i\cdot\boldsymbol{u}\neq 0$, and

$$f_0^{(\mathrm{eq})}=\rho[(1-\alpha)-\boldsymbol{u}^2]=(1-\alpha),$$

$$f_i^{(\mathrm{eq})}=\frac{1}{6}\rho[\alpha+2\boldsymbol{c}_i\cdot\boldsymbol{u}+4(\boldsymbol{c}_i\cdot\boldsymbol{u})^2-\boldsymbol{u}^2]=\frac{1}{6}\alpha. \tag{14}$$

Consequently,

$$f_{\bar{\imath}}^{(\mathrm{eq})}=f_i^{(\mathrm{eq})}-\frac{2}{3}\rho\boldsymbol{c}_i\cdot\boldsymbol{u}=\frac{1}{6}\alpha-\frac{2}{3}\rho\boldsymbol{c}_i\cdot\boldsymbol{u},$$

and Eq. (10) becomes

$$2h_0'(1-\alpha)=h_i'(\alpha/6)+h_{\bar{\imath}}'(\alpha/6-2\rho\boldsymbol{c}_i\cdot\boldsymbol{u}/3) \quad \text{for } i\neq 0.$$

The above equality and Eq. (13) immediately lead to

$$h_{\bar{\imath}}'(\alpha/6)=h_{\bar{\imath}}'(\alpha/6-2\rho\boldsymbol{c}_i\cdot\boldsymbol{u}/3) \quad \text{for } i\neq 0. \tag{15}$$

Because $\rho\boldsymbol{c}_i\cdot\boldsymbol{u}\neq 0$, the above equality contradicts the assumption that $h_{\bar{\imath}}'$ is strictly increasing (for $h_{\bar{\imath}}$ to be strictly convex).

It remains to find a state $(\rho,\boldsymbol{u})$ satisfying Eqs. (14) and $\rho\boldsymbol{c}_i\cdot\boldsymbol{u}\neq 0$ for $i\neq 0$ simultaneously. Note that the flow velocity $\boldsymbol{u}$ can be orthogonally decomposed as $\boldsymbol{u}^2=u_\parallel^2+u_\perp^2$, where $u_\parallel:=\boldsymbol{c}_i\cdot\boldsymbol{u}$ and $u_\perp:=|\boldsymbol{u}-u_\parallel\hat{\boldsymbol{c}}_i|$, and $\hat{\boldsymbol{c}}_i$ is the unit vector parallel to $\boldsymbol{c}_i$. From Eqs. (14), we observe ρ and $u_\parallel$ depend on $u_\perp$ only through $u_\perp^2$. Therefore, if $\rho(u_\perp^2)$ and $u_\parallel(u_\perp^2)$ are monotonic in a neighborhood of $(\rho,\boldsymbol{u})=(1,\mathbf{0})$, ρ and $u_\parallel$ can be uniquely expressed in terms of $u_\perp^2$ (the implicit function theorem). From Eqs. (14), we have

$$\left.\frac{\partial u_\parallel}{\partial u_\perp^2}\right|_{u_\perp=0}=\frac{2\alpha-1}{2(1-\alpha)}\neq 0,$$

if $\alpha\neq 1/2$. Thus, in the neighborhood of $(\rho,\boldsymbol{u})=(1,\mathbf{0})$, we are guaranteed to find a state $(\rho,\boldsymbol{u})$ to satisfy $\boldsymbol{c}_i\cdot\boldsymbol{u}\not\equiv 0$ for $i\neq 0$ and Eqs. (14) simultaneously.

When $\alpha=1/2$, the equilibria of Eqs. (12) become

$$f_0^{(\mathrm{eq})}=\frac{1}{2}\rho(1-2\boldsymbol{u}^2),$$

$$f_i^{(\mathrm{eq})}=\frac{1}{12}\rho[1+4\boldsymbol{c}_i\cdot\boldsymbol{u}+8(\boldsymbol{c}_i\cdot\boldsymbol{u})^2-2\boldsymbol{u}^2], \quad i\neq 0.$$

At the two chosen states, $\rho=1$ and $\boldsymbol{u}=(0,0)$, and $\rho=2$ and $(u_\parallel,u_\perp)=(1/2,0)$, Eq. (10), respectively, yields

$$2h_0'(1/2)=h_i'(1/12)+h_{\bar{\imath}}'(1/12),$$

$$2h_0'(1/2)=h_i'(3/4)+h_{\bar{\imath}}'(1/12),$$

for $i\neq 0$. Consequently, we have

$$h_i'(3/4)=h_i'(1/12) \quad \text{for } i\neq 0.$$

Again, this contradicts the strict convexity assumption of h_i. Hence, we have proven the nonexistence of a local *H* theorem for the D2Q7 model.

Comments regarding the proof are in order at this point. Let us summarize the conditions under which we accomplish the proof: (a) the LBE model is in the general form of Eq. (1); (b) the discrete velocity set $\{\boldsymbol{c}_i\}$ has suitable symmetries; (c) the collision operator $\mathbf{J(f)}$ satisfies certain conservation constraints; and (d) the equilibria $\{f_i^{(\mathrm{eq})}\}$ are polynomials. We should also stress that the proof does not require any specific knowledge of the form of the collision operator $\mathbf{J(f)}$, and that the key step of the proof [Eq. (6)] does not rely on any knowledge of the equilibria $\{f_i^{(\mathrm{eq})}\}$. But the exact values of $\{f_i^{(\mathrm{eq})}\}$ at two points in the space of ρ and $\boldsymbol{u}$ are required. For this reason, the proof does not applied for the exponential equilibria in which $a(\rho,\boldsymbol{u})$ and $\boldsymbol{b}(\rho,\boldsymbol{u})$ are not known exactly for arbitrary value $\boldsymbol{u}\neq\mathbf{0}$, in general. The proof is applicable to the equilibria that are explicit functions of ρ and $\boldsymbol{u}$ satisfying the conservation constraints *exactly*, such as higher order polynomials of $\boldsymbol{u}$ than the second order. The proof can be readily extended to other athermal LBE models: the six-velocity model on a triangular lattice (D2Q6) and the nine-velocity model on a square lattice (D2Q9) in two dimensions, and the fifteen-velocity model (D3Q15), the nineteen-velocity model (D3Q19), and the twenty-seven-velocity model (D3Q27) on a cubic lattice in three dimensions, with the multiple-relaxation-time (MRT) model [4–6], of which the single-relaxation-time or Bhatnagar-Gross-Krook (BGK) model [33] is a special case, or other types of *linear* collision operators.

It is important to place the present effort in the perspective of existing work [19–32]. So far, previous works [20–32] have been restricted to the lattice BGK models [2,3], and the main effort has been focused on the construction of the equilibria that admit an *H* theorem, either analytically [21–31] or numerically [32]. Such equilibria usually are nonpolynomial types (e.g., exponentials [20]). To obtain the correct hydrodynamics, the lowest order Taylor expansions of these nonpolynomial equilibria must be identical to the correct polynomial equilibria. These nonpolynomial equilibria invariably compromise the conservation laws, or make the collision process *implicit*, which can degrade not only the computational efficiency, but also, given that there are only a few discrete velocities in the LBE models [19], the numerical accuracy of the method, or bring in other spurious effects [34]. The entropic LBE scheme based on numerical construction of a entropy function [32] has the severe drawbacks of unknown numerical dissipation and heavy computational overhead (CPU time of such a scheme in two dimensions increases by about two orders of magnitude). Although the theoretical significance of these works are recognized, they have hardly made any impact in practice.

Should we accept as a fact of life that an *H* theorem is simply not a part of the lattice Boltzmann equation for good reasons, then we must deal with the numerical instability associated with the LBE method by other means. The remedies we offer here must not only be effective, but also computationally efficient. Such remedies should be based on our understanding of the origin (or the causes) of the instability. Due to the simple algebraic strucuture of the existing athermal and thermal lattice Boltzmann models, certain eigenvalues of the linearized collision operator coalesce spuriously. For the athermal cases, such coalescences occur near $k=\pi$ in the wave number $\boldsymbol{k}$ space, so that the athermal LBE models are prone to numerical instability initiated by small-scale fluctuations. This effect is further amplified in the lattice BGK schemes which may over-relax all the modes with a single parameter τ when $\tau<1$. This problem can be effectively mitigated if the MRT models [4–6] are used, and with careful implementations to suppress compressible effects [6].

As for the thermal LBE models, the numerical instability is a much more severe problem. It has been shown recently that the energy mode and shear mode of the linearized collision operator of the thermal LBE models coalesce spuriously in a wide range of wave numbers k along certain directions [35]. This coupling is highly anisotropic and cannot be eliminated by increasing the number of discrete velocities. This means the thermal LBE models are prone to instabilities due to fluctuations on a continuous range of scales. So far, we find that the best remedy for this problem is to use the hybrid lattice Boltzmann method that solves the mass and momentum conservation laws by the MRT-LBE method, and the temperature equation by finite difference or other techniques [35].

In conclusion, we have proven that an H theorem does not exist for the athermal lattice Boltzmann models with polynomial equilibria satisfying the conservation laws exactly and explicitly. We discuss some issues pertinent to the numerical instabilities of the lattice Boltzmann methods, and suggest remedies such as the MRT and hybrid lattice Boltzmann schemes [35] that can mitigate the numerical instabilities observed in the LBE simulations. The extension of the proof to the thermal LBE models with polynomial equilibria is under way by the authors.

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