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Nonexistence of *H* Theorem for Some Lattice Boltzmann Models

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In this paper, we provide a set of *sufficient* conditions under which a lattice Boltzmann model does not admit an H theorem. By verifying the conditions, we prove that a number of existing lattice Boltzmann models does not admit an H theorem. These models include D2Q6, D2Q9 and D3Q15 athermal models, and D2Q16 and D3Q40 thermal (energy-conserving) models. The proof does not require the equilibria to be polynomials.

KEY WORDS: Lattice Boltzmann equation; H-theorem.

1. INTRODUCTION

The lattice Boltzmann equation (LBE)[1,2] has emerged as an effective method for computational fluid dynamics (CFD) (cf. a recent review[3] and refs. therein). The most notable feature of the lattice Boltzmann equation is its direct connection to a discretization of the Boltzmann equation,[4,5] rather than to discretizations of the Navier–Stokes equations. The kinetic origin of the LBE method immediately leads to the question whether or not the H theorem associated with the Boltzmann equation is preserved in the lattice Boltzmann equation, after the drastic approximations made to derive it.[4,5] The H theorem has many important ramifications and is directly related to the stability of the LBE method. Therefore it has been a subject of considerable research interest (cf. refs. 6–10 and references therein). It seems to be intuitive that the LBE models with relaxation collision operators and polynomial equilibria do not admit an

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H theorem,[7,8] because it is easy to demonstrate that some LBE models become linearly unstable under certain conditions.[11] However, only very recently was a rigorous proof given.[12]

There has also been an effort to construct LBE models which admit an H theorem.[6,9,10] This has been done in two ways. One is to analytically construct the equilibria which admit an H theorem.[6,9] The other is to construct an collision process which maximizes a given Lyapunov functional numerically.[10] These "entropic" LBE models are aimed to ensure an absolute numerical stability in LBE algorithms. However, these "entropic" LBE models have severe drawbacks.[13,12]

The present paper is a continuation of our previous work,[12] in which we rigorously proved that a class of the LBE models with polynomial equilibria does not admit an H theorem. In this paper we generalize our previous result to provide a set of *sufficient* conditions under which an LBE model does not admit an H theorem. The proof does not require the equilibria to be polynomials. The theorem can also be used to verify some existing results. In particular, we narrow the validity domain of the H theorem given in ref. 6 for a class of LBE models with nonpolynomial equilibria.

The remainder of the paper is organized as follows. Section 2 contains our main results including a lemma and a theorem. The lemma states that the H function must be of a certain canonical form and the theorem proves that an LBE model does not admit an H theorem if it satisfies a set of *sufficient* conditions. Section 3 provides several examples of LBE models with no H theorems. These examples include D2Q9, D3Q15 and D2Q6 athermal LBE models, and D2Q16 and D3Q40 thermal (energy-conserving) models. Section 4 addresses the validity domain of the H theorem for an LBE model with nonpolynomial equilibria. We find the validity domain is smaller than the positivity domain of the equilibria. Finally, Section 5 concludes the paper.

2. MAIN RESULTS

On a D-dimensional lattice $\delta_x\mathbb{Z}_D$ with discrete time $t_n \in \delta_t\mathbb{N}_0$, the lattice Boltzmann equation reads as

$$\mathbf{f}(\boldsymbol{x}_k + \boldsymbol{c}\delta_t, t_n + \delta_t) = \mathbf{f}(\boldsymbol{x}_k, t_n) + \mathbf{J}(\mathbf{f}(\boldsymbol{x}_k, t_n)). \tag{1}$$

In Eq. (1), the bold-face symbols denote column vectors in $\mathbb{R}^Q$:

$$\mathbf{f}(\boldsymbol{x}_k+\boldsymbol{c}\delta_t,t_n+\delta_t):=(f_0(\boldsymbol{x}_k,t_n+\delta_t),\ldots,f_N(\boldsymbol{x}_k+\boldsymbol{c}_N\delta_t,t_n+\delta_t))^\top$$
$$\mathbf{f}(\boldsymbol{x}_k,t_n):=(f_0(\boldsymbol{x}_k,t_n),\ldots,f_N(\boldsymbol{x}_k,t_n))^\top$$
$$\mathbf{J}(\mathbf{f}(\boldsymbol{x}_k,t_n)):=(J_0,\ldots,J_N)^\top,$$

$\{f_i\}$ and $\{J_i\}$ are the single particle distribution functions and collision terms, respectively, and the discrete velocity set $\{\boldsymbol{c}_i\}$ has Q *distinctive* elements, and it may or may not include the zero velocity $\boldsymbol{c}_0=\mathbf{0}$. If $\boldsymbol{c}_0$ is included, then the discrete velocity set is $\{\boldsymbol{c}_i|i=0,1,\ldots,N\}$ and the total number of velocities is $Q=N+1$; otherwise, the velocity set is $\{\boldsymbol{c}_i|i=1,\ldots,N\}$ and $Q=N$.

We assume that the discrete velocity set has the symmetry property that, for every $\boldsymbol{c}_j\in\{\boldsymbol{c}_i\}$, there is a unique $\boldsymbol{c}_{\bar{j}}\in\{\boldsymbol{c}_i\}$ such that

$$\boldsymbol{c}_{\bar{j}}=-\boldsymbol{c}_j. \tag{2}$$

In addition, the lattice $\delta_x\mathbb{Z}_D$ has the following property

$$\boldsymbol{c}_i\delta_t+\boldsymbol{x}_j\in\delta_x\mathbb{Z}_D \quad \forall\boldsymbol{x}_j\in\delta_x Z_D. \tag{3}$$

The evolution of the lattice Boltzmann equation (1) can be decomposed as two steps, collision and advection:

$$\text{collision:}\quad \tilde{\mathbf{f}}(\boldsymbol{x}_k,t_n)=\mathbf{f}(\boldsymbol{x}_k,t_n)+\mathbf{J}(\mathbf{f}(\boldsymbol{x}_k,t_n)), \tag{4a}$$
$$\text{advection:}\quad \mathbf{f}(\boldsymbol{x}_k+\boldsymbol{c}\delta_t,t_n+\delta_t)=\tilde{\mathbf{f}}(\boldsymbol{x}_k,t_n). \tag{4b}$$

In what follows we shall restrict ourselves to a *finite* and *periodic* lattice space. An H theorem for Eq. (1) implies that there exists a *strictly* convex function $H=H(\mathbf{f})$ with the following two properties:

(a) The advection has no effect on the total entropy;

(b) $\mathbf{J}(\mathbf{f}^{(\mathrm{eq})})=\mathbf{0}$ iff $\mathbf{f}^{(\mathrm{eq})}$ minimizes H with given constraints.

The property (a) of H allows us to prove the following lemma.

Lemma 2.1. Assume the first-order derivatives $H_{f_i}:=\partial H/\partial f_i$ of the entropy function $H=H(\mathbf{f})$ exist. Then the above property (a) implies that $H(\mathbf{f})$ must be of the canonical form

$$H(\mathbf{f})=\sum_i h_i(f_i). \tag{5}$$

The proof of this lemma is similar to that in ref. 12 where H is required to be smooth, whereas here H is assumed to have only first-order derivatives H_{f_i}. Because this alters the proof little, we refer interested readers to our previous paper (see ref. 12) for details.

We note that the (strict) convexity of $H(\mathbf{f})$, equivalent to that of the h_i's, is not used in the proof of Lemma 2.1. We also note that although Eq. (5) has been motivated by plausible arguments, for the most part, generally it has simply been taken as a key assumption (e.g., refs. 7, 10).

As is well known, the property (b) of $H(\mathbf{f})$ implies that the equilibria $\mathbf{f}^{(\mathrm{eq})}$ must satisfy

$$h_i'(f_i^{(\mathrm{eq})}) = a + \boldsymbol{b}\cdot\boldsymbol{c}_i + c\,|\boldsymbol{c}_i|^2 \qquad \forall i. \tag{6}$$

Here $a = a(\rho, \boldsymbol{u}, e)$, $\boldsymbol{b} = \boldsymbol{b}(\rho, \boldsymbol{u}, e)$ and $c = c(\rho, \boldsymbol{u}, e)$ are the Lagrange multipliers corresponding to the conservation constraints

$$\rho = \sum_i f_i, \quad \rho\boldsymbol{u} = \sum_i \boldsymbol{c}_i f_i, \quad \rho e = \sum_i \frac{1}{2}|\boldsymbol{c}_i - \boldsymbol{u}|^2 f_i, \tag{7}$$

where ρ, $\boldsymbol{u}$ and e are the density, flow velocity and specific energy, respectively. Obviously, for athermal models, the energy conservation constraint is removed, and hence we have only two Lagrange multipliers $a = a(\rho, \boldsymbol{u})$ and $\boldsymbol{b} = \boldsymbol{b}(\rho, \boldsymbol{u})$.

For most LBE models, the equilibria $\mathbf{f}^{(\mathrm{eq})}$ are not constructed based on Eq. (6). Instead, they are constructed to satisfy the conservation constraints alone. The equilibria so obtained are usually polynomials in the conserved variables and they may not admit an H theorem. To clarify this, we prove the following theorem.

Theorem 2.2. Consider an LBE model with equilibria $\mathbf{f}^{(\mathrm{eq})} = \mathbf{f}^{(\mathrm{eq})}(S)$. If there exist two states S_1 and S_2, and two discrete velocities $\boldsymbol{c}_i$ and $\boldsymbol{c}_j$ such that

$$f_i^{(\mathrm{eq})}(S_1) \neq f_i^{(\mathrm{eq})}(S_2), \quad f_l^{(\mathrm{eq})}(S_1) = f_l^{(\mathrm{eq})}(S_2) \tag{8}$$

for $l \in \{\bar{\imath}, j, \bar{\jmath}\}$ (and $|\boldsymbol{c}_i| = |\boldsymbol{c}_j|$ for thermal models), then the LBE model does not admit an H theorem.

Proof. The proof is accomplished by contradiction. Assume there exists an H theorem. By Lemma 2.1, the entropy function $H(\mathbf{f})$ must be of the form (5) where the h_i's are strictly convex.

For brevity, we consider only the athermal case, where

$$h_i'(f_i^{(\mathrm{eq})}) = a + \boldsymbol{b}\cdot\boldsymbol{c}_i. \tag{9}$$

Because $f_l^{(\mathrm{eq})}(S_1) = f_l^{(\mathrm{eq})}(S_2)$ for $l \in \{\bar{\imath}, j, \bar{\jmath}\}$, Eq. (9) leads to

$$\begin{aligned}
a(S_1) + \boldsymbol{b}(S_1)\cdot\boldsymbol{c}_{\bar{\imath}} &= a(S_2) + \boldsymbol{b}(S_2)\cdot\boldsymbol{c}_{\bar{\imath}},\\
a(S_1) + \boldsymbol{b}(S_1)\cdot\boldsymbol{c}_j &= a(S_2) + \boldsymbol{b}(S_2)\cdot\boldsymbol{c}_j,\\
a(S_1) + \boldsymbol{b}(S_1)\cdot\boldsymbol{c}_{\bar{\jmath}} &= a(S_2) + \boldsymbol{b}(S_2)\cdot\boldsymbol{c}_{\bar{\jmath}}.
\end{aligned}$$

Since $\boldsymbol{c}_{\bar{\jmath}} = -\boldsymbol{c}_j$, we add the last two equalities above to obtain $a(S_1) = a(S_2)$. Thus, the first equality gives $\boldsymbol{b}(S_1)\cdot\boldsymbol{c}_{\bar{\imath}} = \boldsymbol{b}(S_2)\cdot\boldsymbol{c}_{\bar{\imath}}$ and thereby $\boldsymbol{b}(S_1)\cdot\boldsymbol{c}_i = \boldsymbol{b}(S_2)\cdot\boldsymbol{c}_i$. Consequently, we have

$$a(S_1) + \boldsymbol{b}(S_1)\cdot\boldsymbol{c}_i = a(S_2) + \boldsymbol{b}(S_2)\cdot\boldsymbol{c}_i,$$

therefore $h_i'(f_i^{(\mathrm{eq})}(S_1)) = h_i'(f_i^{(\mathrm{eq})}(S_2))$ because of Eq. (9). Then the strict monotonicity of h_i' due to the strict convexity of h_i immediately leads to $f_i^{(\mathrm{eq})}(S_1) = f_i^{(\mathrm{eq})}(S_2)$. This contradicts the assumption that $f_i^{(\mathrm{eq})}(S_1) \neq f_i^{(\mathrm{eq})}(S_2)$. Hence the proof is complete. ∎

Theorem 2.2 provides a set of *sufficient* conditions under which a given LBE model does not admit an H theorem. We note that the proof of Theorem 2.2 does not require any specific knowledge of $\mathbf{f}^{(\mathrm{eq})}$.

3. LBE MODELS WITHOUT *H* THEOREM

In this section, we apply Theorem 2.2 to a number of athermal and thermal (energy-conserving) LBE models to show that these models do not admit an H theorem. For this purpose, we will always choose S_1 to be a quiescent state of a nonzero constant density $\rho = \rho_0 \neq 0$ (and a constant energy e_0 for thermal models) and $\boldsymbol{u} = \boldsymbol{0}$. To find $S_2 = (\rho, \boldsymbol{u})$ or $S_2 = (\rho, e, \boldsymbol{u})$ for athermal and thermal models, respectively, we choose two discrete velocities $\boldsymbol{c}_i$ and $\boldsymbol{c}_j$ and solve the following algebraic equations:

$$f_l^{(\mathrm{eq})}(S_2) = f_l^{(\mathrm{eq})}(S_1) \qquad \text{for} \quad l \in \{\bar{\imath}, j, \bar{\jmath}\}. \tag{10}$$

The solutions of above equations are then used to check if $f_i^{(\mathrm{eq})}(S_1) \neq f_i^{(\mathrm{eq})}(S_2)$, and then if the conditions of Theorem 2.2 are satisfied.

3.1. Athermal Models

For models considered here, the equilibria can be written as[4,5]:

$$f_i^{(\mathrm{eq})} = w_i\,\rho\left\{\gamma_i + \frac{(\boldsymbol{c}_i\cdot\boldsymbol{u})}{c^2} + \frac{1}{2}\left(\frac{(\boldsymbol{c}_i\cdot\boldsymbol{u})^2}{c^4} - \frac{\boldsymbol{u}\cdot\boldsymbol{u}}{c^2}\right)\right\}, \tag{11}$$

where w_i, γ_i and c are parameters to be specified.

3.1.1. The D2Q9 Model

For this model, the discrete velocities are

$$\boldsymbol{c}_i = \begin{cases} (0,0), & i=0, \\ (\pm 1, 0),\ \ (0,\pm 1), & i\in\{1,\ 2,\ 3,\ 4\}, \\ (\pm 1,\pm 1), & i\in\{5,\ 6,\ 7,\ 8\}; \end{cases} \tag{12}$$

$w_0 = 4/9$, $w_{1,2,3,4} = 1/9$ and $w_{5,6,7,8} = 1/36$; $\gamma_0 = \alpha > 0$, $\gamma_{1,2,3,4} = \beta > 0$ and $\gamma_{5,6,7,8} = \gamma = 9 - 4(\alpha+\beta) > 0$; and $c = 1/\sqrt{3}$.

We choose $S_1 = (\rho, u_1, u_2) = (\rho_0, 0, 0)$ with $\rho_0 \neq 0$ and two velocities $\boldsymbol{c}_i = \boldsymbol{c}_1 := (1,\ 0)$ and $\boldsymbol{c}_j = \boldsymbol{c}_0 := (0,\ 0)$. To find another state $S_2 = (\rho, \boldsymbol{u}) \equiv (\rho, u_1, u_2)$, we solve the following equations

$$f_l^{(\mathrm{eq})}(S_2) = f_l^{(\mathrm{eq})}(S_1) \qquad \text{for} \quad l\in\{0,\ \bar{1}\} = \{0,\ 3\}. \tag{13}$$

Substituting S_1 and S_2 into Eq. (13), we have

$$\begin{aligned} \rho\left(\alpha - \frac{3}{2}|\boldsymbol{u}|^2\right) &= \alpha\rho_0, \\ \rho\left(\beta + 3\boldsymbol{u}\cdot\boldsymbol{c}_{\bar{1}} + \frac{9}{2}(\boldsymbol{u}\cdot\boldsymbol{c}_{\bar{1}})^2 - \frac{3}{2}|\boldsymbol{u}|^2\right) &= \beta\rho_0. \end{aligned}$$

These equations have solutions

$$\begin{aligned} \rho &= \frac{2\alpha\rho_0}{2\alpha - 3u^2}, \qquad u^2 := |\boldsymbol{u}|^2 = u_1^2 + u_2^2, \\ u_1 &= \frac{\alpha - \sqrt{\alpha^2 + (2\alpha+\beta)(\alpha-\beta)u_2^2}}{2\alpha+\beta} \equiv u_1(u_2^2). \end{aligned}$$

Clearly, $u_1 = u_1(u_2^2)$ is well defined for $u_2^2 \ll 1$ and $u_1(0) = 0$. Thus, $\rho = \rho(u_2^2)$ is also well defined for $u_2^2 \ll 1$. Moreover, it is not difficult to see that $u_1(u_2^2) \neq 0$ if $u_2^2 \neq 0$ provided that $\alpha \neq \beta$. For $u_1 = u_1(u_2^2) \neq 0$, it is easy to see that $f_1^{(\mathrm{eq})}(S_2) \neq f_1^{(\mathrm{eq})}(S_1)$ for $S_2 = (\rho(u_2^2), u_1(u_2^2), u_2)$ with any u_2 satisfying $0 < u_2^2 \ll 1$. Then the conditions of Theorem 2.2 are satisfied and therefore no H theorem exists for the D2Q9 model provided that $\alpha \neq \beta$.

Similarly, by taking $\boldsymbol{c}_i = \boldsymbol{c}_5 = (1,\ 1)$ and $\boldsymbol{c}_j = \boldsymbol{c}_0 = (0,\ 0)$, we can show that no H theorem exists when $5\alpha + 4\beta \neq 9$.

If $\alpha = \beta$ and $5\alpha + 4\beta = 9$, then $\alpha = \beta = 1$ and the equilibrium (11) is the second-order Taylor expansion of the Maxwellian.[4,5] In this case, we choose $\boldsymbol{c}_i = \boldsymbol{c}_5 = (1,\ 1)$, $\boldsymbol{c}_j = \boldsymbol{c}_0 = (0,\ 0)$, $S_1 = (1, 0, 0)$ and $S_2 = (3/2, 1/3, 1/3)$ and compute

$$\begin{aligned}
&f_0^{(\mathrm{eq})}(S_1) = f_0^{(\mathrm{eq})}(S_2) = \frac{4}{9},\\
&\frac{1}{36} = f_5^{(\mathrm{eq})}(S_1) \neq f_5^{(\mathrm{eq})}(S_2) = \frac{7}{36},\\
&f_{\bar{5}}^{(\mathrm{eq})}(S_1) = f_{\bar{5}}^{(\mathrm{eq})}(S_2) = \frac{1}{36}, \qquad \boldsymbol{c}_{\bar{5}} = \boldsymbol{c}_7.
\end{aligned}$$

Hence we show that the D2Q9 model does not admit an H theorem when $\gamma_i > 0$ in the equilibria (11).

Note that in the last part of the proof, we use a relative large velocity $\boldsymbol{u}$ of $u = \sqrt{2}/3$, although $\mathbf{f}^{(\mathrm{eq})}$ remain positive with this value of u.

Although it is customary to set $\gamma_i > 0$ in the equilibria Eq. (11), it is not necessary. One can set, for example, $\alpha = -3/2$, $\beta = 3$ and $\gamma = 3$.[14] In this case, we take $\boldsymbol{c}_i = \boldsymbol{c}_5 = (1,\ 1)$, $\boldsymbol{c}_j = \boldsymbol{c}_6 = (-1,\ 1)$, $S_1 = (1, 0, 0)$ and $S_2 = (10/9, 1/3, 1/3)$ to compute

$$\frac{7}{36} = f_5^{(\mathrm{eq})}(S_2) \neq f_5^{(\mathrm{eq})}(S_1) = f_l^{(\mathrm{eq})}(S_2) = \frac{1}{12}$$

for $l \in \{\bar{5}, 6, \bar{6}\} = \{7, 6, 8\}$. Thus we complete the proof that the D2Q9 model does not admit an H theorem for plausible values of the parameters $\{\gamma_i\}$ in its equilibria.

3.1.2. The D3Q15 Model

For this 3-dimensional model, the 15 discrete velocities are

$$\boldsymbol{c}_i = \begin{cases} (0, 0), & i = 0,\\ (\pm 1, 0, 0),\ \ (0, \pm 1, 0),\ \ (0, 0, \pm 1), & i \in \{1,\ \dots,\ 6\},\\ (\pm 1, \pm 1, \pm 1), & i \in \{7,\ \dots,\ 15\}, \end{cases} \tag{14}$$

$w_0 = 2/9$ and $\gamma_0 = \alpha$, $w_i = 1/9$ and $\gamma_i = \beta$ for $i \in \{1,\ \dots,\ 6\}$, and $w_i = 1/72$ and $\gamma_i = (9 - 2\alpha - 6\beta)$ for $i \in \{7,\ \dots\ 15\}$. And $\alpha > 0$, $\beta > 0$ and $(\alpha + 3\beta) < 9/2$. For this model $c = 1/\sqrt{3}$.

We choose two velocities: $\boldsymbol{c}_i = \boldsymbol{c}_1 = (1, 0, 0)$ and $\boldsymbol{c}_j = \boldsymbol{c}_0 = (0, 0, 0)$, and two states $S_1 = (\rho_0, 0, 0, 0)$ with $\rho_0 \neq 0$ and $S_2 = (\rho, \boldsymbol{u}) \equiv (\rho, u_1, u_2, u_3)$ as an solution of

$$f_l^{(\mathrm{eq})}(S_2) = f_l^{(\mathrm{eq})}(S_1) \qquad \text{for} \quad l \in \{0, \bar{1}\} = \{0, 4\},$$

which are

$$\rho\left(\alpha - \frac{3}{2}|\boldsymbol{u}|^2\right) = \alpha\rho_0,$$
$$\rho\left(\beta + 3\boldsymbol{u}\cdot\boldsymbol{c}_{\bar{1}} + \frac{9}{2}(\boldsymbol{u}\cdot\boldsymbol{c}_{\bar{1}})^2 - \frac{3}{2}|\boldsymbol{u}|^2\right) = \beta\rho_0.$$

The general solutions of these equations are

$$\rho = \frac{2\alpha\rho_0}{2\alpha - 3u^2}, \qquad u^2 := |\boldsymbol{u}|^2 = u_1^2 + u_2^2 + u_3^3,$$
$$u_1 = \frac{\alpha - \sqrt{\alpha^2 + (2\alpha + \beta)(\alpha - \beta)u_\perp^2}}{2\alpha + \beta}, \qquad u_\perp^2 := u_2^2 + u_3^3.$$

Thus the conditions of Theorem 2.2 are met when $\alpha \neq \beta$. Furthermore, by taking $\boldsymbol{c}_i = \boldsymbol{c}_7 = (1, 1, 1)$ and $\boldsymbol{c}_j = \boldsymbol{c}_0 = (0, 0, 0)$, we can show that no H theorem exists when $\alpha + 2\beta \neq 3$.

When $\alpha = \beta$ and $\alpha + 2\beta = 3$, then $\alpha = \beta = 1$ and the equilibrium is the second-order Taylor expansion of the Maxwellian.[4,5] In this case we take $\boldsymbol{c}_i = \boldsymbol{c}_7 = (1, 1, 1), \boldsymbol{c}_j = \boldsymbol{c}_0 = (0, 0, 0), S_1 = (\rho_0, 0, 0, 0)$ with $\rho_0 \neq 0$ and $S_2 = (\rho, \boldsymbol{u}) = (9/7, 2/9, 2/9, 2/9)$ to show that

$$f_0^{(\mathrm{eq})}(S_1) = f_0^{(\mathrm{eq})}(S_2) = \frac{2}{9},$$
$$\frac{1}{72} = f_7^{(\mathrm{eq})}(S_1) \neq f_7^{(\mathrm{eq})}(S_2) = \frac{1}{72} + \frac{1}{14},$$
$$f_{\bar{7}}^{(\mathrm{eq})}(S_1) = f_{\bar{7}}^{(\mathrm{eq})}(S_2) = \frac{1}{72},$$

where $\boldsymbol{c}_7 = (1, 1, 1)$ and $\boldsymbol{c}_{\bar{7}} = \boldsymbol{c}_{13} = (-1, -1, -1)$. Thus, the D3Q15 model does not admit an H theorem.

3.1.3. The D2Q6 Model

Here the discrete velocities are

$$\boldsymbol{c}_i = (\cos(\pi(i-1)/3), \sin(\pi(i-1)/3)), \quad i = 1, 2, \ldots, 6 \tag{15}$$

and the equilibria are given by Eq. (11) with $w_i = 1/6$, $\gamma_i = 1$ and $c = 1/\sqrt{2}$.

For this model, we choose $\boldsymbol{c}_i = \boldsymbol{c}_5 = (-1/2, -\sqrt{3}/2)$, $\boldsymbol{c}_j = \boldsymbol{c}_1 = (1, 0)$, $S_1 = (1, 0, 0)$ and $S_2 = (3, 0, -1/\sqrt{3})$. Then we compute

$$\frac{7}{6} = f_5^{(\mathrm{eq})}(S_2) \neq f_5^{(\mathrm{eq})}(S_1) = f_l^{(\mathrm{eq})}(S_k) = \frac{1}{6} \quad \text{for } l \in \{\bar{5}, 1, \bar{1}\} = \{2, 1, 4\}.$$

Hence, by using the velocity $\boldsymbol{u} = (0, -1/\sqrt{3})$, we show that the D2Q6 model does not admit an H theorem.

3.2. Thermal (Energy-Conserving) Models

We now consider the thermal LBE models introduced in ref. 15. These models have no zero velocity and the equilibria can be written as

$$f_i^{(\mathrm{eq})} = \rho \left\{ \phi_i + \psi_i (\boldsymbol{c}_i \cdot \boldsymbol{u}) + \chi_i (\boldsymbol{c}_i \cdot \boldsymbol{u})^2 \right\}. \tag{16}$$

Here $u^2 := \boldsymbol{u} \cdot \boldsymbol{u}$ and

$$\phi_i = \phi_i(e, u^2) = A_i(e) + G_i(e)u^2 + E_i(e)u^4, \tag{17a}$$

$$\psi_i = \psi_i(e, u^2, (\boldsymbol{c}_i \cdot \boldsymbol{u})^2) = M_i(e) + Q_i(e)u^2 + H_i(e)(\boldsymbol{c}_i \cdot \boldsymbol{u})^2, \tag{17b}$$

$$\chi_i = \chi_i(e, u^2) = K_i(e) + R_i(e)u^2, \tag{17c}$$

where A_i, G_i, E_i, M_i, Q_i, H_i, K_i and R_i are quadratic polynomials of e, and they only depend on $|\boldsymbol{c}_i|$.[15]

3.2.1. D2Q16 Thermal Model

The D2Q16 model on a square lattice has 4 speeds: 1, $\sqrt{2}$, 2 and $2\sqrt{2}$. For the purpose here, we use the speed 1 velocities to demonstrate nonexistence of H theorem. When $e = 1$, we have $A_i = 1/5$, $G_i = 1/6$, $E_i = 1/8$, $M_i = -1/3$, $Q_i = -1/2$, $H_i = 1/3$, $K_i = -1/3$ and $R_i = -1/6$ for $|\boldsymbol{c}_i| = 1$, $i \in \{1, 2, 3, 4\}$.

By taking $\boldsymbol{c}_i = \boldsymbol{c}_1 = (1, 0)$, $\boldsymbol{c}_j = \boldsymbol{c}_2 = (0, 1)$, $S_1 = (\rho, e, u_1, u_2) = (1, 1, 0, 0)$ and $S_2 = (24/59, 1, 1, 0)$, we find

$$\frac{1}{5} - \frac{24}{59} = f_1^{(\mathrm{eq})}(S_2) \neq f_1^{(\mathrm{eq})}(S_1) = f_l^{(\mathrm{eq})}(S_k) = \frac{1}{5}, \quad \forall\ k \in \{1, 2\}$$

and $l \in \{\bar{1}, 2, \bar{2}\} = \{3, 2, 4\}$. Hence the conditions of Theorem 2.2 are met and therefore H theorem does not exist for this model.

3.2.2. D3Q40 Thermal Model

The D3Q40 model on a cubic lattice has 5 speeds: 1, $\sqrt{2}$, $\sqrt{3}$, 2 and $2\sqrt{3}$. When $e = 8/3$, we have $A_i = -3403/2430$, $G_i = -23/48$, $E_i =$

$-513/8960$, $M_i = Q_i = 0$, $H_i = 1/192$, $K_i = 0$ and $R_i = -3/448$ for $|\boldsymbol{c}_i| = \sqrt{3}$, $i \in \{19, \ldots, 26\}$. We choose two velocities: $\boldsymbol{c}_i = \boldsymbol{c}_{21} = (-1, -1, 1)$ and $\boldsymbol{c}_j = \boldsymbol{c}_{19} = (1, 1, 1)$, and two macroscopic states $S_1 = (1, 8/3, 0, 0, 0)$ and $S_2 = (\rho, 8/3, u_1, u_2, u_3)$ which is the solution of

$$f_l^{(\mathrm{eq})}(S_2) = f_l^{(\mathrm{eq})}(S_1), \qquad l \in \{\bar{\imath}, j, \bar{j}\} = \{23, 19, 25\}.$$

The above equality leads to the following set of equations:

$$u_1 + u_2 + u_3 = 0, \tag{18a}$$

$$\rho\left(\frac{3403}{2430} + \frac{23}{48}u^2 + \frac{513}{8960}u^4\right) = \frac{3403}{2430}, \tag{18b}$$

$$7(u_1 + u_2 - u_3)^3 - 9(u_1 + u_2 - u_3)^2 u^2 = 0. \tag{18c}$$

The solutions of Eqs. (18a) and (18c) are

$$u_2 = u_2(u_1) = \frac{(7 - 9u_1) - \sqrt{(9u_1 + 7)^2 - 324u_1^2}}{18},$$

$$u_3 = u_3(u_1) = \frac{-(7 + 9u_1) + \sqrt{(9u_1 + 7)^2 - 324u_1^2}}{18}.$$

The above two functions of u_1 are well defined in the vicinity of $u_1 = 0$ and vanish at $u_1 = 0$. Moreover, they are smooth and $u_3(u_1)$ does not vanish for $u_1 \neq 0$. Thus Eq. (18b) determines ρ as a function $\rho(u_1)$ of u_1.

Now we take $S_2 = (\rho(u_1), 8/3, u_1, u_2(u_1), u_3(u_1))$, which is completely determined by u_1, with a small but non-zero u_1 to compute

$$\begin{aligned} f_i^{(\mathrm{eq})}(S_2) - f_i^{(\mathrm{eq})}(S_1) &= 2\rho\psi_i(8/3, u^2) \\ &= \rho(u_1)\frac{(u_3(u_1) - u_2(u_1) - u_1)^3}{96} \\ &= \frac{\rho(u_1)u_3^3(u_1)}{12} \neq 0. \end{aligned}$$

Hence, by Theorem 2.2, there exists no H theorems for this particular model. We note that the above proof does not employ a large velocity, as in some of the previous cases.

4. DISCUSSION OF ATHERMAL MODELS WITH NONPOLYNOMIAL EQUILIBRIA

Now we consider a class of athermal LBE models constructed in ref. 6 by explicitly solving Eq. (6) with $h_i(x) = (2/3)x^{3/2}$. Then we have

$$f_i^{(\mathrm{eq})} = (a + \boldsymbol{b} \cdot \boldsymbol{c}_i)^2, \tag{19}$$

where a and $\boldsymbol{b}$ are the Lagrange multipliers determined by the conservation constraints in Eq. (7). The symmetric discrete velocity set $\{\boldsymbol{c}_i\}$ is so chosen that $\sum_i \boldsymbol{c}_{i\alpha}\boldsymbol{c}_{j\beta} = Qc_s^2\delta_{\alpha\beta}$, where subscripts α and β denote the Cartesian coordinates in the D-dimensional space, hence $c_s^2 := \sum_i |\boldsymbol{c}_i|^2/(DQ)$.

The Lagrange multipliers can be explicitly obtained as

$$a = \sqrt{\rho R/Q}, \qquad \boldsymbol{b} = \frac{\rho \boldsymbol{u}}{2aQc_s^2}. \tag{20}$$

Thus, the equilibria are

$$f_i^{(\mathrm{eq})}(\rho, \boldsymbol{u}) = \frac{\rho}{Q}\left\{R + \frac{\boldsymbol{c}_i \cdot \boldsymbol{u}}{c_s^2} + \frac{(\boldsymbol{c}_i \cdot \boldsymbol{u})^2}{4c_s^4 R}\right\}, \tag{21}$$

where $R = \frac{1}{2}\left(1 + \sqrt{1 - M^2}\right)$ and $M := u/c_s$. Note that R, thereby the model, is well defined for $M \leqslant 1$.

In ref. 6, the LBGK model with the above equilibria is shown to admit an H theorem provided the model is under-relaxed. However, the domain of validity for the H theorem, among other things, has not been addressed. It is simply assumed in ref. 6 and subsequent papers along the same line (cf. [9] and references therein) that the positivity of the equilibria, i.e., $M \leqslant 1$, is sufficient to ensure an H theorem. Here we would like to point out that, in fact, the valid domain of the H theorem is smaller than the positive domain of the equilibria.

Since $\sqrt{f_i^{(\mathrm{eq})}} = a + \boldsymbol{b} \cdot \boldsymbol{c}_i$, we have

$$a + \boldsymbol{b} \cdot \boldsymbol{c}_i \geqslant 0 \quad \forall\ i\,,$$

which is equivalent to

$$|\boldsymbol{c}_i \cdot \boldsymbol{u}| \leqslant 2Rc_s^2 \quad \forall\ i,$$

by using the expressions of a and $\boldsymbol{b}$ given in Eq. (20). Moreover, the last inequality is equivalent to

$$M \leqslant \min_{i:\,|\boldsymbol{c}_i| \geqslant c_s} \frac{2c_s|\boldsymbol{c}_i|}{c_s^2 + |\boldsymbol{c}_i|^2} = M_{\min}. \tag{22}$$

Because there always exists at least one $\boldsymbol{c}_i$ such that $|\boldsymbol{c}_i| > c_s$, the above bound on M is strictly lower than the positivity requirement $M \leqslant 1$. Thus, the validity domain of the H theorem may be smaller than the positivity domain of $\mathbf{f}^{(\mathrm{eq})}$, as indicated in ref. 6.

In fact, we can show that the H theorem does not hold if the model has a pair of discrete velocities $\boldsymbol{c}_i$ and $\boldsymbol{c}_j$ such that $\boldsymbol{c}_i \cdot \boldsymbol{c}_j = 0$ and $|\boldsymbol{c}_i| \geqslant 2c_s$ (e.g., D3Q15 model). This can be demonstrated as follows. With $\boldsymbol{c}_i$ and $\boldsymbol{c}_j$ thus chosen, we take $S_1 = (\rho, \boldsymbol{u}) = (\rho_0, \mathbf{0})$ with $\rho_0 \neq 0$ and

$$S_2 = (\rho,\, \boldsymbol{u}) = \Big((1-\theta)^{-1}\rho_0, \theta\boldsymbol{c}_i\Big), \quad \theta := \frac{4c_s^2}{4c_s^2 + |\boldsymbol{c}_i|^2},$$

to compute

$$\frac{9}{Q}\rho_0 = f_i^{(\mathrm{eq})}(S_2) \neq f_i^{(\mathrm{eq})}(S_1) = f_l^{(\mathrm{eq})}(S_k) = \frac{1}{Q}\rho_0$$

for $l \in \{\bar{\imath}, j, \bar{\jmath}\}$ and $k \in \{1, 2\}$. Therefore, the conditions of Theorem 2.2 are satisfied and the H theorem does not hold. We note that $M = \theta|\boldsymbol{c}_i|/c_s \in (M_{\min}, 1]$ at the flow velocity $\boldsymbol{u} = \theta\boldsymbol{c}_i$.

5. CONCLUSIONS

In this paper, we find a set of sufficient conditions under which a LBE model does not have an H theorem. By verifying the conditions, we rigorously prove that the H theorem is not admitted by a number of athermal and thermal (energy-conserving) lattice Boltzmann models. In addition, we narrow the validity domain of the H theorem in [6] for a model with non-polynomial equilibria by using our analysis. Our analysis does not require the equilibria to be polynomials, thus the present work extends our previous results.[12]

For some models, our analysis involves flow velocities with relatively large amplitude u. The value of u certainly exceeds the bound determined by the linear stability analysis.[11] It would be important to confirm our nonexistence results without using the large velocities. This is left for future research.

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