Comment on "Maximum Entropy Principle for Lattice Kinetic Equations"

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In a recent Letter [1], Karlin *et al.* proposed a class of athermal lattice Bhatnagar-Gross-Krook (LBGK) models which purportedly admit an H theorem when the LBGK equation is under-relaxed and the equilibrium $f_i^{(\mathrm{eq})}$ is positive. Since then a considerable number of papers on "entropic lattice Boltzmann equation" (ELBE) has been published (cf. [2–4]). In this comment we would like to point out that the positivity condition $f_i^{(\mathrm{eq})} > 0$ does not ensure an H theorem. We can prove that there exists no H theorem in some positivity domain of $f_i^{(\mathrm{eq})}$, and that the validity domain of the H theorem is *strictly* smaller than the positivity domain [5, 6].

For a lattice Boltzmann equation (LBE) with N distinctive discrete velocities in d-dimensions (denoted as DdQN), the discrete velocity set $\{\boldsymbol{c}_i | i = 1, 2, \ldots, N\}$ is assumed to have the following symmetry property: $\sum_i c_{i\alpha} c_{i\beta} = N c_s^2 \delta_{\alpha\beta}$, where $c_s > 0$ is a constant and $c_{i\alpha}$ is a Cartesian component of $\boldsymbol{c}_i$. We shall assume that $\{\boldsymbol{c}_i\}$ is symmetric, *i.e.*, $\{\boldsymbol{c}_i\} = -\{\boldsymbol{c}_i\}$. The strictly convex function $h_i(x) = \frac{2}{3} x^{3/2}$ for $x > 0$, together with the (athermal) conservation constraints $\sum_i f_i^{(\mathrm{eq})} = \rho$ and $\sum_i \boldsymbol{c}_i f_i^{(\mathrm{eq})} = \rho \boldsymbol{u}$, is used to obtain $f_i^{(\mathrm{eq})}$ by solving [1]

$$h_i'(f_i^{(\mathrm{eq})}) = \sqrt{f_i^{(\mathrm{eq})}} = a + \boldsymbol{b} \cdot \boldsymbol{c}_i, \tag{1}$$

where a and $\boldsymbol{b}$ are the Lagrange multipliers, and ρ and $\boldsymbol{u}$ are the flow density and velocity, respectively. Equation (1) yields the following solution for $f_i^{(\mathrm{eq})}$:

$$f_i^{(\mathrm{eq})}(\rho, \boldsymbol{u}) = \frac{1}{N} \rho \left\{ R + \frac{\boldsymbol{c}_i \cdot \boldsymbol{u}}{c_s^2} + \frac{(\boldsymbol{c}_i \cdot \boldsymbol{u})^2}{4 c_s^4 R} \right\}, \tag{2}$$

where $R = \left(1 + \sqrt{1 - M^2}\right)/2$ and $M := u/c_s$.

For $M \leq 1$, R, hence the model, is well defined. The following inequality is claimed to hold for the model:

$$\sum_k \sum_{i=1}^{N} h_i(f_i(\boldsymbol{x}_k, t_{n+1})) \leq \sum_k \sum_{i=1}^{N} h_i(f_i(\boldsymbol{x}_k, t_n)) \tag{3}$$

for all $t_n \in \delta_t \mathbb{N}_0 := \delta_t \{0, 1, 2, \ldots\}$, leading to the claim of existence of an H theorem [1].

From Eq. (1), we see clearly that $a + \boldsymbol{b} \cdot \boldsymbol{c}_i \geq 0 \ \forall\ i$, which is equivalent to the following inequality [5, 6]:

$$M \leq \min_{i:\, |\boldsymbol{c}_i| \geq c_s} \frac{2 c_s |\boldsymbol{c}_i|}{c_s^2 + |\boldsymbol{c}_i|^2} = M_{\max}. \tag{4}$$

Because there always exists at least one $\boldsymbol{c}_i$ such that $|\boldsymbol{c}_i| > c_s$, therefore $M_{\max} < 1$. Consequently the above upper bound on M is strictly lower than the positivity criterion $M \leq 1$. Thus, the validity domain of the H theorem seems *strictly* smaller the positivity domain.

To complete our argument, we show that a convex function other than h_i, which leads to an H theorem, does not exist, if there exist $\boldsymbol{c}_i \neq \boldsymbol{c}_j$ such that $\boldsymbol{c}_i \cdot \boldsymbol{c}_j = 0$ and $|\boldsymbol{c}_i| \geq 2 c_s$. This can be done by choosing two macroscopic states $S_1 := (\rho_1, \boldsymbol{u}_1) \neq S_2 := (\rho_2, \boldsymbol{u}_2)$ such that

$$f_i^{(\mathrm{eq})}(S_1) \neq f_i^{(\mathrm{eq})}(S_2), \quad f_k^{(\mathrm{eq})}(S_1) = f_k^{(\mathrm{eq})}(S_2), \tag{5}$$

where $k \in \{\bar{\imath}, j, \bar{\jmath}\}$, and $\boldsymbol{c}_{\bar{\imath}} := -\boldsymbol{c}_i$. The above conditions contradict the strictly convexity of h_i stated by Eq. (1) (cf. Theorem 2.2 in [6]). In particular, for the D3Q15 model with $c_s^2 = 2/3$, by choosing $\boldsymbol{c}_i = (1, 1, 1)$ and $\boldsymbol{c}_j = (0, 0, 0)$, $S_1 = (\rho_0, \boldsymbol{0})$, $\rho_0 \neq 0$, and

$$S_2 = ((1 - \theta)^{-1} \rho_0,\ \theta \boldsymbol{c}_i),\ \theta := 4 c_s^2 / (4 c_s^2 + |\boldsymbol{c}_i|^2) = 8/17,$$

$M = \theta |\boldsymbol{c}_i| / c_s \in (M_{\max}, 1]$, $M_{\max} = 6\sqrt{2}/11$, we can easily show that conditions of (5) are satisfied and thus H theorem does not exist. This proof can be applied to models more general than the LBGK models [5, 6].

There are additional problems in the ELBE which should be noted. First, in order to maintain the H theorem, the relaxation time (the viscosity) in the ELBE is not a constant, therefore the time evolution of such an ELBE is unphysical. Second, $f_i^{(\mathrm{eq})}$ of Eq. (2) has error terms of $O(u^4)$ and beyond which are absent in the polynomial equilibria. And third, the maximum velocity allowed in the ELBE is usually much smaller than that in other models [4]. These conditions and the under-relaxation restriction would make the ELBE inefficient and ineffective for flow simulations.

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