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On the *H*-theorem in lattice kinetic theory (**)

1 - Introduction

Over the past decade the lattice approach to hydrodynamics has received considerable attention as an efficient alternative to discretization of the Navier-Stokes equations for the numerical solution of hydrodynamic problems [**1**]. In particular, in the Lattice Boltzmann method [**2**], one considers populations of fictitious particles moving about in a discrete lattice and colliding on lattice sites according to simplified rules designed in such a way as to recover hydrodynamic behaviour in the large-scale limit.

The state of the system is then described by a discrete distribution function $N_i(\boldsymbol{r}, t)$, where $i = 1, \ldots, b$ labels discrete velocities $\boldsymbol{c}_i$, associated with outgoing links at each site $\boldsymbol{r}$ of a regular and sufficiently isotropic lattice.
Populations are updated at discrete time steps t according to a simple stream-and-collide first-order equation,

$$N_i(\boldsymbol{r} + \boldsymbol{c}_i, t + 1) - N_i(\boldsymbol{r}, t) = \Delta_i. \tag{1}$$

In the following, we restrict our attention to the isothermal Navier-Stokes equation. For this case, the collision integral Δ_i must obey only the local conser-

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vation laws

$$\sum_{i=1}^{b} \{1, c_{i\alpha}\} \Delta_i = 0 \tag{2}$$

for the local hydrodynamic fields, i.e., the density $\varrho = \sum_{i=1}^{b} N_i(\boldsymbol{r}, t)$, and the momentum $\varrho u_\alpha = \sum_{i=1}^{b} c_{i\alpha} N_i(\boldsymbol{r}, t)$.

Here $\alpha = 1, \ldots, d$ labels the Cartesian components of d-dimensional vectors. If the long-time large-scale limit of Eq. (1) recovers the Navier-Stokes equation, then hydrodynamics is implemented in a fairly simple, fully discrete kinetic picture.

In the following, we denote $\boldsymbol{N}$ as the b-dimensional vector of populations in kinetic space.

An important part of any realization of the Lattice Boltzmann method is the problem of the local equilibrium $\boldsymbol{N}^{eq}$.

From the perspective of classical kinetic theory [3], local equilibria are found as local minima of a convex function $H(\boldsymbol{N})$, subject to constraints fixed by the hydrodynamic fields,

$$\sum_{i=1}^{b} \{1, c_{i\alpha}\} N_i^{\mathrm{eq}} = \{\varrho, \varrho u_\alpha\}. \tag{3}$$

The convex function H (called the entropy function in the sequel) plays the role of the Boltzmann H-function in classical kinetic theory.

In addition, in order to recover the Navier-Stokes equation up to second-order accuracy in u, the local equilibrium must fulfill the condition

$$\sum_{i=1}^{b} c_{i\alpha} c_{i\beta} N_i^{\mathrm{eq}} = \varrho u_\alpha u_\beta + \varrho c_s^2 \delta_{\alpha\beta}, \tag{4}$$

where c_s is the constant speed of sound.

One of the main open questions of the Lattice Boltzmann method is: *Do there exist entropy functions such that the corresponding local equilibria satisfy simultaneously the additional condition* (4) *to the order of accuracy of the method*?

Following ref. [4], such entropy functions will be named *perfect*, in that they erase any effect of the underlying lattice discreteness. Besides the theoretical interest on its own, this question is relevant to the practical issue of numerical stability of the Lattice Boltzmann method.

The Boltzmann entropy function is perfect in the context of classical continu-

um Boltzmann equation, which is the only kinetic theory known so far where the above question is answered.

Indeed, if the classical definition of local equilibria is relaxed, it is possible to introduce a local equilibrium *ansatz* $\widetilde{N}^{eq}$ (typically, a second-order polynomial in u_α) which satisfies both conditions (3) and (4), regardless of any difference in their origin.

The choice of the ansatz is usually not unique, and different realizations may differ drastically: some are relatively stable while others are not.

On the other hand, if the local equilibrium is supported by *some* entropy function, then the Lattice Boltzmann method can be equipped with the H-theorem, and the stability problem can be studied in a more controlled way.

The first problem in constructing the local equilibrium in the Lattice Boltzmann method is as follows: The seemingly 'natural' choice for the entropy functional as the Boltzmann entropy is not solvable exactly, that is, the local equilibrium cannot be found as an explicit function of the local hydrodynamic fields (unlike the classical case of continuous velocities and local Maxwell distribution function).

This is not a mere technicality, but a basic problem related to phase-space discreteness. In fact, Galilean invariance (G-invariance), a basic symmetry of classical mechanics, requires kinetic equilibria to depend on the relative speed $\vec{v} - \vec{u}$ (sometimes called «peculiar» speed) rather than on the molecular speed $\vec{v}$ itself.

On the other hand, in the continuum, entropy additivity imposes a Maxwellian dependence $e^{-\left(\frac{v-u}{v_T}\right)^2}$, where $v_T \equiv \sqrt{k_B T/m}$ is the thermal speed setting the natural scale for molecular fluctuations around the fluid speed $\vec{u}$. Since the Maxwellian is a trascendental function, large departures from *global* equilibria ($\vec{u} = 0$) require a large (virtually infinite) number of terms in the series expansion:

$$e^{-\left(\frac{v-u}{v_T}\right)^2} = e^{-\frac{v^2}{v_T^2}} \sum_{n=0}^{\infty} H_n(v/v_T)(u/v_T)^n \tag{5}$$

where H_n are the Hermite polynomials.

These terms correspond to excitations on top of the uniform «ground state» and are described by higher and higher order polynomials in the velocity variable. It is therefore natural that a finite set of discrete speed can only support a finite number of these excitations, thereby breaking Galilean invariance. On the other hand, G-invariance can certainly be restored if local equilibria are no longer rep-

resented by exponential functions. But then, the H-theorem is no longer valid, at least not in the classical sense.

To attempt a way out of this unconfortable situation, it is useful to distinguish several properties of entropy functions which are almost given for granted in the continuum and which becomes instead highly non trivial in a discrete phase space. These are:

- G-invariance
- Solvability
- Realizability

By solvability we imply the possibility to express the Lagrangean parameters as explicit (analytic) function of the conserved hydrodynamic variables, i.e. density ϱ and flow speed u_α for the case in point.

Realizability applies to the domain of hydrodynamic parameter space where the local equilibria derived by a given lattice entropy are real-valued and in the range $[0, 1]$ (fluid density made 1). Realizability is a necessary (but not sufficient) condition for stability.

2 - Solvable lattice entropies

Following [**5**], we shall first consider a special convex entropy function,

$$H = \sum_{i=1}^{b} N_i \sqrt{N_i}, \tag{6}$$

chosen in such a way that the local equilibrium *is* the explicit function of the hydrodynamic fields. Incidentally, we observe that this is a Tsallis entropy T_q with exponent $q = 3/2$ [**6**].

This construction is merely an illustration to get an idea of what local equilibria derived from a solvable lattice entropy may look like, and how the H-theorem modifies under the discrete time dynamics.

We consider lattices which satisfy usual symmetry requirements, $\sum_{i=1}^{b} c_{i\alpha} = 0$, and $\sum_{i=1}^{b} c_{i\alpha} c_{i\beta} = \xi^2 \delta_{\alpha\beta}$. The following local equilibrium minimizes the function (6), subject to the constraints of fixed ϱ and $\boldsymbol{u}$:

$$N_i^{\mathrm{eq}} = (\varrho/b)[R + c_s^{-2} \boldsymbol{u}\cdot\boldsymbol{c}_i + (4 c_s^4 R)^{-1} (\boldsymbol{u}\cdot\boldsymbol{c}_i)^2]\,. \tag{7}$$

Here $c_s^2 = b^{-1} \xi^2$ is the sound speed squared, and R is a function of the local

Mach number squared, $M^2 = u^2/c_s^2$,

$$R = \frac{1}{2}\left[1 + \sqrt{1 - M^2}\right]. \tag{8}$$

The above equilibria are G-compliant ($R = 1$) only in the limit of vanishing flow, $M \to 0$. At any finite flow speed, a quadratic anomaly in the Mach-number is apparent. This is the typical situation of first-generation Lattice Gas and Lattice Boltzman models.

The equilibrium (7) is positive for $M \leq 1$ but it does not exist, at least not as a real-valued function, for $M > 1$. This means that no collisional drag is able to equilibrate the non-equilibrium gradients produced by supersonic motion. It is worth pointing out that, in a discrete lattice, the distinction between «supersonic» and «superluminal» is less sharp than in ordinary fluids because the sound speed is a comparable fraction of the maximal particle speed (lattice light speed).

This is similar to the relation holding for a relativistic ideal fluid [**7**]. This conveys a flavour of relativity, as also suggested by the equation 8: beyond $M > 1$ local equilibria become purely imaginary, somehow like the mass of a material particle at superluminal speeds.

Relativistic analogies have been noticed pretty early by T. Toffoli [**10**], who speculates that «lattice gas might know more physics they are credited with». The idea is intriguing but, as far as we can judge, quantitatively untenable. Apart from becoming purely imaginary at supersonic/luminal speeds, the lattice relativistic factor R has manifestly little to do with the Lorentz contractor $\sqrt{1 - v^2/c^2}$. In fact, the lattice factor R is dictated solely by the functional form of the entropy 6, not by a quest of frame invariance of the lattice light speed.

Let us proceed with the proof of the discrete H-theorem.

Proof of the discrete H-theorem. We denote by $\Omega = \{N_i | N_i \geq 0,\ |\boldsymbol{u}[N]| < c_s\}$ the set of admissible non-negative populations which can be mapped onto the equilibrium (7).

The knowledge of the local equilibrium in the explicit form can be utilized in a straightforward way by plugging it into the Lattice BGK collision integral [**11**]:

$$\Delta_i = -\omega(N_i - N_i^{eq}[\varrho[\boldsymbol{N}], \boldsymbol{u}[\boldsymbol{N}]]),$$

where ω is the relaxation parameter. In the standard version of the Lattice BGK method, the parameter ω is assumed to take values in the so-called linear stability interval, $\omega \in [0, 2]$. This restriction is dictated by the requirement of the non-

negative viscosity, according to the well-known expression [2]

$$\nu \sim c_s^2(1/\omega - 1/2)\,. \tag{9}$$

The value $\omega = 2$ corresponds to the zero viscosity limit, most relevant to applications to turbulent flows.

In continuum kinetic theory [3], the local entropy production,

$$\sigma = \sum_{i=1}^{b} \left(\frac{\partial H}{\partial N_i} \right) \Delta_i[N]\,,$$

is a non-positive function.

This is sufficient to prove the H-theorem in the *continuum* time case in its usual form: the time derivative of the entropy equals the entropy production, hence it is a decreasing function of time.

The situation is different if time is discrete: For simplicity, let us consider the space-independent version of the Lattice BGK equation:

$$N_i(t+1) = (1-\omega)\, N_i(t) + \omega N_i^{eq}. \tag{10}$$

The average velocity $\boldsymbol{u}$ is a constant, and if the initial population is admissible, and if $0 \leqslant \omega \leqslant 1$, then $N_i(t) \in \Omega$ for all $t \geqslant 0$.

The straightforward application of the convexity inequality gives

$$H(t+1) - H(t) \leqslant \omega[H^{eq} - H(t)]\,. \tag{11}$$

From the variational origin of N_i^{eq} it follows that the right-hand side of Eq. (11) is nonnegative, which proves the H-theorem in the space-independent case for $\omega \in [0, 1]$, the entropy decreases at each time step [5], [8].

The *second half* of the linear stability interval is more difficult, and here we shall mention only the asymptotic result for populations close to the equilibrium [5]:

$$H_q(t+1) - H_q(t) = \frac{(2-\omega)}{2}\, \sigma_q(t)\,. \tag{12}$$

where the subscript q indicates quadratic approximation $H_q = \sum_i (N_i - N_i^{eq})^2$.

In fact, the equation 12 *defines* the entropy production for the Lattice Boltzmann fluid.

Eq. (12) also implies that, close to equilibrium, variation of the entropy per time step is positive if $0 \leqslant \omega \leqslant 2$, that is on the entire linear stability interval.

However, this is deceivingly simple, and a justification is required because $N_i(\omega) = (1-\omega)\, N_i + \omega N_i^{eq}$ may become negative for $\omega > 1$.

A qualitative argument is as follows: If $|\boldsymbol{u}| < c_s$, the equilibrium (7) is positive, and therefore it has a nonempty positive neighborhood U.

Thus, N_i^{eq} has a nonempty neighborhood (U_Ω in the admissible domain $U_\Omega = U \cap P$, where P is the hyperplane of populations with fixed $\boldsymbol{u}$).

This neighborhood U_Ω can be taken small enough to make H_q a valid approximation, and each of the two states $N_i^{\pm} = N_i^{eq} \pm \varepsilon \Delta N_i$ belong to U_Ω. (Then the segment L joining N_i^{+} and N_i^{-} also belongs to U_Ω, and it consists of two parts, $L_{\pm}$ (between $N_i^{\pm}$ and N_i^{eq})).

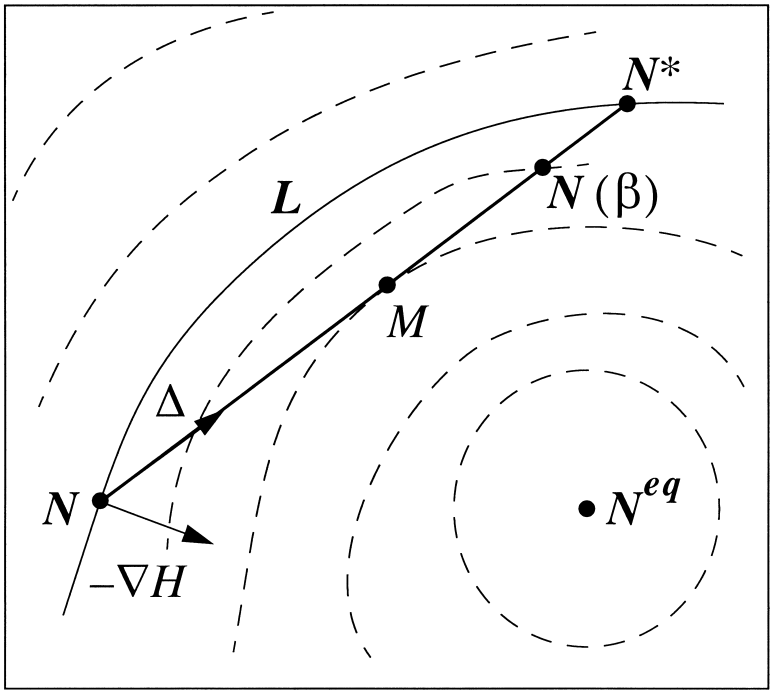

Fig. 1. – Stabilization procedure, bulk case. Curves represent entropy levels, surrounding the local equilibrium $\boldsymbol{N}^{eq}$. The solid curve L is the entropy level with the value $H(\boldsymbol{N}) = H(\boldsymbol{N}^*)$, where $\boldsymbol{N}$ is the initial, and $\boldsymbol{N}^*$ is the conjugate population. The vector $\boldsymbol{\Delta}$ represents the collision integral, the sharp angle between $\boldsymbol{\Delta}$ and the vector $-\boldsymbol{\nabla} H$ reflects the entropy production inequality. The point $\boldsymbol{M}$ is the minimum entropy state on the segment $[\boldsymbol{N}, \boldsymbol{N}^*]$ (see also Ref. [12]). The result of the collision update is represented by the point $\boldsymbol{N}(\beta)$. The choice of β shown corresponds to the «overrelaxation»: $H(\boldsymbol{N}(\beta)) > H(\boldsymbol{M})$ but $H(\boldsymbol{N}(\beta)) < H(\boldsymbol{N})$. The particular case of the BGK collision (not shown) would be represented by a vector $\boldsymbol{\Delta}_{\mathrm{BGK}}$, pointing from $\boldsymbol{N}$ towards $\boldsymbol{N}^{eq}$, in which case $\boldsymbol{M} = \boldsymbol{N}^{eq}$.

Let us take one of the populations $N_i^{\pm}$ (say, N_i^{+}) for the initial condition, and consider H_q at the subsequent time as a function of ω.

This function $H_q(\omega)$ decreases as ω varies from 0 to 1. As ω exceeds 1, the function $H_q(\omega)$ starts *increasing* again but its value remains less than in the initial state N_i^{+}, until ω reaches the value 2. Then $H_q(2) = H_q(0)$, and the update has arrived into N_i^{-}.

If $\omega \in]0, 1]$, populations $N_i(t)$ are confined to the segment L_+, and they tend to N_i^{eq} along a one-sided, local, discrete trajectory.

If $\omega \in [1, 2[$, populations $N_i(t)$ are confined to the segment L. They also tend to N_i^{eq} but in a different way, i.e. by jumping («overrelaxing») back and forth from $L_{\pm}$ to $L_{\mp}$.

This qualitative consideration highlights the entropic origin of the linear stability interval, and indicates the importance of pairs of states with equal entropy. The general case of the H-theorem is qualitatively represented in Figure 1.

This consideration explains why it is impossible to prove the *nonlinear H*-theorem for the standard version of the Lattice BGK equation with a *fixed* stability interval $\omega \in [0, 2]$ on its second half ($\omega \in [1, 2]$): For a generic population taken far away from the local equilibrium, one has to explicitly take into account the deformation of the levels of the entropy function. In the presence of a generic deformation, the two-sided approach to local equilibria may well run away and never converge.

3 - Perfect lattice entropies

Perfect lattice entropies have been discussed already in the literature and consequently we shall only present a brief survey of the main ideas. Perfect entropies can be found which are valid up to the fourth power in the lattice Knudsen number, i.e. the ratio between the lattice spacing and the shortest hydrodynamic scale.

These entropies have the usual *NlogN* form of continuum kinetic theory but, owing to the finite number of speeds, they are *not* solvable, i.e. it is not possible to find an analytic form of the lagrangean parameters as a function of the hydrodynamic fields. Solvability, however, can be regained by expanding the Lagrangean parameters to second order in the Mach number.

A simple example will illustrate the point.

Let us consider a one-dimensional lattice with spacing c. The velocity set at each lattice site consists of three discrete speeds, $c_+ = c$, $c_- = -c$, and $c_0 = 0$.

We consider H-functions of the form

$$H = h_0(N_0) + h_1(N_+) + h_1(N_-)\,. \tag{13}$$

Here h_0 and h_1 are two yet unknown convex functions. The local equilibrium is found as the minimum of H, subject to given hydrodynamic fields ϱ and ϱu.

Denoting by $\mu_{0,1}(x) = [h'_{0,1}(x)]^{-1}$ the inverse of the derivatives of the functions $h_{0,1}(x)$, a formal result of this minimization reads:

$$N_0^{eq} = \mu_0(a)\,, \tag{14}$$

$$N_\pm^{eq} = \mu_1(a \pm \lambda c) \tag{15}$$

The Lagrange multipliers a and λ are related to ϱ and ϱu via the usual mass-momentum-momentum flux constraints:

$$\mu_0(a) + \mu_1(a + \lambda c) + \mu_1(a - \lambda c) = \varrho\,, \tag{16}$$

$$c\mu_1(a + \lambda c) - c\mu_1(a - \lambda c) = \varrho u\,, \tag{17}$$

$$c^2\mu_1(a + \lambda c) + c^2\mu_1(a - \lambda c) = \varrho u^2 + \varrho c_s^2.$$

For the time being, the sound speed c_s is regarded as a free parameter.

Expressing the right hand side of the latter equation in terms of μ_k with the help of the constraints, we find a single non-linear functional equation for the unknowns μ_i $i = 0, 1$.

$$\begin{aligned} T[\mu_0, \mu_1, c_s^2] &= c^2[\mu_1(a + \lambda c) + \mu_1(a - \lambda c)] \\ &- \frac{c^2[\mu_1(a + \lambda c) - \mu_1(a - \lambda c)]^2}{\mu_0(a) + \mu_1(a + \lambda c) + \mu_1(a - \lambda c)} \\ &- c_s^2[\mu_0(a) + \mu_1(a + \lambda c) + \mu_1(a - \lambda c)] = 0\,. \end{aligned} \tag{18}$$

This equation can be solved *approximately* by using a Taylor expansion to order λ^2: $\mu_1(a \pm \lambda c) = \mu_1(a) \pm \mu'_1(a)\lambda c + (1/2)\mu''_1(a)(\lambda c)^2 + \ldots$, where primes denote derivatives in the point a. Upon substituting this expansion into Eq. (19), and requiring that terms of the order λ^0 and λ^2 are equal to zero (terms of the or-

der λ cancel out identically), after some algebra one obtains the following two equations:

$$\mu_0 = 2[(c/c_s)^2 - 1]\,\mu_1, \qquad \mu_1'^2 = (1/2)[(c/c_s)^2 - 1]\,\mu_1\mu_1''. \tag{19}$$

The parameter c_s must now be chosen in such a way that the differential equation in the last line of Eq. (20) admits solutions compatible with the convexity requirement for the H-function (13).

In particular, for $c_s^2 = (1/3)\,c^2$, the resulting differential equation, $\mu_1\mu_1'' = (\mu_1')^2$, has the solution $\mu_1(a) = \exp(a)$, and $\mu_0(a) = 4\exp(a)$.

This means that functions of the form $\mu_1(a \pm \lambda c) = \exp(a \pm \lambda c)$, and $\mu_0(a) = 4\exp(a)$, satisfy Eq. (19) to order λ^4, for arbitrary a.

This solution is the local equilibrium of the convex Boltzmann-like H-function:

$$H = N_0(\ln N_0 - 1 - \ln 4) + N_+(\ln N_+ - 1) + N_-(\ln N_- - 1). \tag{20}$$

Thus, the entropy function (21) is perfect to the order λ^4. Note the different role of the rest population with respect of moving particles in this expression.

As is well known, the Lagrange multipliers behave for small u as follows: $a = a_0 + u^2 a_2 + \dots$, and $\lambda = u\lambda_1 + \dots$, where $a_{0,2}$ and λ_1 are constants. Thus our local equilibrium satisfies condition (4) *not exactly but within the overall accuracy of the Lattice Boltzmann method*. With the Boltzmann-like entropy function (20), the local equilibrium is not known as the explicit function of the hydrodynamic fields.

Nonetheless, it can be shown that when these functions are expanded up to terms of order u^2, and when the higher-order terms are *neglected*, the result is a polynomial quadratic in u. This polynomial satisfies the condition (4) *exactly*, and provides the quadratic local equilibrium ansatz. This remark is quite general: *the second-order expansion of the local equilibrium corresponding to a perfect entropy function is itself the local equilibrium ansatz which satisfies condition* (4) *exactly*.

Interestingly enough, this procedure leads to known faces, such as the D2Q9 equilibria first introduced by Qian and D'Humieres [**11**].

The present analysis provides a more solid theoretical backdrop to these lattice equilibria and (partially) explains their better stability properties as compared to other G-compliant lattice equilibria.

Before concluding, we wish to underscore that all present considerations refer to isothermal lattice models, in which no attempt to track temperature as an independent variable is made.

For an exhaustive discussion of lattice H-theorems for thermal models using a fully non-linear collision operator, the reader is directed to the original work by H. Chen [**15**].

4 - Conclusions

These considerations complete the construction of the Lattice Boltzmann method for isothermal Navier-Stokes equations as a self-contained kinetic theory with the proper H-theorem.

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Abstract

This paper reviews recent results of the entropy-based approach to the Lattice Boltzmann method for simulation of hydrodynamics. Two issues are discussed: Which entropy functions are relevant to hydrodynamics, and how the classical Boltzmann's H-theorem is modified under discrete time dynamics.

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