

H-Theorem and Generalized Semi-Detailed Balance Condition for Lattice Gas Systems

Hudong Chen¹

Received September 23, 1994; final October 25, 1995

For lattice gas systems obeying Fermi–Dirac statistics, an H-theorem can be proved with a more general condition than the semi-detailed balance condition. This new condition allows more flexible transition rates among states, so that it has broader applicability for various lattice gas models, including those which have multiple phase properties.

KEY WORDS: Lattice gases; cellular automata; H-theorem; semi-detailed balance.

1. INTRODUCTION

It has been shown that the lattice gas method (LGM) is an efficient tool for simulating fluid flows.^(1–4) Besides some of its obvious advantages, its convergence and stability properties can be linked to existence of an H-theorem. An H-theorem has been proved by Hénon for lattice gas systems satisfying the so-called semi-detailed balance condition.⁽²⁾ Given an H-theorem, a lattice gas system is guaranteed to approach a unique equilibrium state from any arbitrary perturbations, and hence derivation of hydrodynamics based on the equilibrium distribution is well defined.

In the past few years, a number of lattice gas models have been developed for simulating various types of fluid flows.^(5–8,10,11) However, particle dynamics in these lattice gas systems generally do not obey the semi-detailed balance condition, so that the previous proof of an H-theorem by Hénon no longer applies. In order to provide a solid theoretical justification for these and perhaps various other lattice gas models,⁽¹¹⁾ it is necessary for us to seek an H-theorem with more general conditions than the semi-detailed balance condition.

¹ Exa Corporation, 125 Cambridge Park Drive, Cambridge, Massachusetts 02140.

In this paper, we show that a local H-theorem exists if a generalized semi-detailed balance condition is satisfied. With the generalized condition, transitions among states via collisions can possess preferred directions, and a chemical potential concept can be included. With some straightforward additional constraints, a global H-theorem can also be proved. However, studies remain to be done in order to show the existence of a global H-theorem under more interesting conditions having transition probabilities dependent upon local dynamical properties.

2. LATTICE GAS DYNAMICS AND SEMI-DETAILED BALANCE CONDITION

The evolution of a lattice gas system can be generally described by the equation

$$n_i(\mathbf{x} + \hat{c}_i, t + 1) = n_i(\mathbf{x}, t) + A_i \quad (1)$$

where $n_i(\mathbf{x}, t)$ ($=0$ or 1) represents the particle occupation number for momentum state i on a lattice site \mathbf{x} at time step t . The constant vector \hat{c}_i ($i=0, \dots, b$) is one of b possible speeds of a particle for a given lattice. Interactions among particles are represented by the collision term A_i and its explicit form depends on detailed particle interactions. Averaging the above equation, we have a lattice Boltzmann equation:

$$N_i(\mathbf{x} + \hat{c}_i, t + 1) = N_i(\mathbf{x}, t) + \Omega_i \quad (2)$$

where $N_i(\mathbf{x}, t) \equiv \langle n_i(\mathbf{x}, t) \rangle$ is the single-particle distribution function for momentum state i at site \mathbf{x} and time step t ($0 \leq N_i \leq 1$). The averaged collision term Ω_i ($\equiv \langle A_i \rangle$) has the general form

$$\Omega_i = \sum_{s, s'} (s'_i - s_i) A(s \rightarrow s') P(s) \quad (3)$$

where $s = \{s_i = 0, 1; i = 0, \dots, b\}$ and $s' = \{s'_i = 0, 1; i = 0, \dots, b\}$ are two possible states at a lattice site. $P(s)$ represents the probability of finding state s at a lattice site. $A(s \rightarrow s')$ (≥ 0) is the transition probability from state s to state s' . Once a set of detailed dynamical rules at each lattice site is designed, the explicit form of the transition probability $A(s \rightarrow s')$ ($\forall s, s'$) can be specified. In general, $P(s)$ and $A(s \rightarrow s')$ can depend on dynamical properties of the site of interest itself as well as those of its neighboring sites. By definition, the normalization conditions must be satisfied:

$$\sum_s P(s) = 1 \quad (4)$$

and

$$\sum_{s'} A(s \rightarrow s') = 1, \quad \forall s \tag{5}$$

According to these definitions, we also have

$$N_i = \sum_s s_i P(s)$$

before a collision. But after a collision, the single-particle distribution changes to

$$N'_i = \sum_s s_i P'(s)$$

where $P'(s)$ is the probability of finding the state s after a collision:

$$P'(s') \equiv \sum_s A(s \rightarrow s') P(s) \tag{6}$$

Except for advection, $N_i(\mathbf{x}) \rightarrow N_i(\mathbf{x} + \hat{c}_i)$, it can be realized that all of the dynamics is contained in Eq. (6). Hence, local properties can be understood from this equation alone. Although detailed dynamics depends on specific collisions, it is interesting that fundamental statistical properties can be derived under some general symmetry conditions. Hénon was able to show that an H-theorem can be proved for a lattice gas system as long as the following semi-detailed balance condition (SDBC) is satisfied by the transition probabilities⁽²⁾

$$\sum_s A(s \rightarrow s') = 1, \quad \forall s' \tag{7}$$

That is, for any given destination state s' , the total transition probability from all its source states is the same ($= 1$) as that for any other destination state. With SDBC, the H-theorem indicates that the following function is a nonincreasing function:

$$H = \sum_i [N_i \ln(N_i) + (1 - N_i) \ln(1 - N_i)] \tag{8}$$

at any lattice site. Consequently, a unique equilibrium state is always approached,

$$P^{eq}(s) = \prod_i \bar{N}_i^{s_i} (1 - \bar{N}_i)^{1 - s_i}$$

and the single-particle equilibrium distribution has a general ideal Fermi-gas form,

$$\bar{N}_i = \frac{1}{1 + \exp[\sum_{\alpha} \beta_{\alpha} I_i^{\alpha}]} \quad (9)$$

where I_i^{α} is one of the local invariants under collision,

$$\sum_i I_i^{\alpha}(s'_i - s_i) A(s \rightarrow s') = 0 \quad (10)$$

For example, $I_i^{\alpha} = 1$ or \hat{c}_i corresponds to mass or momentum conservation, respectively. The Lagrange multipliers β_{α} are determined by the local conserved quantities, such as mass and momentum.

Furthermore, a global H-theorem for the system can also be proved, because the global H-function,

$$\mathcal{H} \equiv \sum_{\mathbf{x}} H(\mathbf{x})$$

is invariant under advection.

3. LOCAL H-THEOREM WITH A GENERALIZED CONDITION

Now we show step by step that a local H-theorem can still be proved when SDBC [Eq. (7)] is replaced by a more general condition. These steps are very similar to those of Hénon's.⁽²⁾

Lemma 1. For a transition matrix $A(s \rightarrow s')$ if there exists a positive-definite function $r(s)$ (> 0) such that

$$\sum_s \frac{r(s)}{r(s')} A(s \rightarrow s') = 1, \quad \forall s' \quad (11)$$

then, according to (6), the following inequality holds:

$$f\left(\frac{P'(s')}{r(s')}\right) \leq \sum_s \frac{r(s)}{r(s')} A(s \rightarrow s') f\left(\frac{P(s)}{r(s)}\right) \quad (12)$$

where $f(x)$ is any convex function ($d^2f/dx^2 > 0$).

We refer to Eq. (11) as the generalized semi-detailed balance condition (GSDBC), since SDBC is a special case of it when $r(s) = 1$ ($\forall s$). Moreover,

a condition with unequal transition probabilities between each pair of forward and inverse processes

$$r(s) A(s \rightarrow s') = r(s') A(s' \rightarrow s), \quad \forall s, s'$$

is also a special case of GSDBC but not SDBC.

Proof. For a convex function $f(x)$, there is a general inequality

$$f\left(\frac{\sum_s q(s) P(s)/r(s)}{\sum_s q(s)}\right) \leq \frac{\sum_s q(s) f(P(s)/r(s))}{\sum_s q(s)} \tag{13}$$

where $q(s) (>0)$ is any positive-definite function of s . Let

$$q(s) = \frac{r(s)}{r(s')} A(s \rightarrow s')$$

we have, together with (6) and (11),

$$f\left(\frac{\sum_s q(s) P(s)/r(s)}{\sum_s q(s)}\right) = f\left(\frac{\sum_s [r(s)/r(s')] A(s \rightarrow s') P(s)/r(s)}{\sum_s [r(s)/r(s')] A(s \rightarrow s')}\right) = f\left(\frac{P'(s')}{r(s')}\right)$$

and

$$\begin{aligned} \frac{\sum_s q(s) f(P(s)/r(s))}{\sum_s q(s)} &= \frac{\sum_s [r(s)/r(s')] A(s \rightarrow s') f(P(s)/r(s))}{\sum_s [r(s)/r(s')] A(s \rightarrow s')} \\ &= \sum_s \frac{r(s)}{r(s')} A(s \rightarrow s') f\left(\frac{P(s)}{r(s)}\right) \end{aligned} \tag{14}$$

Hence Lemma 1 is proved.

Lemma 2. The following inequality holds:

$$\sum_{s'} P'(s') \ln \left(\frac{P'(s')}{r(s')}\right) \leq \sum_s P(s) \ln \left(\frac{P(s)}{r(s)}\right) \tag{15}$$

Furthermore, the equality holds when

$$P(s) = \frac{r(s)}{Z} \exp \left[-\sum_{\alpha} \beta_{\alpha} \sum_i I_i^{\alpha} s_i \right] \tag{16}$$

where the local invariant I_i^{α} is described in the previous section. Z is a normalization constant:

$$Z = \sum_s r(s) \exp \left[-\sum_{\alpha} \beta_{\alpha} \sum_i I_i^{\alpha} s_i \right]$$

Proof. Using the inequality in Lemma 1, and choosing $f(x) = x \ln x$, we have

$$P'(s') \ln \left(\frac{P'(s')}{r(s')} \right) \leq \sum_s A(s \rightarrow s') P(s) \ln \left(\frac{P(s)}{r(s)} \right) \quad (17)$$

Summing over s' on both sides of the above and using the normalization condition (5), we prove 15). Furthermore, using the form given in (16) and Eq. (6), then (15) becomes

$$\begin{aligned} \sum_{s'} P'(s') \ln \left[\sum_s \frac{r(s)}{r(s')} A(s \rightarrow s') \exp \left\{ -\sum_\alpha \beta_\alpha \sum_i I_i^\alpha s_i \right\} \right] \\ \leq -\sum_s P(s) \sum_\alpha \beta_\alpha \sum_i I_i^\alpha s_i \end{aligned} \quad (18)$$

But according to (10), we have

$$\exp \left\{ -\sum_\alpha \beta_\alpha \sum_i I_i^\alpha s_i \right\} = \exp \left\{ -\sum_\alpha \beta_\alpha \sum_i I_i^\alpha s'_i \right\}$$

Hence the left-hand side of (18) can be shown to be

$$\begin{aligned} \sum_{s'} P'(s') \ln \left[\sum_s \frac{r(s)}{r(s')} A(s \rightarrow s') \exp \left\{ -\sum_\alpha \beta_\alpha \sum_i I_i^\alpha s'_i \right\} \right] \\ = \sum_{s'} P'(s') \ln \left(\exp \left\{ -\sum_\alpha \beta_\alpha \sum_i I_i^\alpha s'_i \right\} \right) \\ = -\sum_{s'} P'(s') \sum_\alpha \beta_\alpha \sum_i I_i^\alpha s'_i \\ = -\sum_{s'} \sum_s A(s \rightarrow s') P(s) \sum_\alpha \beta_\alpha \sum_i I_i^\alpha s'_i \\ = -\sum_{s'} \sum_s A(s \rightarrow s') P(s) \sum_\alpha \beta_\alpha \sum_i I_i^\alpha s_i \\ = -\sum_s P(s) \sum_\alpha \beta_\alpha \sum_i I_i^\alpha s_i \end{aligned} \quad (19)$$

where the first equal sign requires the use of GSDBC. Therefore, the equality is proved.

In fact, it can also be shown that the probability distribution given in (16) is also a steady-state solution of Eq. (6):

$$P(s') \equiv \sum_s A(s \rightarrow s') P(s)$$

as well as a solution of $\Omega_i = 0$.

Lemma 3. In particular, if $r(s)$ takes a factorized form

$$r(s) = \prod_i^b F_i^{-s_i}, \quad \forall s \tag{20}$$

then the following inequality is satisfied:

$$\sum_s P(s) \ln \left(\frac{P(s)}{r(s)} \right) \geq \sum_i^b \{ N_i \ln(F_i N_i) + (1 - N_i) \ln(1 - N_i) \} \tag{21}$$

The equality holds if and only if

$$P(s) = \prod_i^b N_i^{s_i} (1 - N_i)^{1-s_i} \tag{22}$$

It is realized below that F_i ($i=1, \dots, b$) can be any positive-definite functions of quantities that are unchanged under collisions at a lattice site. For example, F_i could be a function of locally conserved quantities such as local density and momentum,⁽¹⁰⁾ or it could be a function of properties at neighboring sites, such as some functions of scalar product of \hat{c}_i and vector fields which are defined by neighboring distributions.^(6,5,7)

Proof. Since $N_i = \sum_s s_i P(s)$, the right-hand side of (21) can be written as

$$\begin{aligned} & \sum_i^b \{ N_i \ln(F_i N_i) + (1 - N_i) \ln(1 - N_i) \} \\ &= \sum_s P(s) \ln \left[\prod_i^b (F_i N_i)^{s_i} (1 - N_i)^{1-s_i} \right] \end{aligned} \tag{23}$$

Therefore, we only need to show that

$$\sum_s P(s) \ln \left(\frac{r(s) \prod_i^b (F_i N_i)^{s_i} (1 - N_i)^{1-s_i}}{P(s)} \right) \leq 0 \tag{24}$$

Use the property $\ln x \leq x - 1$, we have

$$\ln \left(\frac{r(s) \prod_i^b (F_i N_i)^{s_i} (1 - N_i)^{1-s_i}}{P(s)} \right) \leq \frac{r(s) \prod_i^b (F_i N_i)^{s_i} (1 - N_i)^{1-s_i}}{P(s)} - 1$$

Hence (24) becomes

$$\begin{aligned} \sum_s P(s) \ln \left(\frac{r(s) \prod_i^b (F_i N_i)^{s_i} (1 - N_i)^{1-s_i}}{P(s)} \right) \\ \leq \sum_s r(s) \prod_i^b (F_i N_i)^{s_i} (1 - N_i)^{1-s_i} - 1 \end{aligned} \tag{25}$$

But with the factorized form for $r(s)$ given above, the right-hand side of (25) is equal to zero. Thus, Lemma 3 is proved.

Local H-Theorem. If $r(s) = \prod_i^b F_i^{-s_i}$, the following inequality holds:

$$\begin{aligned} \sum_i^b \{ N_i' \ln(F_i N_i') + (1 - N_i') \ln(1 - N_i') \} \\ \leq \sum_i^b \{ N_i \ln(F_i N_i) + (1 - N_i) \ln(1 - N_i) \} \end{aligned} \tag{26}$$

That is,

$$H = \sum_i^b \{ N_i \ln(F_i N_i) + (1 - N_i) \ln(1 - N_i) \} \tag{27}$$

is a nonincreasing function of $\{N_i, i = 1, \dots, b\}$ under local collisions at each lattice site. The single-particle distribution function N_i corresponding to the minimum H has the following Fermi-Dirac form:

$$N_i^{\text{eq}} = \frac{1}{1 + F_i \exp[\sum_\alpha \beta_\alpha I_i^\alpha]} \tag{28}$$

where I_i^α is one of the local invariants under collision (such as 1, \hat{c}_i), and the Lagrange multipliers β_α are determined by the local conserved quantities, such as mass and momentum.

Proof. Using results in Lemma 2 and 3, we can easily proved (27).⁽²⁾ Moreover, let us write

$$\Delta N_i \equiv N_i - N_i^{\text{eq}}$$

Then it can be shown that

$$\begin{aligned}
 \Delta H &\equiv \sum_i^b \{N_i \ln(F_i N_i) + (1 - N_i) \ln(1 - N_i)\} \\
 &\quad - \sum_i^b \{N_i^{\text{eq}} \ln(F_i N_i^{\text{eq}}) + (1 - N_i^{\text{eq}}) \ln(1 - N_i^{\text{eq}})\} \\
 &= \sum_i^b \left\{ N_i^{\text{eq}} \left(1 + \frac{\Delta N_i}{N_i^{\text{eq}}} \right) \ln \left(1 + \frac{\Delta N_i}{N_i^{\text{eq}}} \right) + (1 - N_i^{\text{eq}}) \right. \\
 &\quad \left. \times \left(1 - \frac{\Delta N_i}{1 - N_i^{\text{eq}}} \right) \ln \left(1 - \frac{\Delta N_i}{1 - N_i^{\text{eq}}} \right) + \Delta N_i \ln \left(\frac{F_i N_i^{\text{eq}}}{1 - N_i^{\text{eq}}} \right) \right\} \quad (29)
 \end{aligned}$$

But the last term vanishes because of conservation properties,

$$\sum_i^b I_i^\alpha \Delta N_i = 0$$

and

$$\ln \left(\frac{F_i N_i^{\text{eq}}}{1 - N_i^{\text{eq}}} \right) = - \sum_\alpha \beta_\alpha I_i^\alpha$$

Furthermore, using an inequality like (13), we have

$$\begin{aligned}
 \Delta H &\geq \sum_i^b N_i^{\text{eq}} \left(1 + \frac{\Delta N_i}{N_i^{\text{eq}}} \right) \ln \left(\frac{\sum_i^b N_i^{\text{eq}} (1 + (\Delta N_i / N_i^{\text{eq}}))}{\sum_i^b N_i^{\text{eq}}} \right) + \sum_i^b (1 - N_i^{\text{eq}}) \\
 &\quad \times \left(1 - \frac{\Delta N_i}{1 - N_i^{\text{eq}}} \right) \ln \left(\frac{\sum_i^b (1 - N_i^{\text{eq}}) (1 - (\Delta N_i / (1 - N_i^{\text{eq}})))}{\sum_i^b (1 - N_i^{\text{eq}})} \right) = 0 \quad (30)
 \end{aligned}$$

Therefore, the local H-theorem is proved.

From the above analysis, we see that a local H-theorem can still be proved with a more general semi-detailed balance condition. The probability function $P(s)$ approaches a factorized equilibrium form in terms of the single-particle distribution N_i if the rate $r(s)$ is factorized. But more generally, the equilibrium has the form given in Lemma 2. Indeed, it can be easily shown that the single-particle equilibrium distribution function (28) is a direct result of

$$N_i^{\text{eq}} = \sum_s s_i P^{\text{eq}}(s)$$

where $P^{\text{eq}}(s)$ has the form given by (16) with a factorized $r(s)$ defined by (20).

4. GLOBAL H-THEOREM

Unlike SDBC, a global H-theorem is not always implied by the local H-theorem above. The reason is that for a general collision invariant $F_i(\mathbf{x})$, its value changes under advection. We write the global H-function as

$$\mathcal{H} \equiv \sum_{\mathbf{x} \in \mathcal{L}} \sum_i^b \{ N_i(\mathbf{x}) \ln(F_i N_i(\mathbf{x})) + (1 - N_i(\mathbf{x})) \ln(1 - N_i(\mathbf{x})) \} \quad (31)$$

This, in general, is not invariant under particle advectons,

$$N_i(\mathbf{x}) \rightarrow \tilde{N}_i(\mathbf{x}) \equiv N_i(\mathbf{x} - \hat{c}_i) \quad (32)$$

unless $\{F_i\}$ satisfies

$$\tilde{F}_i(\mathbf{x}) = F_i(\mathbf{x} - \hat{c}_i), \quad i = 1, \dots, b \quad (33)$$

where $\tilde{F}_i(\mathbf{x})$ has the same functional form as $F_i(\mathbf{x})$ but uses $\{\tilde{N}_j(\mathbf{y}); j = 1, \dots, b; \mathbf{y} \in \mathcal{L}\}$ as possible variables in place of $\{N_j(\mathbf{y}); j = 1, \dots, b; \mathbf{y} \in \mathcal{L}\}$. Obviously, (33) is trivially satisfied in SDBC because it has $F_i \equiv 1$. Consequently, if a lattice gas system satisfies GSDBC and (33), a global H-theorem exists. However, although condition (33) is more general than the SDBC, even more interesting cases are for $\{F_i\}$ to be dependent on more complex dynamical properties.

The change of the global H-function due to advection is

$$\begin{aligned} \Delta \mathcal{H} \equiv & \sum_{\mathbf{x} \in \mathcal{L}} \sum_i^b \{ \tilde{N}_i(\mathbf{x}) \ln(\tilde{F}_i \tilde{N}_i(\mathbf{x})) + (1 - \tilde{N}_i(\mathbf{x})) \ln(1 - \tilde{N}_i(\mathbf{x})) \} \\ & - \sum_{\mathbf{x} \in \mathcal{L}} \sum_i^b \{ N_i(\mathbf{x}) \ln(F_i N_i(\mathbf{x})) + (1 - N_i(\mathbf{x})) \ln(1 - N_i(\mathbf{x})) \} \end{aligned} \quad (34)$$

Using (32), and renaming the dummy index \mathbf{x} , we can immediately see that

$$\begin{aligned} \Delta \mathcal{H} &= \sum_{\mathbf{x} \in \mathcal{L}} \sum_i^b \{ N_i(\mathbf{x} - \hat{c}_i) \ln(\tilde{F}_i(\mathbf{x})) - \{ N_i(\mathbf{x}) \ln(F_i(\mathbf{x})) \} \\ &= \ln \left(\prod_{\mathbf{x} \in \mathcal{L}} \prod_i^b \left[\frac{\tilde{F}_i(\mathbf{x} + \hat{c}_i)}{F_i(\mathbf{x})} \right]^{N_i(\mathbf{x})} \right) \end{aligned} \quad (35)$$

Thus, $\Delta \mathcal{H} \leq 0$ requires

$$\prod_{\mathbf{x} \in \mathcal{L}} \prod_i^b \tilde{F}_i(\mathbf{x})^{N_i(\mathbf{x} - \hat{c}_i)} \leq \prod_{\mathbf{x} \in \mathcal{L}} \prod_i^b F_i(\mathbf{x})^{N_i(\mathbf{x})} \quad (36)$$

Or,

$$\sum_{\mathbf{x} \in \mathcal{L}} \sum_i^b \tilde{\psi}_i(\mathbf{x}) N_i(\mathbf{x} - \hat{c}_i) \leq \sum_{\mathbf{x} \in \mathcal{L}} \sum_i^b \psi_i(\mathbf{x}) N_i(\mathbf{x}) \tag{37}$$

where ψ_i is defined as

$$F_i(\mathbf{x}) \equiv \exp[\psi_i(\mathbf{x})] \tag{38}$$

Equation (37) indicates that ψ_i plays the role of some kind of chemical potential. Therefore, a global H-theorem exists if advections always decrease the overall chemical potential energy, $U = \sum_{\mathbf{x} \in \mathcal{L}} \sum_i^b \psi_i(\mathbf{x}) N_i(\mathbf{x})$, of the system. In other words, if the choice of F_i is made such that (37) is satisfied, then an equilibrium should correspond to a minimum value of U , and a global H-theorem exists. Unlike the cases obeying SDBC, the above equilibrium state is more interesting since it may not necessarily have a spatially homogeneous distribution, which is more applicable to modeling flows with multiple phases. Nevertheless, it seems obvious that condition (37) cannot be satisfied with arbitrarily given N_i . Hence, nontrivial couplings of local equilibrium distributions and advection combined with proper choice of F_i is needed in order to guarantee a global H-theorem. This is subject to further study.

To conclude this section, it is perhaps illuminating to give a simple but specific example of a lattice gas model with seven momentum states on a hexagonal lattice.^(1,3) We define momentum states $i = 1-6$ to be the moving particle states of equal speed along the six possible directions, while momentum state 0 is a rest particle state of zero velocity. If we let $F_i = e^{-a_m}$ for $i = 1, \dots, 6$ and $F_0 = e^{-a_0}$, then, according to Eq. (20), we have the transition probability $A(s \rightarrow s')$ and its inverse related by

$$A(s \rightarrow s') / A(s' \rightarrow s) = e^{a_m s'_m + a_0 s'_0} / e^{a_m s_m + a_0 s_0} \tag{39}$$

where s_0 and s'_0 are, respectively, the rest particle occupation numbers in local lattice states s and s' . Similarly, s_m and s'_m are, respectively, the total moving particle numbers in local lattice states s and s' , namely

$$s_m \equiv \sum_{i=1}^6 s_i$$

$$s'_m \equiv \sum_{i=1}^6 s'_i$$

If collisions are particle conserving, then

$$s_m + s_0 = s'_m + s'_0$$

and Eq. (39) becomes

$$\frac{A(s \rightarrow s')}{A(s' \rightarrow s)} = e^{(a_m - a_0)(s_0 - s'_0)} \quad (40)$$

Hence, suppose $a_0 > a_m$; we see that $A(s \rightarrow s') > A(s' \rightarrow s)$ whenever $s'_0 > s_0$. That is, the higher rest particle occupying state is preferred. Obviously, Eq. (39) is a special case of GSDBC [as defined in (11)]. However, because of the unequal forward and inverse transition probabilities, the original semi-detailed-balance condition is violated. According to the proofs given in the previous section, a local H-theorem exists for this system, and, using Eq. (28), the corresponding equilibrium distributions can be easily written down, with explicit dependence on a_m and a_0 . From these forms, we can immediately interpret a_m and a_0 as effective chemical potentials of moving and rest particles, respectively. Furthermore, based on the analysis provided in this section, we see that a global H-theorem exists for this system if a_m and a_0 are not functions of space.

5. DISCUSSION

We have shown an H-theorem with a generalized condition (GSDBC). This condition has a wider applicability to lattice gas systems which do not simply have ideal Fermi-gas equations of state.

Further studies involve generalizing the above analysis to cases in which (a) the transition ratio $r(s)$ is nonfactorizable and (b) a global H-theorem can be proved with $r(s)$ depending on local dynamics. Also, it should be interesting to examine whether the existing lattice gas models obey the generalized condition given in this paper.^(5-8,10,11)

The generalized semi-detailed balance condition has a wider applicability to lattice gas modeling of various fluid flows. In fact, as we know, many existing lattice gas models do not obey the original semi-detailed balance condition and yet give good macroscopic results,^(5,9,10) even though some of their model constructions as well as theoretical derivations of hydrodynamics use mean-field approximations. In fact, the generalized condition (GSDBC) does not violate the semi-detailed balance condition in a strict physical sense, if we imagine each lattice state s to be a representation of some kind of intermediate macrostate containing a number of "true" microstates. In this representation, the quantity $r(s)$ can then be related to the degeneracy of the macrostate s . Therefore, the semi-detailed balance condition at the "true" microlevel is not violated. However, it is important to emphasize that, though the semi-detailed balance is still satisfied in a strict physical sense, the "true" microstates are

never explicitly followed in any lattice gas models. They are merely used as a tool for theoretically understanding various lattice gas models. In this sense, the generalized condition is different from the more restricted original condition, since in lattice gas models we always deal with lattice states. Furthermore, with the generalized condition, additional physics is introduced into lattice gas formulations when $r(s)$ is dynamical.

ACKNOWLEDGMENTS

The author wishes to thank Drs. Kim Molvig and Chris Teixeira for their useful discussions.

REFERENCES

1. U. Frisch, B. Hasslacher, and Y. Pomeau, *Phys. Rev. Lett.* **56**:1505 (1986).
2. U. Frisch, D. d'Humières, B. Hasslacher, P. Lallemand, Y. Pomeau, and J.-P. Rivet, *Complex Systems* **1**:649 (1987).
3. S. Wolfram, *J. Stat. Phys.* **45**:471–526 (1986).
4. K. Molvig, P. Donis, J. Myczkowski, and G. Vichniac, In *Discrete Kinetic Theory, Lattice Gas Dynamics and Foundations of Hydrodynamics*, R. Monaco, ed., (World Scientific, Singapore, 1988).
5. D. H. Rothman and J. M. Keller, *J. Stat. Phys.* **52**:1119 (1988); A. K. Gunstensen, D. H. Rothman, S. Zaleski, and G. Zanetti, *Phys. Rev. A* **43**:4320 (1991).
6. H. Chen, S. Chen, G. Doolen, Y. C. Lee, and H. Rose, *Phys. Rev. A* **40**:2850 (1989).
7. C. Appert and S. Zaleski, *Phys. Rev. Lett* **64**:1 (1990).
8. B. Dubrulle, U. Frisch, M. Hénon, and J.-P. Rivet, *J. Stat. Phys.* **59**:1187 (1990).
9. S. Chen, G. D. Doolen, K. Eggert, D. Grunau, and E. Y. Loh, *Phys. Rev. A* **43**:7053 (1991).
10. C. Teixeira, Pg.D. Thesis, MIT (1992).
11. G. D. Doolen, ed., *Lattice Gas Methods for PDE's: Theory, Applications and Hardware (Physica D 47)* (North-Holland, Amsterdam, 1991).