Journal of Statistical Physics, Vol. 68, Nos. 3/4, 1992

Biased Lattice Gases with Correlated Equilibrium States

H. J. Bussemaker[1] **and M. H. Ernst**[1]

The approach to and structure of the equilibrium state is studied for a 7-bit lattice gas with biased forward and backward transition rates by means of mean field theory and computer simulations. If the rate constants obey the factorizability and the detailed balance conditions, the occupations of different velocity directions are uncorrelated, an H-theorem is valid, and a nonuniversal equilibrium state exists that depends explicitly on the transition rates. In case the above conditions are not satisfied, the H-theorem is no longer valid, and mean field theory also predicts nontrivial velocity correlations in postcollision states. The simulations are mainly concentrated on the time dependence of pre- and postcollision velocity correlations on a single node, and on slowly increasing fluctuations that might indicate metastable behavior.

KEY WORDS: Velocity correlations in equilibrium; lattice gas automata; biased transition rates; detailed balance; H-theorem; nonuniversal equilibrium; metastabilities.

1. INTRODUCTION

How can a system of point particles with strictly local dynamics have equilibrium distributions in which different velocities are correlated? In their search for lattice gas models with large Reynolds numbers Dubrulle *et al.*[1] have introduced *strongly biased collision dynamics*, where certain in-states scatter into out-states, but the reverse transitions are forbidden. For instance, the out-states on a single node may be biased in favor of pairs of particles leaving under certain angles. These velocity correlations may persist through subsequent propagation steps, leading to in-states in which the occupations of velocity channels are correlated. Simulations of Dubrulle *et al.* and Hénon[2] on the pseudo-4-dimensional FCHC model

[1] Institute for Theoretical Physics, University of Utrecht, The Netherlands.

0022-4715/92/0800-0431$06.50/0

have shown the existence of such correlations, but a theoretical explanation does not exist.

To motivate the research reported here, we quote from ref. 1: "An immediate objective is therefore to understand how these correlations are created, and then, if possible, to invent appropriate remedies in order to decrease the size of the correlations." We formulate the problem in the broader context of interest for models of fluids and chemical reactions.

The basic question is therefore: given a time evolution that consists of two processes, (i) collisions or reactions, and (ii) propagation, possibly diffusive, why does a bias between forward and backward transitions induce a steady state with correlations?

Clearly, an asymmetry or bias in the transition probabilities $A_{\sigma s}$ and $A_{s\sigma}$ from state s to state σ and vice versa may lead to a detailed balance situation, $A_{\sigma s}p_0(s) = A_{s\sigma}p_0(\sigma)$, with $p_0(s)$ the appropriate equilibrium distribution. As we shall discuss, it appears to be the incompatibility of several possible transitions (collisions, reactions), occurring simultaneously in the system, that leads to the violation of the detailed balance conditions. If two types of reactions are incompatible, more complicated cyclic processes are required to sustain the equilibrium state.[3] These cyclic reactions (probably ring collisions) involve the collision/reaction step as well as the propagation step. The biased transitions may create strong correlations directly after the transition. The propagation step will move the individual particles/reactants to different positions, thus forming a new pretransition state. One expects that free streaming partially destroys the correlations on the same node.

In order to study these fundamental issues, we have constructed a 7-bit lattice gas automaton on a triangular lattice, which has the maximum possible number of 20 continuously adjustable forward and backward rate constants. It contains of course the FHP I, II, and III models as special cases. The present model is related to the biased triangular lattice gas with 6 moving and 3 rest particles introduced by d'Humières *et al.*,[4] which has one adjustable parameter. Lattice gases with adjustable rate constants have also been used in the literature[5,6] to increase the so-called non-Galilean factor $G(\rho)$ (see ref. 7) to a value close to unity.

If the biased transition rates allow the existence of a *completely factorized* equilibrium state, an H-theorem exists that guarantees the uniqueness and stability of an equilibrium state that does not contain any correlations. This state may be nonuniversal, in the sense that it depends explicitly on the transition rates.

If the transition rates are incompatible, the H-theorem is no longer valid and there exist in general on- and off-node correlations between different velocity channels.

In a separate publication[8] we have developed a mean field theory based on the assumption that there exist only weak correlations between different nodes in the lattice gas. This approach leads to the nonlinear Boltzmann equation, and to an approximate description of the post-collision correlations, created by the biased collision rules. Precollision correlations are vanishing in the mean field approximation.

The main goal of this paper is to investigate the behavior of velocity correlations close to and in the final equilibrium state by means of computer simulations, to compare the results with the predictions of mean field theory, and to asses the limits of its validity.

The paper is organized as follows. Section 2 contains a brief summary of the mean field theory for biased lattice models.[8] The details for the 7-bit triangular lattice gas are worked out in Section 3. Simulation results are presented and analyzed in Section 4. The main emphasis is on velocity correlations in systems with incompatible transition rates and on the appearance of metastable behavior. Section 5 ends with a summary and outlook.

2. MEAN FIELD THEORY

Before presenting a summary of the mean field theory, we give some basic definitions. A lattice gas automaton (LGA) is a collection of N indistinguishable particles which are, at integer times ($t = 0, 1, 2, \ldots$), located at the nodes $\mathbf{r}$ of a regular d-dimensional lattice with $V = L^d$ nodes and with periodic boundary conditions.

At each node there is a (small) set of allowed velocities $\{\mathbf{c}_i\}$ (e.g., nearest neighbor vectors), where $i = 1, 2, \ldots, b-1$. The label $i = 0$ refers to a rest particle with $\mathbf{c}_0 = 0$. The *state* of a node is described by the set of occupation numbers $s(\mathbf{r}) = \{s_i(\mathbf{r});\ i = 0, 1, 2, \ldots, b-1\}$, where $s_i(\mathbf{r})$ takes the values 0 or 1. There are 2^b possible states at a node.

The time evolution of the lattice gas automaton consists of a collision step and a propagation step. The *stochastic* collision rules only involve particles at the same node $\mathbf{r}$ and are given in terms of a $2^b \times 2^b$ matrix $A_{\sigma s}$ of *transition probabilities*[2] from an in-state $s(\mathbf{r})$ to an out-state $\sigma(\mathbf{r})$ with normalization, for all s,

$$\sum_{\sigma} A_{\sigma s} = 1 \tag{2.1}$$

The collision rules conserve the number of particles $\rho(s(\mathbf{r})) = \sum_i s_i(\mathbf{r})$ and momentum $\mathbf{g}(s(\mathbf{r})) = \sum_i \mathbf{c}_i s_i(\mathbf{r})$ per node. In the subsequent free streaming,

[2] Notice that the order of labels in $A_{\sigma s}$ is reversed with respect to ref. 7.

step particles are moved to the nearest neighbor nodes in the direction of their velocities.

Next we introduce the phase space or Γ-space as the set of all 2^{bV} *configurations* $\mathbf{s} = \{s(\mathbf{r}_1), s(\mathbf{r}_2),..., s(\mathbf{r}_V)\}$ and consider an *ensemble* with a probability distribution $\mathscr{P}(\mathbf{s}, t)$. Its time evolution is given by the Liouville equation.[7,8] In the present paper the main emphasis is on the *single-node distribution function*, defined as

$$p(s(\mathbf{r}), t) = \sum_{\boldsymbol{\sigma}} \delta(s(\mathbf{r}), \sigma(\mathbf{r}))\, \mathscr{P}(\boldsymbol{\sigma}, t) \tag{2.2}$$

where $\delta(s, \sigma) = \prod_j \delta(s_j, \sigma_j)$ is a product of Kronecker deltas. By integrating out the redundant variables in the Liouville equation for the collision step, one obtains the *exact* relation

$$p'(\sigma, t) = \sum_{s} A_{\sigma s}\, p(s, t) \tag{2.3}$$

It connects the *precollision* distribution p at a single node to the *post-collision* one, $p' = Ap$.

The free streaming step will be accounted for only within mean field theory and only for a spatially uniform system. As we are interested in the structure of and approach to the final equilibrium state, we restrict further discussions to spatially uniform nonequilibrium systems where the mean field occupation numbers

$$f_j(\mathbf{r}, t) = \sum_{s(\mathbf{r})} s_j(\mathbf{r})\, p(s(\mathbf{r}), t) \tag{2.4}$$

are translationally invariant. The basic assumption in the mean field description is the neglect of off-node correlations, i.e., $\mathscr{P}(\mathbf{s}, t) = \prod_{\mathbf{r}} p(s(\mathbf{r}), t)$. On the basis of this assumption we have argued in ref. 8 that the *precollision distribution* $p(s, t)$ in mean field theory is given by the *completely factorized* form (without any correlations)

$$p(s, t) = \prod_j [f_j(t)]^{s_j} [1 - f_j(t)]^{1 - s_j} \tag{2.5}$$

and that the mean field occupation number $f_j(t)$ satisfies the nonlinear Boltzmann equation (NLBE) for the spatially uniform case,

$$\Delta f_i(t) \equiv f_i(t+1) - f_i(t) = I_i(f(t)) \tag{2.6}$$

The nonlinear collision term is defined as[7]

$$I_i(f) = \sum_{\sigma, s} (\sigma_i - s_i)\, A_{\sigma s} \prod_j f_j^{s_j} (1 - f_j)^{1 - s_j} \tag{2.7}$$

The factorized form,

$$p_0(s) \equiv p(s, \infty) = \prod_j [f_j(\infty)]^{s_j} [1 - f_j(\infty)]^{1-s_j} \tag{2.8}$$

denotes the single-node distribution in the steady state, and $f_j(\infty)$ the corresponding mean occupation number. Here we only consider basic equilibria of systems that are macroscopically at rest, i.e., the total momentum is vanishing. The existence of a unique and stable equilibrium solution $f_j(\infty)$ follows within mean field theory from an H-theorem. However, the NLBE will not obey such a theorem for an arbitrary chosen set of transition rates $A_{\sigma s}$. We have shown in ref. 8 that the NLBE for *biased lattice models satisfies an H-theorem* provided the *factorized* single-node distribution (2.8) is invariant under collisions, i.e., the factorized form (2.8) is a right eigenvector of the asymmetric transition matrix with eigenvalue unity,

$$\sum_s A_{\sigma s} p_0(s) = p_0(\sigma) \tag{2.9}$$

Condition (2.9), imposed on the factorized form (2.8), is referred to as the *factorized equilibrium condition*, and guarantees the existence of a factorized equilibrium state without any velocity correlations. It is a very restrictive condition on the transition rates. For instance, consider the 7-bit FHP model in basic equilibrium, where

$$f_j(\infty) = \begin{cases} f_0 \equiv z_0/(1+z_0) & (j=0) \\ f \equiv z/(1+z) & (j=1, 2, \ldots, 6) \end{cases} \tag{2.10}$$

by lattice symmetries. Then the factorized form (2.8) contains only two free parameters (f_0, f) or (z_0, z), which have to satisfy the $2^7 = 128$ conditions in (2.9). What are the most important consequences of (2.9)?

(i) If the factorized equilibrium condition (2.9) *cannot* be satisfied for given transition rates, there exist *on- and off-node correlations* between the occupations of the different velocity channels in pre- and postcollision steady states.[8]

(ii) If the factorized equilibrium condition (2.9) is *satisfied*, the fully factorized distribution $\mathscr{P}_0(\mathbf{s}) = \prod_{\mathbf{r}} p_0(s(\mathbf{r}))$ with p_0 as defined in (2.8), is an exact solution of the Liouville equation. Pre- and postcollision distributions are identical and *velocity correlations are absent*. However, the equilibrium distribution has in general a *nonuniversal form* that depends explicitly on the transition rates. In the unbiased LGCAs the Γ-space

distribution has a universal form, as it depends only on the total conserved quantities, not on the rate constants.

For the biased 7-bit FHP models one has the nonuniversal distributions,

$$\begin{aligned} p_0(s) &= q^{-1} z_0^{s_0} z^{\rho(s) - s_0} \\ \mathscr{P}_0(\mathbf{s}) &= Q^{-1} z_0^{N_0(\mathbf{s})} z^{N(\mathbf{s}) - N_0(\mathbf{s})} \\ &= Q^{-1} \exp[\psi_0 N_0(\mathbf{s}) + \alpha N(\mathbf{s})] \end{aligned} \tag{2.11}$$

where $\psi_0 = \ln(z_0/z)$, $\alpha = \ln z$, and $N_0(\mathbf{s}) = \sum_r s_0(\mathbf{r})$ is the (nonconserved) total number of rest particles. The normalization factors are $q = (1+z_0)(1+z)^6$ and $Q = q^V$.

(iii) When does a *universal equilibrium form* apply? Consider the special case $f_j(\infty) = f$ for all j ($j = 0, 1, 2, \ldots, b-1$); then the steady-state distribution satisfies (2.11) with $\psi_0 = 0$, i.e.,

$$\begin{aligned} p_0(s) &= q^{-1} z^{\rho(s)} \\ \mathscr{P}_0(\mathbf{s}) &= Q^{-1} \exp[\alpha N(\mathbf{s})] \end{aligned} \tag{2.12}$$

The Γ-space distribution has the *universal form* of the Gibbs' distribution in ensemble theory. To determine when this special case is realized, one inserts $p_0(s)$ of (2.12) into condition (2.9), which reduces on account of the conservation laws to the *universality condition*,

$$\sum_s A_{\sigma s} = 1 \tag{2.13}$$

as has been derived in ref. 8 under more general conditions. This universality condition is in fact a *necessary* condition for the Liouville equation to have universal equilibrium solutions that depend on the configuration $\mathbf{s}$ only through global invariants, such as total number of particles, total momentum, and total energy in thermal models. In ref. 7 the above condition is called the "semi-detailed balance condition."

(iv) The *factorized* equilibrium state $p_0(s)$ in (2.8) may obey the even more restrictive condition of *detailed balance*, which reads in its standard form[3]

$$A_{\sigma s} p_0(s) = A_{s\sigma} p_0(\sigma) \qquad (\forall \sigma, s) \tag{2.14}$$

It implies (2.9) on account of the normalization (2.1). The above condition represents $2^{b-1}(2^b - 1)$ compatibility relations, imposed on the 2^b components of $p_0(s)$ for given rate constants.

As we shall see in the next section, for the biased 7-bit model the factorized equilibrium condition (2.9) and the detailed balance condition

are equivalent. The reason is that our biased model has at most *two* equivalence classes per family (see Section 3). However, in models with more equivalence classes per family, condition (2.14) is more restrictive than (2.9).

As shown in ref. 8, the factorized detailed balance solution does have a universal form if the symmetry condition

$$A_{\sigma s} = A_{s\sigma} \tag{2.15}$$

is satisfied. We want to point out that in ref. 7 the terminology "detailed balance" is used in the very restricted meaning (2.15), which guarantees a detailed balance with respect to the universal equilibrium distribution.

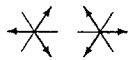
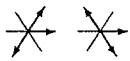
In the next sections these different conditions will be investigated analytically and by computer simulations for the biased FHP model. In fact, we shall find factorized equilibrium solutions that do obey the detailed balance condition (2.14), although the transition rates are not symmetric, and do *not* satisfy the symmetry condition (2.15).

3. BIASED FHP MODELS

3.1. Families and Equivalence Classes

The general considerations of the previous sections will be applied to the 7-bit FHP model defined on the triangular lattice. The set of velocity vectors $\{\mathbf{c}_i\}$ consists of the nearest neighbor lattice vectors ($i = 1, 2, \ldots, 6$) and a rest particle ($i = 0$ with $\mathbf{c}_0 = 0$). There are $2^7 = 128$ possible states $s = \{s_0, s_1, \ldots, s_6\}$ per node, shown in Table I for states with $\rho(s) \leqslant 3$ and $g_x \leqslant g_y \leqslant 0$.[9] The remaining states can be obtained from Table I by interchanging particles and holes and by applying symmetry operations. At a node, the number of particles $\rho(s)$, the x momentum $g_x(s) = \frac{1}{2} p_x(s)$, and y momentum $g_y(s) = \frac{1}{2}\sqrt{3}\, p_y(s)$ are conserved during collisions. Nonvanishing transition rates $A_{\sigma s}$ from an input state s to an output state σ can exist only between states belonging to the same *family*,[10] i.e., within the set of states having the same conserved quantities ρ, g_x, and g_y. Therefore the states are ordered in 20 different families, characterized by the label $\mathcal{F} = (\rho, p_x, p_y)$, with $p_x \geqslant p_y \geqslant 0$. These 20 families are not linked by lattice symmetries. Ten of them are shown in the rows of Table I. The transition matrix $A_{\sigma s}$ therefore has a block diagonal form $A_{\sigma s}\delta_{\mathcal{F}\mathcal{F}'}$, diagonal in the family label $\mathcal{F}$. There are 12 families with only one state, in which $A_{\sigma s}(\mathcal{F}) = \delta_{\sigma s}$ is one-dimensional. The families $\mathcal{F} = (220)$ and $\mathcal{F} = (520)$ are 2-state families, where $A_{\sigma s}(\mathcal{F})$ is a 2×2 matrix. There are four 3-state families $\mathcal{F} = (200)$, (320), (420), (500) with a 3×3 block matrix, and two 5-state families $\mathcal{F} = (300)$ and (400) with a 5×5 block matrix.

Table I. Families $\mathscr{F} = (\rho, p_x, p_y)$ and Equivalence Classes $\mathscr{C}_n$[a]

$\mathscr{F} = (\rho, p_x, p_y)$	$\mathscr{C}_1(\mathscr{F})$	$\mathscr{C}_2(\mathscr{F})$
(0, 0, 0)		
(1, 0, 0)		
(1, 2, 0)		
(2, 0, 0)		
(2, 2, 0)		
(2, 3, 2)		
(3, 0, 0)		
(3, 2, 0)		
(3, 3, 2)		
(3, 4, 0)		

[a] Families with $4 \leqslant \rho(s) \leqslant 7$ follow from a duality transformation.

Furthermore, the states within a family $\mathscr{F}$ are divided into equivalence classes[10] $\mathscr{C}_n(\mathscr{F})$ with $n = 1, 2, \ldots$. All states within one equivalence class are linked by lattice symmetries (rotations, reflections). A family in the 7-bit model contains at most two equivalence classes, $\mathscr{C}_1(\mathscr{F})$ and $\mathscr{C}_2(\mathscr{F})$, respectively without and with a rest particle. As the collision rules must preserve these symmetries, the transition rates between *different* states with the same momentum within the *same* equivalence class are all *equal*.

3.2. Detailed Balance Conditions

We first make a remark on eigenvectors $p_0(\mathscr{F})$ of a block matrix with eigenvalue unity, $A(\mathscr{F})\, p_0(\mathscr{F}) = p_0(\mathscr{F})$, which are of interest in view of the condition (2.9) for the existence of a factorized equilibrium state. For an equilibrium system at rest all components of $p_0(s)$ within the same

equivalence class are equal due to the lattice symmetries, i.e., $p_0(s) = p_n$ for $s \in \mathscr{C}_n(\mathscr{F})$ $(n = 1, 2, \ldots)$.

After this remark, we illustrate the block matrix for the 3-state family $\mathscr{F} = (200)$ (which consists of only one equivalence class), together with the relevant eigenvector. The $\mathscr{F} = (200)$ block of the factorized equilibrium condition (2.9) then reads

$$p_0(200) = A(200)\, p_0(200) = \begin{pmatrix} 1-2q & q & q \\ q & 1-2q & q \\ q & q & 1-2q \end{pmatrix} \begin{pmatrix} p_1 \\ p_1 \\ p_1 \end{pmatrix} \tag{3.1}$$

where $0 \leqslant q \leqslant \frac{1}{2}$. This equation reduces to an identity, and the (200) block of condition (2.9) does not impose any constraints.

From similar arguments we deduce for the 5-state family $\mathscr{F} = (300)$ with two equivalence classes, that the (300) block of condition (2.9) requires

$$p_0(300) = A(300)\, p_0(300)$$
$$= \begin{pmatrix} 1-q-3w & q & v & v & v \\ q & 1-q-3w & v & v & v \\ w & w & 1-2r-2v & r & r \\ w & w & r & 1-2r-2v & r \\ w & w & r & r & 1-2r-2v \end{pmatrix} \begin{pmatrix} p_1 \\ p_1 \\ p_2 \\ p_2 \\ p_2 \end{pmatrix} \tag{3.2}$$

where all entries are positive. In the (300) block there are 4 independent rate constants: the *intraclass* rates $q(\mathscr{F})$ inside class $\mathscr{C}_1(\mathscr{F})$ without rest particles, and $r(\mathscr{F})$ inside class $\mathscr{C}_2(\mathscr{F})$ with rest particles, and the *interclass* rates $v(\mathscr{F})$ and $w(\mathscr{F})$. By convention $w(\mathscr{F})$ denotes the transition probability from a state in class $\mathscr{C}_1(\mathscr{F})$ to one in $\mathscr{C}_2(\mathscr{F})$, and $v(\mathscr{F})$ the probability for the reverse transition. Condition (3.2) then reduces to the *contracted* 2×2 form,

$$\begin{pmatrix} p_1 \\ p_2 \end{pmatrix} = \begin{pmatrix} 1-3w & 3v \\ 2w & 1-2v \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \end{pmatrix} \tag{3.3}$$

or

$$w(300)\, p_1(300) = v(300)\, p_2(300) \tag{3.4}$$

which is the DB condition. This equation (3.4) represents a subset of the detailed balance (DB) conditions (2.14) for all states s and σ belonging to

the class $\mathscr{C}_1(300)$ and $\mathscr{C}_2(300)$, respectively. In all models with a maximum of two equivalence classes per family the factorized equilibrium condition (2.9) and the DB condition are identical.[3] The DB condition in its contracted form depends on the *interclass* transition rates v, w, but does *not* depend on the *intraclass* rates q, r. The same applies to the components $p_0(\mathscr{F})$ of the equilibrium distribution $p_0(s)$. In the absence of any interclass transitions the equilibrium distribution would have the *universal Gibbs form*. The interclass transition rates determine the explicit form of $p_0(\mathscr{F})$ and may therefore lead to nonuniversal equilibrium states.

By repeating the above arguments it follows that the subset of DB conditions for $\mathscr{F}$ blocks consisting of families with a single equivalence class do not impose any constraints on $p_0(\mathscr{F})$. The six families (see Table I) with two equivalence classes, having respectively states with *and* without rest particles, will give a total of six DB constraints,

$$w(\mathscr{F})\, p_1(\mathscr{F}) = v(\mathscr{F})\, p_2(\mathscr{F}) \tag{3.5}$$

Unbiased lattice gases have equal forward and backward rates, $v(\mathscr{F}) = w(\mathscr{F})$ (some of which may vanish) for all $\mathscr{F}$, and the equilibrium state becomes again the universal Gibbs state (2.12): the universality condition (2.13) or "semi-detailed balance condition" of ref. 7 is satisfied. These unbiased models include the FHP I, II, and III models.[9] *Biased* FHP models are the collection of all possible 7-bit models on the triangular lattice with $v(\mathscr{F}) \neq w(\mathscr{F})$ for at least one $\mathscr{F}$ value.

The explicit form of the equilibrium states in the biased FHP models can be determined by inserting the factorized form $p_0(s)$ in (2.11) into condition (2.9). In particular, we have for the components in (3.5), $p_1(\mathscr{F}) = z^{\rho(s)}$ and $p_2(\mathscr{F}) = z_0 z^{\rho(s)-1}$, referring, respectively, to states without and with a rest particle. These factorized forms with two parameters (z_0, z) or (f_0, f) have in fact only *one* free parameter if the average density $\rho = f_0 + 6f$ is prescribed. They yield in combination with the factorizability condition six DB conditions,

$$v(\mathscr{F})\, z_0 = w(\mathscr{F})\, z \tag{3.6}$$

where $\mathscr{F} = (220)$, (300), (320), (420), (400), or (520) labels the six families in Table I that contain two equivalence classes. In *biased* FHP models $v(\mathscr{F}_1) \neq w(\mathscr{F}_1)$ for at least one family, say $\mathscr{F}_1$. So condition (3.6) for $\mathscr{F}_1$ together with the condition

$$\rho = f_0 + 6f = \frac{z_0}{1+z_0} + \frac{6z}{1+z} \tag{3.7}$$

[3] In a 13-bit LGA on a triangular lattice or in the isometric FCHC model there are many more equivalence classes in certain families.

completely fixes the equilibrium distribution (2.11) with parameters z_0 and z. The five additional requirements in (3.6) can be obeyed if the rate constants either satisfy

$$v(\mathscr{F})/w(\mathscr{F}) = v(\mathscr{F}_1)/w(\mathscr{F}_1) \tag{3.8}$$

or

$$v(\mathscr{F}) = w(\mathscr{F}) = 0 \tag{3.9}$$

If the rate constants indeed obey all six DB equations, then (3.6) in combination with (3.7) gives a quadratic equation for z. Hence f_0 and f are known. In this case the equilibrium state is in detailed balance with respect to the *nonuniversal* fully factorized Γ-space distribution (2.11). The nonuniversal parameter

$$\psi_0 = \ln(z_0/z) = \ln[w(\mathscr{F}_1)/v(\mathscr{F}_1)] \tag{3.10}$$

depends explicitly on the transition probabilities. In the fully factorized equilibrium state (2.11) there *do not exist any velocity correlations* before or after collision. If the more restrictive universality condition (2.13) holds, the equilibrium state is in detailed balance with respect to the universal equilibrium distribution (2.11) with $\psi_0 = \ln(z_0/z) = 0$.

In more general FHP models the six DB conditions (3.6) together with the factorized form (2.8) are *incompatible*, so no fully factorized equilibrium exists, and velocity correlations do exist. In particular any *self-dual* biased FHP model cannot obey the DB conditions and shows therefore velocity correlations. The argument goes as follows: let family $\bar{\mathscr{F}}_1$ be the dual of family $\mathscr{F}_1$, appearing in (3.10). For the self-dual model, $v(\bar{\mathscr{F}}_1) = w(\mathscr{F}_1)$ and $v(\mathscr{F}_1) = w(\bar{\mathscr{F}}_1)$. For a DB model $z_0/z = w(\mathscr{F}_1)/v(\mathscr{F}_1) = w(\bar{\mathscr{F}}_1)/v(\bar{\mathscr{F}}_1)$. Consequently, for a biased model, where $v(\mathscr{F}_1) \neq w(\mathscr{F}_1)$, these two relations are incompatible.

3.3. Mean Field Averages and Correlations

Suppose that conditions (2.8) and (2.9) cannot be satisfied simultaneously. Then there exist velocity correlations in the pre- and postcollision states. However, mean field theory still assumes in all cases vanishing precollision correlations, but predicts a nonvanishing postcollision correlation. The question, to be tested by computer simulations, is therefore: is this prediction relevant and to what extent does the relevance depend on the size of the precollision correlations?

The basic idea underlying the mean field theory is that biased collision

rules create postcollision correlations among the velocities of particles on the same node, which are destroyed, perhaps only partially, by the subsequent free streaming step. The resulting on-node precollision correlations may still be sufficiently small so that the mean field theory of Section 2 applies. This would then yield the time dependence of the average occupations $f_j(t)$ and a nontrivial prediction for the postcollision distribution $p'(s, t)$ and for the resulting velocity correlations.

We first consider the collision term $I_i(f)$ in (2.7) of the NLBE in a spatially uniform nonequilibrium state which is macroscopically at rest, i.e., $f_j(t) = f_0(t)$ for $j = 0$ and $f_j(t) = f(t)$ for $j = 1, 2, ..., 6$, with $f_0(t) + 6f(t) = \rho$ a constant. Hence, there is only *one* unknown, say $f_0(t)$. The collision term $I_i(f(t))$ contains the factorized single-node distribution function $p(s, t)$ in (2.5) of the precollision state. For *intraclass* $(s \to \sigma)$ transitions, one has $p(s, t) = p'(\sigma, t)$, and $A_{\sigma s} = A_{s\sigma}$. One shows with the help of these properties that all terms in (2.7) referring to *intraclass* transitions give a vanishing contribution to the collision term. It therefore contains only gain and loss terms coming from *interclass* transitions in which the number of rest particles changes (see Table I).

The equilibrium distribution (2.10) is obtained by solving the stationary NLBE, $I_j(f(\infty)) = 0$, where we can restrict ourselves to $j = 0$. More explicitly,

$$\sum_{\sigma, s} (\sigma_0 - s_0) A_{\sigma s} z_0^{s_0} z^{\rho(s) - s_0} = 0 \tag{3.11}$$

where we have used $p_0(s)$ in (2.11). By setting the sum of all loss terms equal to the sum of all gain terms, one finds

$$\frac{z_0}{z} = \frac{w_{220} + z(w_{300} + 2w_{320}) + z^2(w_{400} + 2w_{420}) + z^3 w_{520}}{v_{220} + z(v_{300} + 2v_{320}) + z^2(v_{400} + 2v_{420}) + z^3 v_{520}} \tag{3.12}$$

where $v_{\mathscr{F}}$ and $w_{\mathscr{F}}$ are short for $v(\mathscr{F})$ and $w(\mathscr{F})$. In biased models the forward and backward transition rates are unequal in at least one family. Equation (3.12) combined with $\rho = f_0 + 6f$ reduces to a polynomial of degree 5 in z. If the rate constants in (3.12) satisfy the detailed balance requirements (3.8)–(3.9), the mean field equation (3.12) also reduces to (3.6). Some comments follow.

Physically acceptable solutions have positive real z_0 and z with $0 < \rho < 7$. If detailed balance conditions are satisfied, it can be shown that the equilibrium distribution is stable and unique (although it may be nonuniversal) and independent of the initial conditions on account of the H-theorem. If detailed balance conditions are violated, an H-theorem is lacking, and it might happen, in principle at least, for special choices of the

transition probabilities that $f_j(t)$ converges to different fixed-point solutions $f_j(\infty)$, depending on the initial conditions.

If the symmetry between particles and holes is maintained by the dynamics, as can be guaranteed by choosing self-dual rate constants, a detailed balance equilibrium cannot exist, as discussed in the previous subsection. The precollision correlations may still be sufficiently small, so that the factorized form of $p_0(s)$ is still a reasonable Ansatz. However, because the DB conditions (3.5) are not satisfied, the postcollision distribution $p_0'(s)$ cannot be factorized and the occupations of the different velocity channels are correlated.

The analytic form of $f_0(t)$ as a function of ρ, the time scales, and nonuniformities in the approach to equilibrium can be understood on the basis of the nonlinear Boltzmann equation, as we shall illustrate for a simple example of a nonuniversal detailed balance model, where only the interclass rates $v(220)=v$ and $w(220)=w$ are nonvanishing. Here the NLBE has the form

$$\Delta f_0 = \{w(1-f_0)\, f - v f_0(1-f)\}\, f(1-f)^4 \tag{3.13}$$

where $\Delta f \equiv f(t+1)-f(t)$ denotes a forward finite difference. The solution shows that $f_0(t)$ converges to a stable equilibrium distribution $f_0(\infty)$ for any initial value $f_0(0)$, where $0<f_0<1$. For $v=0$, $w>0$ one has

$$f_0(\infty) = \begin{cases} \rho & \text{if } 0 \leqslant \rho \leqslant 1 \\ 1 & \text{if } 1 \leqslant \rho \leqslant 7 \end{cases} \tag{3.14}$$

For $v>0$, $w=0$ one has

$$f_0(\infty) = \begin{cases} 0 & \text{if } 0 \leqslant \rho \leqslant 6 \\ \rho - 6 & \text{if } 6 \leqslant \rho \leqslant 7 \end{cases} \tag{3.15}$$

For $v=w>0$ one has the universal equilibrium distributions $f_0(\infty)=f(\infty)=\frac{1}{7}\rho$ of the models FHP I, II, and III.[9] For v, $w>0$ and $v\neq w$ the population $f_0(\infty)$ is the solution of a quadratic equation [see (3.6) and (3.7)] with ρ as a parameter,

$$(v-w)\, f_0^2 + [(w-v)\,\rho + 6v + w]\, f_0 - w\rho = 0 \tag{3.16}$$

Note that this equation only depends on v and w through the ratio w/v. For *all detailed balance models* the dependence of f_0 on ρ is described by the same equation (3.16).

The detailed predictions on time and density dependence of the mean occupation numbers, and the velocity correlations before and after collision, will be compared with computer simulations in the next section.

4. SIMULATION RESULTS

4.1. Description of Simulations

In this section we compare the results of computer simulations with the detailed balance considerations and the mean field theory. The simulations have been performed on a 50×50 triangular lattice. In each realization the *initial state* was prepared by distributing *exactly* $N_i = \rho V/7$ $(i = 0, 1, 2, \ldots, 6)$ particles in the velocity channel with label i, in a random, but spatially uniform manner over the lattice. Hence it could be guaranteed that the initial ensemble contains realizations with exactly the same number of particles $N(\mathbf{s}) = \rho V$ and with momentum $\mathbf{P}(\mathbf{s}(\cdot)) = 0$.

To study the equilibrium values of averages and correlations between channel occupations, most measurements are carried out after 200 time steps. We measure in fact the 2^7 components of the single-node distribution function $p(s, t)$ and $p'(s, t)$, respectively. Their number reduces by lattice symmetries from 128 to 26 independent components (see Table I).

The components $p(s, t)$ and $p'(s, t)$ are obtained by averaging over all 50^2 nodes and over all configurations linked by lattice symmetries. At each density we have averaged over an initial ensemble of 20 different realizations.

The precollision occupations numbers $\langle s_i \rangle = f_i$ are then obtained from (2.4). The covariances $C_{ij}(t)$ measure the precollision correlations[4] at time t between the occupations of different velocity directions on the same node,

$$C_{ij} = \frac{\langle \delta s_i \delta s_j \rangle}{\langle s_i \rangle \langle s_j \rangle} = \frac{\sum_s s_i s_j p(s)}{f_i f_j} - 1 \tag{4.1}$$

Furthermore, f_j' and C_{ij}' denote postcollision values. There are only *four* different correlations, i.e., C_{01}, C_{12}, C_{13}, and C_{14}, due to the lattice symmetries. In mean field theory precollision correlations are assumed to be vanishing.

The number of collisional parameters equals 20 [8 intraclass $q(\mathscr{F})$, $r(\mathscr{F})$, and 12 interclass $v(\mathscr{F})$, $w(\mathscr{F})$], and therefore the parameter space is much too large to be investigated systematically. According to the detailed balance considerations of Section 3 and the mean field theory of Section 2, detailed balance equilibria are *independent* of *intraclass* transition rates. However, we have observed that the correlations may depend on intraclass transition rates in case the transition rates do not obey detailed balance.

[4] The correlation functions $\mathscr{C}_{ij}$ defined by Dubrulle *et al.*[1] are related to (4.1) as $C_{ij} = [(1/f_i - 1)(1/f_j - 1)]^{1/2} \mathscr{C}_{ij}$.

With a total of about 50 different sets we hope to have studied a representative collection of parameter sets that covers most essential features of the model. The transition rates for the sets discussed in this paper are given in Table II.

Figures 1 and 2 show why we have chosen the relatively long relaxation time of 200 time steps for measuring the mean occupations and the correlations between the different velocity channels.

Figure 1 shows the mean occupation of rest particles $f_0(t)$ as a function of ρ over the full density range $(0 \leqslant \rho \leqslant 7)$ at different times $(t = 0, 2, 20, 200)$ for the biased triangular lattice gas with the parameter set #28, both from simulations and from mean field theory. The corresponding rate constants are listed in Table II. The initial configuration was selected from the completely factorized initial distribution $\mathscr{P}(\mathbf{s}, 0)$ in (2.8), specified by $f_j(0) = \frac{1}{7}\rho$ for $j = 0, 1, ..., 6$. The velocity correlations reported in ref. 1 for the FCHC model were measured using the same initial nonequilibrium ensemble. In *unbiased* models $f_0 = \frac{1}{7}\rho$ represents the (universal) equilibrium value. The density of moving particles is always given by $f = \frac{1}{6}(\rho - f_0)$.

Comparison of Table II with (3.8) shows that column #28 contains four incompatible ratios $v(\mathscr{F})/w(\mathscr{F})$, so that set #28 violates detailed balance and is not factorizable. The set is *self-dual*, which accounts for the symmetry $(f_0, \rho) \leftrightarrow (1 - f_0, 7 - \rho)$. The linear portions $f_0 = \frac{1}{7}\rho$ for $\rho < 0.7$

Table II. Transition Rates for the Parameter Sets Used in This Paper, for the FHP III Model, and for the HLS model of Ref. 4

Set	FHP	HLS	#3	#7	#10	#13	#26	#28	#29	#30	#38	#39
$v/w(220)$	1/1	x/1	1/0	0/1	0.01/0.99	0/0	0/1	0/1	0/1	0/1	0/1	0/1
$v/w(300)$	0/0	0/0	0/0	0.4/0	0.4/0	0/0.2	0.4/0	0.4/0	0.4/0	0.4/0	0.1/0	0/0
$v/w(320)$	0.5/0.5	0/1	0/0	0/0	0/0	0.1/0	0/0	0/0	0/0	0/0	0.15/0	0.2/0
$v/w(420)$	0.5/0.5	0/0.5	0/0	0/0	0/0	0/0.1	0/0	0/0	0/0	0/0	0/0.15	0/0.2
$v/w(400)$	0/0	0/0	0/0	0/0.4	0/0.04	0.2/0	0/0.4	0/0.4	0/0.4	0/0.4	0/0.1	0/0
$v/w(520)$	1/1	0/1	0/1	1/0	0.99/0.01	0/0	1/0	1/0	1/0	1/0	1/0	1/0
$q(200)$	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5
$q(300)$	1	1	1	1	1	0.4	1	1	1	1	1	1
$q(320)$	0.5	0	0.5	0	1	1	0	0.5	0.9	1	0	0
$q(400)$	0.5	0.5	0.5	0	0.1	0.5	0.1	0.1	0.1	0.1	0.1	0.1
$r(300)$	0.5	0	0.5	0.1	0.1	0.5	0.1	0.1	0.1	0.1	0.1	0.1
$r(420)$	0.5	0	0.5	0	1	1	0	0.5	0.9	1	0	0
$r(400)$	1	5	1	1	1	0.4	1	1	1	1	1	1
$r(500)$	0.5	0.5	0.5	0	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5

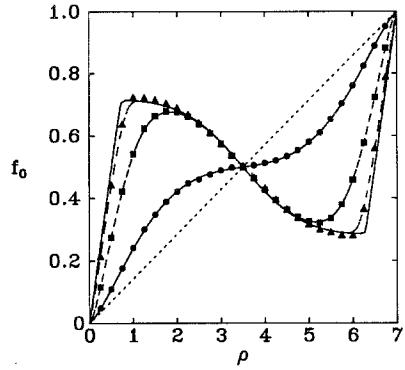


Fig. 1. Mean occupation number of rest particles f_0 versus density ρ for set #28 at different times. Mean field theory at $t=0$ (dotted), $t=2$ (solid), $t=20$ (dashed), and $t=200$ (dashed-dotted) compared with computer simulation results at $t=2$ (●), $t=20$ (■), and $t=200$ (▲). The mean field result at $t=10^4$ (solid line) is barely different from that at $t=200$.

(at $t=200$) and its self-dual image denote equilibria with essentially only rest particles.

On the basis of kinetic theory $f_0(t)$ and $f(t)$ are expected to relax to equilibrium in a few mean free times. The approach to equilibrium is non-uniform as a function of density, as is clearly visible in Fig. 1 for $0.5<\rho<1.5$ and $5.5<\rho<6.5$. Inside the density interval $2.0<\rho<5.0$ the distribution function does indeed equilibrate after about 20 time steps.

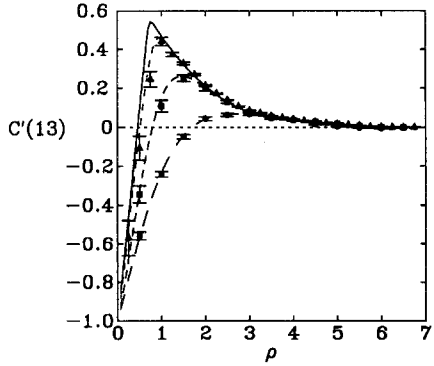


Fig. 2. Postcollision correlations C'_{13} on a single node between velocity directions differing by 120 deg, versus ρ for set #28 at $t=2$, 20, and 200; mean field values and simulation data (see Fig. 1 for meaning of symbols). The mean field result at $t=10^4$ is again barely different from that at $t=200$.

The time dependence of the simulated values of $f_0(t)$ is *at all times in excellent agreement* with the solution of the NLBE. This is surprising in view of the medium size velocity correlations observed in the precollision state ($C_{12} \simeq 0.04$ at $\rho = 3$ and $t = 200$ in Fig. 2). The existence of these correlations indicates a violation of the basic assumption (2.5) of precollision factorization under which the Boltzmann equation has been derived.

4.2. Velocity Correlations

4.2.1. Postcollision States. *Detailed balance models*, including the biased lattice gases obeying detailed balance with respect to a non-universal equilibrium distribution, do not have any velocity correlations before or after the collisions, as discussed in Section 3. This has been tested for the unbiased FHP III model and for more than ten different parameter sets in biased models that obey the DB condition (3.5). It was found that the simulated values of the pre- and postcollision correlation functions C_{ij} and C'_{ij} are smaller than 1% over the whole density range, although the error bars start to increase for $\rho < 1$.

Next we consider Figs. 3 and 4. They show for the specific sets #28 and #13 the full collection of two-channel correlation functions (as a function of density) after 200 time steps. Similar measurements have been carried out for about 50 different parameter sets. As can be seen from Table II, for sets #28 and #13 the ratios $v(\mathscr{F})/w(\mathscr{F})$ do not satisfy the DB condition (3.5). In addition, the basic assumption (2.5) of the *mean field theory* on factorizability is *violated.* The existence of correlations with maxima of $C_{12} \simeq +0.04$ (#28 at $\rho \simeq 3$) and $C_{14} \simeq +0.05$ (#13 at $\rho \simeq 1$) in the precollision state shows that the corresponding single-node distribution function $p_0(s)$ is not factorized. Figures 3 and 4 show the measured values C'_{ij} of the postcollision correlations at $t = 200$ compared with the mean field predictions at $t = 200$ (solid line). Surprisingly, the simulated and theoretical values of C'_{ij}, with two exceptions, agree essentially within error bars, although we are dealing with very large postcollision correlations with extrema of $C'_{13} \simeq +0.5$ (#28) and $C'_{13} \simeq -0.06$ (#13). In the two exceptional cases the qualitative form of C'_{12} (#28) and C'_{14} (#13) are still correctly predicted by the mean field theory. The deviations from mean field theory in C_{12} are simply enhanced in C'_{12} by the biased collision rules. The ratio $R \equiv C'_{12}|_{\text{sim.}}/C'_{12}|_{\text{m.f.}} \simeq 2$ in set #28. In fact after 200 time steps the ratios $R = 1.8$–3, 1.4–1.6, 1.2–1.4, and less than 1.1 were found with the frequencies 2%, 3%, 5%, and 90%, respectively, in excellent agreement with the mean field predictions, even though the factorizability assumption was satisfied only in 43% of the sets.

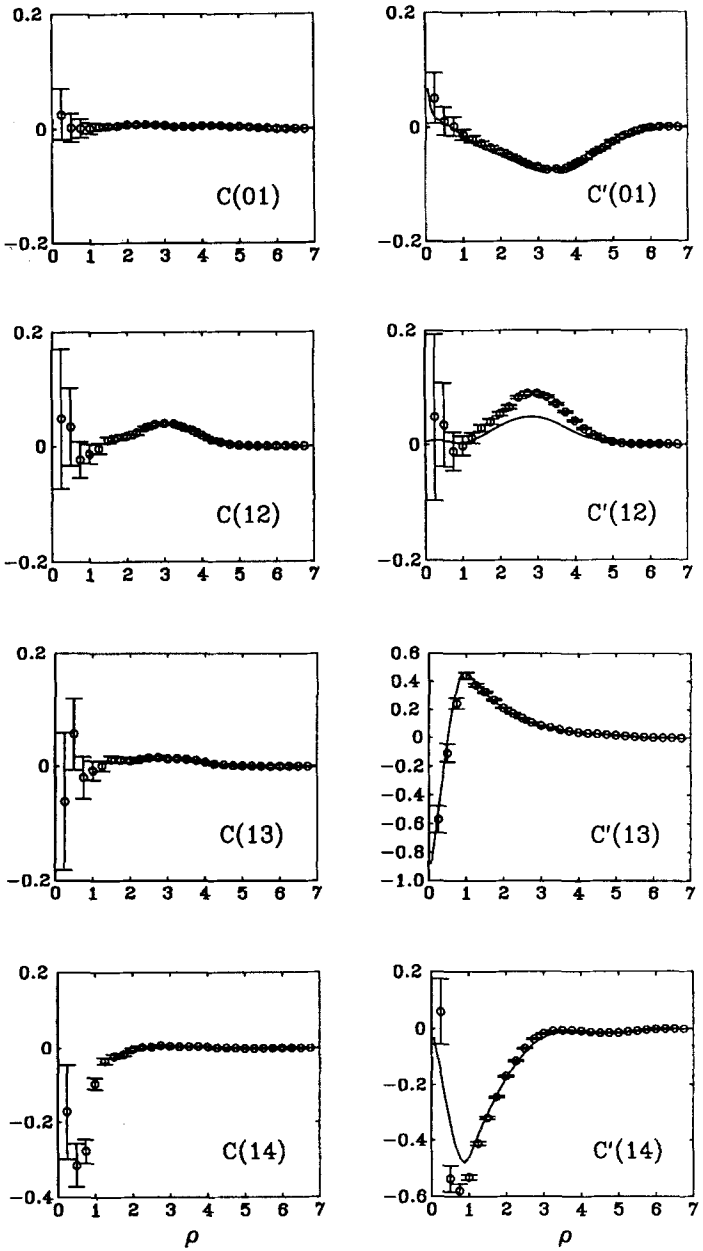


Fig. 3. Simulation data for single-node precollision correlations C_{ij} (left column) and postcollision correlations C'_{ij} (right column) versus ρ at $t = 200$ for set #28. The solid line in the right column gives the theoretical values calculated using mean field theory.

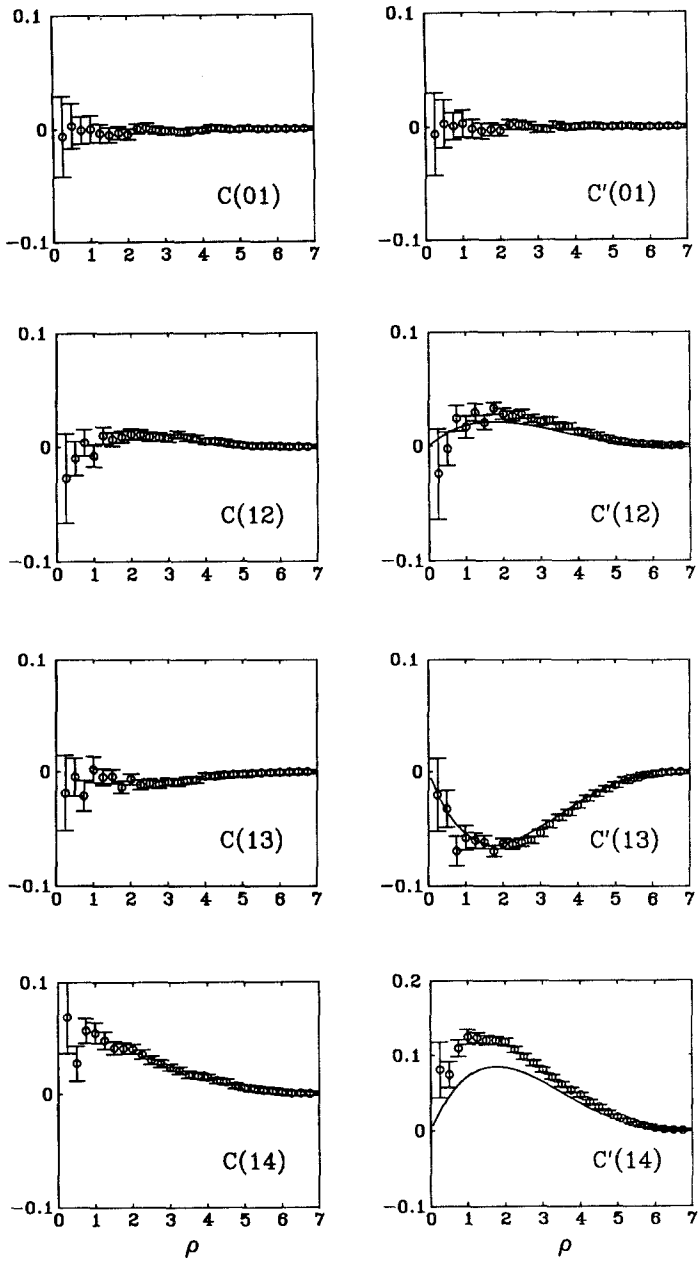


Fig. 4. Simulation data for single-node precollision correlations C_{ij} (left column) and postcollision correlations C'_{ij} (right column) versus ρ at $t = 200$ for set #13. The solid line in the right column gives the theoretical values calculated using mean field theory.

The small or large deviations between simulations and mean field theory in postcollision correlations occur only in C'_{12} and C'_{14}. The latter *always* occur in non-detailed balance models where $v(220) = w(220) = 0$, and *not* in other cases. Regarding the correlations C'_{01} and C'_{13}, there is good agreement for all ρ and for all t. In general, if mean field and simulation results are different, the theory always underestimates the magnitude of the postcollision correlations.

4.2.2. Precollision Correlations. The postcollision distribution generates the precollision distribution through the free streaming step. A comparison of the pre- and postcollision simulation data in Fig. 3 shows that the free streaming step (which moves each particle at node **r** to a *different* nearest neighbor node) is quite efficient in destroying single-node correlations generated by the biased collision rules. The enormous correlations $C'_{12} \simeq +0.5$ (#28) and $C'_{14} \simeq +0.13$ (#13) after 200 time steps at $\rho \simeq 1$ are reduced to a level of 4% in a single streaming step. Almost total destruction of large postcollision correlations has been observed for several parameter sets. For instance, the large correlations $C'_{13} \simeq +0.45$ and $C'_{14} \simeq -0.45$ in set #10, and $C'_{12} \simeq +0.25$ and $C'_{14} \simeq +0.4$ in set #39, all centered around $\rho \simeq 1$, are reduced to the 5% level in the precollision state.

However, not all correlations are absent in the precollision steady state, but it appears difficult to predict the type, size, or even sign of the surviving precollision correlations from the calculated postcollision correlations. Only two types of postcollision correlations appear to be rather persistent under free streaming for very different sets of model parameters: (i) a large positive or negative correlation C'_{12} is only partially destroyed by free streaming and (ii) the simultaneous occurrance of negative correlations $C'_{13} \simeq -1 + A\rho$ ($A \simeq 1$) and $C'_{14} \simeq -B\rho$ ($1 \leqslant B \leqslant 2$) at low densities yields a typical precollision correlation $C_{14} \simeq -1 + A\rho$ ($A \simeq 1$), as in Fig. 3.

We also investigate the suggestion that average occupations $f_0(t)$ differing from the universal equilibrium value $f_0(\infty) = \frac{1}{7}\rho$ of the unbiased models are the cause of velocity correlations in pre- and postcollision states. This suggestion is false, as we shall see. Inspection of Table I shows that it is possible to exactly compensate the loss of rest particles in an $\mathscr{F}_1$ collision by a gain term in an $\mathscr{F}_2$ collision. For instance, take $\mathscr{F}_1 = (300)$ and $\mathscr{F}_2 = (320)$. The condition $f_0(\infty) = f(\infty) = \frac{1}{7}\rho$, or equivalently $z_0 = z$ in (3.12), can be satisfied by setting all rates $v(\mathscr{F}) = w(\mathscr{F}) = 0$ for $\mathscr{F} \neq (300)$, (320), and requiring balancing collision rates,

$$w(300) + 2w(320) = v(300) + 2v(320) \tag{4.2}$$

This condition is satisfied by the choice $2v(320) = w(300) = 0.2$ of the self-dual set #13, which still violates the detailed balance conditions

(3.8)–(3.9). By duality we obtain $v(400) = 2w(420) = 0.2$. The simulations yield average occupation numbers that are at all times in excellent agreement with $f_0(t) = \frac{1}{7}\rho$. However, the simulations show a sizable precollision correlation after 200 time steps with a maximum of $C_{14} \simeq +0.05$ at $\rho \simeq 1$. The simulated values of postcollision correlations, with extrema $C'_{12} \simeq +0.03$, $C'_{13} \simeq -0.06$, and $C'_{14} \simeq +0.12$ for $1 < \rho < 2$, are in good agreement with the mean field predictions, except for the correlation between opposite channels, where mean field theory predicts a maximum $C'_{14} \simeq +0.08$ for $1 < \rho < 2$ at $t = 200$.

In the mean field theory and detailed balance considerations equilibrium distributions can only depend on the *interclass* transition rates. However, simulations show that in non-detailed balance models the equilibrium distribution also depends on the *intraclass* rates. We have performed five sets of simulations at $t = 200$, where $q(320)$ was gradually changed from 0 to 1, with all other rates kept fixed. In doing so, the maximum of $C_{12} \simeq +0.1$ in set #30 gradually decreases via set #28 to $C_{12} \simeq +0.02$ in set #26, all other precollision correlations disappear, the postcollision correlation C'_{12} is reduced to its mean field value, whereas the remaining correlations C'_{01}, C'_{13}, and C'_{14} remain essentially unchanged and are in good agreement with mean field theory. A theory for these precollision correlations is totally lacking.

Precollision correlations in basic equilibria of FCHC models have also been reported by Dubrulle *et al.*[1] and Hénon.[2] We make a brief comparison. In the so-called semi-detailed balance version of the FCHC model the measured correlations are below noise level (less than 0.7%) in the reduced density range $0.32 < \rho/24 < 0.5$.[1] In the versions of the FCHC model that violate semi-detailed balance, positive and negative correlations between different directions ranging from 5% to 22% are observed at a reduced density $\rho/24 \simeq 0.5$, dropping toward lower densities. In the triangular models the correlations C_{12} and C_{13} tend to be largest around the half-filled lattice, too, but C_{01} and C_{14} tend to have their extrema for $1 \leqslant \rho \leqslant 2$. In the 27-bit FCHC-8 model, which has three rest particles, the correlation C_{01} is below noise level. A similar tendency is present here, except in set #3 and a closely related set, where a *large negative* correlation $C_{01} \simeq -0.1$ at $\rho \simeq 1$ has been observed. In their analysis of velocity correlations in the FCHC model *strong negative correlations* of -0.11, -0.08, and -0.22 [see also footnote to Eq. (4.1)] have been associated with the *pseudo-4-dimensional geometry* of the FCHC models contained in a macroscopic slab of size $L \times L \times L \times 2$. Our simulations of set #3 with only two nonvanishing interclass rates $v(220) = 1$ and $w(420) = 1$ show that strong negative correlations can be of dynamic origin also.

In other non-detailed balance FCHC models Hénon[2] has observed

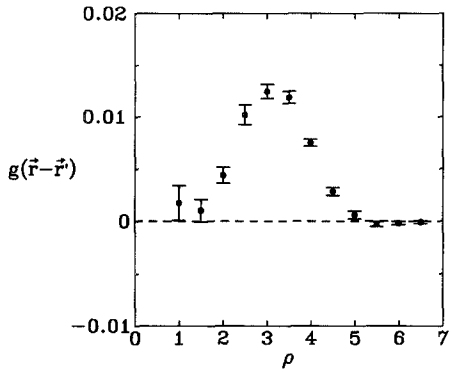


Fig. 5. Pair correlation function $G(\mathbf{r}-\mathbf{r}')$ versus ρ for set #28, where $\mathbf{r}$ and $\mathbf{r}'$ are nearest neighbors.

velocity correlations of 20–30% on the same node, vanishing correlations between nearest neighbor nodes, and 2–3% correlations between next nearest neighbor nodes. We have also observed correlations between the occupations of two velocity channels on different nodes. It appears that nearest and next nearest neighbor correlations are typically of the same size. Even after summing over all velocity channels at both nodes, so that positive and negative correlations largely cancel, a small positive correlation of about 1–2% (sets #28–30) remains. The function so obtained is the pair correlation function $G(\mathbf{r}-\mathbf{r}')$ defined as

$$\rho^2 G(\mathbf{r}-\mathbf{r}') = \langle \delta\rho(\mathbf{r})\, \delta\rho(\mathbf{r}') \rangle = \sum_{ij} \langle \delta s_i(\mathbf{r})\, \delta s_j(\mathbf{r}') \rangle \tag{4.3}$$

This function, for nearest neighbor sites, is shown in Fig. 5 for set #28 as a function of density. We have not yet performed systematic simulations of such properties, nor do we have a theoretical explanation.

4.3. Metastable States

There are some indications of metastable behavior that bares some similarity to that observed by Hénon in a low-speed equilibrium.[11] We have performed simulations of pre- and postcollision correlations up to $t = 1000$ for a few different parameter sets (#3, 7, 28, 30, 38). In the majority of sets the correlations seem to have settled to a stationary value after about 200 time steps. However, in set #30, C_{12} and C'_{12} seem to be nonstationary even after 200 time steps, although all remaining correlations are wellbehaved (see, for instance, Fig. 2). We have observed the following

maxima in C_{12}: 0.04 ($t=20$), 0.09 ($t=200$), 0.17 ($t=500$), and 0.29 ($t=1000$); and in C'_{12}: 0.09 ($t=20$), 0.14 ($t=200$), 0.21 ($t=500$), and 0.32 ($t=1000$). All maxima are located at $\rho \simeq 3$. For set #28, which differs from set #30 only through $q(320)$ and $r(420)$, a similar metastable behavior is observed, although the correlations are much smaller ($C_{12} \simeq 0.13$ and $C'_{12} \simeq 0.17$ at $t=2000$). The similarity with Hénon's metastable states is that in his simulations the correlation range of the region where the spatial symmetry is broken also keeps growing on very long time scales. In the present simulations a possible breaking of spatial symmetries cannot be observed because of the applied spatial averaging.

An explanation for the increasing fluctuations is totally lacking. We are currently investigating possible scenarios. Will the fluctuations finally settle for a stationary value or are we observing a metastable state that finally will make a transition to a different stable equilibrium? What is the dependence on the initial state? Is the chosen initial distribution perhaps in the attraction basin of some metastable state? Will slight modifications of the control parameters/rate constants stimulate transitions to stable equilibria?

5. SUMMARY AND OUTLOOK

With the help of computer simulations and mean field theory we have studied both the approach to and the structure of the stationary state in biased lattice gases. This has been done by considering the mean occupation number $f_j(t)$ and the equal-time pre- and postcollision correlations $C_{ij}(t)$ and $C'_{ij}(t)$ in (4.1) between different velocity channels. The mean field theory is based on the assumption that the occupation numbers on different nodes are uncorrelated, and yields a nontrivial prediction for the on-node velocity correlations $C'_{ij}(t)$ directly after collision. The simulations were carried out on a biased 7-bit triangular lattice gas with many continuously variable transition probabilities. In all cases the simulated occupation numbers are in excellent agreement with the mean field predictions. With respect to the velocity correlations, theory and simulations compare favorably only if the conditions (2.8) and (2.9) are satisfied simultaneously. In case of the 7-bit lattice gas, condition (2.9) is identical to the condition of detailed balance (3.5) or (3.8)–(3.9). In detailed balance models velocity correlations before and after collisions are absent in the steady state; both in the simulations (less than 1%) and in the theory, there exists an H-theorem and a nonuniversal equilibrium distribution (2.11) that depends explicitly on the transition probabilities $A_{\sigma s}$. If, in addition, the universality condition (2.13)—called "semi-detailed balance" in ref. 7—is satisfied, then the steady state distributions depend only on global

invariants and have the same universal form (2.12) as the Gibbs distribution in ensemble theory.

Next, we consider the case that condition (2.8) and condition (2.9) or the detailed balance condition (3.8)–(3.9) are not satisfied. In that case the transition probabilities/collision processes are incompatible. The mean field theory assumes of course that precollision correlations $C_{ij}(t)$ are absent, but predicts nonvanishing postcollision correlations $C'_{ij}(t)$, which can be of appreciable size (see solid lines in Figs. 2–4). As long as precollision C_{ij} remain on the order of a few percent, the postcollision correlations in theory and simulations are in excellent agreement. However, we have also observed many cases of large precollision correlations. We have not yet been able to relate the size sign, or even type of these precollision correlations in any intuitive manner to the chosen transition rates.

In a few cases of incompatible transition rates, we have observed possible metastable behavior in the pre- and postcollision correlations. New features of growing correlations appear only after 1000 or even after 2000 time steps. Simulations for larger times have not yet been carried out.

The problem of incompatible rate constants has relevance not only for fluid models, but also for chemical reactions (law of mass action). Correlations created by incompatible transitions (collisions/reactions) may only be partially destroyed by the intermediate propagation steps. It is not important whether the propagation step is ballistic (as in fluids and gas-phase reactions) or diffusive.

ACKNOWLEDGMENTS

It is a pleasure for M.H.E. to thank U. Frisch, M. Hénon, and J. P. Rivet for stimulating discussions that led to the work reported here, and to thank l'Observatoire de Nice for its hospitality during March 1991, when this research was started. We further acknowledge stimulating discussions with J. W. Dufty, J. L. Lebowitz, R. Brito, A. Noullez, and J. Somers, the hospitality of the Physics Department of the University of Florida in Gainesville, where part of this work was done, and support for M. H. E. from a NATO Travel Grant. H.J.B. is financially supported by the Stichting voor Fundamenteel Onderzoek der Materie (FOM), which is sponsored by de Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO).

REFERENCES

1. B. Dubrulle, U. Frisch, M. Hénon, and J.-P. Rivet, *J. Stat. Phys.* **59**:1187 (1990).
2. M. Hénon, Private communication.
3. N. G. van Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, Amsterdam, 1985).

4. D. d'Humières, P. Lallemand, and G. Searby, *Complex Systems* **1**:633 (1987).
5. G. Searby, V. Zehnlé, and B. Dénet, in *Discrete Kinetic Theory, Lattice Gas Dynamics and Foundations of Hydrodynamics*, R. Monaco, ed. (World Scientific, Singapore, 1988).
6. C. Burges and S. Zaleski, *Complex Systems* **1**:31 (1987).
7. U. Frisch, D. d'Humières, B. Hasslacher, P. Lallemand, Y. Pomeau, and J.-P. Rivet, *Complex Systems* **1**:649 (1987) [reprinted in G. Doolen, ed., *Lattice Gas Methods for Partial Differential Equations* (Addison-Wesley, Singapore, 1990)].
8. H. J. Bussemaker and M. H. Ernst, to be published.
9. D. d'Humières and P. Lallemand, *Complex Systems* **1**:599 (1987).
10. M. Hénon, *Complex Systems* **1**:475 (1987).
11. M. Hénon, *J. Stat. Phys.*, this issue.