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Algebraic Spatial Correlations in Lattice Gas Automata Violating Detailed Balance

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In this paper we discuss the existence of generic long-range correlations in spatially homogeneous and stable equilibrium states of closed lattice gas automata whose stochastic collision rules violate the symmetry conditions of detailed balance and in addition satisfy local conservation laws. Such correlations occur even though the collision rules are strictly local and invariant under all symmetries of the lattice. First a phenomenological (Langevin equation) approach is discussed. Next we present a theoretical analysis on the basis of an approximate microscopic (ring kinetic) theory. This theory is used to calculate the amplitude of $r^{-\alpha}$ tails in the spatial correlations, and the result is compared with computer simulations.

KEY WORDS: Long-range spatial correlations; violation of detailed balance, fluctuation-dissipation theorem, lattice gas automata.

1. INTRODUCTION

As highlighted in a recent review by Dorfman *et al.*[1] a major theme in nonequilibrium statistical mechanics during the past few decades has been the question of under what conditions the correlations in fluids consisting of molecules with short-range interactions only can become long-ranged. The existence of generic long-range spatial correlations in nonequilibrium stationary states of condensed matter is by now well understood. It is intimately connected with the existence of long-time tails in Green–Kubo-type time correlation functions. It seems that necessary conditions for the existence of such algebraic correlations are (i) the existence of local conservation laws and corresponding slow (diffusive or hydrodynamic) modes (ii) lack of detailed balance, and (iii) some degree of anisotropy, due either

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to an underlying lattice or to an external driving field or a gradient imposed by external reservoirs.

Classical fluids in thermal equilibrium are described by the Gibbs distribution. The spatial correlations are short ranged and extend only over the range of the forces, unless parameters are chosen such that the system is near a critical point. However, if a temperature gradient or a shear rate is applied across the system, the system approaches a spatially nonuniform steady state that breaks the spatial isotropy of the continuous fluid. Under these conditions generic long-range density correlations exist in the fluid. Theoretical explanations of this phenomenon have been given in the literature, based on fluctuating hydrodynamic equations, mode coupling approximations, or ring kinetic theory.[1]

In driven diffusive systems the imposed bias fields or reservoirs may give rise to phase separation and pattern formation. On the other hand, the biased dynamics may also allow for a spatially *uniform* nonequilibrium steady state with long-range spatial correlations. Theoretical explanations for the latter case are based on the fluctuating diffusion equation or on microscopic theories.[2–5]

In this paper we consider a lattice gas automaton (LGA) as a many-body system with stochastic interactions of *zero range* that are described by asymmetric transition probabilities $A_{s\sigma} \neq A_{\sigma s}$ different for forward and backward transitions. These transmission probabilities are defined more precisely in Section 4.1 when the microscopic definitions of the LGA are introduced. In the context of LGAs the symmetry $A_{s\sigma} = A_{\sigma s}$ is called *detailed balance*, and the lack of this symmetry is called *violation* of detailed balance. The LGAs under consideration in this paper are *closed* (say, periodic boundary conditions) and fully isolated from the influence of external reservoirs, imposed gradients, or bias fields, and will approach for *long times* a stable and spatially uniform stationary state that we call an *equilibrium* state. We will show in Section 2 that closed systems of LGAs lacking detailed balance may also be viewed as effective or mathematical models for open systems driven by artificial reservoirs.

It is the purpose of this paper to show that the equilibrium state of such LGAs exhibits *long-range correlations*. The existence of such algebraic spatial correlations in closed LGAs has never been observed or discussed in the literature. If an LGA obeys the detailed balance symmetry $A_{s\sigma} = A_{\sigma s}$, then the coefficients of the algebraic tails vanish, and so do all spatial correlations.

Here we demonstrate the existence of these long-range correlations both from the fluctuating Langevin equation as well as from kinetic equations. Furthermore, we obtain microscopic expressions for the coefficients appearing in the algebraic tails of the spatial correlations, which can be

evaluated for large classes of LGAs and for arbitrary state variables (density, etc.), and we show some preliminary evidence that the predictions on long-range correlations from ring kinetic theory are in agreement with computer simulations.

Our conclusion will be that this equilibrium state is different from the Gibbs state of thermal equilibrium, in which the range of spatial correlations is on the order of the range of the interactions. We occasionally refer to these states as non-Gibbsian equilibrium states.

In the context of LGAs as models for fluids, Dubrulle *et al.*[6] were the first to introduce LGAs with local collision rules that violate the constraints of detailed or semi-detailed balance.[7] This was done to construct models with a large Reynolds number. The emphasis nowadays is more on non-detailed balance models as tools to study the kinetics of phase separation and pattern formation.[8] In the present paper we consider, however, non-detailed balance LGAs that approach a stable and spatially uniform non-Gibbsian equilibrium state. Computer simulations[6, 9, 10] have revealed the existence of local velocity correlations and nonlocal spatial correlations in such equilibrium states.

In general, long-range correlations between fluctuations in local densities, $\delta x_i = x_i - \langle x_i \rangle$, are measured through the correlation functions $\mathscr{G}_{ij}(\mathbf{r}, \mathbf{r}', t) = \langle \delta x_i(\mathbf{r}, t)\, \delta x_j(\mathbf{r}', t) \rangle$. An interesting property of LGAs lacking detailed balance is that they exhibit the same type of *long-range* correlations as those discussed in refs. 1–5. These spatial correlations may be studied at different levels of microscopic detail. The coarsest description uses a macroscopic phenomenological equation (diffusion, Navier–Stokes, reaction–diffusion) with a Langevin noise term added to it. Here the transport coefficients and noise strengths are phenomenological input in the theory. The symmetry properties of tensors determine the type of long-range correlations that may occur. The Langevin description is conceptually the simplest, but nevertheless it captures all essential features. In Section 3 this approach is summarized and extended to describe momentum correlations in fluid-type models.

A theoretical understanding of the spatial correlations in the uniform equilibrium state of LGAs without detailed balance was totally lacking until recently, when the present authors developed ring kinetic theory for non-detailed balance (NDB) LGAs in ref. 11 and gave a quantitative explanation of the spatial correlations at short distances, as measured in computer simulations of NDB LGAs. In the theory of dense gases and fluids, ring kinetic theory dates from the late 1960s and early 1970s.[12] In the context of LGAs satisfying detailed balance, ring kinetic theory had already been applied to explain the observed long-time tails in the velocity autocorrelation function of fluid-type LGA[13] and to calculate the correc-

tions to mean field transport coefficients caused by sequences of correlated binary collisions, the so-called ring collisions.[13, 14]

In Section 4 the ring kinetic theory for NDB LGAs of ref. 11 is analyzed to obtain the behavior of the spatial correlations *at large distances*. This analysis clearly shows the existence of generic long-range correlations in the non-Gibbsian equilibrium state of NDB LGAs. In this fully microscopic statistical mechanical description the combined effects of noise strengths and transport coefficients are calculated from the theory. This is a great advantage over the Langevin equation approach. Section 5 deals with an example of a non-detailed balance LGA: a fluid-type model with local mass and momentum conservation whose dynamics obeys all the symmetries of the triangular lattice. We end with a discussion.

2. NDB LGA AS DRIVEN DIFFUSIVE SYSTEM

To understand the relation between a non-detailed balance LGA and a driven diffusive system, it is instructive to view the former models as effective models in which the different collision rules (transition probabilities) can be interpreted as coupled chemical reactions sustained by artificial reservoirs that impose prescribed forward and backward rate constants. To make this more explicit, we consider the following coupled chemical reactions:

$$X + A \underset{k_-}{\overset{k_+}{\rightleftarrows}} B, \qquad 2X + C \underset{k'_-}{\overset{k'_+}{\rightleftarrows}} X + D \tag{2.1}$$

Let x, a, b, etc., denote the concentrations of X, A, B, etc., and let k_+, k_-, k'_+, and k'_- be the rate constants. Then the rate equation for the concentration x is

$$\dot{x} = (k_- b - k_+ xa) + (k'_- dx - k'_+ x^2 c) \tag{2.2}$$

In a closed system similar equations can be written for $\dot{a}$, $\dot{b}$, $\dot{c}$, $\dot{d}$.

Suppose we contrain the system by artificial reservoirs that keep the concentration of a, b, c, d constant (open system), and we determine the stationary solution of (2.2) by setting $\dot{x} = 0$. The stationary solution, denoted by x_0, describes a detailed balance equilibrium state if the contributions $(\cdots)$ of the individual reactions on the right-hand side of (2.2) vanish separately for $x = x_0$, i.e., if x_0 satisfies the more restrictive detailed balance conditions:

$$k_+ x_0 a = k_- b, \qquad k'_+ x_0^2 c = k'_- x_0 d \tag{2.3}$$

These conditions are sufficient for the existence of a stationary state, but by no means necessary. In general the stationary state x_0 of this driven thermodynamic system will not satisfy the detailed balance conditions (2.3)

(except in the very special case where $k_-b/k_+ = k'_-d/k'_+c$). Hence, the stationary state is referred to as a non-detailed balance state.

Alternatively, we may describe the reactions in (2.1) in the open system as

$$X \underset{\beta}{\overset{\alpha_+}{\rightleftarrows}} \varnothing, \qquad 2X \underset{\beta'}{\overset{\alpha'}{\rightleftarrows}} X \tag{2.4}$$

where $\alpha = k_+ a$, $\beta = k_- b$, $\alpha' = k'_+ c$, and $\beta' = k'_- d$, and consider these equations as defining an effective model of a *closed* N-particle system. The equilibrium state of this closed system is a non-detailed balance state.

The kinetic equation (2.2) only describes the time evolution of the global concentration. To describe the local concentration $x(\mathbf{r}, t)$, one may introduce the spatial dependence by adding a diffusion term $D_X \nabla^2 x$ to the right-hand side of (2.2), where D_X is the diffusion coefficient of the substance X.

To make the parallel with the Boltzmann equation description of LGAs, one needs to generalize the one-component case (2.2) to a multi-component case with local concentrations $\{x_i(\mathbf{r}, t);\ i = 1, 2, \ldots, b\}$. Then the chemical reactions (2.4) correspond to collisions between particles in different one-particle states i with velocity $\mathbf{c}_i$ and the reaction–diffusion equation corresponds to the nonlinear lattice Boltzmann equation for LGAs. The stationary solution $x_i(\mathbf{r}, \infty) = x_i^0$ with $i = 1, 2, \ldots, b$ is obtained by setting the total collision term equal to zero and solving for x_i^0. If x_i^0 does not make the individual collision terms in (2.2) vanish, i.e., does not satisfy the analog of (2.3)—which is the relation $A_{s\sigma} = A_{\sigma s}$ (see Section 4.1)—then x_i^0 describes a non-detailed balance state, and we call the model a non-detailed balance LGA.

Of course, the parallel is not complete, as the spatial dependence evolves in the reaction–diffusion equations through diffusive propagation, and in the corresponding lattice Boltzmann equation through ballistic propagation.

To continue the parallel between the reaction–diffusion equation and the lattice Boltzmann equation at the fluctuation level, one may add a Langevin noise term to the lattice Boltzmann equation (as has been done in refs. 15 and 16). The transport coefficients are then determined by the theory, but the noise strength is phenomenological input. This parallel, however, will not be pursued any further.

The above arguments illustrate how the behavior of a closed LGA without the detailed balance contraints, isolated from external fields and reservoirs, can be viewed as an open, driven thermodynamic system. In this sense NDB LGAs can be interpreted as generalizations of driven diffusive systems.

3. THE LANGEVIN EQUATION APPROACH

3.1. Driven Diffusion

In this subsection we recapitulate the basic theory of nonequilibrium Langevin models for driven diffusion, as described in refs. 2–4. In such systems one is dealing with a conserved scalar field (mass density, concentration). Different types of generic long-range correlations may occur in such systems, depending on the degree of spatial anisotropy.

We start with an example in which the symmetry between the coordinate axes is broken; without loss of generality we use a two-dimensional representation with x–y anisotropy. Consider a locally conserved density $h(\mathbf{r}, t) = \langle \hat{h}(\mathbf{r}, t) \rangle$. On average its long-wavelength components satisfy a diffusion equation with an anisotropic diffusion tensor, $D_{\alpha\beta} = D_\alpha \delta_{\alpha\beta}$. To account for long-wavelength fluctuations, one adds to this equation a Langevin noise term, which is essentially the divergence of a fluctuating current. After Fourier transformation the Langevin equation reads

$$\partial_t \hat{h}(\mathbf{q}, t) = -(D_x q_x^2 + D_y q_y^2)\, \hat{h}(\mathbf{q}, t) + \hat{\eta}(\mathbf{q}, t) \tag{3.1}$$

The random noise is assumed to be Gaussian with zero mean, $\langle \hat{\eta}(\mathbf{q}, t) \rangle = 0$, and its variance is given by

$$\langle \hat{\eta}(\mathbf{q}, t)\, \hat{\eta}(-\mathbf{q}, t') \rangle = 2(B_x q_x^2 + B_y q_y^2)\, \delta(t - t') \tag{3.2}$$

Again, we have allowed for spatial anisotropy by having two constants B_x and B_y. Both the diffusion coefficients D_α and the noise strengths B_α, are phenomenological coefficients: they are *not* provided by the theory. The stationary susceptibility can be calculated from (3.1) and (3.2) as

$$\chi(\mathbf{q}) = \lim_{t \to \infty} \langle |\hat{h}(\mathbf{q}, t)|^2 \rangle = \frac{B_x q_x^2 + B_y q_y^2}{D_x q_x^2 + D_y q_y^2} \tag{3.3}$$

as $\mathbf{q} \to 0$. From this expression it can be seen that $\chi(\mathbf{q})$ depends on the direction as $\hat{\mathbf{q}} = \mathbf{q}/|\mathbf{q}|$ of the wave vector, unless the special relation $B_x/D_x = B_y/D_y$ holds.

Once the susceptibility $\chi(\mathbf{q})$ is known, the equal-time density–density correlation function in the stationary state $\mathscr{G}(\mathbf{r})$ can be calculated from

$$\mathscr{G}(\mathbf{r}) = v_0 \int_{1\,\mathrm{BZ}} \frac{d\mathbf{q}}{(2\pi)^d} e^{i\mathbf{q}\cdot\mathbf{r}} \chi(\mathbf{q}) \tag{3.4}$$

where the $\mathbf{q}$-integration extends over the first Brillouin zone and v_0 is the volume of a unit cell in the direct lattice ($v_0 = 1$ on the square lattice and $v_0 = \frac{1}{2}\sqrt{3}$ on the triangular lattice).

Equations (3.1) and (3.2) can be generalized by including higher order gradients. We then have

$$\partial_t \hat{h}(\mathbf{q}, t) = -D(\mathbf{q})\, q^2 \hat{h}(\mathbf{q}, t) + \hat{\eta}(\mathbf{q}, t) \tag{3.5}$$

together with

$$\langle \hat{\eta}(\mathbf{q}, t)\, \hat{\eta}(-\mathbf{q}, t') \rangle = 2B(\mathbf{q})\, q^2 \delta(t - t') \tag{3.6}$$

where $D(\mathbf{q})$ and $B(\mathbf{q})$ are now general functions of $\mathbf{q}$ that can be expanded in powers of q_x^2 and q_y^2. In what follows we will recall how the symmetry properties of the various terms in such an expansion determine the type of long-range correlations that occur[3] and under what conditions such correlations are absent.

If the system satisfies detailed balance, and consequently the equilibrium distribution corresponds to thermodynamic equilibrium, then the equilibrium value of the susceptibility $\chi(\mathbf{q}) \simeq \chi_0$ as $q \to 0$ is known from thermodynamics. Transport coefficients and noise strengths are in this case related by the *fluctuation-dissipation theorem*,

$$B(\mathbf{q}) = \chi_0 D(\mathbf{q}) \tag{3.7}$$

and the correlation function is short ranged, i.e., $\mathcal{G}(\mathbf{r}) = \chi_0 \delta(\mathbf{r})$ unless the system is at a critical point where $\chi(\mathbf{q}) \to \infty$. However, *without* the detailed balance constraint the equilibrium state is not a Gibbs state. In general the susceptibility $\chi(\mathbf{q})$ is then unknown, and there is *no* fluctuation-dissipation theorem imposing a relationship between $B(\mathbf{q})$ and $D(\mathbf{q})$.

Consider expression (3.4): the long-wavelength limit $\chi_0(\hat{\mathbf{q}})$ of the susceptibility is *anisotropic* since generically it depends on the direction along which the limit is taken. Hence, the function $\chi(\mathbf{q})$ is *not continuous* at $\mathbf{q} = \mathbf{0}$. A rescaling of the integration variables in (3.4), viz. $\mathbf{q} = \mathbf{k}/r$, shows that $\mathcal{G}(\mathbf{r}) \simeq E_0(\hat{\mathbf{r}})/r^d$ at large distances. As diffusive modes are correlated over time intervals $t \sim r^2$, the spatial correlations $\sim 1/r^d$ have an intimate connection with the long-time tails $\sim 1/t^{d/2}$ in the velocity and other current–current correlation functions.[1, 17]

The above scenario—$1/r^d$ correlations occurring because the susceptibility $\chi(\mathbf{q})$ is not continuous at $\mathbf{q} = 0$—is realized in purely diffusive LGAs where the collision rules do not satisfy detailed balance and in addition break the rotational lattice symmetry by having different transition probabilities in x and y direction.[2–5]

Even if $\chi(\mathbf{q})$ is continuous at $\mathbf{q} = \mathbf{0}$, weaker singularities at $\mathbf{q} = \mathbf{0}$ may still give rise to algebraic correlations. To make this more specific, we consider a system where the susceptibility has the full symmetry of the

underlying lattice (square, triangular, cubic, etc.). The symmetry properties of the $\mathcal{O}(q^2)$ term in the expansion of $\chi(\mathbf{q})$ involve fourth-rank tensors. On the square lattice, such tensors contain anisotropic parts. Consequently the second $\mathbf{q}$-derivative of $\chi(\mathbf{q})$ is *not continuous*, and again a simple scaling of (3.4) shows that $\mathcal{G}(r) \simeq E_2(\hat{\mathbf{r}})/r^{d+2}$ (see, for instance, ref. 3).

On the triangular lattice fourth-rank tensors are *isotropic* and $1/r^{d+2}$ correlations are absent. We then have to consider the next subleading term in the expansion of $\chi(\mathbf{q})$ which is $O(q^4)$, and involves sixth-rank tensors. Such tensors are not isotropic on any two- or three-dimensional lattice, and it follows that the spatial correlations on a triangular lattice decay as $\mathcal{G}(\mathbf{r}) \simeq E_4(\hat{\mathbf{r}}/r^{d+4}$ with $d=2$. In three dimensions there does not exist any regular lattice on which fourth-rank tensors are isotropic,[18] and spatial correlations in non-detailed balance LGAs with dynamics observing the full lattice symmetries and with only scalar conserved densities are always of the form $\mathcal{G}(\mathbf{r}) \sim 1/r^{d+2}$ with $d=3$.

3.2. Momentum Correlations in Fluid-Type Models

In fluid-type LGAs similar results apply to equal-time correlation functions between the momentum density $\mathbf{g}(\mathbf{r})$ at two different points, i.e., the equilibrium correlation function $\mathcal{G}_{\alpha\beta}(\mathbf{r}) = \langle g_\alpha(\mathbf{r})\, g_\beta(0)\rangle$ behaves as $E(\hat{\mathbf{r}})/r^d$ for large r. The presence of conserved densities of a vectorial character offers a much richer structure of density–density correlation functions than in the case of the driven diffusive systems. In Sections 4 and 5 we obtain the same result on the basis of a fully microcopic theory.

This type of correlation can be understood on the basis of a phenomenological Langevin theory as well, with noise terms added to the hydrodynamic equation (Navier–Stokes equation) describing the time evolution of the flow field on large spatial scales. For our purpose it is sufficient to only consider the symmetry properties of the problem. The quantity $\mathcal{G}_{\alpha\beta}(\mathbf{r})$ is a second-rank tensor field with the full symmetry of the underlying lattice. The same holds for the corresponding susceptibility $\chi_{\alpha\beta}(\mathbf{q})$, which can be decomposed into a longitudinal and a transverse component as

$$\chi_{\alpha\beta}(\mathbf{q}) = \hat{\mathbf{q}}_\alpha \hat{\mathbf{q}}_\beta \chi_{//}(\mathbf{q}) + (\delta_{\alpha\beta} - \hat{\mathbf{q}}_\alpha \hat{\mathbf{q}}_\beta)\, \chi_{\perp\perp}(\mathbf{q}) \tag{3.8}$$

where $\chi_{//}(\mathbf{q})$ and $\chi_{\perp\perp}(\mathbf{q})$ are scalar fields. Let us suppose that the limit $\mathbf{q} \to 0$ of these scalar fields exists, i.e.,

$$\lim_{q\to 0} \chi_{//}(\mathbf{q}) = \chi_{//}, \qquad \lim_{q\to 0} \chi_{\perp\perp}(\mathbf{q}) = \chi_{\perp\perp} \tag{3.9}$$

If the two limits are unequal, $\chi_{//} \neq \chi_{\perp\perp}$, then the tensor field (3.8) is *not continuous* at $\mathbf{q} = \mathbf{0}$. From the microscopic expressions derived in Sections 4 and 5, it follows that the longitudinal and transverse susceptibilities are indeed equal/unequal if the detailed balance symmetry is satisfied/violated. Fourier inversion of the asymptotic form (3.8) and subsequent rescaling ($\mathbf{q} = \mathbf{k}/r$) shows again that generic long-range momentum correlations $\mathcal{G}_{\alpha\beta}(\mathbf{r}) \sim E(\hat{\mathbf{r}}/r^d)$ exist in the uniform equilibrium state on any d-dimensional lattice unless $\chi_{//} = \chi_{\perp\perp}$. In particular, in any two-dimensional LGA fluid on the triangular lattice that violates the detailed balance symmetry, this yields

$$\mathcal{G}_{xx}(\mathbf{r}) = -\mathcal{G}_{yy}(\mathbf{r}) = \frac{\sqrt{3}}{4\pi}(\chi_{//} - \chi_{\perp\perp})\left(\frac{x^2 - y^2}{r^4}\right) \tag{3.10}$$

The above result shows the existence of long-range $1/r^2$ behavior in the spatial correlation between momentum densities at two different points in terms of two susceptibilities $\chi_{//}$ and $\chi_{\perp\perp}$. In the Langevin approach these susceptibilities can be expressed in terms of phenomenological noise strengths and transport coefficients similar to B and D in Section 3.1. In the next section we present a microscopic theory which allows us to derive general formulas for the phenomenological coefficients $E_n(\hat{\mathbf{r}})$. These formulas can be calculated for general LGAs of diffusive or fluid type. As an application we present in Section 5 a triangular LGA fluid for which $\chi_{//}$ and $\chi_{\perp\perp}$ will be calculated explicitly.

4. MICROSCOPIC THEORY

4.1. Detailed Balance

We consider an LGA defined on a regular d-dimensional lattice $\mathcal{L}$ with periodic boundary conditions, containing $V = L^d$ nodes. On each node $\mathbf{r} \in \mathcal{L}$ there exists a set of allowed velocity channels $\mathbf{c}_i$ ($i = 1, 2, \ldots, b$), where i labels nearest neighbor lattice vectors, and possibly rest particles. The system evolves at discrete time steps $t = 0, 1, \ldots$. The microscopic configuration of the system at time t is given in terms of occupation numbers $s_i(\mathbf{r}, t) = \{0, 1\}$ (Fermi exclusion rule) denoting the absence or presence of a particle in velocity channel $(\mathbf{r}, \mathbf{c}_i)$. The state of node $\mathbf{r}$ is denoted by $s(\mathbf{r}, t) = \{s_i(\mathbf{r}, t);\ i = 1, 2, \ldots, b\}$. The dynamics of the LGA consists of a collision step followed by a propagation step. The collision step is performed at all nodes simultaneously, and is defined by the strictly local transition probabilities $A_{s\sigma}$ from a precollision state s at a single node to a post-collision state σ at the same node. The transition matrix is normalized, $\sum_\sigma A_{s\sigma} = 1$, and invariant under the full group of symmetry operations of the underlying lattice.

Certain conservation laws must be obeyed by $A_{s\sigma}$. In case only the local mass or number of particles is conserved in a collision, the local density is a slowly varying quantity, and we are dealing with a purely diffusive model. If momentum is also conserved in a collision, the local momentum density or flow velocity is slowly varying, and we are dealing with an athermal fluid. If in addition energy—which may be purely kinetic or internal—is conserved, then the local energy density or temperature is a slowly varying quantity as well, and we are dealing with a thermal fluid. The ring kinetic theory in this section is presented in a general framework so as to cover all such cases.

After these definitions, we devote the remainder of this subsection to a careful description of what is meant by "detailed balance" in the context of LGAs, as many different authors are using different generalizations of this concept. A lattice gas is said to have the *detailed balance symmetry* if the single node transition matrix has the extra symmetry

$$A_{s\sigma} = A_{\sigma s} \qquad (\forall s, \sigma) \tag{4.1}$$

in addition to lattice symmetries and conservation laws. To make the analogy with the standard concept of 'detailed balance' as used in kinetic equations as close as possible, one may express the nonlinear binary collision term[19] of the Boltzmann equation for a gas with stochastic interactions in terms of a transition rate $A(\mathbf{c}_1\mathbf{c}_2 \mid \mathbf{c}_1^*\mathbf{c}_2^*)$ from an in-state $(\mathbf{c}_1\mathbf{c}_2)$ to an out-state $(\mathbf{c}_1^*\mathbf{c}_2^*)$. This A is the analog of $A_{s\sigma}$. Here the detailed balance symmetry is

$$A(\mathbf{c}_1\mathbf{c}_2 \mid \mathbf{c}_1^*\mathbf{c}_2^*) = A(-\mathbf{c}_1^* - \mathbf{c}_2^* \mid -\mathbf{c}_1 - \mathbf{c}_2) \tag{4.2}$$

We apply this to a binary collision in an LGA, and observe that the dynamics of an LGA is invariant under all symmetries of the lattice, including *inversion*. Therefore the minus sign in (4.2) can be removed, resulting in

$$A(\mathbf{c}_1\mathbf{c}_2 \mid \mathbf{c}_1^*\mathbf{c}_2^*) = A(\mathbf{c}_1^*\mathbf{c}_2^* \mid \mathbf{c}_1\mathbf{c}_2) \tag{4.3}$$

which is the direct analog of (4.1). Similar arguments apply to n-tuple collisions in LGAs.

Frisch *et al.*[7] have shown the following: if a LGA satisfies the detailed balance symmetry (4.1), then the Liouville equation admits a completely factorized equilibrium distribution $\mathscr{D}(\mathbf{s}) = \prod_{\mathbf{r}} F_0(s(\mathbf{r}))$ without spatial correlations, where $\mathscr{D}(\mathbf{s})$ is the Γ-space distribution. A microstate $\mathbf{s}$ is defined as the set of occupation numbers $\mathbf{s} = \{s(\mathbf{r}); \mathbf{r} \in \mathscr{L}\} = \{s_i(\mathbf{r}); \mathbf{r} \in \mathscr{L}, i = 1, 2, \ldots, b\}$. Maximization of the entropy furthermore suggests that $F_0(s)$

with $s=\{s_i;\ i=1, 2,..., b\}$ should also be factorized over the separate velocity channels, i.e.,

$$F_0(s)=\prod_i (f_i^0)^{s_i}(1-f_i^0)^{1-s_i} \tag{4.4}$$

Then one can show that the average occupation number f_i^0 of a single-particle state $\{\mathbf{r}, \mathbf{c}_i\}$ in equilibrium necessarily takes the form of the Fermi distribution. In case the number of particles, momentum, and energy are conserved, the Fermi distribution reads

$$f_i^0=\langle s_i(\mathbf{r})\rangle_{\text{eq}}=[1+\exp(-\alpha-\boldsymbol{\gamma}\cdot\mathbf{c}_i+\beta\varepsilon_i)]^{-1} \tag{4.5}$$

It contains three parameters α, $\boldsymbol{\gamma}$, and $-\beta$, which are conjugate to the collisional invariants $a_i=\{1, \mathbf{c}_i, \varepsilon_i\}$, where the energy ε_i of a particle in channel $\mathbf{c}_i$ can be purely kinetic, $\varepsilon_i=\frac{1}{2}c_i^2$, but it may include internal energy. If energy or momentum is not conserved, then the conjugate parameter β or γ should be set equal to zero.

Moreover, $F_0(s)$ above can be written in the equivalent form

$$F_0(s)=\frac{\exp[\alpha\rho(s)+\boldsymbol{\gamma}\cdot\mathbf{g}(s)-\beta e(s)]}{\sum_{s'}\exp[\alpha\rho(s')+\boldsymbol{\gamma}\cdot\mathbf{g}(s')-\beta e(s')]} \tag{4.6}$$

where the locally conserved quantities

$$\begin{pmatrix}\rho(s)\\ \mathbf{g}(s)\\ e(s)\end{pmatrix}=\sum_i\begin{pmatrix}1\\ \mathbf{c}_i\\ \varepsilon_i\end{pmatrix}s_i \tag{4.7}$$

are respectively the number of particles, momentum, and energy corresponding to state s. This can be verified by carrying out the s' summation in the denominator and using the explicit form (4.5) of the Fermi distribution f_i^0. For later reference we quote a further consequence of the detailed balance symmetry, namely

$$F_0(s)\,A_{s\sigma}=A_{\sigma s}F_0(\sigma)\qquad(\forall s, \sigma) \tag{4.8}$$

This is implied by (4.1) and (4.6) together with the conservation laws.

From the previous results we also infer that the Γ-space distribution over microstates $\mathbf{s}=\{s_i(\mathbf{r});\ \mathbf{r}\in\mathscr{L},\ i=1, 2,..., b\}$ is the Gibbs distribution,

$$\mathscr{D}(\mathbf{s})=\prod_{\mathbf{r}}F_0(s(\mathbf{r}))=\frac{\exp[\alpha N(\mathbf{s})+\boldsymbol{\gamma}\cdot\mathbf{P}(\mathbf{s})-\beta H(\mathbf{s})]}{\mathscr{Z}_{\text{gr}}(\alpha, \gamma, \beta)} \tag{4.9}$$

where the global invariants $N(\mathbf{s})$, $\mathbf{P}(\mathbf{s})$, and $H(\mathbf{s})$ are, respectively, the total number of particles, the total momentum, and the total energy. The partition function $\mathscr{Z}_{gr}$ is defined such that $\sum_{\mathbf{s}} \mathscr{D}(\mathbf{s}) = 1$. To verify that the Gibbs distribution (4.9) is indeed a stationary solution of the Liouville equation,[7] one needs the property that the Gibbs distribution $\mathscr{D}(\mathbf{s})$ is invariant under the separate action of the collision step and the propagation step.

There is no proof that the relevant equilibrium distribution is always of the form (4.9) when N, $\mathbf{P}$, and H form the complete set of global invariants, but computer simulations provide strong numerical evidence that the single-particle distribution has the Fermi form and that spatial and velocity correlations are absent in the equilibrium state.

The present interpretation of detailed balance is in agreement with that of van Kampen[20]: a physical system approaches for long times a unique thermodynamic equilibrium state. If an LGA is to model a physical system, the transition matrix should be consistent with this equilibrium distribution. A sufficient condition[2] to guarantee this is the detailed balance symmetry, which has the form (4.1) in the present paper.

If an LGA violates the detailed balance symmetry we call it an NDB model. As we shall see in the next sections, the equilibrium state of an NDB model is not given by the factorized Gibbs form (4.9), but exhibits long-range algebraic correlations. According to the discussion in Section 2, such LGAs may be considered as effective or mathematical models describing driven physical systems.

In the LGAs considered in this paper all global invariants are strictly sums over one-particle states $\{\mathbf{r}, \mathbf{c}_i\}$. Consequently there are no correlations between occupation numbers at the same or at different nodes in the Gibbs state (4.9) of LGAs that satisfy the detailed balance symmetry (4.1), and all multiparticle distributions factorize in equilibrium, or, equivalently, all correlation functions vanish. The pair correlation function, for instance, has the diagonal form

$$\mathscr{G}_{ij}(\mathbf{r}-\mathbf{r}') = \langle \delta s_i(\mathbf{r})\, \delta s_j(\mathbf{r}') \rangle_{eq} = \delta_{ij}\delta(\mathbf{r},\mathbf{r}') f_i^0(1-f_i^0) \tag{4.10}$$

where the fluctuations are defined as $\delta s_i(\mathbf{r}) = s_i(\mathbf{r}) - f_i^0$ and $\delta(\mathbf{r}, \mathbf{r}')$ is a d-dimensional Kronecker delta.

The above discussion does not exclude the possibility that one can construct *mathematical* models that violate the detailed balance symmetry,

[2] A weaker condition that still guarantees the existence of a Gibbsian equilibrium state is the *semi*-detailed balance or Stueckelberg condition, $\sum_s A_{s\sigma} = 1$. However in all specific models used in the literature for analytic calculations or computer simulations, the semi-detailed balance condition is equivalent to (4.1) except in the face-centered hypercubic (FCHC) models discussed by Hénon.[9]

but nevertheless possess a completely factorized (be it non-Gibbsian) equilibrium state.[21] This can be done as follows: one chooses a set $\{f_i^0\}$, different from the Fermi distribution, and constructs an LGA with a transition matrix $A_{s\sigma}$ that satisfies the symmetry relation $F_0(s)\, A_{s\sigma} = F_0(\sigma)\, A_{\sigma s}$ for all s and σ, with $F_0(s)$ given by the product form (4.4). This type of symmetry relation is a mathematical extension of (4.5) and is referred to as "detailed balance with respect to a given equilibrium distribution f_i^0." We will not consider this extension in the present paper.

4.2. Ring Kinetic Theory

In a very recent paper Bussemaker *et al.*[11] have derived a coupled set of kinetic equations: the generalized Boltzmann equation for the single-particle distribution function and the ring kinetic equation for the pair correlation function. The equations apply to LGAs with zero range interactions *with* or *without* the detailed balance symmetry. The methods used to obtain these kinetic equations are similar to the ones used to study classical fluids.

The LGAs studied in the remainder of this paper violate the detailed balance symmetry, and are assumed to approach for long times a spatially uniform and stable equilibrium state. The single particle distribution function and the pair correlation function in that equilibrium state are

$$\begin{aligned} f_i^0 &= \langle s_i(\mathbf{r}) \rangle_{\text{eq}} \\ \mathscr{G}_{ij}(\mathbf{r}-\mathbf{r}') &= \langle \delta s_i(\mathbf{r})\, \delta s_j(\mathbf{r}') \rangle_{\text{eq}} \end{aligned} \tag{4.11}$$

with $\delta s_i(\mathbf{r}) = s_i(\mathbf{r}) - f_i^0$ and $i, j = \{1, 2, ..., b\}$. They can be obtained from the stationary solution of the kinetic equations of ref. 11, which constitute a coupled set of nonlinear equations that can be solved *numerically* for general LGAs. This has been shown in ref. 11 by two applications to LGAs without the detailed balance symmetry: (i) the pair correlation function $\mathscr{G}(\mathbf{r})$ in a one-dimensional model of interacting random walkers, and (ii) the correlation $\mathscr{G}_{ij}(\mathbf{r}=0)$ between particles in velocity channels $\mathbf{c}_i$ and $\mathbf{c}_j$ on the same node of a triangular LGA fluid. In both cases the predictions of ring kinetic theory were in good agreement with the results of computer simulations.

The purpose of this section is to show *analytically* that the ring kinetic theory of ref. 11 yields for *large distances* the algebraic tails $\sim 1/r^2$ of the correlation functions that were predicted by the phenomenological Langevin equation of Section 3 and to calculate the coefficients of these tails explicitly from the microscopic theory.

The numerical analysis of Bussemaker *et al.* has also shown that the fully self-consistent solution of the nonlinear coupled kinetic equations is only slightly different [less than 1% for the average occupation f_i^0, and less than 10% for the pair correlation function $\mathscr{G}_{ij}(\mathbf{r}-\mathbf{r}')$] from a simple perturbative solution called the simple ring approximation. In this paper we therefore restrict ourselves to this approximation, where f_i^0 is determined as the stationary solution of the nonlinear Boltzmann equation. As shown in ref. 11, the Fourier transform of the pair correlation function $\mathscr{G}_{ij}(\mathbf{r})$ is then given as

$$\hat{\mathscr{G}}_{ij}(\mathbf{q}) \equiv \chi_{ij}(\mathbf{q}) = \left[\frac{1}{1-s(\mathbf{q})\omega} s(\mathbf{q})\, B \right]_{ij} \tag{4.12}$$

or equivalently,

$$\hat{\mathscr{C}}_{ij}(\mathbf{q}) \equiv \Delta\chi_{ij}(\mathbf{q}) = \left[\frac{1}{1-s(\mathbf{q})\omega} s(\mathbf{q})\, E \right]_{ij} \tag{4.13}$$

where we also introduced the excess correlation function

$$\begin{aligned} \mathscr{C}_{ij}(\mathbf{r}) &\equiv \mathscr{G}_{ij}(\mathbf{r}) - \mathscr{G}_{ij}^d(\mathbf{r}) \\ \mathscr{G}_{ij}^d(\mathbf{r}) &= \delta(\mathbf{r}, \mathbf{0})\, \delta_{ij}\, g_i^0 \\ g_i^0 &= f_i^0(1-f_i^0) \end{aligned} \tag{4.14}$$

The two source terms in (4.12) and (4.13) are given by

$$E_{ij} \equiv B_{ij} - [(1-\omega)\, \mathscr{G}^d(\mathbf{0})]_{ij} \simeq \Omega_{ij}^{20} \tag{4.15}$$

The approximate equality in (4.15) refers to the simple ring approximation and the Ω-coefficients are defined as

$$\Omega_{ij}^{20} \equiv \sum_{s\sigma} (\delta\sigma_i \delta\sigma_j - \delta s_i \delta s_j)\, A_{s\sigma} F_0(s) \tag{4.16}$$

Here $\delta\sigma_i = \sigma_i - f_i^0$ and $F_0(s)$ is given by (4.4) with f_i^0 replaced by the solution of the nonlinear Boltzmann equation, which differs from the Fermi distribution. If, however, relation (4.8) is valid, which is a direct consequence of the detailed balance symmetry (4.1) and the conservation laws, then it is automatically guaranteed that the set of coefficients Ω_{ij}^{20} is vanishing. Consequently $\hat{\mathscr{C}}_{ij}(\mathbf{q})$ in (4.13) vanishes, and $\hat{\mathscr{G}}_{ij}(\mathbf{q})$ in (4.12) reduces to the diagonal form $\mathscr{G}_{ij}^d(\mathbf{r}=\mathbf{0})$ in (4.14).

The terms $(1-\omega)$ and $(1-s(\mathbf{q})\omega)$ in the above equations are matrices whose rows and columns are labeled by a pair of labels (ij)

with $i, j \in \{1, 2, ..., b\}$; similarly, $\mathscr{G}(\mathbf{q})$, $\chi(\mathbf{q})$, $\mathscr{C}(\mathbf{q})$, B, E, and Ω^{20} can be considered as vectors and $(s(\mathbf{q})B)_{ij} = s_{ij}(\mathbf{q})\, B_{ij} = \exp[i\mathbf{q}\cdot(\mathbf{c}_j - \mathbf{c}_i)]\, B_{ij}$. In fact, $s(\mathbf{q})\omega$ is a direct product of two matrices,

$$s_{ij}(\mathbf{q})\, \omega_{ij,kl} = \{e^{-i\mathbf{q}\cdot\mathbf{c}_i}(1+\Omega)_{ik}\}\{e^{+i\mathbf{q}\cdot\mathbf{c}_j}(1+\Omega)_{jl}\} \tag{4.17}$$

where Ω_{ij} is the linearized Boltzmann collision operator, $[\exp(i\mathbf{q}\cdot\mathbf{c})]_{ij} = \delta_{ij}\exp(i\mathbf{q}\cdot\mathbf{c}_i)$ is a diagonal matrix, and

$$\Omega_{ij} = \sum_{s\sigma} (\sigma_i - s_i)\, A_{s\sigma} F_0(s)\, \delta s_j / g_j^0 \tag{4.18}$$

In case $A_{s\sigma}$ satisfies the detailed balance symmetry (4.1), then one can show directly that the matrix $\Omega_{ij} g_j^0$ is indeed symmetric. Without this symmetry it is in general nonsymmetric.

To calculate $\Delta\chi_{ij}(\mathbf{q})$ in (4.13) for *small* $\mathbf{q}$ we perform a spectral decomposition of the product matrix in (4.17) and consider the eigenvalue problem (in matrix notation),

$$e^{-i\mathbf{q}\cdot\mathbf{c}}(1+\Omega)\,\psi_\mu(\mathbf{q}) = \Lambda_\mu(\mathbf{q})\,\psi_\mu(\mathbf{q}) \tag{4.19}$$

where $\psi_\mu(\mathbf{q})$ is a right eigenvector with label μ and eigenvalue $\Lambda_\mu(\mathbf{q})$. Let $\phi_\mu(\mathbf{q})$ be the corresponding left eigenvector. These eigenvectors form a complete biorthonormal set, satisfying

$$\langle \phi_\mu(\mathbf{q}) \mid \psi_\nu(\mathbf{q}) \rangle \equiv \sum_i \phi_{\mu i}(\mathbf{q})\, \psi_{\nu i}(\mathbf{q}) = \delta_{\mu\nu} \tag{4.20}$$

The eigenvalues $\Lambda_\mu(\mathbf{q})$ and eigenvectors $\psi_\mu(\mathbf{q})$, $\phi_\mu(\mathbf{q})$ at small $\mathbf{q}$ can be calculated by standard perturbation theory for degenerate eigenvalues. This was already done for closely related LGAs with a symmetric $\Omega_{ij} g_i^0$,[22, 23] and with a nonsymmetric one.[24]

Before writing the spectral decomposition of (4.12) or (4.13), we restrict our discussion to spatial correlation functions between *conserved* densities,

$$\mathscr{G}_{ab}(\mathbf{r}) = \sum_{ij} a_i b_j \mathscr{G}_{ij}(\mathbf{r}) \equiv \langle ab \mid \mathscr{G}(\mathbf{r}) \rangle \tag{4.21}$$

where $a_i, b_i = 1$ in purely diffusive LGAs, and $a_i, b_i \in \{1, \mathbf{c}_i\}$ in athermal LGA fluids, and $a_i, b_i \in \{1, \mathbf{c}_i, \frac{1}{2}\mathbf{c}_i^2\}$ in thermal LGA fluids. On account of (4.12)–(4.14) this implies for the corresponding susceptibilities

$$\begin{aligned} \chi_{ab}(\mathbf{q}) &= \chi_{ab}^d + \Delta\chi_{ab}(\mathbf{q}) \\ \chi_{ab}^d &= \sum_i a_i b_i f_i^0 (1 - f_i^0) \end{aligned} \tag{4.22}$$

The spectral decomposition of the relevant excess susceptibilities then becomes

$$\Delta\chi_{ab}(\mathbf{q}) = \sum_{ij} a_i b_j \hat{\mathscr{C}}_{ij}(\mathbf{q}) = \sum_{\mu\nu} \frac{\langle ab \mid \psi_\mu(\mathbf{q})\psi_\nu(-\mathbf{q})\rangle\langle \phi_\mu(\mathbf{q})\,\phi_\nu(-\mathbf{q}) \mid s(\mathbf{q})E\rangle}{1-\Lambda_\mu(\mathbf{q})\,\Lambda_\nu(-\mathbf{q})} \tag{4.23}$$

As we are interested in the behavior of the excess susceptibility for small $\mathbf{q}$, the $\mu\nu$ summation in (4.23) can be restricted to terms with a vanishing denominator where eigenvalues $\Lambda_\mu(\mathbf{q}) \to 1$ as $\mathbf{q} \to 0$, i.e., to products of slow (hydrodynamic or diffusive) modes.

In purely diffusive models there is only a diffusive mode ($\mu = D$) with $\Lambda_D(\mathbf{q}) = 1 - Dq^2 + \cdots$, with D the diffusion coefficient. In an athermal LGA fluid there are sound modes ($\mu = \sigma = \pm$) with $\Lambda_\sigma(\mathbf{q}) = 1 - i\sigma v_s q - \Gamma q^2 + \cdots$, and shear modes ($\mu = \perp$) with $\Lambda_\perp(\mathbf{q}) = 1 - \nu q^2 + \cdots$, where the speed of sound v_s, the sound damping coefficient Γ, and the shear viscosity ν can all be explicitly calculated from (4.19) using perturbation theory.

Expression (4.23) is the main new result of this paper. It provides a *microscopic* expression for the *phenomenological* coefficients entering in the Langevin description of long-range correlations in non-detailed balance LGAs. The advantages of the microscopic theory are evident: (i) one can calculate the phenomenological coefficients of Section 3 for a microscopic model, and (ii) one can show from the general expression (4.23) that all $\Delta\chi_{ij}(\mathbf{q})$ vanish if the detailed balance symmetry is obeyed, as is demonstrated below (4.16).

5. APPLICATION: A FLUID-TYPE LGA

As an illustration we apply our microscopic theory to an LGA fluid without detailed balance. In this model, which is defined on the triangular lattice, each node may contain a rest particle and six moving particles. The transition probabilities $A_{s\sigma}$ between states with a rest particle and those without are asymmetric. Even with the requirement that the model satisfy all symmetries of the triangular lattice, it still contains 20 independent transition probabilities.[10] In ref. 11 ring kinetic theory was applied to such a model, and it was found that short-range correlations are very well predicted by this theory.

Consider the simple choice of parameters shown in Fig. 1, where only two different types of collisions are shown. Let f_0 and f denote the average occupation numbers for rest particles and moving particles, respectively. They are related by $f_0 + 6f = \rho$, with ρ the average occupation of a node.

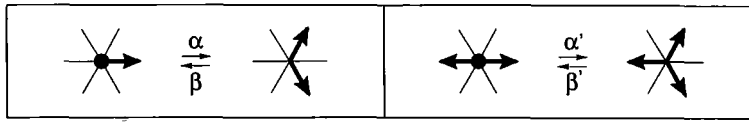

Fig. 1. Typical collision rules for a triangular LGA fluid lacking the detailed balance symmetry.

If the detailed balance symmetry (4.1) holds, which in this case would imply that $\alpha = \beta$ and $\alpha' = \beta'$ in Fig. 1, then the equilibrium state is completely factorized,[3] and $f_0 = f = \rho/7$.

If the momentum density in an LGA is conserved, it qualifies as a model for fluid flow, in which the local flow velocity is a slowly varying hydrodynamic variable. If in addition the microscopic transition probabilities $A_{s\sigma}$ violate the detailed balance symmetry (4.1), there exist long-range $1/r^2$ correlations (3.10) in the equilibrium state, as shown in Section 2.2. In the Langevin theory of Section 3 the limiting values for $\mathbf{q} \to 0$ of the longitudinal and transverse susceptibilities $\chi_{//}$ and $\chi_{\perp\perp}$ are expressed in terms of phenomenological noise strengths and transport coefficients. The ring kinetic theory of Section 4 provides an explicit expression (4.23) for the dominant small-$\mathbf{q}$ behavior of these susceptibilities. Using perturbation theory, one can calculate the amplitude of the algebraic spatial tail analytically in terms of the transition matrix $A_{s\sigma}$. Thus we have a completely microscopic theory for the long-range correlations occurring in such LGAs. Its detailed evaluation is very elaborate, and will be given in ref. 25. Here we will only quote the final result of the calculation. The transverse susceptibility, the calculation of which only involves a pair of shear modes, is given by

$$\chi_{\perp\perp} = 3f(1-f) - \left(\frac{3}{4\nu}\right)\frac{E_{13}}{\omega_\nu^2} \tag{5.1}$$

The second term on the right hand side of (5.1) is a non-detailed balance correction to the result $\chi^d_{\perp\perp} = 3f(1-f)$ that holds for detailed balance models. The longitudinal susceptibility is given by

$$\chi_{//} = 3f(1-f) + \frac{3}{4}\left(v_s^2 - \frac{1}{\omega_\zeta}\right)\frac{E_{10}}{\Gamma\omega_\zeta} - \left(\frac{3}{8\Gamma}\right)\frac{E_{12}}{\omega_\nu^2} \tag{5.2}$$

It contains the same detailed balance contribution $\chi^d_{//} = 3f(1-f)$, but a

[3] In the special case when $\alpha/\beta = \alpha'/\beta'$ there still exists a completely factorized but non-Gibbsian state with $f_0 \neq f$. However, for generic choices of parameters that lack detailed balance symmetry, this will not occur, and the equilibrium state contains correlations.

different non-detailed balance correction, which is determined by pairs of sound modes.

The nonvanishing E_{ij} in (5.1) and (5.2) are defined in (4.15). Furthermore, v_s is the speed of sound and ν and Γ are, respectively, the shear viscosity and sound damping coefficient. These transport coefficients in our microscopic theory are obtained from the (mean-field) eigenvalue problem (4.19)

$$\begin{aligned} \nu &= \frac{1}{4}\left(\frac{1}{\omega_\nu}-\frac{1}{2}\right) \\ \Gamma &= \frac{1}{2}\nu+\frac{1}{2}\left(\frac{1}{2}-v_s^2\right)\left(\frac{1}{\omega_\zeta}-\frac{1}{2}\right) \end{aligned} \tag{5.3}$$

where ω_ν and ω_ζ are the eigenvalues of $-\Omega_{ij}$ in (4.18) related to shear and bulk viscosity.

From (5.1) and (5.2) it should be clear that $\chi_{//}$ generically differs from $\chi_{\perp\perp}$, unless E_{10} and E_{13} are both vanishing as a consequence of the detailed balance symmetry. This provides an explicit example of long-range $1/r^d$ correlations in the equilibrium state of NDB fluid-type LGAs on the basis of a microscopic theory, together with a quantitative prediction for the magnitude of the spatial correlations.

To test the predictions of the ring approximation for long-range correlations we have performed computer simulations. Previous computer simulations have already confirmed the predictions of ring kinetic theory for short ranged correlations in ref. 11. A particular choice of parameters was made for the collisions shown in Fig. 1 together with other collisions that obey the lattice symmetries and conservation laws.[25] The complete set of transition rates was chosen such that the model is invariant under exchange of particles and holes. Consequently, at the half-filled lattice we have $f_0 = f = 1/2$ by symmetry. However, away from half-filling $f_0 \neq f$.

Figure 2 shows the pair correlation between the x components of the momentum densities at two nodes, separated by r lattice spacings in the x direction, $\mathscr{G}_{xx}(r, 0) = \langle g_x(r, 0)\, g_x(0, 0)\rangle_{\text{eq}}$, in the half filled lattice. The solid (zigzag) line connects the points of integer r values and represents the result of an exact numerical evaluation of the ring expression (4.12) and of subsequent numerical Fourier inversion using the method of ref. 11. The straight (dashed) line with slope -2 represents the asymptotic tail (3.10), combined with the analytic results (5.1) and (5.2) for the susceptibilities, evaluated at the specific model parameters and densities used in the simulations. The exact ring theory (zigzag) starts to approach the asymptotic theory (dashed) for $r > 5$, thus demonstrating the consistency of the asymptotic and numerical evaluations of the theoretical results.

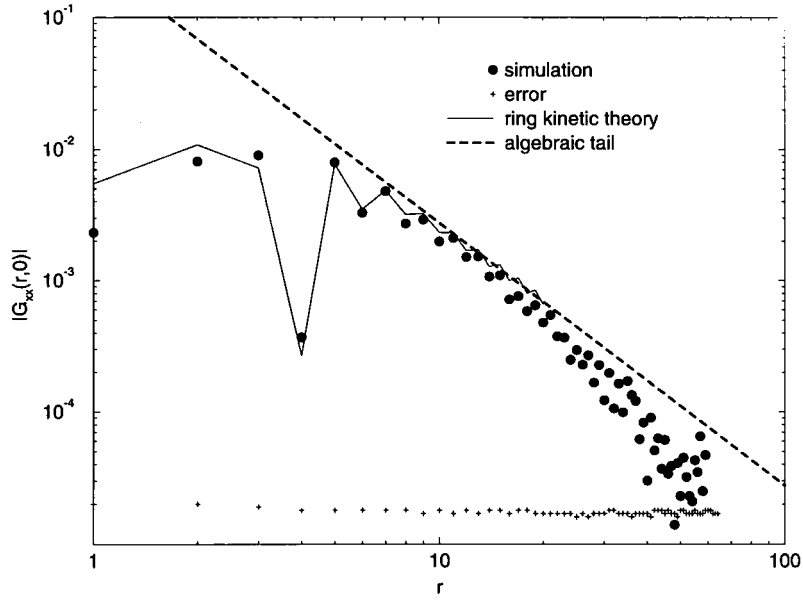

Fig. 2. Momentum–momentum correlation function $\mathscr{G}_{xx}(r, 0)$ between nodes separated by a vector $\mathbf{r} = (r, 0)$ parallel to the x-axis as a function of r in a triangular LGA without detailed balance, at half-filling, with system size 256×256 and equilibration time 2000. Comparison of exact ring theory (zigzag line), asymptotic ring theory (dashed line), and simulations (black dots). Simulation errors are indicated by the plus signs at the bottom of the figure.

The zigzagging is related to the parity of r and is a consequence of a spurious conservation law, the staggered total momentum.[29] It will be discussed in ref. 25. The simulations refer to a 256×256 system with periodic boundary conditions; an average was made over several runs in which the system was prepared at random at $t = 0$ and then equilibrated during 2000 time steps before measurements of the pair correlation function were made using a fast Fourier transform method. Figure 2 shows the comparison between theory and simulations (black circles). For r larger than about 10 lattice spacings the decay becomes algebraic, $\mathscr{G}_{xx}(r, 0) \simeq -E/r^2$, as predicted by the analysis of Section 3.2. There is good agreement between this analytic result and the simulations for r in the range between 10 and 20. The faster decay of the simulation data for r larger than 20 is due to the fact that the system, even after 2000 time steps, has not yet reached equilibrium on those scales. This is not surprising since the long-range correlations are caused by slow, diffusive processes acting on large temporal and spatial scales. An estimate for the spatial scale r_0 involved is

$r_0 = (\nu t)^{1/2} \simeq 20$, where the mean-field estimate, $\nu \simeq 0.2$ at half-filling, has been used.

A reason for the small systematic deviations in the range $10 < r < 20$ might be the use of mean-field or Boltzmann values for the transport coefficients ν and Γ and related eigenvalues ω_ν and ω_ζ in the evaluation of (5.1) and (5.2). In principle one should use renormalized transport coefficients. All these effects will be analyzed in more detail in ref. 25.

6. CONCLUSION

Lattice gas automata with strictly local collision rules that lack detailed balance have a non-Gibbsian equilibrium state containing equal-time spatial correlations. In this paper we have shown that the existence of local invariants (number and momentum density) necessarily leads to the existence of generic long-range correlations in equilibrium, i.e., to algebraic decay of the pair correlation function for large distances.

Our analysis is based on a microscopic theory in which the behavior of the wavevector-dependent susceptibility is obtained from a ring kinetic equation describing the evolution of the pair correlation function. The long-range behavior of the pair correlation function follows from an analysis of the small-wavenumber behavior of the susceptibility. The exponent that defines the algebraic decay for long distances is obtained from the symmetry properties of tensors of various rank. The analysis can be performed at the level of a Langevin equation in which fluctuation strengths and transport coefficients are phenomenological parameters. However, the microscopic theory presented in Section 4 makes it possible to *calculate* these quantities starting from the definition of the model. We have provided here well-defined expressions from which the amplitude of the algebraic tails can be calculated.

The strength of the arguments based on the Langevin equation is that for large classes of models at arbitrary densities there exist algebraic tails $\mathcal{G}(\mathbf{r}) \simeq E_n(\hat{\mathbf{r}})/r^n$ with phenomenological coefficients $E_n(\hat{\mathbf{r}})$ that are in general nonvanishing *unless* there exist an additional symmetry which forces these coefficients to vanish. This additional symmetry is the *detailed balance* relation. If detailed balance is satisfied, then the anisotropic part $\Delta\chi(\mathbf{q})$ of the susceptibility is vanishing by construction.

The strength of our microscopic theory in Section 4 is that we derive explicit expressions for the anisotropic parts $\Delta\chi(\mathbf{q})$ of the susceptibilities which in general are only vanishing if the detailed balance symmetry is obeyed. There is an intimate connection between the long-range correlations that occur in non-Gibbsian equilibrium states of LGAs lacking detailed balance on the one hand and nonequilibrium steady states of driven thermo-

dynamic systems on the other hand. We have used techniques that are well-known in the context of the kinetic theory of fluids or nonequilibrium Langevin equations for driven diffusive systems.[1-5]

From the point of view of using LGAs as tools to study transport phenomena in spatially extended systems this paper contains the important message that generic scale invariance is a necessary consequence of violation of the detailed balance symmetry. Alternatively, we have argued that NDB LGAs can be interpreted as effective models for driven systems. Explicit microscopic analysis is facilitated in the case of LGAs due to the fact that space, time, and velocity are all discrete. For long times NDB LGAs approach a non-Gibbsian state containing long-range correlations without the necessity of external driving fields or reservoirs. In nonuniform steady states with imposed gradients the spatial correlations are much longer ranged,[26-28] but such cases have not been considered here.

As an application we discussed in Section 5 the occurrence of momentum correlations of the type $1/r^2$ in a two-dimensional fluid-type LGA violating detailed balance. These correlation are not caused by a dynamics breaking the triangular symmetry of the underlying lattice, but by a spontaneous fluctuation of vector type, the local momentum density, that breaks the rotational symmetry of the system. To our knowledge this type of correlation has not been discussed in the literature.

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