Kinetic theory for lattice-gas cellular automata

T. R. Kirkpatrick
Institute for Physical Science and Technology, University of Maryland, College Park, Maryland 20742

M. H. Ernst
Institute for Theoretical Physics, University of Utrecht, P.O. Box 80006, 3508 TA Utrecht, The Netherlands
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The kinetic theory for lattice-gas cellular automata is extended beyond Boltzmann's mean-field approximation by including correlated ring-type collisions. This theory provides explicit expressions for time-correlation functions for all times in terms of a ring collision integral. We also obtain some exact results for time-correlation functions for short times. In particular, deviations from the Boltzmann equation result observed in computer simulations of the velocity-autocorrelation function of three-dimensional systems after two time steps are explained. For long times the results obtained reduce to those found using phenomenological mode-coupling theory.

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I. INTRODUCTION

Although lattice-gas cellular automata (LGCA's) as models for nonequilibrium fluids have been extensively studied since 1986 [1–5], the kinetic theory of these systems beyond the Boltzmann mean-field approximation of uncorrelated collisions is nonexistent. As far as the transport coefficients are concerned, there are no compeling reasons for such an extension, because the transport coefficients measured in computer simulations of LGCA's are *at all densities* in good agreement with the predictions of the Boltzmann equation [6].

However, in the past few years deviations from the Boltzmann prediction have been observed in the behavior of time-correlation functions at *long* [7–11], *intermediate* [9], and *short* [8,10] *times*. Best known are the observed *long-time tails*, $\sim t^{-d/2}$, in d-dimensional systems, whereas the Boltzmann equation predicts an exponential decay of correlations. Of course, the long-time tails have been explained in quantitative detail by the phenomenological mode-coupling theory [7,9,11], but this theory has never been derived or justified on the basis of the microdynamic equation for any LGCA.

Furthermore, at short and intermediate times extensive computer simulations on the velocity-autocorrelation function (VACF) show unexplained deviations from the Boltzmann-equation result already after *two* time steps in three-dimensional simulations [8,10], while in one-, two-, and four-dimensional systems [8,10] there are only deviations from the Boltzmann-equation result after three time steps.

One expects, of course, that sooner or later sequences of correlated collisions, which are neglected in the Boltzmann approximation, will give observable contributions to the time-correlation functions with increasing density. But why should three dimensions be qualitatively different from one, two, or four dimensions?

The goal of this paper is to present a fundamental extension of the kinetic theory for LGCA's beyond the Boltzmann equation by accounting for correlated ring collisions. Our theory will not only provide a formal derivation and justification of the long-time mode-coupling theory, as is done in Sec. V, but it also gives an explicit expression in Sec. IV for the short and intermediate time behavior of the time-correlation functions at $t=1,2,3,\ldots$ in terms of ring collision integrals, analogous to the case of continuous fluids [12]. In Sec. III we will explain why the measured results for time-correlation functions after two time steps in *three-dimensional* systems show deviations from Boltzmann, which are absent in the simulations for $d\neq 3$. These three-dimensional result will be related to the peculiar properties of the quasi-three-dimensional face-centered-hypercubic (FCHC) model [13] that will be discussed in Sec. II. In this section we also discuss the microdynamic evolution equations for general d-dimensional LGCA's.

II. FORWARD AND BACKWARD MICRODYNAMICS

Lattice gases are defined on a regular or periodic lattice in a d-dimensional space. We consider a system of N particles in a box of dimension L_α lattice spacings wide in the αth direction ($\alpha=x_1,x_2,\ldots,x_d$). We use units where the lattice constant is unity so that the total number of sites in the system is equal to its volume and is given by $V=L_{x_1}L_{x_2}\cdots L_{x_d}$. In general we assume periodic boundary conditions. A b-bit lattice-gas model is defined as follows. It contains a set of b different velocity channels $\mathbf{c}_i$ per lattice site $\mathbf{r}$, which includes the nearest neighbors and possibly a rest particle with zero speed, $\mathbf{c}_i=0$. The occupation number $n_i(\mathbf{r},t)$ of the ith velocity channel can only take the values 0 ("empty") or 1 ("occupied") (Fermi exclusion rule). Collisions occur only among particles at a single node ("point particles"). For a complete review of lattice-gas dynamics see Ref. [1].

The time evolution of a LGCA consists of a collision step over a time interval (t^-,t^+) with $t^\pm=t\pm\varepsilon$ ($\varepsilon\downarrow 0$) and a propagation step over the interval (t^+,t^-+1). The collision step can be represented by,

$$n_i(\mathbf{r},t^+)=n_i(\mathbf{r},t^-)+I_i(n(t^-)) , \tag{2.1}$$

and the propagation step by

$$n_i(\mathbf{r},t^+)=n_i(\mathbf{r}+\mathbf{c}_i,t^-+1)\equiv S_i n_i(\mathbf{r},t^-+1) . \tag{2.2}$$

A combination of both equations yields the *forward evolution* equation ($t>0$),

$$n_i(\mathbf{r}+\mathbf{c}_i,t^-+1)=n_i(\mathbf{r},t^-)+I_i(n(t^-)) ,$$

or

$$n_i(\mathbf{r},t^-+1)=S_i^{-1}n_i(\mathbf{r},t^-)+S_i^{-1}I_i(n(t^-)) . \tag{2.3}$$

In a b-bits model the collision term $I_i(n)$ is a polynomial of degree b in the occupation numbers n_k, each of which refers to a different velocity channel. Its explicit form has been discussed extensively in the literature [13,5]. The collision rules may be deterministic or stochastic and in general conserve particle number and momentum but not energy. Therefore, the LGCA's discussed in the present paper have no temperature (athermal models). Thermal LGCA's with nontrivial energy conservation and with the proper symmetry of the isotropic fluid are still lacking.

The quantities of interest in this paper are the equilibrium time-correlation functions, $\langle n_i(t)n_j(0)\rangle = \langle n_i(0)n_j(-t)\rangle$, which depend only on the time difference. It is also convenient to have a backward evolution equation, expressing $n_j(-t)$ in terms of $n_j(0)$. As the collision rules are invariant under the reversal of velocities $\mathbf{c}_i$, the backward collision and streaming steps can be represented by

$$\begin{aligned} n_i(\mathbf{r},-t^-)&=n_i(\mathbf{r},-t^+)+I_i(n(-t^+)) ,\\ n_i(\mathbf{r},-t^+)&=n_i(\mathbf{r},+\mathbf{c}_i,-t^-+1)\\ &=S_{in_i}(\mathbf{r},-t^-+1) . \end{aligned} \tag{2.4}$$

A combination of both expressions yields the *backward evolution* equation ($t>0$)

$$n_i(\mathbf{r},-t^--1)=S_i n_i(\mathbf{r},-t^-)+I_i(Sn(-t^-)) . \tag{2.5}$$

From now on we write $n_i(\mathbf{r},t)\equiv n_i(\mathbf{r},t^-)$ and all occupation numbers refer to precollisional states.

For use in later sections it is convenient to expand the collision operator $I_i(n)$ in Eqs. (2.3) and (2.5) into fluctuations around equilibrium,

$$\delta n_i(\mathbf{r},t)=n_i(\mathbf{r},t)-\langle n_i\rangle=n_i(\mathbf{r},t)-f . \tag{2.6}$$

Here $\langle\ \rangle$ denotes an average over an equilibrium ensemble, and $\langle n_i\rangle=f=\rho/b$ is independent of the velocity c_i in athermal LGCA's and is equal to the *reduced density* ($0\le f\le 1$). Expansion of the collision operator yields,

$$I_i(n)=\sum_{\lambda=1}^{b-1}\Omega_{ii_1}^{(\lambda)\cdots i_\lambda}\delta n_{i_1}\delta n_{i_2}\cdots\delta n_{i_\lambda} , \tag{2.7}$$

where the relation $I_i(f)=0$ and the Einstein summation convention have been used. Equation (2.7) defines the coefficients $\Omega_{ii_1}^{(\lambda)\cdots i_\lambda}$. They have the following *properties* that will be frequently used later on:

(i) $\Omega_{ii_1}^{(\lambda)\cdots i_\lambda}$ is symmetric in $(i_1\ldots i_\lambda)$.

(ii) $\Omega_{ii_1}^{(\lambda)\cdots i_\lambda}$ vanishes if $\lambda=b$ and if at least one pair of indices out of $(i\cdots i_\lambda)$ is equal [see below Eq. (2.3)].

(iii) $\Omega_{ik}^{(1)}$ is the linearized Boltzmann collision operator which has the additional symmetry $\Omega_{ik}^{(1)}=\Omega_{ki}^{(1)}$.

These symmetry relations can be derived from the symmetry of the collision rules under interchange of ingoing and outgoing particles.

In order to be able to understand why three dimensions is special, it is important to note that all LGCA's are contained in a macroscopic box with periodic boundary conditions and with $V=L^d$ sites, except for $d=3$ [13]. The reason is that there does not exist a regular space lattice in three dimensions, on which fourth-rank tensors, such as the viscosity, are isotropic so that the Navier-Stokes equations have the required symmetry of the isotropic fluid [14,15]. D'Humières, Lallemand, and Frisch [14] therefore introduced the FCHC model that gives the three-dimensional (3D) fluid symmetry, by considering a quasi-three-dimensional slab with $2V=L\times L\times L\times 2$ sites, embedded in a four-dimensional (4D) simple cubic lattice. Further, only *even* sites ($r_x+r_y+r_z+r_t=$even) are accessible, so that the number of available sites is $V=L^3$. There are 24 allowed velocity states per node,

$$(\pm1,\pm1,0,0),\quad(\pm1,0,\pm1,0),\quad(0,\pm1,\pm1,0) ,$$

$$(\pm1,0,0,\pm1),\quad(0,\pm1,0,\pm1),\quad(0,0,\pm1,\pm1) .$$

It will turn out that the observed non-Boltzmann-type correlations in 3D LGCA's after two time steps are actually a *finite-size effect,* caused by the very small linear extent of two lattice spacings in the fourth (unphysical) dimension. These correlations are therefore of *geometric,* rather than dynamic origin.

To analyze these geometric correlations, it is convenient to consider a simpler quasi-one-dimensional strip in the Frisch-Hasslacher-Pomeau (FHP) model [13], two lattice spacings wide in the y direction, embedded in a two-dimensional (2D) triangular lattice and shown in Fig. 1. The model allows six velocity states per site (FHP-I) and possibly an additional rest particle (FHP-II and -III) [16].

The main object of study will be the time-correlation function of the fluctuation $\langle\delta n_i(\mathbf{r},t)\delta n_j(\mathbf{r}',t')\rangle$, which depends only on $(\mathbf{r}-\mathbf{r}')$ and $(t-t')$. Its equal time value is

$$\langle\delta n_i(\mathbf{r},0)\delta n_j(\mathbf{r}',0)\rangle=\kappa\delta_{ij}\delta(\mathbf{r},\mathbf{r}') , \tag{2.8}$$

where δ_{ij} and $\delta(\mathbf{r},\mathbf{r}')$ are Kronecker deltas and where κ is determined by Fermi statistics, i.e.,

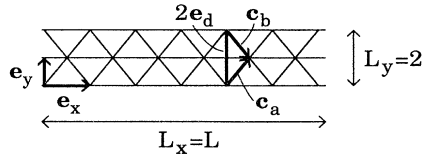

FIG. 1. Quasi-one-dimensional strip with periodic boundary conditions with periods $L_z=L$ and $L_y=2$, and $\mathbf{e}_x=\mathbf{c}_1$, $\mathbf{c}_a=\mathbf{c}_2$, and $\mathbf{c}_b=\mathbf{c}_6$.

$$\kappa=\langle(\delta n_i)^2\rangle=\langle n_i^2\rangle-\langle n_i\rangle^2=f(1-f)\ . \tag{2.9}$$

The normalized time-correlation function is referred to as the kinetic propagator,

$$\Gamma_{ij}(\mathbf{r},t)\kappa=\langle\delta n_i(\mathbf{r},t)\delta n_j(\mathbf{0},0)\rangle \tag{2.10}$$

with $\Gamma_{ij}(\mathbf{r},0)=\delta_{ij}\delta(\mathbf{r},0)$. Its Fourier transform is denoted by

$$\hat{\Gamma}_{ij}(\mathbf{q},t)\kappa=\sum_{\mathbf{r}} e^{-i\mathbf{q}\cdot\mathbf{r}}\Gamma_{ij}(\mathbf{r},t)\kappa$$
$$=V^{-1}\langle n_i(\mathbf{q},t)n_j^*(\mathbf{q},0)\rangle\ , \tag{2.11}$$

where $n_i(\mathbf{q},t)$ is the Fourier transform of $\delta n_i(\mathbf{r},t)$ and the asterisk denotes complex conjugation.

All two-point time-correlation functions can be expressed in terms of the kinetic propagator. For instance, the van Hove function or density-density correlation function is

$$\langle\delta\rho(\mathbf{r},t)\delta\rho(\mathbf{0},0)\rangle=\sum_{i,j}\Gamma_{ij}(\mathbf{r},t)\kappa\ , \tag{2.12}$$

where $\delta\rho=\sum_i\delta n_i$ is the microscopic density fluctuation. Another example is the single-site velocity-correlation function,

$$\langle g_x(\mathbf{r},t)g_x(\mathbf{r},0)\rangle=\sum_{i,j}c_{ix}c_{jx}\Gamma_{ij}(\mathbf{r}=\mathbf{0})\kappa$$
$$=\frac{1}{V}\sum_{q}\sum_{i,j}c_{ix}c_{jx}\hat{\Gamma}_{ij}(\mathbf{q},t)\kappa\ , \tag{2.13}$$

where $\mathbf{g}(\mathbf{r},t)=\sum_i\mathbf{c}_i n_j(\mathbf{r},t)$ is the microscopic momentum density and $\hat{\Gamma}(\mathbf{q})$ is the Fourier transform of $\Gamma(\mathbf{r})$. Additional important time-correlation functions are the current-current correlation functions or Green-Kubo integrands,

$$\phi(t)=V^{-1}\langle J(t)J(0)\rangle$$
$$=\sum_{ij}j(c_i)j(c_j)\hat{\Gamma}_{ij}(\mathbf{0},t)\kappa\ , \tag{2.14}$$

where the total current is

$$J(t)=\sum_{r,i}j(c_i)\delta n_i(\mathbf{r},t)\ . \tag{2.15}$$

The one-particle currents $j(c_i)$, corresponding to the shear viscosity η and to the bulk viscosity ζ, are, respectively, $j_\eta(c_i)=c_{ix}c_{iy}$ and $j_\zeta(c_i)=d^{-1}c_i^2-c_0^2$, where d is the number of dimensions and c_0 is the sound velocity for the LGCA under consideration [17].

III. SHORT-TIME BEHAVIOR

In principle we have now introduced the basic definitions needed to calculate the kinetic propagator $\Gamma_{ij}(\mathbf{r},t)=\Gamma_{ji}(-\mathbf{r},-t)$. The last equality follows from the translational invariance in space and time of the equilibrium state. To calculate $\Gamma(t)$ one can iterate the forward or backward equation t times. In doing so one generates an enormous number of terms, and one needs to develop a systematic kinetic theory to account for the different sequences of uncorrelated and correlated collisions, such as ring collisions.

In the present section we use exact methods to study the short-time behavior of the propagator $\Gamma(t)$. Subsequent sections will be devoted to its long-time behavior. The kinetic propagator after a *single time step* follows directly from Eqs. (2.10) and (2.3),

$$\Gamma_{ij}(\mathbf{r},1)\kappa=\left\langle\delta n_j(\mathbf{0})S_i^{-1}\left[\delta n_i(\mathbf{r})+\sum_{\lambda=1}^{b}\Omega^{(\lambda)}_{ii_1\cdots i_\lambda}\delta n_{i_1}(\mathbf{r})\cdots\delta n_{i_\lambda}(\mathbf{r})\right]\right\rangle, \tag{3.1}$$

where $\delta n(\mathbf{r})$ is short for $\delta n(\mathbf{r},0)$. Consider the first term inside the average which yields

$$\langle\delta n_j(\mathbf{c}_i)\delta n_i(\mathbf{r})\rangle=\kappa\delta_{ij}\delta(\mathbf{r},\mathbf{c}_i) \tag{3.2}$$

on account of Eqs. (2.2) and (2.8). In addition we have used translational invariance to replace $\delta n_j(0)S_i^{-1}$ inside the average by $S_i\delta n_j(0)=\delta n_j(\mathbf{c}_i)$.

The next set of correlation functions contains the fluctuations,

$$\langle\delta n_j(\mathbf{c}_i)\delta n_{i_1}(\mathbf{r})\cdots\delta n_{i_\lambda}(\mathbf{r})\rangle=\kappa\delta_{\lambda_1}\delta_{ji_1}\delta(\mathbf{r},\mathbf{c}_i)\ . \tag{3.3}$$

The labels $i_1,\ldots,i_\lambda$ are all different on account of the property (ii) below Eq. (2.7). The kinetic propagator after *one time step* then becomes

$$\Gamma_{ij}(\mathbf{r},1)=(\delta_{ij}+\Omega^{(1)}_{ij})\delta(\mathbf{r},\mathbf{c}_i)\ . \tag{3.4}$$

Its Fourier transform is

$$\hat{\Gamma}_{ij}(\mathbf{q},1)=e^{-i\mathbf{q}\cdot\mathbf{c}_i}(\delta_{ij}+\Omega^{(1)}_{ij})\ . \tag{3.5}$$

It shows that $\Gamma(1)$ is exactly given by the linearized Boltzmann collision operator.

Next we consider the propagator after two time steps, which would be given by Eq. (3.1) with $\delta n_k(\mathbf{r},0)$ replaced by $\delta n_k(\mathbf{r},1)$. The last quantity should subsequently be expressed in $\delta n_l(\mathbf{r},0)$, using the forward equation (2.3) a second time. This second iteration of Eq. (2.3) yields a huge number of terms. For a b-bits model the total number of terms in $\Gamma(2)$ is

$$\sum_{l=1}^{b-1}(b+1)^l=\frac{1}{b}[(1+b)^b-b-1]\ , \tag{3.6}$$

which is approximately 2×10^4 for $b=6$ (FHP model) and 10^{12} for $b=24$ (FCHC model). Fortunately there ex-

ists a simpler method to calculate $\Gamma(2)$ by using the stationarity of the equilibrium state, i.e.,

$$\Gamma_{ij}(\mathbf{r},2)\kappa=\langle \delta n_i(\mathbf{r},1)\delta n_j(\mathbf{0},-1)\rangle \ , \tag{3.7}$$

and applying the forward equation (2.3) to the first factor inside the average and the backward equation (2.5) to the second factor, yielding only a total of $(1+b)^2$ terms. This yields in combination with Eq. (2.7),

$$\Gamma_{ij}(\mathbf{r},2)\kappa=\left\langle \left[S_i^{-1}\left[\delta n_i(\mathbf{r})+\sum_{\lambda=1}^{b}\Omega^{(\lambda)}_{ii_1\cdots i_\lambda}\delta n_{i_1}(\mathbf{r})\cdots\delta n_{i_\lambda}(\mathbf{r})\right]\right]\right.$$
$$\left.\times\left[S_j\delta n_j(\mathbf{0})+\sum_{\mu=1}^{b}\Omega^{(\mu)}_{jj_1\cdots j_\mu}[S_{j_1}\delta n_{j_1}(\mathbf{0})]\cdots[S_{j_\mu}\delta n_{j_\mu}(\mathbf{0})]\right]\right\rangle . \tag{3.8}$$

On account of property (ii) below Eq. (2.7) the nonvanishing terms in Eq. (3.8) contain the same number of δn's originating from $\delta n(\mathbf{r},1)$ as from $\delta n(\mathbf{0},-1)$, yielding,

$$\Gamma_{ij}(\mathbf{r},2)\kappa=(\delta_{ik}+\Omega^{(1)}_{ik})(\delta_{jl}+\Omega^{(1)}_{jl})\langle\delta n_k(\mathbf{r}-\mathbf{c}_i)\delta n_l(\mathbf{c}_l)\rangle$$
$$+\sum_{\lambda=2}^{b}\Omega^{(\lambda)}_{ii_1\cdots i_\lambda}\Omega^{(\lambda)}_{jj_1\cdots j_\lambda}\langle\delta n_{i_1}(\mathbf{r}-\mathbf{c}_i)\cdots\delta n_{i_\lambda}(\mathbf{r}-\mathbf{c}_i)\delta n_{j_1}(\mathbf{c}_{j_1})\cdots\delta n_{j_\lambda}(\mathbf{c}_{j_\lambda})\rangle \ . \tag{3.9}$$

Using Eqs. (2.8) the first term in Eq. (3.9) is

$$\Gamma_{ij}(\mathbf{r},2)=(\delta_{ik}+\Omega^{(1)}_{ik})(\delta_{jk}+\Omega^{(1)}_{jk})\delta(\mathbf{r},\mathbf{c}_i+\mathbf{c}_k) \ , \tag{3.10}$$

or in Fourier language,

$$\hat{\Gamma}_{ij}(\mathbf{q},2)=e^{-i\mathbf{q}\cdot\mathbf{c}_i}(\delta_{ik}+\Omega^{(1)}_{ik})e^{-i\mathbf{q}\cdot\mathbf{c}_k}(\delta_{kj}+\Omega^{(1)}_{kj}) \ , \tag{3.11}$$

where the symmetry property (iii), quoted below Eq. (2.7), has been used. Below we will show that all terms in Eq. (3.9) with $\lambda\geq 2$ *are vanishing provided* the macroscopic periodicity cell is more than *two* lattice spacings wide in every space directions. Therefore, $\Gamma(2)$, as given by Eqs. (3.10) and (3.11), is *exact* for sufficiently large systems. Furthermore, it is correctly given by the Boltzmann approximation, i.e., $\hat{\Gamma}(\mathbf{q},2)=[\hat{\Gamma}(\mathbf{q},1)]^2$ using a matrix notation.

We consider the remaining terms in Eq. (3.9) starting with $\lambda=2$, which contains the fluctuation formula

$$\langle\delta n_{i_1}(\mathbf{r}-\mathbf{c}_i)\delta n_{j_2}(\mathbf{r}-\mathbf{c}_i)\delta n_{j_1}(\mathbf{c}_{j_1})\delta n_{j_2}(\mathbf{c}_{j_2})\rangle$$
$$=\kappa^2(\delta_{i_1j_1}\delta_{i_2j_2}+\delta_{i_1j_2}\delta_{i_2j_1})\delta(\mathbf{r},\mathbf{c}_i+\mathbf{c}_{j_1})\delta(\mathbf{r},\mathbf{c}_i+\mathbf{c}_{j_2}) \tag{3.12}$$

with $i_1\neq i_2$ and $j_1\neq j_2$. The constraints imposed on $\mathbf{r}$ yield $\delta(\mathbf{c}_{j_1},\mathbf{c}_{j_2})=1$ and require $\mathbf{c}_{j_1}=\mathbf{c}_{j_2}$. However, $\Omega^{(2)}_{jj_1j_2}$ vanishes if $j_1=j_2$ and the total contribution of the $(\lambda=2)$ term in Eq. (3.9) vanishes. The same argument applies to all other contributions with $\lambda>2$.

So far we have not taken the periodic boundary conditions into account. Suppose that the system is contained in a macroscopic periodicity cell with periods I_α $(\alpha=x_1,x_2,\ldots,x_d)$. Then the spatial δ functions in Eqs. (3.10) and (3.12) should be replaced by $\bar{\delta}$, defined as

$$\bar{\delta}(\mathbf{r},\mathbf{r}')=\begin{cases}1 & \text{if } \mathbf{r}'=\mathbf{r}+\sum_{\alpha=x_1}^{x_d}M_\alpha L_\alpha e_\alpha\\ 0 & \text{otherwise},\end{cases} \tag{3.13}$$

where $(\mathbf{e}_\alpha,\alpha=x_1,x_2,\ldots,x_d)$ represents a set of vectors in the independent directions and $M_\alpha=(0,\pm1,\pm2,\ldots)$. Suppose all periods $L_\alpha>2$, then the conditions imposed by $\bar{\delta}(\mathbf{c}_{j_1},\mathbf{c}_{j_2})=1$ cannot be met, and all terms in Eq. (3.9) with $\lambda\geq 2$ are still vanishing.

However, if the periodic box in one space direction, say $\mathbf{e}_d$, would *only be two lattice spacings wide,* the condition $\bar{\delta}(\mathbf{c}_{j_1},\mathbf{c}_{j_2})=1$ can be met with $j_1\neq j_2$, and $\mathbf{c}_{j_1}=\mathbf{c}_{j_2}\pm(\mathbf{c}_a-\mathbf{c}_b)$ and there exist nonvanishing contributions to Eq. (3.9) given by

$$\delta\Gamma_{ij}(\mathbf{r},2)=2\kappa^2\Omega_{ij_1j_2}\Omega_{jj_1j_2}\bar{\delta}(\mathbf{c}_{j_1},\mathbf{c}_{j_2})\bar{\delta}(\mathbf{r},\mathbf{c}_i+\mathbf{c}_{j_1}) \ . \tag{3.14}$$

As an example we show in Fig. 1 how Eq. (3.14) applies to a quasi-one-dimensional strip. Here $\mathbf{e}_x$ and $\mathbf{e}_y$ are unit vectors in the x and y directions. The dimensions of the system are $L_x=L(\to\infty)$ in the x direction and $L_y=2$ in the y direction. The lattice is a triangular lattice and we show a pair (ab) of velocity vectors, $\mathbf{c}_a$ and $\mathbf{c}_b$, satisfying $\mathbf{c}_a-\mathbf{c}_b=2\mathbf{e}_d$. The condition imposed by the first $\bar{\delta}$ function in Eq. (3.14) has the following set of four solutions:

$$\begin{aligned}&(\mathbf{c}_{j_1}=\pm\mathbf{c}_a,\quad \mathbf{c}_{j_2}=\pm\mathbf{c}_b) \ ,\\ &(\mathbf{c}_{j_1}=\pm\mathbf{c}_b,\quad \mathbf{c}_{j_2}=\pm\mathbf{c}_a) \ ,\end{aligned} \tag{3.15}$$

contributing to Eq. (3.14). Subsequently one must sum over all possible pairs (ab), satisfying $c_a-c_b=2\mathbf{e}_d$.

The terms with $\lambda>2$ can be analyzed similarly and one finds that the λth term,

$$(\lambda!)\kappa^\lambda\Omega^{(\lambda)}_{ij_1\cdots j_\lambda}\Omega^{(\lambda)}_{jj_1\cdots j_\lambda}\bar{\delta}(\mathbf{c}_{j_1},\mathbf{c}_{j_2})\cdots\bar{\delta}(\mathbf{c}_{j_1},\mathbf{c}_{j_\lambda})$$
$$\times\bar{\delta}(\mathbf{r},\mathbf{c}_i+\mathbf{c}_{j_1}) \tag{3.16}$$

is vanishing, because two intermediate $\bar{\delta}$ functions cannot be satisfied simultaneously since $\mathbf{c}_{j_2}\neq\mathbf{c}_{j_3}\neq\cdots\neq\mathbf{c}_{j_\lambda}$.

Collecting results from Eqs. (3.14) and (3.15) we find for the kinetic propagator $\Gamma(2)$ in a quasi-$(d-1)$-

dimensional system, contained in a d-dimensional slab of linear dimensions $L^{d-1}\times 2$,

$$\hat{\Gamma}_{ij}(\mathbf{q},2)=[[\hat{\Gamma}(\mathbf{q},1)]^2]_{ij} +4\kappa e^{-i\mathbf{q}\cdot\mathbf{c}_i}\sum_{(ab)}(\Omega^{(2)}_{iab}e^{-i\mathbf{q}\cdot\mathbf{c}_a}\Omega^{(2)}_{jab} +\Omega^{(2)}_{i\bar{a}\bar{b}}e^{+i\mathbf{q}\cdot\mathbf{c}_a}\Omega^{(2)}_{j\bar{a}\bar{b}}) , \tag{3.17}$$

where we sum over all parts (ab), satisfying $\mathbf{c}_a-\mathbf{c}_b=2\mathbf{e}_d$, and $\bar{j}$ denotes the label referring to the velocity $-\mathbf{c}_j$ when j denotes $\mathbf{c}_j$. In deriving Eq. (3.17) we have also used the relation $\exp[i\mathbf{q}\cdot(\mathbf{c}_a-\mathbf{c}_b)]=1$, as implied by periodic boundary conditions. As an illustration we mention that the FHP model of Fig. 1 has one pair (a,b), with $\mathbf{c}_a=\mathbf{c}_2$ and $\mathbf{c}_b=\mathbf{c}_6$, and that the FCHC model has three pairs (ab) with $\mathbf{c}_a=\mathbf{e}_\beta+\mathbf{e}_d$ and $\mathbf{c}_b=\mathbf{e}_\beta-\mathbf{e}_d$ $(\beta=x,y,z)$.

As a further illustration we have applied the result given by Eq. (3.17) for the excess geometric correlations, to calculate at time $t=2$ the correction to the Boltzmann value of the stress-stress correlation function for a 1D strip (see Fig. 1) of the FHP-I model (FHP-I has no rest particles). This has been done in Appendix A.

The values of $\Gamma(t)$ for $t=3,4,\ldots$ involve rings and more complicated collisions that have not been considered here. In the subsequent sections on long-time behavior the ring collisions will be analyzed in more detail.

IV. RING KINETIC EQUATION

To study the long-time behavior of the kinetic propagator $\langle\delta n_1(\mathbf{r},t)\delta n_{1'}(0,0)\rangle$, we derive a formal identity that expresses the time evolution of this correlation function in terms of higher-order ones. Finally we do a loop expansion with a one-loop diagram, the *ring integral,* that gives the long-time tails.

We start from the forward microdynamic Eq. (2.3) combined with the fluctuation expansion, Eq. (2.7), and represent each $\delta n_l(\mathbf{r},t)$ by a Fourier series

$$\delta n_l(\mathbf{r},t)=\frac{1}{V}\sum_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{r}}n_l(\mathbf{q},t) , \tag{4.1}$$

and we use the relation

$$\frac{1}{V}\sum_{\mathbf{r}}e^{-i\mathbf{r}\cdot(\mathbf{q}-\mathbf{q}')}=\delta(\mathbf{q},\mathbf{q}') . \tag{4.2}$$

The Fourier transform of Eq. (2.3) then becomes

$$e^{i\mathbf{q}\cdot\mathbf{c}_i}n_i(\mathbf{q},t+1)=n_i(\mathbf{q},t)+\Omega^{(1)}_{ik}n_k(\mathbf{q},t)+\sum_{\lambda=2}^{b}V^{1-\lambda}\sum_{\mathbf{q}_1\cdots\mathbf{q}_\lambda}\delta\left[\mathbf{q},\sum_{p=1}^{\lambda}\mathbf{q}_p\right]\Omega^{(\lambda)}_{ii_1\cdots i_\lambda}\left[\prod_{p=1}^{\lambda}n_{ip}(\mathbf{q}_p,t)\right] , \tag{4.3}$$

where we have used that the streaming operator S_i becomes diagonal in the Fourier representation $S_i(\mathbf{q})=\exp(i\mathbf{q}\cdot\mathbf{c}_i)$. To proceed we introduce a discrete Laplace transform,

$$\tilde{n}_i(\mathbf{q},z)=\sum_{t=0}^{\infty}e^{-zt}n_i(\mathbf{q},t) . \tag{4.4}$$

The microdynamic Eq. (4.3) can then be written as

$$L_{ik}(\mathbf{q},z)\tilde{n}_k(\mathbf{q},z)=e^{z+i\mathbf{q}\cdot\mathbf{c}_i}n_i(\mathbf{q},0)+\sum_{t=0}^{\infty}e^{-zt}\sum_{\lambda=2}^{b}V^{1-\lambda}\sum_{\mathbf{q}_1\cdots\mathbf{q}_\lambda}\delta\left[\mathbf{q},\sum_{p=1}^{\lambda}\mathbf{q}_p\right]\Omega^{(\lambda)}_{ii_1\cdots i_\lambda}\prod_{p=1}^{\lambda}n_{i_p}(\mathbf{q}_p,t) . \tag{4.5}$$

Here we introduced the wave number and frequency-dependent Boltzmann collision operator $L_{ik}(\mathbf{q},z)$, which reads in matrix notation

$$L(\mathbf{q},z)=e^{z+i\mathbf{q}\cdot\mathbf{c}}-1-\Omega^{(1)} , \tag{4.6}$$

with the convention that a function $A(\mathbf{c})$ represents a diagonal matrix with $A_{ij}(\mathbf{c})=A(\mathbf{c}_i)\delta_{ij}$. The symmetry of all three terms on the right-hand side (rhs) of Eq. (4.6) under (ij) interchange implies that $L(\mathbf{q},z)$ is a *symmetric* matrix.

After multiplying Eq. (4.5) with L^{-1} and inserting Eq. (4.5) into the discrete Laplace transform of Eq. (2.11), we obtain the result

$$\tilde{\Gamma}_{ij}(\mathbf{q},z)\kappa=\kappa[L^{-1}(\mathbf{q},z)]_{ij}e^{z+i\mathbf{q}\cdot\mathbf{c}_j} +\sum_{t=0}^{\infty}e^{-zt}\sum_{\lambda=2}^{b}v^{-\lambda}\sum_{\mathbf{q}_1\cdots\mathbf{q}_\lambda}\delta\left[\mathbf{q},\sum_{p=1}^{\lambda}\mathbf{q}_p\right][L^{-1}(\mathbf{q},z)]_{ii'}\Omega^{(\lambda)}_{i'i_1\cdots i_\lambda}\left\langle\left[\prod_{p=1}^{\lambda}n_{i_p}(\mathbf{q}_p,t)\right]n_j^*(\mathbf{q},0)\right\rangle . \tag{4.7}$$

This formula expresses the (11)-correlation function, Γ_{ij}, in terms of the $(\lambda 1)$-correlation function with $\lambda=2,3,\ldots,b$. In the first term on the rhs we have used that the Fourier transform of Eq. (2.8) equals $V\delta_{ij}\kappa$. This first term is in fact the Boltzmann approximation to the kinetic propagator, i.e.,

$$\tilde{\Gamma}^0(\mathbf{q},z)\equiv\sum_{t=0}^{\infty}e^{-zt}\hat{\Gamma}^0(\mathbf{q},t) =(e^{z+i\mathbf{q}\cdot\mathbf{c}}-1-\Omega^{(1)})^{-1}e^{z+i\mathbf{q}\cdot\mathbf{c}} . \tag{4.8}$$

Expansion in a geometric series yields then

$$\hat{\Gamma}^0(\mathbf{q},t)=[e^{-i\mathbf{q}\cdot\mathbf{c}}(1+\Omega^{(1)})]^t . \tag{4.9}$$

The results given by Eqs. (4.8) and (4.9) have been used extensively in the literature [18,19] to calculate Green-Kubo formulas and current-current correlation functions in LGCA's within the Boltzmann approximation.

By employing stationarity of equilibrium averages, $\langle A(t)B(0)\rangle=\langle A(0)B(-t)\rangle$, we use the backward evolution equation (2.5) to further reduce Eq. (4.7). For that purpose we define

$$\bar{n}_j(\mathbf{q},z)=\sum_{t=0}^{\infty} e^{-zt}n_j(\mathbf{q},-t) . \tag{4.10}$$

Now the Laplace transform in the last term of Eq. (4.7) can be carried out, i.e.,

$$\sum_{t=0}^{\infty} e^{-zt}\langle n_{i_1}(\mathbf{q}_1,0)\cdots n_{i_\lambda}(\mathbf{q}_\lambda,0)n_j^*(\mathbf{q},-t)\rangle = \langle n_{i_1}(\mathbf{q}_1,0)\cdots n_{i_\lambda}(\mathbf{q}_\lambda,0)\bar{n}_j^*(\mathbf{q},z)\rangle . \tag{4.11}$$

By manipulations similar to the ones used in deriving Eq. (4.5) we obtain from the backward dynamic equation (2.5)

$$\bar{n}_j^*(\mathbf{q},z)=e^{z+i\mathbf{q}\cdot\mathbf{c}_j}[L^{-1}(\mathbf{q},z)]_{jj'}n_{j'}^*(\mathbf{q},0) + \sum_{t=0}^{\infty} e^{-zt}\sum_{\mu=2}^{b} e^{i\mathbf{q}\cdot j}[L^{-1}(\mathbf{q},z)]_{jj'}\Omega^{(\mu)}_{j'j_1\cdots j_\mu}V^{1-\mu}\sum_{\mathbf{q}_1'\cdots\mathbf{q}_\mu'}\delta\left[\mathbf{q},\sum_{p=1}^{\mu}\mathbf{q}_p'\right]\prod_{p=1}^{\mu}[S_{j_p}^{-1}(\mathbf{q}_p')n_{j_p}^*(\mathbf{q}_{p'}',-t)] . \tag{4.12}$$

We note that this equation for the complex conjugate of the backward equation contains exactly the same inhomogeneous symmetric Boltzmann operator $L(\mathbf{q},z)$ as the forward equation (4.7). Next we insert Eq. (4.12) into Eq. (4.11) and observe that the term containing $n_{j'}^*(\mathbf{q},0)$ yields a vanishing contribution because $i_1\neq i_2=\cdots\neq i_\lambda$.

The remaining terms in Eq. (4.11) yield in combination with Eq. (4.7)

$$\tilde{\Gamma}_{ij}(\mathbf{q},z)\kappa=\tilde{\Gamma}^0_{ij}(\mathbf{q},z)\kappa + \sum_{\lambda=2}^{b}\sum_{\mu=2}^{b}V^{1-\lambda-\mu}\sum_{\mathbf{q}_1\cdots\mathbf{q}_\lambda}\sum_{\mathbf{q}_1'\cdots\mathbf{q}_\mu'}\sum_{t=0}^{\infty}e^{-zt}L^{-1}_{ii'}\Omega^{(\lambda)}_{i'i_1\cdots i_\lambda}e^{i\mathbf{q}\cdot\mathbf{c}_j}L^{-1}_{jj'}\Omega^{(\mu)}_{j'j_1\cdots j_\mu}$$
$$\times\delta(\mathbf{q},\mathbf{q}_1+\cdots\mathbf{q}_\lambda)\delta(\mathbf{q},\mathbf{q}_1'+\cdots+\mathbf{q}_\mu')S_{j_1}^{-1}(\mathbf{q}_1')\cdots S_{j_\mu}^{-1}(\mathbf{q}_\mu')$$
$$\times\langle n_{i_1}(\mathbf{q}_1,t)\cdots n_{j_\lambda}(\mathbf{q}_\lambda,t)n_{j_1}^*(\mathbf{q}_1',0)\cdots n_{j_\mu}^*(\mathbf{q}_\mu',0)\rangle , \tag{4.13}$$

where $L=L(\mathbf{q},z)$. The formal (unclosed) equation of motion for Γ expresses the (11) correlation in terms of the $(\lambda\mu)$ correlation functions with $(\lambda,\mu=2,3,\ldots,b)$.

In the subsequent part of this section we will introduce a *factorization approximation* that converts Eq. (4.13) into a closed equation for $\Gamma(\mathbf{q},t)$. The basic idea is that Fourier components of occupation numbers are approximately distributed as a Gaussian, at least for small wave numbers, as a consequence of the law of large numbers. Further, we note that by constructing higher-order hierarchy equations and by using factorization approximations in these equations a systematic loop expansion can be developed. The factorization approximation used here gives the one-loop theory exactly. In the Gaussian decoupling approximation the higher-order correlation functions can be expressed in products of pair-correlation functions and all higher cumulants are neglected.

Next we observe that the $(\lambda\mu)$ correlations in Eq. (4.13) are only nonvanishing in the Gaussian approximation if every i label out of $(i_1,\ldots,i_\lambda)$ is paired to a j label out of $(j_1,\ldots,j_\mu)$. Consequently $\lambda=\mu$ and the $(\lambda\lambda)$ correlations factor into a sum of products of $\Gamma(t)$. For the (22)-correlation function we obtain in this manner

$$\langle n_1(\mathbf{q}_1,t)n_2(\mathbf{q}_2,t)n_{1'}^*(\mathbf{q}_1',0)n_{2'}^*(\mathbf{q}_2,0)\rangle = V^2\kappa^2(\mathbf{q}_1,\mathbf{q}_1')\delta(\mathbf{q}_2,\mathbf{q}_2')\hat{\Gamma}_{11}(\mathbf{q}_1,t)\hat{\Gamma}_{22},(\mathbf{q}_2,t) + V^2\kappa^2\delta(\mathbf{q}_1,\mathbf{q}_2')\delta(\mathbf{q}_2,\mathbf{q}_1')\hat{\Gamma}_{12},(\mathbf{q}_1,t)\hat{\Gamma}_{21},(\mathbf{q}_2,t) . \tag{4.14}$$

For the time being we neglect all higher-order terms with $\lambda>2$ in Eq. (4.13). As will be shown in the next section, the terms with $\lambda=2$ yield the two-mode contributions, yielding long-time tails $\sim t^{-d/2}$ in current correlation functions. The terms with $\lambda=3$ yield three mode contributions with subleading long-time tails $\sim t^{-d}$, where d is the number of dimensions. Also note that the $\lambda=3,4,5,\ldots$ terms are all higher order in a loop expansion then the $\lambda=2$ terms and should not be retained without also improving the approximation given by Eq. (4.14).

Insertion of Eq. (4.14) into Eq. (4.13) and using that $L(\mathbf{q},z)$ is a symmetric matrix gives

$$\tilde{\Gamma}_{ij}(\mathbf{q},z)=\tilde{\Gamma}^0_{ij}(\mathbf{q},z)[L^{-1}(\mathbf{q},z)]_{ii'}\Omega^{(2)}_{i'12}\tilde{R}_{12,1'2'}(\mathbf{q},z)\Omega^{(2)}_{j',1'2'}[L^{-1}(\mathbf{q},z)]_{j'j}e^{i\mathbf{q}\cdot\mathbf{c}_j} , \tag{4.15}$$

where $\tilde{R}(\mathbf{q},z)$ is the discrete Laplace transform, defined in Eq. (4.4), of the ring collision integral,

$$R_{12,1'2'}(\mathbf{q},t)=\frac{2\kappa}{V}\sum_{\mathbf{q}'}\hat{\Gamma}_{11'}(\mathbf{q}',t)S_{1'}^{-1}(\mathbf{q}')\hat{\Gamma}_{22'}(\mathbf{q}-\mathbf{q}',t)S_{2'}^{-1}(\mathbf{q}-\mathbf{q}') . \tag{4.16}$$

The structure of the ring integral given by Eq. (4.15) is a discrete time convolution. It describes a Boltzmann propagator (L^{-1}), a collision (Ω), two independently propagating particles ($\Gamma S^{-1})(\Gamma S^{-1}$), and a subsequent correlated collision (Ω) followed by a Boltzmann propagator (L^{-1}). We further observe that $R_{12,1'2'}(\mathbf{q},t)$ vanishes for $t=0$. The formal reason is that $\sum_q \exp[i\mathbf{q}\cdot(\mathbf{c}_{1'}-\mathbf{c}_2)]=V\delta_{1'2'}$, whereas $1'\neq 2'$ because of $\Omega^{(2)}_{j1'2'}$. Physically the reason is that the $(1'2')$ collision, denoted by $\Omega^{(2)}_{j1'2'}$ cannot be followed by a second collision, denoted by $\Omega^{(2)}_{i12}$, between the same pair, if the particles are only freely propagating during the intermediate time interval t. Therefore $t\geq 1$, allowing that particle 1 and/or 2 can at least suffer one intermediate collision with another fluid particle. Of course in a $(d-1)$-dimensional slab, which is only two lattice spacings wide in the dth dimension, $R_{12,1',2'}(\mathbf{q},0)\sim\bar{\delta}(\mathbf{c}'_1,\mathbf{c}'_2)$ is in general nonvanishing [see Eqs. (3.13)–(3.15)]. It gives rise to the excess geometric correlations, discussed in Sec. III. This is the standard structure of the ring collision term in the kinetic theory of continuous fluids [12].

Including all λ terms in Eq. (4.13) in the Gaussian approximation leads similarly to the result

$$\tilde{\Gamma}_{ij}(\mathbf{q},z)=\tilde{\Gamma}^0_{ij}(\mathbf{q},z)+\sum_{\lambda=2}^{b} L^{-1}_{ii'}\Omega^{(\lambda)}_{i'12\cdots\lambda}e^{i\mathbf{q}\cdot\mathbf{c}_j}L^{-1}_{jj'}\Omega^{(\lambda)}_{j'1'2'\cdots\lambda'}\tilde{R}^{(\lambda)}_{12\cdots\lambda,1'2'\cdots\lambda'}(\mathbf{q},z)\ , \tag{4.17}$$

where

$$R^{(\lambda)}_{12\cdots\lambda,1'2'\cdots\lambda'}(\mathbf{q},t)=\frac{\lambda!\kappa^{\lambda-1}}{V^{\lambda-1}}\sum_{q_1\cdots q_\lambda}\delta(\mathbf{q},\mathbf{q}_1+\cdots+\mathbf{q}_\lambda)\prod_{p=1}^{\lambda}[\hat{\Gamma}_{pp'}(\mathbf{q}_{p'},t)S^{-1}_{p'}(\mathbf{q}_{p'})]\ . \tag{4.18}$$

By extending the arguments below Eq. (4.16) one can show that $R^{(\lambda)}(\mathbf{q},0)=0$ for all $\lambda=2,3,\ldots,b$. The kinetic propagators in Eqs. (4.16) and (4.18) are the full propagators and Eqs. (4.16) or (4.18) give a self-consistent equation from which $\Gamma(\mathbf{q},t)$ can be solved in principle. This equation is referred to as a self-consistent ring equation. In the next section we shall only consider the ring integral $R^{(0)}$ with all Γ's replaced by their Boltzmann approximation, Γ^0 in Eq. (4.9). This approximation is called the simple ring approximation [12].

A particularly interesting application of these results would be the calculation of the current-current correlation function $\phi(t)$ in the ring approximation for all times t, as there exist many simulation data, in particular for the velocity autocorrelation function (VACF) [7–10].

In order to do so we write the correlation function in Eq. (2.14) as $\phi(t)=\mathbf{j}\cdot\hat{\Gamma}(\mathbf{0},t)\cdot\mathbf{j}\kappa$, using a notation with a $b\times b$ matrix $\hat{\Gamma}$ and a b vector $\mathbf{j}(c)$ with components $\mathbf{j}(\mathbf{c}_i)$ $(i=1,2,\ldots,b)$. Combining Eq. (4.15) with Eq. (4.6) at $\mathbf{q}=0$ we obtain for the discrete Laplace transform

$$\begin{aligned}\Phi(z)=&\kappa\mathbf{j}(c)\cdot[1-e^{-z}(1+\Omega^{(1)})]^{-1}\cdot\mathbf{j}(c)\\&+\kappa[\exp(-2z)][\mathbf{j}(c)\cdot[1-e^{-z}(1+\Omega^{(1)})]^{-1}]_i\Omega^{(2)}_{i12}\tilde{R}_{12,1'2'}(\mathbf{0},z)\Omega^{(2)}_{j1'2'}[[1-e^{-z}(1+\Omega^{(1)})]^{-1}\cdot\mathbf{j}(c)]_j\ .\end{aligned} \tag{4.19}$$

In time language the last term involves time convolutions.

A further simplification follows from the observation that $\mathbf{j}(c)$ is an eigenfunction of $\Omega^{(1)}$ for almost all LGCA's, i.e., $\Omega^{(1)}\mathbf{j}(c)=-\lambda\mathbf{j}(c)$, where λ is positive. Consequently $\Omega^{(1)}$ in Eq. (4.19) may be replaced by the corresponding eigenvalue $-\lambda$. This certainly holds for all 4-, 8-, and 9-bits models on the square lattice [14,20,21], for all 6- and 7-bits models on triangular lattice [13], and for all versions of the FCHC models [14,22] in three- and four-dimensional lattices.

As the inverse Laplace transform of $[1-e^{-z}(1-\lambda)]^{-1}$ and $[1-e^{-z}(1-\lambda)]^{-2}$ are, respectively, $(1-\lambda)^t$ and $(t+1)(1-\lambda)^t$, the current correlation function in the ring approximation has the form

$$\phi(t)=(1-\lambda)^t\phi(0)+\kappa\sum_{\tau=1}^{t-1}\tau(1-\lambda)^{\tau-1}j(c_i)\Omega^{(2)}_{i12}R_{12,1'2'}(t-1-\tau)\Omega^{(2)}_{j1'2'}j(c_j)\ . \tag{4.20}$$

In fact the upper limit on the τ summation can be restricted to $\tau=t-2$ in systems with linear dimensions larger than two, because $R_{12,1'2'}(0)=0$ [see below Eq. (4.16)]. This shows again that the Boltzmann result $(1-\lambda)^t$ is exact for $t=2$. As this expression cannot be evaluated analytically, it will be computed numerically in a separate publication [23] for the VACF, and compared with existing simulation data.

The contribution from the ring integral to the total transport coefficient can be obtained from $\tilde{\Phi}(z)$ in Eq. (4.19) by setting $z=0$. This leads to a meaningful result for dimensionalities $d>2$. However, in two-dimensional systems $R(t)$ decays algebraically as $1/t$, as we shall see in the next section. Consequently, $\tilde{R}(z)$ diverges as $\ln(z)$ for $z\to 0$, which is in complete agreement with the fundamental observation for continuous fluids that Navier-Stokes-type hydrodynamics does not exist in two-dimensional systems.

V. LONG-TIME TAILS

In order to analyze the long-time behavior of the ring integral $R^{(\lambda)}(\mathbf{q},t)$ in Eqs. (4.6) and (4.7) we need the slow modes of the kinetic propagator $\hat{\Gamma}^0(\mathbf{q},t)$. We therefore introduce the kinetic eigenvalue problem [24],

$$L(\mathbf{q},z_\mu)a_\mu(\mathbf{q},\mathbf{c})=0\ . \tag{5.1}$$

With the help of Eq. (4.6) it can be rewritten, using ma-

trix notation, as

$$e^{-i\mathbf{q}\cdot\mathbf{c}}(1+\Omega^{(1)})a_\mu(\mathbf{q},\mathbf{c})=e^{z_\mu(q)}a_\mu(\mathbf{q},\mathbf{c}) . \tag{5.2}$$

Once the eigenvalue problem is solved, it follows directly from Eq. (4.9) that $a_\mu(\mathbf{q},\mathbf{c})$ is a *right* eigenfunction of the propagator, i.e.,

$$\hat{\Gamma}^0(\mathbf{q},t)a_\mu(\mathbf{q},\mathbf{c})=e^{z_\mu(q)t}a_\mu(\mathbf{q},\mathbf{c}) . \tag{5.3}$$

We note that $\hat{\Gamma}^0 S^{-1}$ is a symmetric matrix on account of Eq. (4.6). However, $\hat{\Gamma}^0$ is nonsymmetric, so its *left* eigenfunction is

$$\tilde{a}_\mu(\mathbf{q},\mathbf{c})=e^{i\mathbf{q}\cdot\mathbf{c}}a_\mu(\mathbf{q},\mathbf{c}) . \tag{5.4}$$

The spectral decomposition of $\hat{\Gamma}^0$ is then

$$\begin{aligned}\hat{\Gamma}^0_{ij}(\mathbf{q},t)&=\sum_\mu a_\mu(\mathbf{q},\mathbf{c}_i)e^{z_\mu(q)t}\tilde{a}_\mu(\mathbf{q},\mathbf{c}_j)\\&=\sum_\mu a_\mu(\mathbf{q},\mathbf{c}_i)e^{z_\mu(q)t}a_\mu(\mathbf{q},\mathbf{c}_j)e^{i\mathbf{q}\cdot\mathbf{c}_j} ,\end{aligned} \tag{5.5}$$

provided the normalization is chosen such that the Cartesian inner product is

$$a_\mu(\mathbf{q})\cdot a_\nu(\mathbf{q})\equiv\sum_{i=1}^{b} a_\mu(\mathbf{q},\mathbf{c}_i)a_\nu(\mathbf{q},\mathbf{c}_i)=\delta_{\mu\nu} . \tag{5.6}$$

The eigenvalue spectrum of the $b\times b$ matrix $\hat{\Gamma}^0$ contains $(d+1)$ slowly decaying ("soft") hydrodynamic modes with $z_\mu(q)\sim O(z)$ or $O(q^2)$ for small wave numbers (originating from particle and momentum conservation), and $(b-d-1)$ rapidly decaying kinetic modes with $z_\mu(q)\to-\lambda$ as $q\to 0$, where $-\lambda$ is an eigenvalue of $\Omega^{(1)}$ with $1/\lambda$ typically on the order of the mean free time t_0 between collisions. The hydrodynamic modes are linear combinations of the collision invariants $a(\mathbf{c}_i)=(1,\mathbf{c}_i)$.

The eigenvalue problem determined by Eq. (5.1) for the hydrodynamic modes was solved by Brito, Ernst, and Kirkpatrick [24] for small q. There are two sound modes, $(\sigma=\pm)$, $a_\sigma(q,c)=N_\sigma(\hat{\mathbf{q}}\cdot\mathbf{c}+\sigma c_0)$ with $z_\sigma(q)=-iq\sigma c_0-\gamma q^2$, and $(d-1)$ shear modes $a_{\eta i}(q,c)=N_\eta\hat{\mathbf{q}}_{\perp i}\cdot\mathbf{c}$ with $z_\eta(q)=-(\eta/\rho)q^2$, where N_μ is a normalization constant. The vectors $\{\mathbf{q},\mathbf{q}_{\perp i}, i=1,2,\ldots,d-1\}$ form an orthonormal set of unit vectors, with $\mathbf{q}=\mathbf{q}/q$. Furthermore, c_0 is the sound velocity, and η/ρ and γ are the Boltzmann values for the kinematic viscosity and the sound damping constant for the LGCA under consideration [24]. Both transport coefficients include the so-called *collision* and the *propagation* part [13,15].

If we restrict ourselves to the long-time behavior $(t\gg t_0)$ of the kinetic propagator given by Eq. (5.5) and the ring integrals of Eqs. (4.16) and (4.18), the kinetic modes in Eq. (5.5) can be neglected. The analysis below of the ring integral is very similar to the one for the continuous fluid [12].

Using the spectral decomposition given by Eq. (5.5) the simple ring integral $R^{(0)}$ in Eq. (4.16) can be written as

$$R^{(0)}_{12,1'2'}(\mathbf{q},t)=\frac{2\kappa}{V}\sum_{\mathbf{k}}\sum_{\mu\nu}a_\mu(\mathbf{k},\mathbf{c}_1)a_\nu(\mathbf{q}-\mathbf{k},\mathbf{c}_2)e^{[z_\mu(\mathbf{k})+z_\nu(\mathbf{q}-\mathbf{k})]t}a_\mu(\mathbf{k},\mathbf{c}_{1'})a_\nu(\mathbf{q}-\mathbf{k},\mathbf{c}_{2'}) , \tag{5.7}$$

where the $(\mu\nu)$ summations extend only over hydrodynamic modes. In Appendix B the following identity is proved for the hydrodynamic modes [to $O(q^0)$]:

$$\Omega^{(2)}_{i12}a_\mu(\mathbf{c}_1)a_\nu(\mathbf{c}_2)=-\frac{(1-2f)}{2f(1-f)}\Omega^{(1)}_{i1}a_\mu(\mathbf{c}_1)a_\nu(\mathbf{c}_1) . \tag{5.8}$$

It allows us to write Eq. (5.7), using $\kappa=f(1-f)$, as

$$\Omega^{(2)}_{i12}R^{(2)}_{12,1'2'}(\mathbf{q},t)\Omega^{(2)}_{j1'2'}=\Omega^{(1)}_{i1}R^{(0)}_{i1'}(\mathbf{q},t)\Omega^{(1)}_{1'j} , \tag{5.9}$$

and the ring integrals becomes

$$R^{(0)}_{ij}(\mathbf{q},t)=\frac{(1-2f)^2}{2f(1-f)}\frac{1}{V}\sum_{\mathbf{k}}\sum_{\mu\nu}a_\mu(\mathbf{k},\mathbf{c}_i)a_\nu(\mathbf{q}-\mathbf{k},\mathbf{c}_i)e^{[z_\mu(\mathbf{k})+z_\nu(\mathbf{q}-\mathbf{k})]t}a_\mu(\mathbf{k},\mathbf{c}_j)a_\nu(\mathbf{q}-\mathbf{k},\mathbf{c}_j) . \tag{5.10}$$

The above expression is essentially the mode-coupling result. It describes the long-time behavior of the ring integral for times t large compared to the mean free time t_0. For the time-correlation function given by Eq. (4.20) at times $t\gg t_0$ one should consistently neglect the first exponentially decaying term on the rhs of Eq. (4.19) and set $z=0$ in the first and last factor of the second term. Subsequently we substitute Eq. (5.9) into Eq. (4.20), and obtain the long-time behavior of the Green-Kubo correlation function in the simple ring approximation,

$$\begin{aligned}\phi(t)&\simeq\kappa\mathbf{j}\cdot R^{(0)}(\mathbf{0},t)\cdot\mathbf{j}\\&=\frac{1}{2V}\sum_{\mathbf{q}}\sum_{\mu,\nu}|A_{\mu\nu}(\mathbf{q})|^2e^{[z_\mu(\mathbf{q})+z_\nu(\mathbf{q})]t} .\end{aligned} \tag{5.11}$$

The amplitudes are given by

$$\begin{aligned}A_{\mu\nu}(\mathbf{q})&=(1-2f)\sum_i j(\mathbf{c}_i)a_\mu(\mathbf{q},\mathbf{c}_i)a_\nu(-\mathbf{q},\mathbf{c}_i)\\&=V^{-1}\langle J\psi_\mu(\mathbf{q})\psi_\nu(-\mathbf{q})\rangle .\end{aligned} \tag{5.12}$$

The result is *identical* to that of the phenomenological mode-coupling theory for arbitrary density. It has been used by Naitoh *et al.* [9] as the starting point for calculating the long-time tails of correlation functions in LGCA's. The second line in Eq. (5.12) quotes the expression of Naitoh *et al.*, where

$$\psi_\mu(\mathbf{q})=\sum_i a_\mu(\mathbf{q},\mathbf{c}_i)n_i(\mathbf{q})/\sqrt{\chi_{\mu\mu}}\ ,$$
$$\chi_{\mu\mu}=V^{-1}\langle\psi_\mu(\mathbf{q})\psi_\mu(-\mathbf{q})\rangle=f(1-f)\ . \tag{5.13}$$

A discussion of this result is given in the next section.

VI. CONCLUSION

This paper presents a kinetic theory description for fluid-type LGCA's that includes correlated collisions, which are absent in the mean-field-type Boltzmann equation. From these extensions we have obtained a number of interesting results.

(i) Time-correlation functions at time $t=2$ are exactly given by the Boltzmann-equation result, Eq. (3.11), provided the periodic box, containing the particles, is more than two lattice spacings wide in any space direction.

(ii) Due to the severe restriction of isotropy of fourth-rank tensors there exist only *quasi*-3D isotropic LGCA's, the so-called FCHC models [13,14], which are defined on a 3D slab, two lattice spacings wide in the fourth (unphysical) dimension. The geometric correlations given by Eq. (3.16), observed as deviations from the Boltzmann-equation result, appear to be finite-size effects related to the unphysical fourth dimension. The general formula for an arbitrary $(d-1)$ dimensional slab is given in Eq. (3.16) and the explicit evaluation for a 1D strip is given in Appendix A. In a planned separate paper [25] this result will be extended to the velocity-correlation function of a tagged particle and compared with the available 3D computer simulations.

(iii) Within the approximation of the ring kinetic equation we have calculated the current-current correlation function given by Eq. (4.20) in terms of the ring collision integral, Eq. (4.16). This integral has been evaluated numerically [23] for the triangular lattice-gas models, not only at short and intermediate times ($t=1,2,\ldots,20$), but also for asymptotically long times (say $t>20$), where the numerical results approach the long-time tails $1/t$ derived in Sec. V.

(iv) The phenomenological mode-coupling theory, Eqs. (5.10) and (5.11), for LGCA's has been derived from the fundamental microscopic theory, using the methods of kinetic theory.

We next make a number of comments and conclusions on the mode-coupling results for LGCA's. The kinetic theory derivation of the long-time behavior in LGCA's, as presented here, gives a much stronger result than in the case of continuous fluids. This LGCA kinetic theory result is valid for arbitrary density and identical to the result of the phenomenological mode-coupling theory. In continuous fluids, however, the corresponding kinetic theory derivation of Eq. (5.11) is only valid in the limit of low densities [12]. The mode-coupling result, Eq. (5.11), gives the well-known long-time tails $t^{-d/2}$ that have been discussed extensively in the literature [7–11] and are in good agreement with computer simulations of LGCA's for the VACF. For a further discussion of its consequences we refer to the literature [7–11].

In the derivation of the mode-coupling theory one needs to solve a kinetic eigenvalue problem defined by Eq. (5.1). Here we have restricted ourselves to modes that become soft [$z_\mu(q)\to 0$ as $q\to 0$]. In the analysis of Brito, Ernst, and Kirkpatrick [24], it was shown that there exist in many LGCA's additional spurious modes, for which the real part of $z_\mu(q)$ becomes soft, when q approaches special reciprocal-lattice vectors, usually located at the corners of the Brillouin zone. These modes must be included in the mode-coupling formula, Eq. (5.10). The present analysis can be simply extended to include such cases. The spurious soft modes give rise to additional long-time tails [11].

Finally it can be shown, starting from the spectral decomposition given by Eq. (5.5) and using an analysis similar to the one in Sec. V for the two-mode contributions, that the ring integral $R^{(\lambda)}$ in Eq. (4.18), involving λ one-particle propagators, reduces to a long-time result similar to (5.10), involving λ slow modes instead of just two. The leading long-time tail, however, is only determined by the two-mode terms. The three-mode contributions ($\lambda=3$) yield a subleading tail $\sim t^{-d}$.

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APPENDIX A

In this appendix we use Eq. (3.17) to calculate at time $t=2$ the correction to the Boltzmann value of the stress-stress correlation function for a quasi-one-dimensional strip of the FHP-I model. To this end we define the correlation function

$$\phi^{(l)}(t)=\mathbf{j}_i^{(l)}\hat{\Gamma}_{ij}(\mathbf{q}=\mathbf{0},t)\mathbf{j}_j^{(l)}\ , \tag{A1}$$

with $\mathbf{j}_i$ a momentum flux. For a two-dimensional system there are two independent fluxes,

$$\mathbf{j}_i^{(1)}=c_{ix}c_{iy} \tag{A2a}$$
$$\mathbf{j}_i^{(2)}=\tfrac{1}{2}(c_{ix}^2-c_{iy}^2)\ , \tag{A2b}$$

and we note that for a spatially isotropic two-dimensional system one has $\phi^{(1)}(t)=\phi^{(2)}(t)$. However, it is clear that for the finite 2D system shown in Fig. 1 one does not necessarily have $\phi^{(1)}(t)=\phi^{(2)}(t)$.

The second term in Eq. (3.17) gives the correction to the Boltzmann value of the stress-stress correlation function at $t=2$. We define this contribution by $\delta\phi^{(l)}(2)$. The

Eqs. (3.17) and (A1) and the discussion below Eq. (3.17) gives

$$\delta\phi^{(l)}(2)=4f(1-f)[(\mathbf{j}_i^{(l)}\Omega_{126}^{(2)})^2+(\mathbf{j}_i^{(l)}\Omega_{i35}^{(2)})^2] . \quad \text{(A3)}$$

The matrix elements $\Omega_{ijk}^{(2)}$ in Eq. (A3) have been tabulated in Ref. [15]. Using these results yields

$$\delta\phi^{(1)}(2)=0 , \quad \text{(A4a)}$$

$$\delta\phi^{(2)}(2)=18f^3(1-f)^5 . \quad \text{(A4b)}$$

APPENDIX B

In this appendix we indicate how Eq. (5.8) can be derived for a general LGCA. We begin by considering a particular binary collision, labeled a, operator for particles with velocity i and j for a generic b-bits LGCA,

$$I_i^{(a)}(f)=\left[\prod_{l\neq i,j}^{b}\bar{f}_l^*\right]f_i^*f_j^*-\left[\prod_{l\neq i,j}^{b}\bar{f}_l\right]f_if_j . \quad \text{(B1)}$$

Here $\bar{f}_i\equiv 1-f_i$, $f_i=f(\mathbf{c}_i)$ is a general nonequilibrium single-particle distribution function and the asterisk denotes post-collisional velocities. The factors $\bar{f}$ in Eq. (B1) enforce the Fermi exclusion rule. For reasons that will become clear, we next define

$$F_i=\frac{f_i}{\bar{f}_i} , \quad \text{(B2a)}$$

so that Eq. (B1) can be written

$$I_i^{(a)}(f)=\left[\prod_{l}^{b}f_l\right](F_i^*F_j^*-F_iF_j) . \quad \text{(B2b)}$$

Next, let us suppose that f is a (fermion) local equilibrium distribution of the form

$$f_i^{(LE)}=\frac{1}{1+\exp(\mathbf{b}\cdot\mathbf{a}_i)} . \quad \text{(B3)}$$

Here $\mathbf{a}_i$ ($=1$ or $\mathbf{c}_i$) is a collision invariant and $\mathbf{b}$ is the thermohydrodynamic variable conjugate to $\mathbf{a}_i$: $\mathbf{b}=b_{\text{eq}}+\delta b=\{\nu,\gamma\}$ with ν proportional to the chemical potential, γ proportional to the macroscopic flow velocity, and b_{eq} is the equilibrium value of $\mathbf{b}$.

To obtain a useful identity we use that $I_i^{(a)}$ vanishes if f is replaced by $f^{(LE)}$, as can be seen by using momentum conservation, and

$$F_i^{(LE)}=\exp(-\mathbf{b}\cdot\mathbf{a}_i) . \quad \text{(B4a)}$$

This gives

$$I_i^{(a)}(f^{(LE)})=0 . \quad \text{(B4b)}$$

We next use Eq. (B3) in Eq. (B2) and expand in powers of δb. To zeroth and linear order only trivial identities are obtained. To quadratic order one finds

$$(a_{\mu,i}^*a_{\nu,i}^*+a_{\mu,j}^*a_{\nu,j}^*-a_{\mu,i}a_{\nu,i}-a_{\mu,j}a_{\nu,j}) .$$
$$=-(a_{\mu,i}^*a_{\nu,j}^*+a_{\mu,j}^*a_{\nu,i}^*-a_{\mu,i}a_{\nu,j}-a_{\mu,j}a_{\nu,i}) . \quad \text{(B5)}$$

To make use of Eq. (B5) we relate this equation to the expansion given by Eq. (2.7). For our particular (ij) binary collision the operator $\Omega_{ij}^{(1)}$ in Eq. (2.7) is given by

$$\Omega_{ij}^{(a)}\delta f_j=f(1-f)^{b-3}(\delta f_i^*+\delta f_j^*-\delta f_i-\delta f_j) . \quad \text{(B6)}$$

Similarly, the operator $\Omega_{ijk}^{(2)}$ for the binary collision (ij) is

$$\Omega_{ijk}^{(a)}\delta f_j\delta f_k=-f(1-f)^{b-4}\left[\sum_k\delta f_k\right](\delta f_i^*+\delta f_j^*-\delta f_i-\delta f_j)$$
$$+f(1-f)^{b-4}[(\delta f_i^*)^2+(\delta f_j^*)^2-(\delta f_i)^2-(\delta f_j)^2]+(1-f)^{b-4}(\delta f_i^*\delta f_j^*-\delta f_i\delta f_j) . \quad \text{(B7)}$$

Now let us suppose that δf is a collision invariant. The first term on the rhs of Eq. (B7) then vanishes due to the conservation laws. The second term on the rhs of this equation is proportional to the linearized collision operator given by Eq. (B6). Similarly, Eq. (B5) can be used to relate the final term on the rhs to Eq. (B6). Combining these terms yields

$$\Omega_{i12}^{(a)}a_\mu(\mathbf{c}_i)a_\nu(\mathbf{c}_2)=-\frac{(1-2f)}{2f(1-f)}\Omega_{i1}^{(a)}a_\mu(\mathbf{c}_i)a_\nu(\mathbf{c}_1) . \quad \text{(B8)}$$

Summing over all possible binary collisions then proves Eq. (5.8) for this type of collision. The same consideration can be used to prove Eq. (5.8) for triple- and higher-order collisions.

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