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Hydrodynamics and Time Correlation Functions for Cellular Automata

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Hydrodynamic excitations in lattice gas cellular automata are described in terms of equilibrium time correlation functions for the local conserved variables. For large space and time scales the linearized hydrodynamic equations are obtained to Navier–Stokes order. Exact expressions for the associated susceptibilities and transport coefficients are identified in terms of correlation functions. The general form of the time correlation functions for conserved densities in the hydrodynamic limit is given and illustrated by some examples suitable for comparison with computer simulation. The transport coefficients are related to time correlation functions for the conserved fluxes in a way analogous to the Green–Kubo expressions for continuous fluids. The general results are applied for a one-component fluid and several types of binary diffusion. Also discussed are the effects of unphysical slow modes such as staggered particle or momentum densities.

KEY WORDS: Cellular automata; lattice gases; mode coupling theory; staggered modes; Green–Kubo relations; viscosity; diffusion.

1. INTRODUCTION

The discovery of lattice gas cellular automata capable of reproducing Navier–Stokes hydrodynamics as a continuum limit has opened a number of interesting lines of study (see ref. 1 for an overview of recent developments).(2) In one direction, it appears that solutions to the nonlinear hydrodynamic equations under various physical boundary conditions can be studied efficiently by construction of computing machines specialized to implement the simple dynamics of cellular automata (CA). Here, we consider a complementary use of CA as models to study the rela-

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tionship of macrodynamics to its underlying microdynamics for systems with many degrees of freedom. Thus, we take seriously the CA as models for a fluid, and apply standard methods of nonequilibrium statistical mechanics to investigate the conditions under which hydrodynamic equations can be expected to apply and the relationship of the parameters of these equations to the microdynamics. The use of continuous time lattice models (e.g., the lattice Lorentz gas) has proved fruitful in clarifying many aspects of fluid dynamics, such as anomalous memory effects in low dimensions. We believe the additional simplifications of CA will allow an even more penetrating analysis of how the macroscopic fluid dynamics results from its underlying microdynamics.

In the following we limit attention to CA that admit an equilibrium state and a relatively small number of globally conserved variables. We assume that "spurious" conserved variables arising from an oversimplified dynamics, but without physical significance, have been eliminated from the CA or otherwise isolated. In this context, the local microscopic conservation laws provide the basis for macroscopic hydrodynamics on a space and time scale large compared to that for the lattice. The class of CA considered here consist of point particles. This excludes certain other CA, such as the hard hexagon or MDMD model of Colvin *et al.*,(3) which include collisional transfer contributions not included in our description. For the analysis given here, no further details of the microdynamics is required. In particular, the results apply for both deterministic and stochastic dynamics. Also, we do not restrict the fluid to be isotropic, so that CA leading to hydrodynamics with lower symmetry than the Navier–Stokes equations are included in our discussion.

For states near equilibrium the deviations of the local conserved variables from their equilibrium values are expected to obey the linearized hydrodynamic equations (on the appropriate space and time scale). There is then a formally exact relationship of these deviations to the equilibrium space and time correlation function for the microscopic conserved densities that allows identification of linearized hydrodynamics with the long-time dynamics of the correlation functions. This relationship was first expressed in a general form by Onsager,(4) and has been exploited extensively to describe properties of both real and model fluids.(5–8) Our objective here is to show that the time correlation function method applies to CA as well, and to develop some of its consequences for this case.[3] Although the results are limited to linear hydrodynamic equations, a broad field of study is indicated in this context both by simulation of the correlation functions

[3] Preliminary reports of some of our results are given elsewhere.(9,10)

and their evaluation by standard many-body methods. In the last section, we discuss several qualitative and quantitative problems that would be of interest to address by this method.

In Section 2, the conserved variables and their correlation functions are introduced. The consequences of the conservation laws for the correlation functions are obtained and used to define a formally exact set of equations for the correlation functions. The continuum limit of these equations is then obtained to Navier–Stokes order (second order in the spatial gradients). The coefficients in this expansion are the thermodynamic susceptibilities (e.g., sound velocity) and the transport coefficients. In general, the susceptibilities can be evaluated exactly if there are no correlations between lattice sites in the equilibrium enesemble, as is true for all current CA considered. The hard-hexagon model(3) is an exception. The transport coefficients are given by discrete-time sums over time correlation functions for the fluxes associated with the conserved variables. This result is similar to the Green–Kubo expressions(11) for transport coefficients in real fluids or solids, with some important differences. The hydrodynamic limit of the correlation functions can be calculated from the solution to these linear equations, and some examples are given. We stress the importance of simulating these functions for low-dimensional systems where the hydrodynamics is expected to be anomalous.(12)

Section 3 is devoted to evaluation of the time correlation functions in the hydrodynamic limit (long time and large wavelength). Two cases are considered. The correlation functions of local conserved densities are expressed in terms of the hydrodynamic modes.(13) The second case considered is correlation functions of the conserved currents which characterize the Green–Kubo expressions for the transport coefficients. Their long-time dependence is calculated on the basis of hydrodynamic mode coupling theory,(12, 14, 15) retaining the dominant two-mode contribution. The formulation is general and includes the case of spurious slow modes (see Section 5).

In Section 4 application of the general results to CA models for a one-component fluid(16) is discussed, and expressions for the viscosities are obtained. Most of the results for transport coefficients in this section are new, although there are other derivations of Green–Kubo expressions in the literature for specific coefficients and specific models.(16–21) In many cases we find discrepancies with the results given here. These differences are also noted and discussed. Closest to our derivation is the projection operator method given recently by Zanetti,(22) who has obtained independently some of the results presented here.

As noted above, the simplicity of CA dynamics often leads to spurious conservation laws without physical significance at the macroscopic level.

However, they introduce additional slow modes and associated transport coefficients that must be accounted for. In Section 5 we consider the application of the time correlation function method to the description of such spurious conservation laws. Specifically, we describe the diffusive modes arising from the conservation of staggered momentum densities in the two-dimensional FHP model on a hexagonal lattice, discovered recently by Zanetti.(22) Green–Kubo expressions for new diffusion coefficients are obtained for lattice gases and for the FHP model. Some differences from the results of Zanetti are noted.

Several types of diffusion are considered in Section 6: tagged particle diffusion, diffusion in a two-color mixture of mechanically identical particles, and binary diffusion in a two-component mixture. Finally, a number of comments are offered in the last section to motivate further study of the correlation functions introduced here.

2. GREEN–KUBO RELATIONS

Hydrodynamics is a macroscopic manifestation of the microscopic conservation laws. We consider only CA fluids consisting of point particles. In that case the microscopic equation of motion for the occupation numbers has the general form

$$n(\mathbf{c}, \mathbf{r}+\mathbf{c}; t+1) = n(\mathbf{c}, \mathbf{r}; t) + I(c \mid n) \tag{2.1}$$

The nonlinear collision term $I(c \mid n)$ only takes the values 0, ± 1, and describes dynamics that can be deterministic or stochastic. Beyond this general form, no further restrictions are required on the collision term except that it supports a set of conservation laws (e.g., number, momentum) whose local densities are given by the vector $A(\mathbf{r}, t) = \{A_\alpha(\mathbf{r}, t)\}$,

$$A(\mathbf{r}, t) = \sum_c a(\mathbf{c})\, n(\mathbf{c}, \mathbf{r}; t) \tag{2.2}$$

Here $\mathbf{r}$ is the position vector of a lattice site, $\mathbf{c}$ is a velocity vector for a particle at that site, where $|\mathbf{c}|$ may take different values 0, 1, ..., and t is an integer-valued time. These local densities are constructed from collisional invariants, $a(\mathbf{c}) = \{a_\alpha(\mathbf{c})\}$ (e.g., mass $a_\alpha = 1$, momentum $a_\alpha = \mathbf{c}$), satisfying $\sum_c a(\mathbf{c})\, I(c \mid n) = 0$, and from the occupation number for the velocity state $\mathbf{c}$ on site $\mathbf{r}$ at time t, $n(\mathbf{c}, \mathbf{r}; t)$. The microscopic conservation law for the lattice gases can be written

$$\sum_c a(\mathbf{c})[n(\mathbf{c}, \mathbf{r}+\mathbf{c}; t+1) - n(\mathbf{c}, \mathbf{r}; t)] = 0 \tag{2.3}$$

The details of how the dynamics for $n(\mathbf{c}, \mathbf{r}; t)$ is generated and the structure of the lattice are unimportant for the analysis of this section. The only restriction beyond existence of the conserved variables A is an equilibrium distribution that is spatially uniform.(16) The results obtained here are therefore quite general, applying to both deterministic and stochastic dynamics, to lattices with anisotropic hydrodynamics, and to single-speed and multiple-speed models.

The matrix of equilibrium correlation functions for the conserved variables is defined by[4]

$$G(\mathbf{r}, t; \mathbf{r}', t') = \langle \delta A(\mathbf{r}, t)\, \delta A(\mathbf{r}', t') \rangle \tag{2.4}$$

with $\delta A = A - \langle A \rangle$. The brackets denote an average over the equilibrium distribution of values for $n(\mathbf{c}, \mathbf{r}; t) = 0$ or 1 for all $\mathbf{c}$ and $\mathbf{r}$. This distribution is taken to be stationary and has the translational invariance of the lattice. It follows that G depends only on the differences $\mathbf{r} - \mathbf{r}'$ and $t - t'$. A Fourier representation is introduced by

$$G(\mathbf{k}, t) = \sum_{\mathbf{r}} [\exp(-i\mathbf{k} \cdot \mathbf{r})]\, G(\mathbf{r}, t; \mathbf{0}, 0) = \langle A(\mathbf{k}, t) | A(\mathbf{k}) \rangle \tag{2.5}$$

where the inner product is defined as

$$\langle F | G \rangle = V^{-1} \langle \delta F\, \delta G^* \rangle \tag{2.6}$$

The asterisk denotes complex conjugation, $A(\mathbf{k}, t)$ is the Fourier transform of the conserved variable, and V is the total number of sites in the lattice.

These correlation functions describe the relaxation of spontaneous fluctuations in the equilibrium state. In addition, they represent the nonequilibrium dynamics of the average conserved variables for states near equilibrium through the relationship(5–8)

$$\langle \delta A(\mathbf{k}, t) \rangle_{\text{ne}} = G(\mathbf{k}, t)\, G^{-1}(\mathbf{k}, 0) \langle \delta A(\mathbf{k}, 0) \rangle_{\text{ne}} \tag{2.7}$$

where $\langle \delta A \rangle_{\text{ne}} = \langle A \rangle_{\text{ne}} - \langle A \rangle$ and $\langle \cdots \rangle_{\text{ne}}$ denotes an average over the initial nonequilibrium ensemble. The linearized hydrodynamic equations correspond to the dynamics of $\langle \delta A(\mathbf{k}, t) \rangle_{\text{ne}}$ for large t and small $\mathbf{k}$,

$$\left(\frac{\partial}{\partial t} + ik\Omega + k^2 \Lambda + \cdots \right) \langle \delta A(\mathbf{k}, t) \rangle_{\text{ne}} = 0 \tag{2.8}$$

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[4] This definition of G is the transpose of the correlation matrix introduced in ref. 10. It has the advantage of being more directly related to the response function and hydrodynamic modes [see (2.7) below]. However, since the eigenvalues of a matrix and its transpose are the same, the expressions for the transport coefficients and modes given in ref. 10 agree with those obtained here.

The time derivative occurs because (2.8) is valid only for large times in which a continuum limit applies. Also, the dots on the left side indicate terms higher order in k. Navier–Stokes-order hydrodynamics results from retaining only terms up through order k^2. The matrix Ω describes the reversible (Euler) dynamics, while Λ desicrbes Navier–Stokes-order dissipation. The elements of Λ are the transport coefficients. Comparison of Eqs. (2.7) and (2.8) shows that these matrices can be identified from an analysis of the equilibrium time correlation functions. This basic result is Onsager's regression hypothesis, that the long-time decay of long-wavelength components of the equilibrium fluctuations follows the macroscopic laws (2.8). The correlation function method is therefore an efficient way to obtain exact expressions for Ω and Λ without explicit consideration of the nonequilibrium state. This is in contrast to other methods based on a Chapman–Enskog expansion of the distribution function or on the Landau–Lifschitz method of fluctuating hydrodynamic equations with a Langevin force added.

The analysis is straightforward and makes use only of the conservation laws and stationarity. The details have been given elsewhere,(10) so only the primary results will be quoted here. There are three steps in the derivation. First, the discrete Laplace transform of $G(\mathbf{k}, t)$ is introduced by

$$\tilde{G}(\mathbf{k}, s) = \sum_{t=1}^{\infty} e^{-st} G(\mathbf{k}, t-1) \tag{2.9}$$

Next, the conservation laws are used to obtain a formally exact equation for $\tilde{G}$,

$$[e^s - 1 + L(\mathbf{k}, s)]\, \tilde{G}(\mathbf{k}, s) = G(\mathbf{k}, 0) \tag{2.10}$$

The matrix $L(\mathbf{k}, s)$ is given in terms of the correlation functions for the local conserved densities and their fluxes. The dispersion relation

$$\mathrm{Det}[e^s - 1 + L(\mathbf{k}, s)] = 0 \tag{2.11}$$

identifies the fluctuation spectrum for these correlation functions. The hydrodynamic excitations are defined to be those solutions to (2.11) for which $s = -\omega(k) \to 0$ as $\mathbf{k} \to 0$. Expanding to Navier–Stokes order (second order in k), Eq. (2.11) simplifies to

$$\mathrm{Det}[s + ik\Omega + k^2\Lambda] = 0 \tag{2.12}$$

The Euler matrix Ω and susceptibility matrix χ are given by

$$\Omega = \langle J | A \rangle \chi^{-1}, \qquad \chi \equiv \langle A | A \rangle \tag{2.13}$$

Here, J is the longitudinal current associated with the conserved density A, defined by

$$J(t) = \sum_{\mathbf{r},c} c_l a(\mathbf{c})\, \delta n(\mathbf{c}, \mathbf{r}; t), \qquad c_l = \hat{\mathbf{k}} \cdot \mathbf{c} \tag{2.14}$$

The transport or Navier–Stokes matrix Λ is given by the small-s limit of the Green–Kubo relation,

$$\Lambda(s) = \sum_{t=0}^{\infty}{}^{*}\, e^{-st}\phi(t) \equiv \sum_{t=0}^{\infty} e^{-st}\phi(t) - \frac{1}{2}\phi(0) \tag{2.15}$$

In writing (2.12) it has been assumed that $\Lambda(0)$ is bounded (for dimensionality $d \leqslant 2$ this is not the case; see Section 3). The asterisk indicates that the $t=0$ term has a weight of 1/2. Here we have introduced the matrix of current–current correlation functions,

$$\phi(t) = \langle J(t) \,|\, J \rangle \chi^{-1} - \Omega^2 = \langle \hat{J}(t) \,|\, \hat{J} \rangle \chi^{-1} \tag{2.16}$$

and used the relation $\langle J | A \rangle = \langle A | J \rangle$. Also, $\hat{J}$ denotes the "subtracted" flux,

$$\hat{J} = J - A \langle A | A \rangle^{-1} \langle A | J \rangle = J - A\Omega^{+} \tag{2.17}$$

The subtracted flux is seen to be that part of J that is orthogonal to the conserved densities A. As shown in ref. 10, the term $\phi(0)/2$ in (2.15) originates completely from the Euler or reversible part; in particular, a term $-\Omega^2/2$ comes from the small-s expansion of $e^s - 1 \simeq s + s^2/2$, where $s^2/2$ is replaced effectively by $-k^2\Omega^2/2$. This corresponds to eliminating the second time derivatives of slow hydrodynamic variables with the help of the Euler equations. The term $\Lambda^p \equiv -\phi(0)/2$ is referred to as the propagation part of the transport matrix. It is purely kinematic and only contains static correlations. We also note that the subtracted parts in Eqs. (2.15)–(2.17) are constant in time.

Equations (2.12)–(2.15) are the primary results of this section. They are exact expressions for the matrices in the hydrodynamic equations (2.8) in terms of equilibrium correlation functions, provided the small-s limit of $\Lambda(s)$ remains finite. The dispersion relations (2.12) show that the matrix of correlation functions $G(\mathbf{k}, t) = \langle A(\mathbf{k}, t) \,|\, A(\mathbf{k}) \rangle$ obeys for long times and small k the linear equations

$$\left(\frac{\partial}{\partial t} + ik\Omega + k^2 \Lambda \right) G(\mathbf{k}, t) = 0 \tag{2.18}$$

This in turn yields the linearized hydrodynamic equations (2.8)

The evaluation of the susceptibility and Euler matrices χ and Ω is easily performed for a given CA since the occupation numbers for different states $\{\mathbf{c}, \mathbf{r}\}$ at equal times are uncorrelated in the equilibrium state,(16)

$$\langle \delta n(\mathbf{c}, \mathbf{r})\, \delta n(\mathbf{c}', \mathbf{0}) \rangle = K\, \delta_{\mathbf{r},\mathbf{0}}\, \delta_{c,c'}, \qquad K = f(1-f) = \rho(b-\rho)/b^2 \tag{2.19}$$

Here f and $\rho = bf$ are the average occupation per state $\{\mathbf{c}, \mathbf{r}\}$ and per site $\mathbf{r}$, respectively, where b is the number of velocity states per site. The relation (2.19) guarantees that the susceptibility matrix χ and the Euler matrix Ω are k independent,

$$\chi_{\alpha\beta} \equiv \langle A_\alpha(\mathbf{k}) \,|\, A_\beta(\mathbf{k}) \rangle = K \sum_c a_\alpha(c)\, a_\beta(c) \tag{2.20}$$

$$(\Omega\chi)_{\alpha\beta} = \langle J_\alpha(\mathbf{k}) \,|\, A_\beta(\mathbf{k}) \rangle = K \sum_c c_l a_\alpha(c)\, a_\beta(c) \tag{2.21}$$

Further reduction of χ and Ω requires specification of the *CA*. Evaluation of the matrix Λ for the transport coefficients is more difficult and involves a detailed analysis of the many-body dynamics.

3. HYDRODYNAMIC MODES AND MODE COUPLING THEORY

In this section the long-time and long-wavelength limits of time correlation functions are calculated using methods developed for continuous fluids. For the correlation matrix of conserved densities $G(\mathbf{k}, t)$, this simply involves solution to the linearized hydrodynamic equations (2.18). Evaluation of the current correlation functions $\langle \hat{J}(t) \,|\, \hat{J} \rangle$ in this limit is somewhat more difficult. Here we apply the mode coupling theory of Kadanoff and Swift(14) developed for critical dynamics and adapted by Ernst *et al.*(15) for fluids away from critical points. The basic idea is that products of two, three,..., microscopic fluctuations $\delta A(\mathbf{k}, t)\, \delta A(\mathbf{q}, t)$... are slow modes of the system with hydrodynamic components contributing to the current correlation functions.

We first consider the hydrodynamic modes by diagonalizing the matrix in Eq. (2.18), assuming for the time being that $\Lambda(s)$ remains finite as $s \to 0$ (this can be assured by considering a large but finite system, although possibly at the expense of some system-size dependence; see discussion below). The eigenvalues are the roots $s = -\omega_\mu$ of the secular equation, where μ labels l modes if Eq. (2.12) is an $l \times l$ determinant. If $L(\mathbf{k}, s)$ in (2.11) and $\Lambda(s)$ in (2.12) are regular functions of k and s at small values of their arguments, then the roots of the secular equations (2.11) and (2.12) can be expanded in a power series in k,

$$\omega_\mu(k) = ic_\mu k + \lambda_\mu k^2 \tag{3.1}$$

where c_μ is the sound velocity of a propagating mode and λ_μ is the damping constant or diffusivity. It is possible to show that the sound velocities are real and that the damping constants, given in the form of Green–Kubo expressions, are positive.(8) For diffusive modes $c_\mu = 0$. The corresponding right and left eigenfunctions are to lowest order in k linear combinations of the conserved densities (2.1) that are specified below. They are defined by

$$\begin{aligned}(ik\Omega + k^2\Lambda)\,\psi^\mu(\mathbf{k}) &= \omega_\mu(k)\,\psi^\mu(\mathbf{k})\\ (ik\Omega + k^2\Lambda)^+\,\tilde{\psi}^\mu(\mathbf{k}) &= \omega_\mu^*(k)\,\tilde{\psi}^\mu(\mathbf{k})\end{aligned} \tag{3.2}$$

These eigenfunctions form a biorthogonal set $\psi^\nu_\alpha(k)[\tilde{\psi}^\mu_\alpha(\mathbf{k})]^* = \delta_{\mu\nu}$, Also , it is easily shown that $\psi^\mu_\alpha(\mathbf{k}) = \chi_{\alpha\beta}\tilde{\psi}^\mu_\beta(\mathbf{k})$, to the relevant order in k. An associated set of phase functions is constructed from the same linear combinations of the conserved densities that diagonalize the macroscopic hydrodynamic equations,

$$|\psi^\mu\rangle = \tilde{\psi}^\mu_\alpha\,|A_\alpha\rangle, \qquad |\tilde{\psi}^\mu\rangle = (\tilde{\psi}^\mu_\alpha)^*\,|A_\alpha\rangle \tag{3.3}$$

with the property $\langle\psi^\mu|\tilde{\psi}^\nu\rangle = \delta_{\mu\nu}$. Explicit expressions for the coefficients $\tilde{\psi}^\mu_\alpha$ are given in the next section. Since they turn out to be real, there is no distinction between $|\psi^\mu\rangle$ and $|\tilde{\psi}^\mu\rangle$, and the tilde can be deleted. If the matrix (2.4) is written as

$$G(\mathbf{k}, t) = \langle A(\mathbf{k}, t)\,|\,A(\mathbf{k})\rangle \equiv \langle A(\mathbf{k})|\,\mathscr{I}_t\,|A(\mathbf{k})\rangle \tag{3.4}$$

then its time evolution for large t can be represented as

$$\mathscr{I}_t \simeq \sum_\mu |\psi^\mu(\mathbf{k})\rangle\, e^{-\omega_\mu(k)t}\langle\psi^\mu(\mathbf{k})| \tag{3.5}$$

Equation (3.4) with the long-time approximation (3.5) is the Landau–Placzek theory(13) for CA fluids,

$$G_{\alpha\beta}(\mathbf{k}, t) = \sum_\mu M^\mu_{\alpha\beta}(\mathbf{k})e^{-\omega_\mu(k)t} \tag{3.6}$$

where the single-mode strength factors are

$$M^\mu_{\alpha\beta}(\mathbf{k}) = \langle A_\alpha(\mathbf{k})\,|\,\psi^\mu(\mathbf{k})\rangle\langle\psi^\mu(\mathbf{k})\,|\,A_\beta(\mathbf{k})\rangle \tag{3.7}$$

Since the matrix Ω is easily determined for any given CA, it is straightforward to determine the sound velocities and eigenvectors. Calculation of the transport coefficients is more difficult since it requires analysis of the time evolution of the CA. Equations (2.14) and (3.3) provide an appropriate formulation of transport that is suitable for study both by simulation and analytical means.

Equation (3.6) shows that the correlation functions $G_{\alpha\beta}(\mathbf{k}, t)$ provide a direct probe of linearized hydrodynamics by simulation of fluctuations in the equilibrium state. Present efforts are directed primarily at simulation of various nonequilibrium states with emphasis on effects due to nonlinear hydrodynamics. Here we want to stress the complementary problem of determining the form of linearized hydrodynamics in low dimensions. The simple structure of (3.1) is valid only if the transport coefficients λ_i exist in the $s \to 0$ limit indicated in (2.14). However, for fluid-type models with dimensionality $d \leqslant 2$ it is expected that the transport coefficients diverge in this limit for an unbounded system, or that $L(\mathbf{k}, s)$ in (2.11) or $\Lambda(s)$ in (2.12) are nonanalytic functions of s at the origin.

Related correlation functions that have been studied by simulation are the single-site correlation functions $G(\mathbf{r}, t; \mathbf{r}, 0) \equiv C(t)$, which are space independent due to translational invariance. These correlation functions can be written in a form suitable for study of their hydrodynamic limit as

$$C(t) \equiv V^{-1} \sum_{\mathbf{k}} G(\mathbf{k}, t) \tag{3.8}$$

where the $\mathbf{k}$ summation extends over the first Brillouin zone. The long-time behavior of this function should be dominated by the contributions from small k, for which the hydrodynamic limit (3.5) applies. The expression (3.6) gives directly

$$C_{\alpha\beta}(t) = V^{-1} \sum_{\mathbf{k}, \mu} M^{\mu}_{\alpha\beta}(\mathbf{k}) e^{-\omega_\mu(k) t} \tag{3.9}$$

The strength factors $M^{\mu}_{\alpha\beta}$ can be calculated from (3.7) once the CA fluid is specified and the local conserved densities are identified. Purely diffusive modes (with $c_\mu = 0$) contribute in (3.9) terms proportional to $t^{-d/2}$; the terms involving sound modes decay faster. We note that this long-time tail is characteristic of single-site correlation functions, which decay like the solution of a diffusion equation evaluated at the origin. This tail is not related to the so-called "long-time tails" of the current–current correlation functions (2.15), which originate from a coupling of two hydrodynamic modes. The former tail is contained already in the low-density Boltzmann approximatin; the latter is not. One needs a kinetic equation with additional many-particle collisions (ring collisions).

In the preceding part of this section we have been assuming that the

Navier–Stokes transport coefficients exist and that the hydrodynamic propagators, defined as

$$G_{\mu}(\mathbf{k}, t) = \langle \psi^{\mu}(\mathbf{k}, t) | \psi^{\mu}(\mathbf{k}) \rangle, \qquad G_{\mu}(\mathbf{k}, 0) = 1 \tag{3.10}$$

decay as pure exponentials in the long-wavelength limit. For dimensionality $d \leqslant 2$ this need not be true. In the remaining part of this section we formulate a self-consistent mode coupling theory in terms of these propagators. This is obtained in two steps. First, the Laplace transform of the propagators is expressed in terms of the eigenvalues as $[s + ikc_{\mu} + k^2 \lambda_{\mu}(\mathbf{k}, s)]\, \tilde{G}_{\mu}(\mathbf{k}, s) = 1$, where $\lambda_{\mu}(\mathbf{k}, s)$ may depend on the direction of $\mathbf{k}$ but not its magnitude. Next, the eigenvalues are expressed as functionals of $G_{\mu}(\mathbf{k}, t)$ through an asymptotic analysis of the Green–Kubo expressions for $\lambda_{\mu}(\mathbf{k}, s)$. These two expressions then must be solved simultaneously.

Within the present context, it is straightforward to extend the mode coupling theory developed for continuous fluids to CA fluids to determine the long-wavelength, long-time behavior of the current–current correlation function matrix associated with the Green–Kubo expressions (2.15),

$$\langle \hat{J}(\mathbf{k}, t) | \hat{J}(\mathbf{k}) \rangle = \langle \hat{J}(\mathbf{k}) | \mathscr{I}_t | \hat{J}(\mathbf{k}) \rangle$$

The currents may still depend on the direction $\hat{k}$ of the wavevector $\mathbf{k}$ but not on its length. Mode coupling theory is a generalization of (3.5) that identifies the slow dynamics of a variable with its dependence on the local conserved densities and their products. Since the currents $\hat{J}$ are orthogonal to linear combinations of these densities, it is necesssary to retain terms up through bilinear combinations,

$$\begin{aligned} \mathscr{I}_t \simeq & \sum_{\mu} |\psi^{\mu}(\mathbf{k})\rangle\, G_{\mu}(\mathbf{k}, t) \langle \psi^{\mu}(\mathbf{k})| \\ & + (2V)^{-1} \sum_{\mathbf{q}, \mu, \nu} |[\psi^{\mu}(\mathbf{q})\, \psi^{\nu}(\mathbf{k}-\mathbf{q})]\rangle\, G_{\mu}(\mathbf{q}, t)\, G_{\nu}(\mathbf{k}-\mathbf{q}, t) \\ & \times \langle [\psi^{\mu}(\mathbf{q})\, \psi^{\nu}(\mathbf{k}-\mathbf{q})]| + \cdots \end{aligned} \tag{3.11}$$

Here, $[\psi\psi]$ denotes the part of $\psi\psi$ orthognal to $|1\rangle$ and $|\psi\rangle$. The long-time behavior of the current–current correlation function is therefore given by

$$\langle \hat{J}_{\alpha}(\mathbf{k}, t) | \hat{J}_{\beta}(\mathbf{k}) \rangle \to (2V)^{-1} \sum_{\mathbf{q}, \mu, \nu} M^{\mu\nu}_{\alpha\beta}(\mathbf{q}, \mathbf{k}-\mathbf{q})\, G_{\mu}(\mathbf{q}, t)\, G_{\nu}(\mathbf{k}-\mathbf{q}, t) \tag{3.12}$$

where the two-mode strength factors are

$$M^{\mu\nu}_{\alpha\beta}(\mathbf{q}, \mathbf{l}) = \langle \hat{J}_{\alpha}(\mathbf{k}) | \psi^{\mu}(\mathbf{q})\, \psi^{\nu}(\mathbf{l}) \rangle \langle \psi^{\mu}(\mathbf{q})\, \psi^{\nu}(\mathbf{l}) | \hat{J}_{\beta}(\mathbf{k}) \rangle \tag{3.13}$$

The hydrodynamic eigenvalues (3.1) and Green–Kubo relations above presume the existence of the small-s limit for $\Lambda(s)$. This is always possible to assure for finite geometry, but the limit may not exist in the large-system-size limit. The source of this difficulty lies in the assumption that the hydrodynamic eigenvalues are analytic in the wavevector k. More generally, the eigenvalue equation (3.2) representing the dispersion relations for the slow excitations must be replaced by the implicit equation

$$\{ik\Omega + k^2\Lambda[\hat{k}, -\omega_\mu(k)]\}\,\psi^\mu(\mathbf{k}) = \omega_\mu(k)\,\psi^\mu(\mathbf{k}) \tag{3.14}$$

where $\Lambda[\hat{k}, s]$ denotes the (possibly nonanalytic) small-s behavior of the Navier–Stokes matrix (2.12) at $s = 0$. To solve this equation, the asymptotic time dependence of the current correlation function $\phi(t)$ can be described using the mode coupling result (3.12). The equation for the hydrodynamic modes is then found to be

$$\begin{aligned}
\omega_\mu(k) &= ic_\mu k + \lambda_\mu(k)k^2 \\
\lambda_\mu(k) &= \lambda_\mu^b + \frac{1}{2}\sum_{t=0} \exp[\omega_\mu(k)t] \\
&\qquad \times \sum_{\mathbf{q},\rho,\nu} A_\mu^{\rho\nu}(\mathbf{q}, \mathbf{k}-\mathbf{q})\, G_\mu(\mathbf{q}, t)\, G_\nu(\mathbf{k}-\mathbf{q}, t)
\end{aligned} \tag{3.15}$$

$$A_\mu^{\rho\nu}(\mathbf{q}, \boldsymbol{l}) = (\tilde{\psi}_\alpha^\mu)\, M_{\alpha\beta}^{\rho\nu}(\mathbf{k}, \boldsymbol{l})\psi_\beta^\mu \tag{3.16}$$

Here $M_{\alpha\beta}^{\rho\nu}$ is the mode couppling amplitude given by (3.13) and λ_μ^b is the "bare" transport coefficient arising from the faster dynamical excitations. The self-consistent equation (3.15) is to be solved for asymptotically small k, and leads to a nonanalytic dependence(7) on k of the hydrodynamic eigenvalues (3.14).

The results of Sections 2 and 3 represent the linearized hydrodynamic modes, susceptibilities, and transport coefficients in their most general form, provided the transport coefficients exist. The hydrodynamic description for the long-time behavior of time correlation functions has also been extended to CA fluids. No specific dimension, lattice structure, or CA dynamics is implied. In subsequent sections, these results are applied to specific models of current interest.

4. SINGLE-COMPONENT FLUID

To illustrate the above results in more detail, we consider a lattice gas for a simple one-component fluid. A restriction to complete isotropy is not necessary and one could include in the discussion both the FHP(16) and HPP(17) models, as we have shown in a preliminary publication.(9) Here, however, we will restrict ourselves to systems where tensors up to fourth rank have the full fluid isotropy. The collisional invariants are those associated with conservation of particle number and all components of the momentum,

$$a_\alpha(c) = \begin{cases} a_n = 1 \\ a_l = \hat{\mathbf{k}} \cdot \mathbf{c} = c_l \\ a_t = \hat{\boldsymbol{\varepsilon}}_t \cdot \mathbf{c} = c_t \qquad (t = 3, \ldots, d+1) \end{cases} \tag{4.1}$$

where $\{\hat{\mathbf{k}}, \hat{\boldsymbol{\varepsilon}}_3, \ldots, \hat{\boldsymbol{\varepsilon}}_{d+1}\}$ is a set of d orthonormal unit vectors. The slow variables are the local densities $A_\alpha(\mathbf{k}, t) = \sum_c a_\alpha(c)\, \hat{\mathbf{n}}(\mathbf{c}, \mathbf{k}; t)$, with $\alpha = \{n, l, t\}$. We assume that all unphysical conservation laws have been eliminated (see, however, Section V) so that (4.1) form the complete set. We first calculate the susceptibility matrix, using (2.20) and (4.1). It is diagonal, $\chi_{\alpha\beta} = \chi_\alpha \delta_{\alpha\beta}$, with

$$\chi_n = \langle A_n | A_n \rangle = bK, \qquad \chi_l = \langle A_l | A_l \rangle = c_0^2 \chi_n, \qquad \chi_t = \chi_l \tag{4.2}$$

where b is the number of velocity states per site, including a possible zero-velocity state (rest particle). Also, c_0 is defined as $bdc_0^2 = \sum_c c^2$ and will appear to be the sound velocity. The constant K is defined in (2.19). The Euler matrix follows from Eq. (2.21) and has only two nonvanishing elements,

$$\langle J_n | A_l \rangle = \langle J_l | A_n \rangle = c_0^2 \chi_n, \qquad \Omega_{nl} = 1, \qquad \Omega_{ln} = c_0^2 \tag{4.3}$$

The eigenvalues and eigenfunctions represent two propagating sound modes, labeled with $\sigma = \pm$, and $d - 1$ nonpropagating shear modes, labeled with t as in (4.1). For dimensionality $d > 2$ the Navier–Stokes transport coefficients exist and the eigenvalues are, for small k,[5]

$$\omega_\sigma(k) = i\sigma c_0 k + \Gamma k^2, \qquad \omega_t(k) = \nu k^2 = (\eta/\rho) k^2 \tag{4.4}$$

and the corresponding eigenfunctions are

$$\begin{aligned} |\psi^\sigma(\mathbf{k})\rangle &= \{c_0 \, |A_n(\mathbf{k})\rangle + \sigma \, |A_l(\mathbf{k})\rangle\}/(2\chi_l)^{1/2} \\ |\psi^t(\mathbf{k})\rangle &= |A_t(\mathbf{k})\rangle/(\chi_l)^{1/2} \end{aligned} \tag{4.5}$$

The subtracted fluxes associated with these eigenfunctions are defined by (2.17), and found to be

$$\begin{aligned} &\hat{J}_n(\mathbf{k}, t) = 0, \qquad \hat{J}_\sigma(\mathbf{k}, t) = \sigma(2\chi_l)^{-1/2} \sum_{\mathbf{r}, c} (c_l^2 - c_0^2)\, \delta n(\mathbf{c}, \mathbf{r}; t) \\ &\hat{J}_t(\mathbf{k}, t) = \chi_l^{-1/2} \sum_{\mathbf{r}, c} c_t c_l \, \delta n(\mathbf{c}, \mathbf{r}; t) \end{aligned} \tag{4.6}$$

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[5] Note that the viscosity defined through $\eta = \rho\nu$ differs from the usual one by a factor $1/v_0$ where v_0 is the volume of the unit cell and ρ is its filling fraction. In the FHP-model $v_0 = \sqrt{3}/2$.

with $\delta n = n - \langle n \rangle$. The sound damping constant Γ and the kinematic viscosity $\nu = \eta/\rho$ follow from (2.14) as the small-s limit of

$$\begin{aligned} \lambda_\sigma(s) = \Gamma(s) &= \sum_{t=0}^{\infty}{}^{*}\, e^{-st} \langle \hat{J}_\sigma(t) \,|\, \hat{J}_\sigma \rangle \\ \lambda_t(s) = \nu(s) &= \sum_{t'=0}^{\infty}{}^{*}\, e^{-st'} \langle \hat{J}_t(t') \,|\, \hat{J}_t \rangle \end{aligned} \tag{4.7}$$

These are the Green–Kubo relations for the one-component CA fluid.

The results (4.7) can be expressed in terms of two scalar viscosities characterizing a viscosity tensor, defined by

$$\eta_{ijlm}(s) = (\rho/\chi_l) \sum_{t=0}^{\infty}{}^{*}\, e^{-st} \langle \hat{J}_{ij}(t) \,|\, \hat{J}_{lm} \rangle \tag{4.8}$$

with the tensor $\hat{J}_{ij}$ given by

$$\hat{J}_{ij}(t) = \sum_{\mathbf{r}, c} (c_i c_j - c_0^2 \delta_{ij})\, \delta n(\mathbf{c}, \mathbf{r}; t) \tag{4.9}$$

The fluxes appearing in Eq. (4.8) are simply related to $\hat{J}_{ij}$ by $(2\chi_l)^{1/2} \hat{J}_l = \hat{k}_i \hat{k}_j \hat{J}_{ij}$ and $\chi_l^{1/2} \hat{J}_t = \hat{\varepsilon}_{ti} \hat{k}_j \hat{J}_{ij}$. Since the fourth-rank tensor η_{ijlm} has the full fluid symmetry, it can be expressed in terms of two independent scalars,

$$\eta_{ijlm} = \eta \left(\delta_{il}\, \delta_{jm} + \delta_{im}\, \delta_{jl} - \frac{2}{d} \delta_{ij}\, \delta_{lm} \right) + \xi\, \delta_{ij}\, \delta_{lm} \tag{4.10}$$

It is easily shown that

$$\Gamma = (2\rho)^{-1} \left[\frac{2(d-1)}{d} \eta + \xi \right] \qquad \text{and} \qquad \nu = \frac{\eta}{\rho}.$$

which identifies η as the shear viscosity and ξ as the bulk viscosity. The Green–Kubo relations for these transport coefficients are therefore given by the small-s limits of

$$\eta(s) = \frac{1}{(d-1)(d+2)} \frac{\rho}{\chi_l} \sum_{t=0}^{\infty}{}^{*}\, e^{-st} \langle \hat{J}_{ij}^0(t) \,|\, \hat{J}_{ij}^0 \rangle \tag{4.11}$$

$$\xi(s) = d^{-2} \frac{\rho}{\chi_l} \sum_{t=0}^{\infty}{}^{*}\, e^{-st} \langle \hat{J}_{ii}(t) \,|'\, \hat{J}_{jj} \rangle \tag{4.12}$$

Here, $\hat{J}_{ij}^0$ denotes the traceless part of $\hat{J}_{ij}$, and a summation convention over repeated indicies is implied.

Several observations can be made from these results. As expected, the shear viscosity vanishes in one dimension. The bulk viscosity vanishes in all dimensions for single-speed models, since $c^2 = dc_0^2 = 1$. This is similar to the case of continuous fluids, where the bulk viscosity vanishes in the absence of statistical correlations (low density, no internal states). For the specific case of the FHP I model, the parameters are $d = 2$, $b = 6$, and $c_0 = 1/\sqrt{2}$. Equation (4.11) then reduces to a result obtained by Rivet for the shear viscosity.(18) The FHP II and III models include a rest particle, so $b = 7$. In this case Eq. (4.11) does not agree with that given by Rivet. Instead, his expression actually represents $\eta + \frac{1}{2}\zeta$. Recently, Zanetti(22) has obtained expressions for the viscosities. His expressions for the shear and bulk viscosities are equivalent to ours.

In Table I we list for the FHP models the values of the propagation parts of the transport coefficients $A^p_{\alpha\beta} = -\phi_{\alpha\beta}(0)/2$ defined below Eq. (2.17). The results agree with those obtained by d'Humieres and Lallemand.(23)

Qian *et al.*(24) have considered a one-dimensional lattice gas CA with five velocities per site ($c = 0, \pm 1, \pm 2$; $b = 5$). There are two collisional invariants ($a_n = 1$, $a_l = c$) and $c_0^2 = 2$. Since the shear viscosity is zero, the bulk and longitudinal viscosities are equal and given by (4.12) with

$$J_{ii}(t) = \sum_{r,c} (c^2 - 2)\, \delta n(c, r; t) \tag{4.13}$$

The corresponding correlation function (4.12) in one dimension is expected to diverge strongly as $s \to 0$ due to memory effects (mode coupling). The resulting sound damping at long wavelengths then will be anomalous.

To illustrate the hydrodynamic result (3.6) for the single-component fluid, we quote the behavior of autocorrelation functions of mass and momentum densities at small k and large t values,

$$\begin{aligned} G_{ll}(\mathbf{k}, t) &= c_0^2 G_{nn}(\mathbf{k}, t) = c_0^2 \chi_n \cos(c_0 k t) e^{-\Gamma k^2 t} \\ G_{tt}(\mathbf{k}, t) &= c_0^2 \chi_n e^{-\nu k^2 t} \end{aligned} \tag{4.14}$$

Table I

Property	FHP I	FHP II, III
b	6	7
c_0	$1/\sqrt{2}$	$\sqrt{3/7}$
$\nu^p = \eta^p/\rho$	$-1/8$	$-1/8$
ξ^p/ρ	0	$-1/28$
κ_1^p	$-1/8$	$-1/8$
κ_2^p	$-1/4$	$-1/4$

A closely related function that has been considered in recent computer simulations on lattice gas cellular automata$^{(3,25)}$ is the single-site velocity correlation function, or correlation function of the flow field, defined as

$$\psi(t) = (dV)^{-1} \sum_{\mathbf{r}} \langle \mathbf{g}(\mathbf{r}, 0) \cdot \mathbf{g}(\mathbf{r}, t) \rangle \tag{4.15}$$

where $\mathbf{g}(r, t) = \sum_c \mathbf{c}n(\mathbf{c}, \mathbf{r}; t)$ is the momentum density. By decomposing $\mathbf{g}$ into contributions from the densities in (4.1), we can write $\psi(t)$ in terms of the hydrodynamic modes [see Eq. (3.9)],

$$\begin{aligned} \psi(t) &= (dV)^{-1} \sum_{k} [(d-1)\, G_{tt}(\mathbf{k}, t) + G_{ll}(\mathbf{k}, t)] \\ &\sim \frac{d-1}{d} c_0^2 \chi_n (4\pi \nu t)^{-d/2} \\ &\quad + d^{-1} c_0^2 \chi_n (4\pi \Gamma t)_1^{-d/2} F_1 \left(\frac{d}{2}, \frac{1}{2}; \frac{-c_0^2 t}{4\Gamma} \right) \end{aligned} \tag{4.16}$$

The k summation in the first equality extends over the first Brillouin zone. For large systems this sum may be replaced by an integration over $\mathbf{k}$ with weight $v_0 V/(2\pi)^d$, where v_0 is the volume of the unit cell. The k integral over G_{ll}, given in the second equality of (4.16), can be identified as a confluent hypergeometric function ${}_1F_1$. The confluent hypergeometric function ${}_1F_1$ decays exponentially for $d =$ odd and algebraically for $d =$ even.$^{(26)}$ For example, with $d = 2$ and "bare" Boltzmann–Enskog values for the transport coefficients,$^{(23)}$ the dominant shear and sound mode contributions are, respectively, $v_0 c_0^2 \chi_n / 8\pi \nu t$ and $-v_0 \chi_n / 4\pi t^2$. The last term is purely kinematic.

5. STAGGERED DENSITIES AS SLOW MODES

Due to the discrete structure of the phase space and the simplified dynamics there exist spurious conservation laws in the HPP and FHP models. For instance, if only binary collisions are allowed, the total momentum along every lattice line is a global invariant. By adding triple collisions, these unphysical conservation laws are eliminated in the FHP model.

However, there exist other classes of global invariants for the CA fluids on which computer simulations have been performed. As a simple example, consider a CA Lorentz gas, where a single particle is moving with unit speed on a square lattice. A fraction ρ of its sites, chosen at random, is occupied by immobile scatterers. The dynamics (deterministic or stochastic) of the moving particle is described by the occupation number $n(\mathbf{c}, \mathbf{r}; t)$ which satisfies number conservation (2.1). If the sites of the square lattice are denoted by $\mathbf{r} = r_x \mathbf{c}_1 + r_y \mathbf{c}_2$, then (given appropriate boundary conditions), the lattice can be divided into two sublattices, depending on whether $\mathbf{r} \cdot \boldsymbol{\beta} = r_x + r_y$ is even or odd, where $\boldsymbol{\beta} = (1, 1)$. Obviously, all particles at time t on one sublattice will be on the other sublattice at time $t + 1$, independent of the scattering rules and independent of the density of scatterers. The difference $\Delta(t)$ between the total number of particles on the odd and even sublattices changes in time as $(-1)^t$ and the global invariant is

$$H = \sum_{\mathbf{r}, c} (-1)^{t + \mathbf{r} \cdot \boldsymbol{\beta}} n(\mathbf{c}, \mathbf{r}; t).$$

The staggered particle density

$$h(\mathbf{r}, t) = \sum_{c} (-1)^{t + \mathbf{r} \cdot \boldsymbol{\beta}} n(\mathbf{c}, \mathbf{r}; t)$$

is a slowly varying quantity that satisfies (2.1). In the large-time and large-wavelength limits, this density satisfies a diffusion equation. The corresponding diffusion coefficient is again given by a Green–Kubo relation, which will be given in Section 6.3. This invariant does not exist on the hexagonal lattice. Similarly, one has for the HPP model on the square lattice as spurious invariants the total staggered number and momentum of the particles,

$$H' = \sum_{\mathbf{r}, c} (-1)^{t + \mathbf{r} \cdot \boldsymbol{\beta}} a(\mathbf{c}) \, n(\mathbf{c}, \mathbf{r}; t)$$

where $a(\mathbf{c}) = \{1, \mathbf{c}\}$.

Recently Zanetti$^{(22)}$ has constructed similar global invariants for the FHP fluid that can be understood from the following one-dimensional example of a fluid with speeds $|c| = 0$ and $|c| = 1$ only. If momentum is conserved in collisions, then

$$H'' = \sum_{r, c} (-1)^{t + r} c n(c, r; t)$$

is a global invariant. Adding particles with speed $|c| = 2$ destroys this invariant. For a more extensive discussion on different types of global invariants in lattice gases we refer to d'Humieres *et al.*$^{(28)}$

For the FHP fluid there are $b = 7$ velocity states per site: $\mathbf{c}_0 = 0$ (rest particle) and $\mathbf{c}_a = \{\cos[\pi(a-1)/3], \sin[\pi(a-1)/3]\}$, with $a = 1, 2, ..., 6$. In this case Zanetti has constructed three global invariants of the type indicated above,

$$H_\beta \equiv \sum_{\mathbf{r}} h_\beta(\mathbf{r}, t) = \sum_{\mathbf{r}, c} (-1)^{t+\hat{\boldsymbol{\beta}}\cdot\mathbf{r}}\, \hat{\boldsymbol{\beta}} \cdot \mathbf{c}n(\mathbf{c}, \mathbf{r}; t) \tag{5.1}$$

where $\boldsymbol{\beta} = \{\boldsymbol{\beta}_1, \boldsymbol{\beta}_2, \text{ or } \boldsymbol{\beta}_3\}$ represents a reciprocal lattice vector with $\boldsymbol{\beta}_a \cdot \mathbf{c}_a = 0$ and $\boldsymbol{\beta}_a \cdot \mathbf{c}_{a\pm 1} = -\boldsymbol{\beta}_a \cdot \mathbf{c}_{a\pm 2} = \pm 1$. Here, $\hat{\boldsymbol{\beta}}$ is a unit vector parallel to $\boldsymbol{\beta}$. Since $\boldsymbol{\beta}_a \cdot \mathbf{r}$ is an integer, it allows us to divide the lattice rows, parallel to $\mathbf{c}_a$, into an even and an odd sublattice. The total $\boldsymbol{\beta}$ momentum on the even sublattice at time t is on the odd sublattice at time $t+1$. Adding particles with speed $|c| \neq 0$ and $|c| \neq 1$ will again destroy this invariant.

The time correlation function of two different staggered momentum densities

$$h_\beta(\mathbf{r}, t) = (-1)^{t+\boldsymbol{\beta}\cdot\mathbf{r}}\, \hat{\boldsymbol{\beta}} \cdot \mathbf{g}(\mathbf{r}, t)$$

at two different space-time points is not translational invariant because of the two sublattices involved. We consider instead its spatial average as the relevant time correlation function for conserved densities to be used in Eq. (5), namely,

$$\begin{aligned} G_{\beta\beta'}(\mathbf{r}, t) &= V^{-1} \sum_{\mathbf{r}'} \langle A_\beta(\mathbf{r} + \mathbf{r}', t)\, A_{\beta'}(\mathbf{r}', 0) \rangle \\ &= (-1)^{t+\boldsymbol{\beta}\cdot\mathbf{r}} \langle g_\beta(\mathbf{r}, t)\, g_{\beta'}(\mathbf{0}, 0) \rangle\, \delta_{\beta\beta'} \end{aligned} \tag{5.2}$$

where $g_\beta = \hat{\boldsymbol{\beta}} \cdot \mathbf{g}$. In the second equality we have used the relation

$$V^{-1} \sum_{r} (-1)^{(\boldsymbol{\beta}+\boldsymbol{\beta}')\cdot\mathbf{r}} = \delta_{\beta\beta'}$$

We will show here that this correlation function satisfies a diffusion equation in the long-wavelength limit,

$$[s + k^2 \Lambda_\beta(\hat{k}, s)]\, \tilde{G}_{\beta\beta}(\mathbf{k}, s) = G_{\beta\beta}(\mathbf{k}, 0) = \chi_t \tag{5.3}$$

where the small-s limit of $\Lambda_\beta(\hat{k}, s)$ is the diffusivity of the staggered mode. Zanetti has derived Green–Kubo relations for these spurious transport coefficients. As we find partial disagreement with his results, we also apply our method to these staggered densities, defined in (5.2). We do so by extending the set of three slow variables (4.1) for the FHP model $A_\alpha(\mathbf{k}, t)$ with $\alpha = \{n, l, t\}$ to include the additional three staggered densities,

$$\begin{aligned} A_\beta(\mathbf{k}, t) &= (-1)^t \sum_{\mathbf{r}, c} [\exp(-i\mathbf{k} \cdot \mathbf{r}) \exp(-\boldsymbol{\beta} \cdot \mathbf{r}\pi i)]\, \hat{\beta} \cdot \mathbf{c}n(\mathbf{c}, \mathbf{r}; t) \\ &= (-1)^t \sum_{c} \hat{\boldsymbol{\beta}} \cdot \mathbf{c}\hat{n}(\mathbf{c}, \mathbf{k} + \pi\boldsymbol{\beta}; t) \end{aligned} \tag{5.4}$$

where $\pi\boldsymbol{\beta}_1$, $\pi\boldsymbol{\beta}_2$, and $\pi\boldsymbol{\beta}_3$ denote corners of the first Brillouin zone or Wigner–Seitz cell on the reciprocal lattice.

Next we consider the 6×6 matrices χ, Ω, and Λ in Eqs. (2.13) and (2.14). The susceptibility matrix remains diagonal and we add to the results (4.2),

$$\chi_\beta = \langle A_\beta | A_\beta \rangle = c_0^2 \chi_n = \chi_l \tag{5.5}$$

For the Euler matrix we have in addition to the results (4.3),

$$\Omega_{\alpha\beta} = \Omega_{\beta\beta'} = 0 \tag{5.6}$$

with $\alpha = \{n, l, t\}$ and $\beta, \beta' = \{\beta_1, \beta_2, \beta_3\}$. It follows from (2.17) and (5.6) that the subtracted currents $\hat{J}_\alpha$ in (4.6), with $\alpha = (n, l, t)$, do not couple to the staggered densities, and are orthogonal to all conserved densities. Therefore the Green–Kubo relations (4.7)–(4.12) for the standard transport coefficients remain valid. It also follows that the currents J_β for the staggered densities have no subtracted component, i.e., in the limit as $|\mathbf{k}| \to 0$,

$$\begin{aligned} \hat{J}_\beta(\hat{k}, t) &= J_\beta(\hat{k}, t) \\ &= \sum_{\mathbf{r}, c} (-1)^{t + \boldsymbol{\beta}\cdot\mathbf{r}}\, \hat{k}\cdot\mathbf{c}\, \hat{\beta}\cdot\mathbf{c}\, \delta n(\mathbf{c}, \mathbf{r}; t) \end{aligned} \tag{5.7}$$

and are also orthogonal to all conserved densities. Next, consider the Navier–Stokes matrix for the transport coefficients Λ. Consider first the submatrix $\Lambda_{\beta\beta'}$. The associated current, given by (5.7), is written in terms of the local microscopic stress,

$$J_\beta(t) = \sum_{\mathbf{r}} (-1)^{t + \boldsymbol{\beta}\cdot\mathbf{r}}\, \hat{k}_i \hat{\beta}_j \sigma_{ij}(\mathbf{r}, t) \tag{5.8}$$

$$\sigma_{ij}(\mathbf{r}, t) = \sum_{c} c_i c_j\, \delta n(\mathbf{c}, \mathbf{r}; t) \tag{5.9}$$

The current correlation function defining $\Lambda_{\beta\beta'}$ is then

$$\begin{aligned} \langle \hat{J}_{\beta'}(t) | \hat{J}_\beta \rangle = V^{-1} &\sum_{\mathbf{r}, \mathbf{r}'} (-1)^{t + \boldsymbol{\beta}\cdot\mathbf{r} + \boldsymbol{\beta}'\cdot\mathbf{r}'} \\ &\times \hat{k}_i \hat{k}_m \hat{\beta}'_j \hat{\beta}_n \langle \sigma_{ij}(\mathbf{r}', t)\, \sigma_{mn}(\mathbf{r}, 0) \rangle \end{aligned} \tag{5.10}$$

Use of translational invariance and the relation

$$V^{-1} \sum_{r} (-1)^{(\boldsymbol{\beta} + \boldsymbol{\beta}')\cdot\mathbf{r}} = \delta_{\beta\beta'}$$

shows

$$\begin{aligned} &\Lambda_{\beta\beta'} = \Lambda_\beta(\hat{k}, s)\, \delta_{\beta\beta'} \\ &\Lambda_\beta(\hat{k}, s) = (\chi_\beta)^{-1} \sum_{t=0}^{*} e^{-st} \sum_{\mathbf{r}} (-1)^{t+\boldsymbol{\beta}\cdot\mathbf{r}} \\ &\qquad \times \hat{k}_i \hat{k}_m \hat{\beta}_j \hat{\beta}_n \langle \sigma_{ij}(\mathbf{0}, 0)\, \sigma_{mn}(\mathbf{r}, t)\rangle \end{aligned} \tag{5.11}$$

It can be shown in a similar fashion that $\Lambda_{\alpha\beta} = \Lambda_{\beta\alpha} = 0$, for $\alpha = \{n, l, t\}$ and $\beta = \{\beta_1, \beta_2, \beta_3\}$. It is clear from (5.11) that the diffusion coefficients Λ_β are in fact components of a fourth-rank tensor associated with the stress autocorrelation function. By arguments similar to those used in the reduction of (4.8) we obtain the $\hat{k}$-dependendent diffusion coefficients,

$$\Lambda_\beta(\hat{k}, s) = \kappa_1(s) + \kappa_2(s)(\hat{\mathbf{k}} \cdot \hat{\boldsymbol{\beta}})^2 \tag{5.12}$$

with Green–Kubo relations for the scalar coefficients,

$$\begin{aligned} \kappa_1(s) &= (4\chi_l)^{-1} \sum_{t=0}^{*} e^{-st} \sum_{\mathbf{r}} (-1)^{t+\boldsymbol{\beta}\cdot\mathbf{r}} \\ &\qquad \times \langle \sigma^0_{ij}(\mathbf{0}, 0)\, \sigma^0_{ij}(\mathbf{r}, t)\rangle \\ \kappa_2(s) &= (4\chi_l)^{-1} \sum_{t=0}^{*} e^{-st} \sum_{\mathbf{r}} (-1)^{t+\boldsymbol{\beta}\cdot\mathbf{r}} \\ &\qquad \times \langle \sigma_{ii}(\mathbf{0}, 0)\, \sigma_{jj}(\mathbf{r}, t)\rangle \end{aligned} \tag{5.13}$$

where σ^0_{ij} denotes the traceless part of σ_{ij} [compare with (4.11) and (4.12) for $d = 2$].

There is a significant difference between Zanetti's result for $\kappa_1 + \kappa_2$ and ours. His expression for the staggered current density appears with σ_{ij} in (5.9) replaced by $\sum_c (c_i c_j - c_0^2\, \delta_{ij})\, \delta n(\mathbf{c}, \mathbf{r}; t)$. Then, for example, his staggered current components involving σ_{ii} and associated transport coefficients vanish for the single-speed FHP model, whereas ours are nonzero. The difference persists for the FHP II and III models as well. The propagation parts for the new diffusion coefficients are $\Lambda^p_{\beta\beta'} = -\frac{1}{2}\phi_{\beta\beta'}(0)$, as defined below (2.17). Table I shows the results for κ^p_1 and κ^p_2 for the FHP models. Our results agree with those of Zanetti, but his equations fail to satisfy the relation $\kappa^p_2 = -\frac{1}{2}\phi_{\kappa_2}(0)$.

6. BINARY DIFFUSION

In this section three types of diffusion are considered. The first is diffusion in a mixture of colored particles, the second is a mixture of particles with different mass, while the third is Lorentz gases and tagged particle diffusion. The color mixture is defined by starting from a lattice gas of identical "white" particles that obey the exclusion principle (no two particles can occupy simultaneously the same state, $\{\mathbf{c}, \mathbf{r}\}$). Next, a particle is painted red with probability x. This system then can be in thermal equilibrium in all respects except for the color distribution. It is somewhat different from a regular binary mixture in lattice gas models, whose exclusion rules are described by occupation numbers $c_1(\mathbf{c}, \mathbf{r}; t)$ and $n_2(\mathbf{c}, \mathbf{r}; t)$ for the two types of particles. In the regular mixture two particles of different types can be in the same state; this is forbidden in the color mixture. The Boolean variables describing the microscopic state will be slightly different in the two cases, as seen below. A Lorentz gas may be considered as a limiting case of a binary mixture with very different masses, vanishing concentration of light (moving) particles, and a finite concentration of heavy (immobile) scatterers. Since the concentration of moving particles is infinitesimal, the interaction between moving particles can be neglected and the exclusion rule for double occupancy removed. Attention then can be restricted to a single moving particle. Exactly the same derivation applies to a tagged particle moving in a gas of untagged particles.

6.1. Color Mixture

To describe the color mixture, a Boolean color variable $\sigma(\mathbf{c}, \mathbf{r}; t) = 1$ for red and 0 for white is associated with every *occupied* velocity state [i.e., $n(\mathbf{c}, \mathbf{r}; t) = 1$]. For density ρ and red particle fraction x we have

$$\rho = \sum_c \langle n(\mathbf{c}, \mathbf{r}; t)\rangle, \qquad \rho x = \sum_c \langle n(\mathbf{c}, \mathbf{r}; t)\, \sigma(\mathbf{c}, \mathbf{r}; t)\rangle \tag{6.1}$$

In addition to the conservation laws (2.2) for total particle number and momentum, there is a conservation law for red particle number,

$$\sum_c \left[n(\mathbf{c}, \mathbf{r}+\mathbf{c}; t+1)\, \sigma(\mathbf{c}, \mathbf{r}+\mathbf{c}; t+1) - n(\mathbf{c}, \mathbf{r}; t)\, \sigma(\mathbf{c}, \mathbf{r}; t)\right] = 0 \tag{6.2}$$

In the single-component case the time correlation function for fluctuations of $\delta n(\mathbf{c}, \mathbf{r}; t)$ is the basic quantity in which all transport properties can be expressed. Here it is necessary to consider the microscopic color fluctuation, defined by

$$\delta\sigma(\mathbf{c}, \mathbf{r}; t) = n(\mathbf{c}, \mathbf{r}; t)[\sigma(\mathbf{c}, \mathbf{r}; t) - x] \tag{6.3}$$

The equal time variance is given by

$$\langle \delta\sigma(\mathbf{c}, \mathbf{r}; t)\, \delta\sigma(\mathbf{c}', \mathbf{r}'; t)\rangle = K'\, \delta_{\mathbf{r},\mathbf{r}'}\, \delta_{c,c'} \tag{6.4}$$

with

$$K' = fx(1-x) = \rho x(1-x)/b \tag{6.5}$$

The variables $\delta\sigma$ and δn are uncorrelated in the sense $\langle \delta n(\mathbf{c}, \mathbf{r}; t)\, \delta\sigma(\mathbf{c}', \mathbf{r}'; t)\rangle = 0$, as follows from (6.3).

The matrix formulation of hydrodynamic fluctuations in Section 2 applies to the color mixture if an additional hydrodynamic variable $\delta A_\sigma(r, t) = \sum_c \delta\sigma(\mathbf{c}, \mathbf{r}; t)$, is included for the local color fluctuation. The corresponding matrices Λ and Ω do not couple this new variable to the dynamics of the mass and momentum fluctuations. Furthermore, $\Omega_{\sigma\sigma}$ vanishes. Therefore, the additional hydrodynamic equation is a diffusion equation,

$$\left(\frac{\partial}{\partial t} + k^2 D_\sigma\right) G_{\sigma\sigma}(\mathbf{k}, t) = 0 \tag{6.6}$$

where

$$G_{\sigma\sigma}(\mathbf{k}, t) = \langle A_\sigma(\mathbf{k}, t) \,|\, A_\sigma(\mathbf{k})\rangle \tag{6.7}$$

The diffusion coefficient for the colored mixture is given by the small-s limit of the Green–Kubo expression,

$$D_\sigma(s) = (d\chi_0 V)^{-1} \sum_{t=0}^{\infty}{}^{*}\, e^{-st} \langle \mathbf{I}_\sigma(t) \cdot \mathbf{I}_\sigma\rangle \tag{6.8}$$

where $\chi_\sigma = \langle A_\sigma | A_\sigma\rangle = bK'$ and K' is defined in (6.5), and where the subtracted flux $\mathbf{I}_\sigma$ is defined by

$$\mathbf{I}_\sigma(t) = \sum_c \mathbf{c}\, n(\mathbf{c}, \mathbf{r}; t)[\sigma(\mathbf{c}, \mathbf{r}; t) - x] \tag{6.9}$$

Equations (6.8) and (6.9) have a structure analogous to those for the continuous fluid case.$^{(8)}$

6.2. Regular Binary Mixture

In the regular binary mixture, local density conservation holds separately for the total mass density of each species, $\sum_c m_s n_s(\mathbf{c}, \mathbf{r}; t)$, with $s = 1$ or 2. The average for each species is denoted by ρ_s, with $\rho = \rho_1 + \rho_2$. In addition, there is conservation of the total momentum density $\sum_{s,c} m_s \mathbf{c}_s n_s(\mathbf{c}, \mathbf{r}; t)$. To describe the model, it is convenient to consider linear combinations of the basic fluctuations defined to be the total mass density fluctuation $\delta\mu$ and a concentration fluctuation δx given by

$$\begin{aligned} \delta\mu(\mathbf{c}, \mathbf{r}; t) &= \sum_s m_s\, \delta n_s(\mathbf{c}, \mathbf{r}; t) \\ \delta x(\mathbf{c}, \mathbf{r}; t) &= (m_1/\chi_1)\, \delta n_1(\mathbf{c}, \mathbf{r}; t) - (m_2/\chi_2)\, \delta n_2(\mathbf{c}, \mathbf{r}; t) \end{aligned} \tag{6.10}$$

where $\chi_s = m_s^2\langle [\delta n(\mathbf{c}, \mathbf{0})]^2\rangle = m_s^2 f_s(1 - f_s)$, with $f_s = \langle n_s\rangle$. The equal time fluctuations are

$$\begin{aligned} \langle \delta\mu(\mathbf{c}', \mathbf{0})\, \delta\mu(\mathbf{c}, \mathbf{r})\rangle &= \delta_{\mathbf{r},\mathbf{0}}\, \delta_{c,c'}\chi \\ \langle \delta\mu(\mathbf{c}', \mathbf{0})\, \delta x(\mathbf{c}, \mathbf{r})\rangle &= 0 \\ \langle \delta x(\mathbf{c}', \mathbf{0})\, \delta x(\mathbf{c}, \mathbf{r})\rangle &= \delta_{\mathbf{r},\mathbf{0}}\, \delta_{c,c'}(\chi')^{-1} \end{aligned} \tag{6.11}$$

where $\chi = \chi_1 + \chi_2$ and $(\chi')^{-1} = \chi_1^{-1} + \chi_2^{-1}$.

The matrix form of hydrodynamic fluctuations in Section 2 is again applicable if the additional hydrodynamic variable $\delta A_x(\mathbf{r}, t) = \sum_c \delta x(\mathbf{c}, \mathbf{r}; t)$ is include. From here on the arguments are very similar to those preceding Eq. (6.7). The only nonvanishing element of Ω connecting the concentration fluctuations δx with fluctuations in the total mass and momentum densities is

$$\Omega_{xl}\chi_l = \hat{k}\cdot\langle \mathbf{J}_x | A_l\rangle = \sum_c (c_1^2 - c_2^2)/d \tag{6.12}$$

Here $\{\mathbf{c}_s\}$ refers to members of the set of b_s lattice vectors corresponding to allowed velocities in species s. If a rest particle is allowed, the vector $\mathbf{c}_s = \mathbf{0}$ is included in the set. Since in general $\mathbf{c}_1 \neq \mathbf{c}_2$, Ω_{xl} is nonvanishing and the longitudinal momentum fluctuations couple to the concentration fluctuations. The proper diffusion coefficient is then obtained by diagonalization of Ω to identify the new hydrodynamic diffusion mode.

For the sake of illustration we now restrict attention to a special case by imposing two simplifying restrictions: (i) the number of velocity states per site is the same for each species, $b_1 = b_2 = b$, yielding $\langle A_x | A_x\rangle = b/\chi'$, and (ii) the mean speed per site $v_s^2 = (db)^{-1}\sum_c c_s^2$ is the same for each species, i.e., $v_1 = v_2 = c_0$. Consequently, $\Omega_{xl} = 0$ and the concentration fluctuation decouples from the other hydrodynamic modes just as for the color diffusion case. The time correlation function $\langle A_x(t) | A_x\rangle$ satisfies a diffusion equation like (6.6) with diffusion coefficient $D(s)$ given by

$$D(s) = (\chi'/bdV) \sum_{t=0}^{\infty}{}^{*}\, e^{-st}\langle \mathbf{I}_x(t)\cdot\mathbf{I}_x\rangle \tag{6.13a}$$

$$= (bd\chi'V)^{-1} \sum_{t=0}^{\infty}{}^{*}\, e^{-st}\langle \mathbf{I}_1(t)\cdot\mathbf{I}_1\rangle \tag{6.13b}$$

The fluxes are given by

$$\mathbf{I}_x(t) \equiv \sum_{\mathbf{r},c} [(m_1\mathbf{c}_1/\chi_1)\, n_1(\mathbf{c}, \mathbf{r}; t) - (m_2\mathbf{c}_2/\chi_2)\, n_2(\mathbf{c}, \mathbf{r}; t)] \tag{6.14a}$$

$$\mathbf{I}_s(t) \equiv \sum_{s'} \sum_{\mathbf{r},c} \left(\delta_{ss'} - \frac{\chi_s}{\chi}\right) m_{s'}\mathbf{c}_{s'} n_{s'}(\mathbf{c}_{s'}, \mathbf{r}; t) \tag{6.14b}$$

with s and $s' = 1, 2$. The equality (6.13b) can be deduced from (6.13a) after some rearrangements using $\mathbf{I}_1 + \mathbf{I}_2 = 0$. The subtracted current in the diffusion coefficient for a binary mixture of continuous fluids$^{(8)}$ differs from (6.14b) in that χ_s/χ is replaced by ρ_s/ρ. This difference can be traced to the lack of equipartition between different species in the lattice gas models to the exclusion rule for two identical particles in the same state, $\{\mathbf{c}_{s'}, \mathbf{r}\}$.

Equations (6.13b) and (6.14a) do not reduce to the diffusion coefficient for the color mixture, given by Eqs. (6.8) and (6.9), if the masses are taken equal $(m_1 = m_2)$ and species 1 is considered "red" and species 2 is considered "white." The reason is that this limit allows a red and white particle to be in the same state, whereas the color mixture does not.

6.3. Lorentz Gas and Tagged Particle Diffusion

In this case the dynamics of a *single* particle (stochastic or deterministic) is described by the occupation number $n(\mathbf{c}, \mathbf{r}; t)$, with the conservation law

$$\sum_{c} [n(\mathbf{c}, \mathbf{r} + \mathbf{c}; t + 1) - n(\mathbf{c}, \mathbf{r}; t)] = 0 \tag{6.15}$$

The only hydrodynamic variable is then $A(\mathbf{r}, t) = \sum_c n(\mathbf{c}, \mathbf{r}; t)$. The equal time correlation of occupation numbers is now simply

$$\langle n(\mathbf{c}', \mathbf{0})\, n(\mathbf{c}, \mathbf{r}) \rangle = (bV)^{-1}\, \delta_{cc'}\, \delta_{\mathbf{r},\mathbf{0}}$$

The correlation function of tagged particle densities or van Hove self-correlation function is then

$$G(\mathbf{k}, t) = \sum_{\mathbf{r},\mathbf{r}'} \sum_{c,c'} \{\exp[-i\mathbf{k}\cdot(\mathbf{r} - \mathbf{r}')]\} \times \langle n(\mathbf{c}', \mathbf{r}': 0)\, n(\mathbf{c}, \mathbf{r}; t) \rangle \tag{6.16}$$

with a susceptibility matrix $\chi(\mathbf{k}) = G(\mathbf{k}, 0) = 1$. Following the analysis of Section 2, it is found to obey a diffusion equation with diffusion coefficient given by the small-s limit of

$$\begin{aligned} D(s) &= d^{-1} \sum_{t=0}^{\infty}{}^{*}\, e^{-st} \langle \mathbf{v}(t)\cdot\mathbf{v}(0) \rangle \\ \mathbf{v}(t) &= \sum_{\mathbf{r},c} \mathbf{c}\, n(\mathbf{c}, \mathbf{r}; t) \end{aligned} \tag{6.17}$$

This expression has already been used in the literature.(27) From the discussion in Section 5 on staggered densities it follows immediately that the staggered density (5.1) in the Lorentz gas on a hypercubic lattice is a slow diffusive mode. The corresponding diffusivity $\kappa(s)$ can be derived in an analogous manner as (5.13). The explicit form of $\kappa(s)$ is obtained from (6.17) by inserting the factor $(-1)^{\boldsymbol{\beta}\cdot(\mathbf{r}+\mathbf{r}')}$ in the summand, where $\boldsymbol{\beta}=(1, 1, 1,..., 1)$ is a d-dimensional vector. This is a new result.

In principle, tagged particle diffusion is a limiting case of the color mixture with a vanishing fraction of tagged "red" particles. This limit is somewhat subtle. However, the above derivation can be repeated verbatim after replacing "moving particle" by "tagged particle." The attractiveness of the method of Section 2 is that the details of the dynamics do not enter in the derivation, and it is not necessary to specify whether the untagged particles are moving or fixed. Therefore, the Green–Kubo relation for the tagged particle diffusion coefficient is also given by Eq. (6.17).

In existing simulations of tagged-particle diffusion in lattice gas cellular automata(29) the diffusion coefficient has been obtained from the mean square displacement, $\langle[\mathbf{r}(t)-\mathbf{r}(0)]^2\rangle \rightarrow 2dDt$, as $t\rightarrow\infty$. Equation (6.17) offers an alternative for direct simulation.

7. DISCUSSION

The time correlation function method developed for continuous fluids has been shown to apply as well to cellular automata. The method focuses attention on time correlation functions for the local conserved densities, which are related to the linearized hydrodynamics for the system considered. The primary results obtained here and some of their implications are summarized in the following comments.

1. The derivation of the linearized hydrodynamic equations and identification of the corresponding sound speeds, susceptibilities, and transport coefficients is quite general. It applies to deterministic and stochastic dynamics, to single-speed and multispeed models (including rest particles), and to lattices for which the macroscopic equations may not have fluid isotropy. The only condition on the dynamics is the existence of local conservation laws (2.2) and an equilibrium state. The specific applications considered here include the FHP models with fluid symmetry, multispeed models (such as FHP II and III and the one-dimensional model of Qian *et al.*(24)), and several cases of binary mixtures. In ref. 9 we have also given the viscosities for the HPP model that does not have fluid symmetry. In this last case our Green–Kubo expression for the longitudinal viscosity

differs from that of ref. 17 by an overall factor and the presence of the propagation part.

2. The space- and time-dependent correlation functions for the conserved variables were determined for long times and small wave vectors by solution of the hydrodynamic equations. These results are valid under the assumption that the transport coefficients exist (see below), which may require that the latter become system-size dependent. Direct simulation of these equilibrium time-dependent fluctuations would provide measurement of both the hydrodynamic modes and the associated coefficients. The related, but k-independent, single-site correlation functions already have been simulated,$^{(25)}$ and have the asymptotic algebraic decay given by Eq. (4.16). It is of interest to illustrate different types of long-time behavior by discussing the single-site correlation function $G_{\beta\beta}(\mathbf{r}=\mathbf{0}, t)$ of the staggered densities, defined in (5.1) for the two-dimensional FHP model. The long-time, long-wavelength (coarse-grained) behavior is given by, according to (3.8), (3.9), and (5.3),

$$G_{\beta\beta}(\mathbf{r}=\mathbf{0}, \mathbf{t}) = V^{-1} \sum_{\mathbf{k}} G_{\beta\beta}(\mathbf{k}, t) \to V^{-1} \sum_{\mathbf{k}} \chi_l \exp[-k^2 \Lambda^0_\beta(\hat{k}) t]$$

$$\simeq v_0 \chi_l [(\kappa_{01} + \kappa_{02})\kappa_{01}]^{-1/2} (4\pi t)^{-1}$$

Here the bare diffusivities $\Lambda^0_\beta(\hat{k}) = \kappa_{01} + \kappa_{02}(\hat{\mathbf{k}} \cdot \hat{\boldsymbol{\beta}})^2$ have been used. The single-site correlation function has additional *fine-grained, long-time behavior*, resulting from the undamped oscillatory staggered modes. This behavior is seen from the identity $G_{\beta\beta}(\mathbf{r}=\mathbf{0}, t) = (-1)^t \psi(t)$, where $\psi(t)$ is the single-site velocity correlation function whose long-time behavior is given in (4.1). Therefore, we obtain a contribution

$$G_{\beta\beta}(\mathbf{r}=\mathbf{0}, t) \simeq v_0 \chi_l (-1)^t (8\pi v_0 t)^{-1}$$

where v_0 is the bare viscosity. The factor $(-1)^t$ is due to a high-frequency undamped mode at $\mathbf{k}=0$, similar to the plasmon mode in a one-component plasma. When coarse graining this fine-grained oscillatory behavior, it yields a vanishing contribution.

3. The transport coefficients are given by formally exact expressions analogous to the Green–Kubo formulas for continuous fluids. They are discrete time sums over time correlation functions of so-called subtracted fluxes, in which the first term at $t=0$ has a relative weight 1/2. Alternatively, if this last restriction is removed, there appears a negative contribution of 1/2 the $t=0$ term, which has been called the "propagation" part of the transport coefficient. It is a vestige of the discrete space-time of the CA that persists at the macroscopic level. The derivation here shows

that no particular significance should be attributed to this part of the transport coefficient. The name "propagating part" is actually inappropriate, as it falsely suggests a relationship with the free-streaming motion of the particles. This is not the case. Such a term is even present in standard random walk models on a uniform lattice. This can be seen by taking the forward-time derivative of Einstein's formula for the mean square displacement and by transforming it into a velocity correlation function by defining a particle velocity as $\mathbf{v}(t) = \Delta_t \mathbf{r}(t)$.

4. The Green–Kubo expressions for the transport coefficients are obtained from the Navier–Stokes matrix Λ in Eq. (2.14). It is possible to show (ref. 8, Chapter 10) that Λ is a positive-definite matrix and consequently that the transport coefficients are positive (when they exist). Positivity is necessary for stability of the hydrodynamic modes. This point is noted in light of certain "measurements" where it seems that negative viscosities have been found.(31)

5. The Green–Kubo expressions for the transport coefficients involve a limit of small s. This limit occurs because these expressions were obtained from the dispersion relation (2.10), leading to $s = s(k) \to 0$ as $k \to 0$. The existence of the transport coefficients in this limit means they are "bulk" or "material" constants. However, by analogy to the case of continuous fluids, it is expected that there will be a slow algebraic decay of the current correlation functions for the Green–Kubo expressions $\sim t^{-d/2}$ for $d \geqslant 2$ and $\sim t^{-2/3}$ for $d = 1$. Long-time tails in the velocity autocorrelation function of a tagged particle in the FHP III fluid have already been observed in computer simulations.(30) They imply a behavior of $\Lambda(s) \sim \ln(s)$ for $d = 2$ and $\Lambda(s) \sim s^{-1/3}$ for $d = 1$.

6. The last observation indicates that the transport coefficients do not exist in dimensions less than or equal to 2. Therefore it is expected that Navier–Stokes hydrodynamics has transport properties that depend intrinsically on the boundary conditions, or alternatively that the hydrodynamic eigenvalues have a more complex structure. This makes the study of linearized hydrodynamics, by theory or simulation, particularly interesting for the low-dimensional CA. Kadanoff *et al.*(32) have investigated the consequences of the small-s divergence in $\Lambda(s) \sim \ln(s)$ by nonequilibrium simulation of Poiseuille flow. Their analysis of the results using mode coupling theory for the long-time tails leads to good agreement. A similar analysis of one-dimensional CAs predicts anomalous sound damping $\sim k^{3/2}$. Indications of this behavior have been seen by Qian *et al.*(24) The self-consistent mode coupling theory to describe these problems has been given in Eqs. (3.14)–(3.16).

7. The general method is applied to a single-component fluid to yield

expressions for the shear (η), bulk (κ), and longitudinal viscosity $\{\eta_l = [2(d-1)/d]\eta + \kappa\}$. The Green–Kubo expressions for bulk viscosity and sound damping constant [Γ in Eq. (4.7)] are new; our formula for the shear viscosity has the same structure as in continuous fluids, i.e., a time correlation function of two traceless, second-rank tensors, as imposed by the isotropic symmetry of fourth-rank tensors. It agrees with Rivet's result for single-speed cellular automata models. For multispeed models Rivet's formula actually represents instead the combination $\eta + \frac{1}{2}\kappa$. We also discuss the discrepancies between Zanetti's results$^{(22)}$ and ours.

8. The theory is also applied to several types of diffusion. We consider binary mixtures where the exclusion rule for double occupancy of a state $\{\mathbf{c}, \mathbf{r}\}$ applies to (i) identical particles only (regular mixtures) and (ii) particles that are identical except for their color (colored mixture). The microscopic description (6.3) and (6.10) in terms of Boolean variables is different in both cases, and so are the diffusion mode, its time correlation function $G(\mathbf{k}, t)$, and the corresponding Green–Kubo formulas (6.8) and (6.13) for the diffusion coefficients D, which are new results.

9. The formalism is further applied to the Lorentz gas, consisting of a single moving particle in a random array of fixed scatterers. The Green–Kubo formula (6.17) for the diffusion coefficient is a discrete time sum of the velocity correlation function,$^{(29)}$ which also applies for the diffusion coefficient of a single tagged particle in a one-component fluid. There exist much simulation data for this correlation function.$^{(25,30)}$

10. The analysis here has been formally exact and has not addressed any particular approximation method for analysis of the many-body dynamics. The equilibrium space-time correlation functions and the Green–Kubo current correlation functions are appropriate quantities for study by various approximation methods known from the study of continuous fluids. For example, a Boltzmann approximation often provides a very good approximation for the transport coefficients of CA, not only at low density (and by duality also at high density), but also at intermediate densities. In lattice gases with reflecting collisions, in which a particle after collision retraces part of its trajectory, there are long memory effects (pathological one-dimensional features) that invalidate the Boltzmann approximation.$^{(27)}$ In these cases improved approximations such as ring resummation or effective medium approximations work considerably better than the Boltzmann equation. There appears to be a wide range of such problems to be studied for CA. Application of methods of nonequilibrium statistical mechanics and kinetic theory to such simple dynamical systems may clarify conditions for their validity and limitations.

11. For the staggered diffusivities the situation is less clear. No calculation, not even a Boltzmann approximation, is available that is free of serious objections.(22) The basic dynamics, even in uncorrelated collisions, has to take into account the interchange of staggered momentum between the two sub lattices. It therefore involves at least two time steps. For a Lorentz gas cellular automaton one can show that the staggered diffusivity and the usual diffusion coefficient are identical.

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