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Green-Kubo Formalism for Lattice Gas Hydrodynamics and Monte-Carlo Evaluation of Shear Viscosities

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Abstract. A Green-Kubo formula, relating the shear viscosity to discrete time correlation functions, is derived via a Liouville equation formalism for a class of non-deterministic lattice gas models. This allows a Monte-Carlo calculation of the viscosity. Preliminary results are presented for the Frisch-Hasslacher-Pomeau two-dimensional lattice gas model.

1. Introduction

When a physical system at thermodynamical equilibrium is subject to a weak large-scale perturbation (say a temperature gradient), a flux of a conjugated quantity (say a heat flux) results, which is linear in the gradient. In an isotropic newtonian fluid, a gradient of velocity creates a *momentum flux*, related by a linear relation involving a fourth-order tensor. Isotropy implies that this tensor is expressible in terms of two scalars, the shear and bulk viscosities. Fluctuation-dissipation theory relates such *transport coefficients* to time-integrated correlation functions. The earliest results in that line was obtained by Einstein in the study of Brownian motion [1]. In the fifties, systematic fluctuation-dissipation relations were developed for classical and quantum mechanical systems by Green [2,3] and Kubo [4].

Cellular automata with discrete state variables attached to a lattice and suitable conservation relations (lattice gases) present thermodynamic equilibria, as continuous systems do, and they can display large-scale hydrodynamic behavior [5,6]. Fluctuation-dissipation relations for lattice gases have been considered in references 6 through 9. Due to discreteness, there are novel features in the theory of transport coefficients, such as "propagation viscosities" [10]. Typically, there are two possible approaches. One is based on "noisy hydrodynamics" [6]. The other one, in the spirit of Green

[3], uses a Liouville equation approach and is developed here for a quite general class of D-dimensional, non-deterministic, one-speed models. For a more restricted class of deterministic two-dimensional models, results were already announced by Frisch and Rivet [11].

In section 2, we formulate the problem; we will use the same notation as in reference [6]; however, in order to make the paper reasonably self-contained, we will reintroduce briefly some of the basic concepts. In section 3, we perturbatively solve the Liouville equation around an equilibrium state and find the discrete Green-Kubo formula for the shear viscosity. In section 4, we show how to use the discrete Green-Kubo formula for a Monte-Carlo calculation of the shear viscosity; numerical results are given only for the simplest FHP model [5,6]. Comparisons are made with theoretical values obtained from the lattice Boltzmann approximation [6,10] and with results of numerical experiments based on relaxation of large scale shear waves [12,13].

2. The class of models and the formalism

In order to avoid heavy notation as much as possible, we limit the following study to the class of non-deterministic, one-speed models whose complete definition is given in reference 6. This includes several two-dimensional and three-dimensional (pseudo-four-dimensional) models known as HPP, FHP-I, and FCHC. We will also give the final results for FHP models with rest-particles, which do not belong to this class. We recall briefly the main features of the one-speed models: unit mass particles are moving with speed c along links of a regular D-dimensional Bravais lattice, where each node is connected to its b nearest neighbors by a set of b vectors $\mathbf{c}_i$, $i = 1, \ldots, b$ of equal modulus c. This set is supposed to verify some further geometric conditions given in reference 6. The fact that two particles with the same velocity vector are not allowed to be at the same node at the same time (exclusion principle) enables us to describe the state of one node at any integer time by a b-bit binary word: $s = \{s_i, i = 1, \ldots, b\}$ where $s_i = 1$ if a particle is present at the node, in the cell corresponding to the velocity vector $\mathbf{c}_i$, and $s_i = 0$ otherwise.

If initial conditions (time $t = 0$) are taken such that all particles are located at the nodes, the free propagation along links ensures that at any integer time[1] t_*, all particles are at the nodes. At any node, incoming particles can perform *local* collisions according to a non-deterministic rule; that is, an input state described by the binary word s will be changed into an output state s' with the transition probability $A(s \to s')$. These transition probabilities are taken node-independent. $A(s \to s')$ is zero if input and output states have different total mass $(\sum_i s_i)$ or momentum $(\sum_i s_i \mathbf{c}_i)$.

The state of the whole lattice $\mathcal{L}$ at integer time t_* may be described by the so-called Boolean field:

[1] As in [6], an index "star" denotes the discrete independent variables.

$$n(t_*) = \Big\{n_i(t_*, \mathbf{r}_*),\, i = 1, .., b;\, \mathbf{r}_* \in \mathcal{L}\Big\}. \tag{2.1}$$

The time evolution of this Boolean field is governed by the *microdynamical equation*, (see [6], section 3.1) which can be formally written using streaming, collision, and evolution operators $\mathcal{S}$, $\mathcal{C}$, and $\mathcal{E}$:

$$n(t_* + 1) = \mathcal{S} \circ \mathcal{C} n(t_*) = \mathcal{E} n(t_*). \tag{2.2}$$

For non-deterministic collision rules, the operator $\mathcal{E}$ is itself non-deterministic. The conservation laws induce two exact relations for the Boolean field:

$$\sum_i n_i(t_* + 1, \mathbf{r}_* + \mathbf{c}_i) = \sum_i n_i(t_*, \mathbf{r}_*), \tag{2.3}$$

$$\sum_i \mathbf{c}_i n_i(t_* + 1, \mathbf{r}_* + \mathbf{c}_i) = \sum_i \mathbf{c}_i n_i(t_*, \mathbf{r}_*). \tag{2.4}$$

The lattice gas may be described statistically by a probability distribution $P(s(.))$ that gives the probability of occurrence of a configuration $s(.) = \{s(\mathbf{r}_*),\, \mathbf{r}_* \in \mathcal{L}\}$. The time-evolution of this probability distribution is given by a Liouville equation (see [6], section 3.3)

$$P\Big(t_* + 1, \mathcal{S} s'(.)\Big) =$$

$$\sum_{s(.)\in\Gamma} \prod_{\mathbf{r}_*\in\mathcal{L}} A[s(\mathbf{r}_*) \to s'(\mathbf{r}_*)]\, P\Big(t_*, s(.)\Big), \quad \forall s'(.) \in \Gamma, \tag{2.5}$$

where Γ denotes the set of all possible configurations of the lattice $\mathcal{L}$. For further use, it is convenient to introduce a global transition probability $A^{(g)}(s \to s')$ which is $\prod_{\mathbf{r}_*\in\mathcal{L}} A[s(\mathbf{r}_*) \to s'(\mathbf{r}_*)]$ and to write equation (2.5) in the more compact form

$$P\Big(t_* + 1, \mathcal{S} s'(.)\Big) = \sum_{s(.)\in\Gamma} A^{(g)}(s \to s')\, P\Big(t_*, s(.)\Big). \tag{2.6}$$

The following mean[2] quantities will be useful in the sequel:

$$\text{mean population:} \quad N_i(t_*, \mathbf{r}_*) = \sum_{s.\in\Gamma} s_i(\mathbf{r}_*) P\Big(t_*, s(.)\Big),$$

$$\text{density:} \quad \rho(t_*, \mathbf{r}_*) = \sum_i N_i(t_*, \mathbf{r}_*),$$

$$\text{mass current (momentum):} \quad \mathbf{j}(t_*, \mathbf{r}_*) = \sum_i \mathbf{c}_i N_i(t_*, \mathbf{r}_*),$$

$$\text{mean velocity:} \quad \mathbf{u}(t_*, \mathbf{r}_*) = \mathbf{j}(t_*, \mathbf{r}_*)/\rho(t_*, \mathbf{r}_*). \tag{2.7}$$

[2] Averaged over the probability distribution $P\Big(s(.)\Big)$

The Liouville equation admits a family of homogeneous factorized *equilibrium solutions* of the form [6]:

$$P^{(eq)}\big(s(.)\big) = \prod_{\mathbf{r}_*\in\mathcal{L}} \prod_i N_i^{(eq)s_i}(1-N_i^{(eq)})^{(1-s_i)}. \tag{2.8}$$

For low-speed equilibria, $N_i^{(eq)}$ may be expressed in terms of the density and mean velocity:

$$N_i^{(eq)}(\rho,\mathbf{u}) = \frac{\rho}{b} + \frac{\rho D}{bc^2}\mathbf{c}_{i\alpha}u_\alpha + O(u^2). \tag{2.9}$$

Averages over the the equilibrium distribution with $\mathbf{u}=0$ will be denoted by angular brackets $\langle\rangle$. *Local equilibria* having the above form but with slowly varying parameters ρ and $\mathbf{u}$ will be the zero-order terms of an expansion in powers of the scale separation ϵ between the lattice constant and the smallest excited scale. As has been shown in reference 6, sections 5 through 7, when the lattice has sufficient isotropy, as we will assume here,[3] hydrodynamical equations are obtained for the density and momentum. The momentum equation involves a kinematic shear viscosity[4]

$$\nu(\rho) = -\frac{bc^4}{D(D+2)}\psi(\rho) - \frac{c^2}{2(D+2)}. \tag{2.10}$$

The coefficient $\psi(\rho)$ relates the first-order perturbation $\epsilon N_i^{(1)}$ of the mean population to the gradient of the mass current $\mathbf{j}=\rho\mathbf{u}$ through [6]

$$\epsilon N_i^{(1)} = \psi(\rho)Q_{i\alpha\beta}\partial_\alpha(\mathbf{j}_\beta),$$

$$\text{where}\quad Q_{i\alpha\beta} = \mathbf{c}_{i\alpha}\mathbf{c}_{i\beta} - \frac{c^2}{D}\delta_{\alpha\beta} \tag{2.11}$$

is the (traceless) microscopic stress-tensor. To determine the viscosity, we must find the shear-induced perturbation of the mean population. As the mean population does not satisfy a closed set of equations,[5] we must revert to the full probability distribution satisfying the Liouville equation.

3. Perturbative resolution of the Liouville equation

Global homogeneous equilibrium distributions are exact steady solutions of the Liouville equation, but local equilibria are not.[6] We will look for a solution of the Liouville equation (2.5) in the form

$$P\big(t_*,s(.)\big) = P^{(0)}\big(t_*,s(.)\big) + \epsilon P^{(1)}\big(t_*,s(.)\big) + O(\epsilon^2), \tag{3.1}$$

[3]The formalism presented here is easily extended to anisotropic cases in terms of an anisotropic viscosity tensor.

[4]The bulk viscosity is zero for one-speed models [6].

[5]Except in the lattice Boltzmann approximation which we are not using here.

[6]Local equilibria have the same dependence in ρ and $\mathbf{u}$ as a global equilibria but with ρ and $\mathbf{u}$ allowed to be space-dependent.

where $P^{(0)}\big(t_*, s(.)\big)$ is a low-speed local equilibrium distribution whose parameters have slow variations on spatial scale ϵ^{-1}. We assume that the perturbation $P^{(1)}$ vanishes initially. Using equation (2.5), we find that the perturbation $P^{(1)}$ satisfies the inhomogeneous Liouville equation

$$P^{(1)}\big(t_* + 1, \mathcal{S}s'(.)\big) - \sum_{s(.)\in\Gamma} A^{(g)}(s \to s')P^{(1)}\big(t_*, s(.)\big) =$$

$$-\epsilon^{-1}\Big[P^{(0)}\big(t_* + 1, \mathcal{S}s'(.)\big) - \sum_{s(.)\in\Gamma} A^{(g)}(s \to s')P^{(0)}\big(t_*, s(.)\big)\Big]. \tag{3.2}$$

We have now to make some straightforward manipulations of the r.h.s of the above equation.

Using the fact that s'_i is 0 or 1 and performing for each value of i the spatial shift $\mathbf{r}_* \to \mathbf{r}_* + \mathbf{c}_i$, we can write $P^{(0)}\big(t_* + 1, \mathcal{S}s'(.)\big)$ in the form

$$P^{(0)}\big(t_* + 1, \mathcal{S}s'(.)\big)$$

$$= \prod_{j,\rho_*}\Big[N_j^{(0)}(t_*+1, \rho_*+\mathbf{c}_i)s'(\rho_*) + \big(1-N_j^{(0)}(t_*+1, \rho_*+\mathbf{c}_i)\big)\big(1-s'(\rho_*)\big)\Big]. \tag{3.3}$$

As the mean populations $N_i^{(0)}$ are supposed to have slow space and time variations, we Taylor-expand all finite differences up to the first order in the gradients, and make the rescalings (see [6], section 5)

$$\partial_t \to \epsilon\partial_{t_1} \quad \text{and} \quad \partial_{\mathbf{r}} \to \epsilon\partial_{\mathbf{r}_1}. \tag{3.4}$$

We thereby obtain

$$P^{(0)}\big(t_* + 1, \mathcal{S}s'(.)\big) = P^{(0)}\big(t_*, s'(.)\big)$$

$$+\epsilon\sum_{j,\rho_*}(\partial_{t_1} + \mathbf{c}_{i\alpha}\partial_{1\alpha})N_j^{(0)}(t_*.\rho_*)\left(P_{j,\rho_*}^{(+eq)}(s'(.)) - P_{j,\rho_*}^{(-eq)}(s'(.))\right)$$

$$+ O(\epsilon^2). \tag{3.5}$$

Here, we have introduced

$$P_{j,\rho_*}^{(+eq)}(s(.))$$

$$= s_j(\rho_*) \prod_{(i',\mathbf{r}'_*)\neq(j,\rho_*)}\Big[N_{i'}^{(eq)}s_{i'}(\mathbf{r}'_*) + (1 - N_{i'}^{(eq)})(1 - s_{i'}(\mathbf{r}'_*))\Big],$$

$$P_{j,\rho_*}^{(-eq)}(s(.))$$

$$= (1 - s_j(\rho_*)) \prod_{(i',\mathbf{r}'_*)\neq(j,\rho_*)}\Big[N_{i'}^{(eq)}s_{i'}(\mathbf{r}'_*) + (1 - N_{i'}^{(eq)})(1 - s_{i'}(\mathbf{r}'_*))\Big], \tag{3.6}$$

which have an interesting interpretation. $P^{(+eq)}_{j,\rho_*}(s(.))$ (respectively $P^{(-eq)}_{j,\rho_*}(s(.))$) is the probability distribution corresponding to a state where all nodes and all cells are occupied with the zero-speed global equilibrium probability, except the ith cell of the node ρ_* which is occupied with probability 1 (respectively 0). These states are referred to as "SBSE" for Single Bit Set Equilibrium (respectively, "SBCE" for Single Bit Cleared Equilibrium).

Note that $P^{(0)}(s'(.))$ is the same as $\sum_{s(.)\in\Gamma} A^{(g)}(s \to s')P^{(0)}(s(.))$, because $P^{(0)}$ has *locally* the same analytic form as $P^{(eq)}$. This allows us to rewrite equation (3.2) for the perturbation $P^{(1)}$ as

$$P^{(1)}\big(t_* + 1, \mathcal{S}s'(.)\big) - \sum_{s(.)\in\Gamma} A^{(g)}(s \to s')P^{(1)}\big(t_*, s(.)\big) =$$

$$-\sum_{j,\rho_*}(\partial_{t_1} + \mathbf{c}_{i\alpha}\partial_{1\alpha})N_i^{(0)}\left[P^{(+eq)}_{j,\rho_*}(s'(.)) - P^{(-eq)}_{j,\rho_*}(s'(.))\right],$$

$$\forall s'(.) \in \Gamma. \tag{3.7}$$

We can now re-express the time derivatives in terms of space derivatives by using the macrodynamical Euler equations ([6], section 5) and the low speed equilibrium form (2.9); the expression $(\partial_{t_1} + \mathbf{c}_{i\alpha}\partial_{1\alpha})N_i^{(0)}$ becomes then $\frac{D}{bc^2}Q_{i\alpha\beta}\partial_{1\alpha}(\rho u_\beta)$ and equation (3.7) becomes

$$P^{(1)}\big(t_* + 1, \mathcal{S}s'(.)\big) - \sum_{s(.)\in\Gamma} A^{(g)}(s \to s')P^{(1)}\big(t_*, s(.)\big) =$$

$$-\frac{D}{bc^2}\sum_{j,\rho_*}\Big(P^{(+eq)}_{j,\rho_*}(s'(.)) - P^{(-eq)}_{j,\rho_*}(s'(.))\Big)Q_{j\alpha\beta}\partial_{1\alpha}(\rho u_\beta),$$

$$\forall s'(.) \in \Gamma. \tag{3.8}$$

In order to solve equation (3.8), we consider the probability distributions $P^{(+eq)}_{j,\rho_*}(t_*, s(.))$ and $P^{(+eq)}_{j,\rho_*}(t_*, s(.))$ obtained after t_* evolution steps, starting from an SBSE and an SBCE. The solution of (3.8) with vanishing initial condition is

$$P^{(1)}\big(t_*, s'(.)\big) =$$

$$-\frac{D}{bc^2}\sum_{\tau_*=0}^{t_*-1}\sum_{j,\rho_*}\Big[P^{(+eq)}_{j,\rho_*}(\tau_*, \mathcal{S}^{-1}s'(.))$$

$$-P^{(-eq)}_{j,\rho_*}(\tau_*, \mathcal{S}^{-1}s'(.))\Big]Q_{j\alpha\beta}\partial_{1\alpha}(\rho u_\beta). \tag{3.9}$$

For further use, we introduce the following notation:

$$N^{(+eq)}(\tau_*; i, \mathbf{r}_*|j, \rho_*) = \sum_{s(.)\in\Gamma} s_i(\mathbf{r}_*) P^{(+eq)}_{j,\rho_*}(\tau_*, s'(.)),$$
$$N^{(-eq)}(\tau_*; i, \mathbf{r}_*|j, \rho_*) = \sum_{s(.)\in\Gamma} s_i(\mathbf{r}_*) P^{(-eq)}_{j,\rho_*}(\tau_*, s'(.)). \tag{3.10}$$

$N^{(+eq)}(\tau_*; i, \mathbf{r}_*|j, \rho_*)$ (respectively, $N^{(-eq)}(\tau_*; i, \mathbf{r}_*|j, \rho_*)$) is the conditional probability to find at time τ_*, a particle at node $\mathbf{r}_*$ in cell i, knowing that at time 0 there was one (respectively none) at node ρ_* in cell j. We can now express the perturbation of mean population $N_i^{(1)}(t_*, \mathbf{r}_*) = \sum_{s'(.)\in\Gamma} s'_i(\mathbf{r}_*) P^{(1)}(t_*, s'(.))$ in the form

$$N_i^{(1)}(t_*, \mathbf{r}_*) =$$
$$-\frac{D}{bc^2} \sum_{\tau_*=0}^{t_*-1} \sum_{j,\rho_*} \Big(N^{(+eq)}(\tau_*; i, \mathbf{r}_*|j, \rho_*)$$
$$-N^{(-eq)}(\tau_*; i, \mathbf{r}_*|j, \rho_*) \Big) Q_{j\alpha\beta} \partial_{1\alpha}(\rho u_\beta). \tag{3.11}$$

We now use the two following identities:

$$N_i^{(eq)} = \frac{\rho}{b} = N^{(+eq)}(\tau_*; i, \mathbf{r}_*|j, \rho_*)\frac{\rho}{b} + N^{(-eq)}(\tau_*; i, \mathbf{r}_*|j, \rho_*)(1-\frac{\rho}{b}), \tag{3.12}$$

$$\langle n_i(\tau_*, \mathbf{r}_*)\, n_j(0, \rho_*)\rangle = N^{(+eq)}(\tau_*; i, \mathbf{r}_*|j, \rho_*) N_j^{(eq)}(0, \rho_*). \tag{3.13}$$

Equation (3.12) expresses that the equilibrium populations can be recovered from transition probabilities. Equation (3.13) expresses the two-point equilibrium probability in terms of the transition probability and the single-point probability. Using (3.12) and (3.13), we can rewrite (3.11) as

$$N_i^{(1)}(t_*, \mathbf{r}_*) = -\frac{Db}{c^2\rho(b-\rho)} \sum_{\tau_*=0}^{t_*-1} \sum_{j,\rho_*} \Big\langle \tilde{n}_i(\tau_*, \mathbf{r}_*) \tilde{n}_j(0, \rho_*) \Big\rangle Q_{j\alpha\beta} \partial_{1\alpha}(\rho u_\beta),$$

$$\tilde{n}_i = n_i - \langle n_i \rangle = n_i - \frac{\rho}{b}. \tag{3.14}$$

The average is over the zero-speed global equilibrium. From the isotropy of fourth-order tensors, it follows that

$$\sum_{i\alpha\beta} Q_{i\alpha\beta} Q_{i\alpha\beta} = \frac{bc^4(D-1)}{D}. \tag{3.15}$$

Using equations (2.10), (2.11), (3.15), reversal and translation invariances, we finally obtain

$$\nu(\rho) = \nu^{(prop)} + \sum_{\tau_*=0}^{t_*-1} \Gamma(\tau_*), \qquad \nu^{(prop)} = -\frac{c^2}{2(D+2)}, \tag{3.16}$$

where

$$\Gamma(\tau_*) =$$

$$\frac{bD}{c^2(D-1)(D+2)}\frac{1}{\rho(b-\rho)}\sum_{\rho_*}\sum_{i,j}\sum_{\alpha\beta}Q_{i\alpha\beta}\Big\langle\tilde{n}_i(\tau_*,\rho_*)\tilde{n}_j(0,0)\Big\rangle Q_{j\alpha\beta} \quad (3.17)$$

is (within a numerical factor) the correlation function of the microscopic stress-tensor. If $\Gamma(\tau_*)$ falls off sufficiently fast as $\tau_* \to \infty$, the summation over τ_* can be extended to infinity. This is the case in three dimensions but not in two, where the viscosity may at best display a quasi-steady plateau as τ_* increases (see section 4), so we will keep a finite upper bound for the time-summation.

Let us now specialize the results for the FHP-I model. We just substitute 6 for b, 2 for D, and 1 for c in the above formulae and get

$$\nu(\rho) = -\frac{1}{8} + \sum_{\tau_*=0}^{t_*-1}\Gamma(\tau_*)$$

$$\Gamma(\tau_*) = \frac{3}{\rho(6-\rho)}\sum_{\rho_*}\sum_{i,j}\sum_{\alpha\beta}Q_{i\alpha\beta}\Big\langle\tilde{n}_i(\tau_*,\rho_*)\tilde{n}_j(0,0)\Big\rangle Q_{j\alpha\beta}. \quad (3.18)$$

For variants of FHP-I called FHP-II and FHP-III [6,14], which include rest particles, a simple generalization leads to

$$\nu(\rho) = -\frac{1}{8} + \sum_{\tau_*=0}^{t_*-1}\Gamma(\tau_*),$$

$$\Gamma(\tau_*) = \frac{49}{6\rho(7-\rho)}\sum_{\rho_*}\sum_{I,J}\sum_{\alpha\beta}(1-\frac{1}{2}\delta_{\alpha\beta})Q_{I\alpha\beta}\Big\langle\tilde{n}_I(\tau_*,\rho_*)n_J(0,0)\Big\rangle Q_{J\alpha\beta},$$

$$Q_{I\alpha\beta} = c_{I\alpha}c_{I\beta} - \frac{3}{7}\delta_{\alpha\beta}. \quad (3.19)$$

The capital indices I and J which take the values $(\star, 1, 2, \ldots, 6)$ refer to the seven possible velocities, namely, the velocity zero ($I = \star$) and the six non-zero velocities of FHP-I.

4. Monte-Carlo calculation of the shear viscosity

In lattice gases as in (continuous) molecular dynamics (MD), there are broadly two strategies for calculating transport coefficients: *macroscopic* strategies involving large-scale gradients and *microscopic* strategies based on Green-Kubo relations. Their relative merits in MD have been recently discussed in reference 15. For lattice gases, macroscopic calculations of the shear viscosity have been performed by d'Humières and Lallemand [13] and by Zanetti [9]. The existence of a discrete analog for lattice gases of

the MD Green-Kubo formula provides us with an alternative numerical procedure. It is our purpose here to describe this path for a simple case, the two-dimensional model FHP-I, which has binary head-on and triple collisions.

Since lattice gases are governed by *local* cellular automata rules, there are some interesting simplifications not present in MD. These are consequences of the following properties concerning equilibrium finite-time correlations:

P1 Finite $L \times L$ periodically wrapped-around lattices and infinite lattices admit the same factorized single-time equilibrium solutions. Multi-time distributions are identical when the maximum time-separation between the arguments is less than $, L/(2c)$, where c is the particle speed (unity for FHP-I model).

P2 The binary equilibrium correlation function $\langle \tilde{n}_i(\tau_*, \rho_*)\tilde{n}(0,0)\rangle$ vanishes if $c|\tau_*| < |\rho_*| < L/2$. (Actually, for the FHP-I model, it vanishes outside of a hexagonal domain of influence $\mathcal{D}(\tau_*)$ inscribed in the circle of radius $c|\tau_*|$.)

The first part of **P1** has been established in reference 6 (section 4.1). For the second part, we observe that multiple-time distributions are expressible in terms of single-time distributions and iterated evolution operators. The evolution operator propagates information at the maximum speed c_o; thus, for time-separation less than $L/(2c)$ no finite-size effects are felt. **P2** is a consequence of **P1** and of the absence of single-time correlations between different nodes.

A consequence of **P1** is that finite-time correlations appearing in the Green-Kubo formula can be evaluated on a sufficiently large finite lattice by ensemble and space averaging. A consequence of **P2** is that the spatial summation over ρ_* in the Green-Kubo formula 3.18 can be restricted to the domain of influence $\mathcal{D}(\tau_*)$; otherwise, as we will see, trouble arises. We have found time averaging to be unreliable even for correlation functions involving only small (or vanishing) time-separations. This may be due to a finite-size effect and/or a bias in the total momentum of the randomly generated initial configuration.

After these preliminaries, we describe a simulation strategy. We combine two kinds of averaging:

spatial averaging over all lattice nodes. All nodes of the lattice are successively shifted to the origin $\mathbf{r}_* = 0$; the results of these elementary experiments are cumulated and divided by the number of nodes L^2.

ensemble averaging in which N elementary experiments are performed. Each elementary experiment involves an independent random generation of the Boolean variables $n_i(0, \mathbf{r}_*)$ with mean $N_i = \rho/6$, the zero-velocity equilibrium value. A small number of samples (typically, N is about 40) ensures an adequately low level of random noise, provided

the spatial summation over ρ_* is restricted to the domain of influence $\mathcal{D}(\tau_*)$. If we simply use (3.18), ignoring that the spatial summation can be restricted to the domain of influence, the results will be far too noisy for realistic values of N. Consider, for example, the $\tau_* = 0$ term of the time-summation; its relative Monte-Carlo noise (the inverse of the signal to noise ratio) is $O(\sqrt{L^2/N})$; this tends to zero when $N \to \infty$ but far too slowly: it is still about 30 for a 64×64 lattice filled with a density $\rho = 1.2$, averaged over $N = 50$ shots. On the other hand, if the summation is restricted to the domain of influence, namely $\rho_* = 0$ for the $\tau_* = 0$ term, the relative Monte-Carlo noise becomes $O(1/\sqrt{N\,L^2})$ which is far smaller. We see how important it is not to sum over terms which are known by **P2** to be zero. For $\tau_* \neq 0$, this is also true, although to a lesser extent since the size of the domain of influence grows like $|\tau_*|$.

Numerical results

The characteristics of the numerical experiments were:

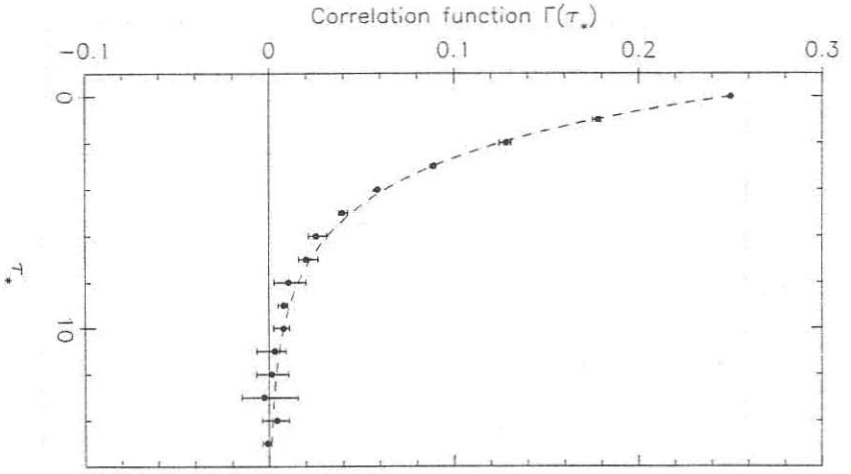
lattice size: 64×64 nodes

averaging over $N = 40$ independent realizations

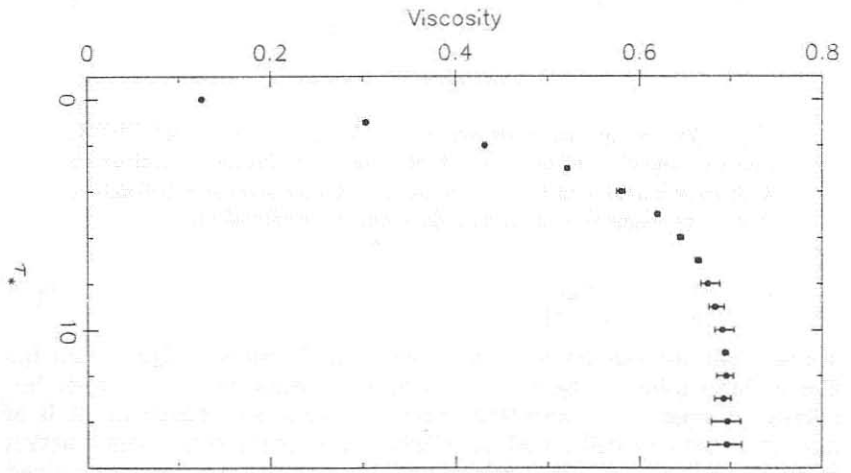
number of time steps $\tau_{max} = 15$.

Three independent experiments (with different seeds for the pseudo-random generator) have been done in order to have an experimental estimate of the Monte-Carlo noise. The function $\Gamma(\tau_*)$ in the expression 3.18 of the kinematic shear viscosity will be referred to as the *correlation function*. The cumulated correlation function up to time $t_* - 1$ plus the propagation viscosity $(-1/8)$ will be referred to as the *viscosity*. Figures 1a and b present for a density per node $\rho = 1$, the correlation function and the viscosity for τ_* between 0 and 15. The black circles are averages over the three experiments. The absolute Monte-Carlo noise grows in a way consistent with our theoretical estimate. Clearly, beyond $\tau_* = 10$, the results are too noisy to be significant, but for our purpose there is no need to go beyond $\tau_* = 10$. The viscosity exhibits beyond $\tau_* = 8$ a plateau defined with an accuracy of about 3 percent at the value $\nu = 0.7 \pm 0.02$. Similarly, evaluated viscosities for various values of the density are represented as black circles (with error bars) on figure 2. The stars (also with error bars) are the viscosities observed by d'Humières and Lallemand [13] from macroscopic simulations with relaxation of shear waves. Whenever both data are available, the error bars overlap except at very low densities. This probably reflects a pathology of the FHP-I model: at low densities, triple collisions are so rare that the dynamics are affected by a spurious invariant that would be present in the absence of triple collisions.

The continuous curve of figure 2 is the viscosity calculated from the lattice Boltzmann approximation [6,10]



a



b

Figure 1: (a) Monte-Carlo simulation of the correlation function of the microscopic stress-tensor for the FHP-I model at density $\rho = 1$. Black circles are data points with error bars. The dashed line is a least square fit of an exponential to the first five points. (b) Viscosity with error bars in the same conditions as figure 1a. The plateau gives the effective kinematic shear viscosity.

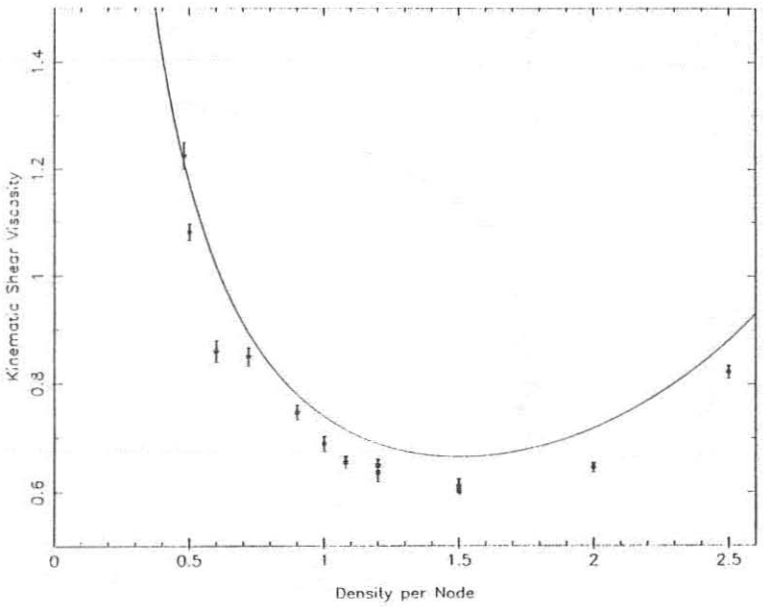


Figure 2: Density dependence of viscosities for the model FHP-I. Black circles with error bars: Monte-Carlo simulations. Black stars with error bars: shear wave simulations of d'Humières and Lallemand [13]. Continuous line: Lattice Boltzmann approximation.

$$\nu = -\frac{1}{8} + \frac{1}{2\rho(6-\rho)^3}. \tag{4.1}$$

We see that the Boltzmann results are 10 to 30 percent higher than the Green-Kubo values. The Boltzmann approximation for the viscosity implicitly assumes an exponentially decaying correlation function. It is of interest to see how well the Monte-Carlo values for the correlation function fit an exponential. The dashed line on figure 1a is an exponential obtained by a least square fit on the low noise data for $\tau_* = 0, 1, 2, 3, 4$. If we now assume that the exponential behavior holds all the way to infinity and sum the geometric series, we obtain a value of the viscosity which lies within a few percent of the Boltzmann value.

The correlation function $\Gamma(\tau_*)$ cannot be exponential all the way to infinity; theoretical arguments on "long time tails" predict that the viscosity for very long times and very large systems is logarithmically divergent [6,7,16,17]. There have been various attempts to find long time tails in lattice gas correlation functions [7,18]. To unambiguously reveal long time tails in simulations of the FHP model is definitely beyond the scope of the

present work.

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References

[1] A. Einstein, *Ann. Phys.*, **17** (1905) 549, **19** (1906) 371.

[2] H. S. Green, *J. Chem. Phys.*, **20** (1952) 1281, **22** (1954) 398.

[3] H. S. Green, *J. Math. Phys.*, **2** (1961) 344.

[4] R. Kubo, *J. Phys. Soc. Jpn.*, **12** (1957) 570.

[5] U. Frisch, B. Hasslacher, and Y. Pomeau, *Phys. Rev. Lett.*, **56** (1986) 1505.

[6] U. Frisch, B. Hasslacher, D. d'Humières, P. Lallemand, Y. Pomeau, and J. P. Rivet, "Lattice gas hydrodynamics in two and three dimensions", *Complex Systems*, **1** (1987) 648.

[7] J. Hardy, Y. Pomeau, and O. de Pazzis, *Phys. Rev.*, **A13** (1976) 1949.

[8] F. Hayot, "Viscosity in lattice gas automata", *Physica D*, in press.

[9] L. Kadanoff, G. McNamara, and G. Zanetti, "Size-dependence of the shear viscosity for a two-dimensional lattice gas", preprint Univ. Chicago (1987).

[10] M. Hénon, "Viscosity of a lattice gas", *Complex Systems*, **1** (1987) 762.

[11] U. Frisch and J. P. Rivet, *Comptes Rendus Acad. Sci. Paris*, **303** (1986) 1065.

[12] D. d'Humières, P. Lallemand, and T. Shimomura, "An experimental study of lattice gas hydrodynamics", Los Alamos Report LA-UR-85-4051 (1985).

[13] D. d'Humières and P. Lallemand, *Physica*, **140A** (1986) 337.

[14] D. d'Humières and P. Lallemand, "Numerical simulations of hydrodynamics with lattice gas automata in two dimensions", *Complex Systems*, **1** (1987) 598.

[15] J. J. Erpenbeck, *Phys. Rev.*, **A35** (1986) 218.

[16] B. J. Alder and T. E. Wainwright, *Phys. Rev.*, **A1** (1970) 18.

[17] Y. Pomeau and P. Résibois, *Phys. Rep.*, **19C** (1975) 64.

[18] N. Margolus, T. Toffoli, and G. Vichniac, *Phys. Rev. Lett.*, **56** (1986) 1694.