

## **Lattice Gas Hydrodynamics in Two and Three Dimensions**

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**Abstract.** Hydrodynamical phenomena can be simulated by discrete lattice gas models obeying cellular automata rules [1,2]. It is here shown for a class of  $D$ -dimensional lattice gas models how the macrodynamical (large-scale) equations for the densities of microscopically conserved quantities can be systematically derived from the underlying exact "microdynamical" Boolean equations. With suitable restrictions on the crystallographic symmetries of the lattice and after proper limits are taken, various standard fluid dynamical equations are obtained, including the incompressible Navier-Stokes equations

in two and three dimensions. The transport coefficients appearing in the macrodynamical equations are obtained using variants of the fluctuation-dissipation theorem and Boltzmann formalisms adapted to fully discrete situations.

## 1. Introduction

It is known that wind or water tunnels can be indifferently used for testing low Mach number flows, provided the Reynolds numbers are identical. Indeed, two fluids with quite different microscopic structures can have the same macroscopic behavior because the *form* of the macroscopic equations is entirely governed by the microscopic conservation laws and symmetries. Although the values of the *transport coefficients* such as the viscosity may depend on the details of the microphysics, still, two flows with similar geometries and identical values for the relevant dimensionless transport coefficients are related by similarity.

Recently, such observations have led to a new simulation strategy for fluid dynamics: fictitious microworld models obeying discrete cellular automata rules have been found, such that two- and three-dimensional fluid dynamics are recovered in the macroscopic limit [1,2]. Cellular automata, introduced by von Neumann and Ulam [3], consist of a lattice, each site of which can have a finite number of states (usually coded by Boolean variables); the automaton evolves in discrete steps, the sites being simultaneously updated by a deterministic or nondeterministic rule. Typically, only a finite number of neighbors are involved in the updating of any site. A very popular example is Conway's Game of Life [4]. In recent years, there has been a renewal of interest in this subject (see, e.g., [5-7]), especially because cellular automata can be implemented in massively parallel hardware [8-10].

The class of cellular automata used for the simulation of fluid dynamics are here called "lattice gas models". Historically, they emerged from attempts to construct discrete models of fluids with varying motivations. The aim of *molecular dynamics* is to simulate the *real* microworld in order, for example, to calculate transport coefficients; one concentrates mass and momentum in discrete particles with continuous time, positions, and velocities and arbitrary interactions [11-14]. Discrete velocity models, introduced by Broadwell [15] (see also [16-20]), have been used mostly to understand rarefied gas dynamics. The velocity set is now finite, space and time are still continuous, and the evolution is probabilistic, being governed by Boltzmann scattering rules. To our knowledge, the first lattice gas model with fluid dynamical features (sound waves) was introduced by Kadanoff and Swift [21]. It uses a master-equation model with continuous time. The first fully deterministic lattice gas model (now known as HPP) with discrete time, positions, and velocities was introduced by Hardy, de Pazzis, and Pomeau [22,23] (see also related work in reference 24). The HPP model, a presentation of which will be postponed to section 2, was

introduced to analyze, in as simple a framework as possible, fundamental questions in statistical mechanics such as ergodicity and the divergence of transport coefficients in two dimensions [23]. The HPP model leads to sound waves, which have been observed in simulations on the MIT cellular automaton machine [8]. The difficulties of the HPP model in coping with full fluid dynamics were overcome by Frisch, Hasslacher, and Pomeau [1] for the two-dimensional Navier-Stokes equations; models adapted to the three-dimensional case were introduced by d'Humières, Lallemand, and Frisch [2]. This has led to rapid development of the subject [25–47]. These papers are mostly concerned with lattice gas models leading to the Navier-Stokes equations. A number of other problems are known to be amenable to lattice gas models: buoyancy effects [48], seismic P-waves [49], magneto-hydrodynamics [50–52], reaction-diffusion models [53–55], interfaces and combustion phenomena [56,57], Burgers' model [58].

The aim of this paper is to present in detail and without unnecessary restrictions the theory leading from a simple class of  $D$ -dimensional "one-speed" lattice gas models to the continuum macroscopic equations of fluid dynamics in two and three dimensions. The extension of our approach to multi-speed models, including, for example, zero-velocity "rest particles", is quite straightforward; there will be occasional brief comments on such models. We now outline the paper in some detail while emphasizing some of the key steps. Some knowledge of nonequilibrium statistical mechanics is helpful for reading this paper, but we have tried to make the paper self-contained.

Section 2 is devoted to various lattice gas models and their symmetries. We begin with the simple fully deterministic HPP model (square lattice). We then go to the FHP model (triangular lattice) which may be formulated with deterministic or nondeterministic collision rules. Finally, we consider a general class of (usually) nondeterministic, one-speed models containing the pseudo-four-dimensional, face-centered-hypercubic (FCHC) model for use in three dimensions [2]. In this section, we also introduce various abstract symmetry assumptions, which hold for all three models (HPP, FHP, and FCHC) and which will be very useful in reducing the complexity of the subsequent algebra.

In section 3, we introduce the "microdynamical equations", the Boolean equivalent of Hamilton's equations in ordinary statistical mechanics. We then proceed with the probabilistic description of an ensemble of realizations of the lattice gas. At this level, the evolution is governed by a (discrete) Liouville equation for the probability distribution function.

In section 4, we show that there are equilibrium statistical solutions with no equal-time correlations between sites. Under some mildly restrictive assumptions, a Fermi-Dirac distribution is obtained for the mean populations which is *universal*, i.e., independent of collision rules. This distribution is parametrized by the mean values of the collision invariants (usually, mass and momentum).

Locally, mass and momentum are discrete, but the mean values of the

density and mass current can be tuned continuously, just as in the “real world”. Furthermore, space and time can be regarded as continuous by considering local equilibria, slowly varying in space and time (section 5). The matching of these equilibria leads to macroscopic PDEs for the conserved quantities.

The resulting “macrodynamical equations”, for the density and mass current, are not invariant under arbitrary rotations. However, in section 6, we show that the essential terms in the macroscopic equations become isotropic as soon as the lattice gas has a sufficiently large crystallographic symmetry group (as is the case for the FHP and pseudo-four-dimensional models, but not for the HPP model).

When the necessary symmetries hold, fluid dynamical equations are derived in section 7. We consider various limits involving large scales and times and small velocities (compared to particle speed). In one limit, we obtain the equations of scalar sound waves; in another limit, we obtain the incompressible Navier-Stokes equations in two and three dimensions. It is noteworthy that Galilean invariance, which does not hold at the microscopic level, is restored in these limits.

In section 8, we show how to determine the viscosities of lattice gases. They can be expressed in terms of equilibrium space-time correlation functions via an adaptation to lattice gases of fluctuation-dissipation relations. This is done with a viewpoint of “noisy” hydrodynamics, which also brings out the crossover peculiarities of two dimensions, namely a residual weak scale-dependence of transport coefficients at large scales. Alternatively, fluctuation-dissipation relations can be obtained from the Liouville equation with a Green-Kubo formalism [43]. Fully explicit expressions for the viscosities can be derived via the “Lattice Boltzmann Approximation”, not needed for any earlier steps. This is a finite-difference variant of the discrete-velocity Boltzmann approximation. The latter, which assumes continuous space and time variables, is valid only at low densities, while its lattice variant seems to capture most of the finite-density effects (with the exception of two-dimensional crossover effects). Further studies of the Lattice Boltzmann Approximation may be found in reference 42. Implications for the question of the Reynolds number are discussed at the end of the section.

Section 9 is the conclusion. Various questions are left for the appendices: detailed technical proofs, inclusion of body forces, catalog of results for various FHP models, proof of an H-theorem for the Lattice Boltzmann Approximation (due to M. Hénion).

## 2. Deterministic and nondeterministic lattice gas models

### 2.1 The HPP model

Let us begin with a heuristic construction of the HPP model [22–24]. Consider a two-dimensional square lattice with unit lattice constant as shown in figure 1. Particles of unit mass and unit speed are moving along the



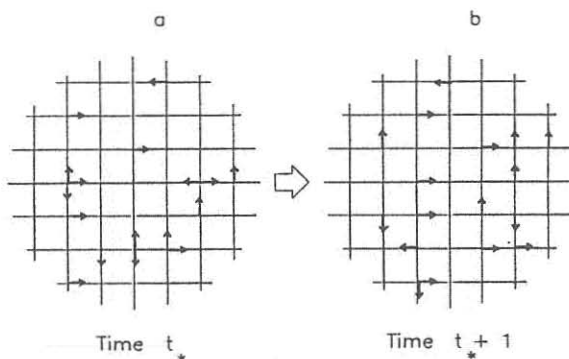


Figure 1: The HPP model. The black arrows are for cell-occupation. In (a) and (b) the lattice is shown at two successive times.

lattice links and are located at the nodes at integer times. Not more than one particle is to be found at a given time and node, moving in a given direction (exclusion principle). When two and exactly two particles arrive at a node from opposite directions (head-on collisions), they immediately leave the node in the two other, previously unoccupied, directions (see figure 2). These deterministic collision laws obviously conserve mass (particle number) and momentum and are the only nontrivial ones with these properties. Furthermore, they have the same discrete invariance group as the lattice.

The above definition can be formalized as follows. We take an  $L$  by  $L$  square lattice, periodically wrapped around (a nonessential assumption, made for convenience). Eventually, we will let  $L \rightarrow \infty$ . At each node, labeled by the discrete vector  $\mathbf{r}_*$ , there are four cells labeled by an index  $i$ , defined modulo four. The cells are associated to the unit vectors  $\mathbf{c}_i$  connecting the node to its four nearest neighbors ( $i$  increases counter-clockwise). Each cell  $(\mathbf{r}_*, i)$  has two states coded with a Boolean variable:  $n_i(\mathbf{r}_*) = 1$  for "occupied" and  $n_i(\mathbf{r}_*) = 0$  for "unoccupied". A *cellular automaton* updating rule is defined on the *Boolean field*  $n_* = \{n_i(\mathbf{r}_*), i = 1, \dots, 4, \mathbf{r}_* \in \text{Lattice}\}$ . It has two steps. Step one is *collision*: at each node, the four-bit states  $(1, 0, 1, 0)$  and  $(0, 1, 0, 1)$  are exchanged; all other states are left unchanged. Step two is *propagation*:  $n_i(\mathbf{r}_*) \rightarrow n_i(\mathbf{r}_* - \mathbf{c}_i)$ . This two-step rule is applied at each integer time,  $t_*$ . An example of implementation of the rule, in which arrows stand for cell-occupation, is shown in figures 1a and b.

Collisions in the HPP model conserve mass and momentum locally,

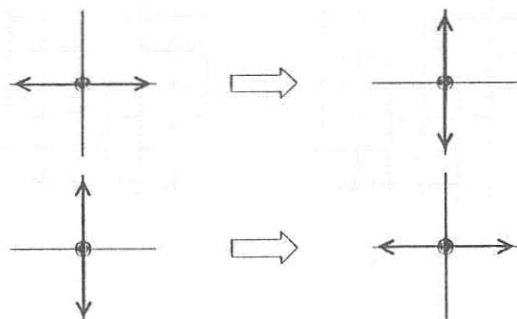


Figure 2: Collision rules for the HPP model.

whereas propagation conserves them globally. (Actually, momentum is conserved along each horizontal and vertical line, resulting in far too many conserved quantities for physical modeling.) If we attribute to each particle a kinetic energy  $\frac{1}{2}$ , the total kinetic energy is also conserved. Energy conservation is, however, indistinguishable from mass conservation and will not play any dynamical role. Models having an energy conservation law independent of mass conservation will not be considered in this paper (see [2,29]).

The dynamics of the HPP model is invariant under all discrete transformations that conserve the square lattice: discrete translations, rotations by  $\frac{\pi}{2}$ , and mirror symmetries. Furthermore, the dynamics is invariant under *duality*, that is exchange of 1's and 0's (particles and holes).

## 2.2 The FHP models

The FHP models I, II, and III (see below), introduced by Frisch, Hasslacher, and Pomeau [1] (see also [25–31,35,38–44,46]) are variants of the HPP model with a larger invariance group. The residing lattice is triangular with unit lattice constant (figure 3). Each node is now connected to its six neighbors by unit vectors  $\mathbf{c}_i$  (with  $i$  defined modulo six) and is thus endowed with a six-bit state (or seven, see below). Updating involves again propagation (defined as for HPP) and collisions.

In constructing collision rules on the triangular lattice, we must consider

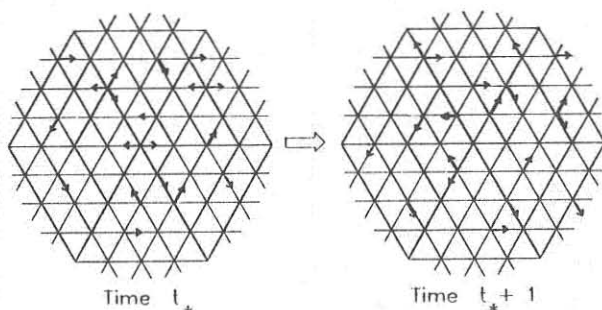


Figure 3: The FHP model with binary head-on and triple collisions at two successive times.

both *deterministic* and *nondeterministic* rules. For a head-on collision with occupied “input channels”  $(i, i + 3)$ , there are two possible pairs of occupied “output channels” such that mass and momentum are conserved, namely  $(i + 1, i + 4)$  and  $(i - 1, i - 4)$  (see figure 4a). We can decide always to choose one of these channels; we then have a deterministic model, which is *chiral*, i.e., not invariant under mirror-symmetry. Alternatively, we can make a nondeterministic (random) choice, with equal probabilities to restore mirror-symmetry. Finally, we can make a pseudo-random choice, dependent, for example, on the parity of a time or space index.

We must also consider *spurious conservation laws*. Head-on collisions conserve, in addition to total particle number, the difference of particle numbers in any pair of opposite directions  $(i, i + 3)$ . Thus, head-on collisions on a triangular lattice conserve a total of four scalar quantities. This means that in addition to mass and momentum conservation, there is a spurious conservation law. The large-scale dynamics of such a model will differ drastically from ordinary hydrodynamics, unless the spurious conservation law is removed. One way to achieve this is to introduce triple collisions  $(i, i + 2, i + 4) \rightarrow (i + 1, i + 3, i + 5)$  (see figure 4b).

Several models can be constructed on the triangular lattice. The simplest set of collision rules with no spurious conservation law, which will be called FHP-I, involves only (pseudo-random) binary head-on collisions and triple collisions. FHP-I is not invariant under duality (particle-hole exchange), but can be made so by inclusion of the duals of the head-on collisions (see figure 4c). Finally, the set of collision rules can be saturated (exhausted) by inclusion of head-on collisions with a “spectator” [59], that is, a particle which remains unaffected in a collision; figure 4d is an example of a head-on collision with a spectator present.

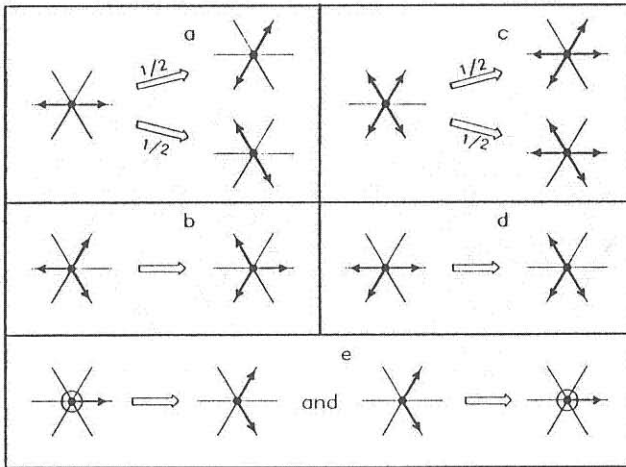


Figure 4: Collision rules for the FHP models: (a) head-on collision with two output channels given equal weights; (b) triple collision; (c) dual of head-on collision under particle-hole exchange; (d) head-on collision with spectator; (e) binary collisions involving one rest particle (represented by a circle).

The model, FHP-II, is a seven-bit variant of FHP-I including a zero-velocity “rest particle”, the additional collision rules of figure 4e, and variants of the head-on and triple collisions of figures 4a and 4b with a spectator rest particle. Binary collisions involving rest particles remove spurious conservations, and do so more efficiently at low densities than triple collisions. Finally, model FHP-III is a collision-saturated version of FHP-II [31]. For simplicity, we have chosen not to cover the theory of models with rest particles in detail.

The dynamics of the FHP models are invariant under all discrete transformations that conserve the triangular lattice: discrete translations, rotations by  $\pi/3$ , and mirror symmetries with respect to a lattice line (we exclude here the chiral variants of the models).

### 2.3 The FCHC four-dimensional and the pseudo-four-dimensional models

Three dimensional regular lattices do not have enough symmetry to ensure macroscopic isotropy [1,2,39]. A suitable four-dimensional model has been introduced by d’Humières, Lallemand, and Frisch [2]. The residing lattice is face-centered-hypercubic (FCHC), defined as the set of signed integers  $(x_1, x_2, x_3, x_4)$  such that  $x_1 + x_2 + x_3 + x_4$  is even. Each node is connected via links of length  $c = \sqrt{2}$  to 24 nearest neighbors, having two coordinates differing by  $\pm 1$ . Thus, the FCHC model has 24-bit states. The 24 possible velocity vectors are again denoted  $c_i$ ; for the index  $i$ , there is no preferred

ordering and we will leave the ordering unspecified. Propagation for the FCHC lattice gas is as usual. Collision rules should conserve mass and four-momentum while avoiding spurious conservations. This can be achieved with just binary collisions, but better strategies are known [32,33]. Non-deterministic rules involving transition probabilities are needed to ensure that the collisions and the lattice have the same invariance group (precise definitions are postponed to section 2.4).

The allowed transformations of the FCHC model are discrete translations and those isometries generated by permutations of coordinates, reversal of one or several coordinates and symmetry with respect to the hyperplane  $x_1 + x_2 + x_3 + x_4 = 0$ .

To model three-dimensional fluids and maintain the required isotropies, we define the pseudo-four-dimensional model [2] as the three-dimensional projection of an FCHC model with unit periodicity in the  $x_4$ -direction (see figure 5). It resides on an ordinary cubic lattice with unit lattice constant. The full four-dimensional discrete velocity structure is preserved as follows. There is one communication channel to the twelve next-nearest neighbors (corresponding to the twelve velocity vectors such that  $v_4$ , the fourth component of the velocity, vanishes) and there are two communication channels to the six nearest neighbors (corresponding respectively to velocities with  $v_4 = \pm 1$ ). During the propagation phase, particles with  $v_4 = \pm 1$  move to nearest neighbor nodes, while particles with  $v_4 = 0$  move to next-nearest neighbors. The collision strategy is the same as for the FCHC model, so that four-momentum is conserved. The fourth component is not a spuriously conserved quantity because, in the incompressible limit, it does not effectively couple back to the other conserved quantities [2].

## 2.4 A general class of nondeterministic models

In most of this paper, we will work with a class of models (generally non-deterministic) encompassing all the above one-speed models. The relevant common aspects of all those models are now listed: there is a regular lattice, the nodes of which are connected to nearest neighbors through links of equal length; all velocity directions are in some sense equivalent and the velocity set is invariant under reversal; at each node there is a cell associated with each possible velocity. This cell can be occupied by one particle at most; particles are indistinguishable; particles are marched forward in time by successively applying collision and propagation rules; collisions are purely local, having the same invariances as the velocity set; and collisions conserve only mass and momentum.

We now give a more formal definition of these one-speed models as cellular automata. Let us begin with the geometrical aspects. We take a  $D$ -dimensional Bravais lattice  $\mathcal{L}$  in  $\mathbb{R}^D$  of finite extension  $O(L)$  in all directions (eventually,  $L \rightarrow \infty$ ); the position vector  $\mathbf{r}_*$  of any node of such a lattice is a linear combination with integer coefficients of  $D$  independent generating vectors [60]. We furthermore assume that there exists a set of

.....  $v_4 = 0$   
 —————  $v_4 = +1 \text{ and } -1$

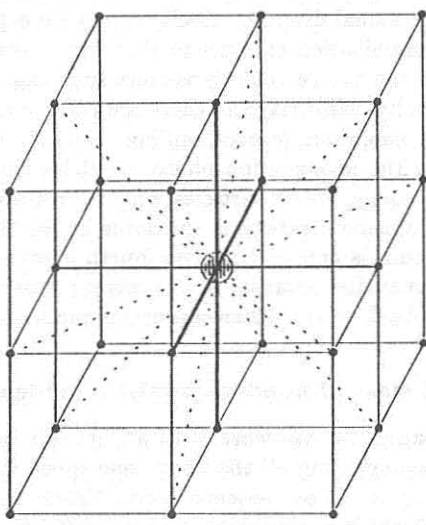


Figure 5: The pseudo-four-dimensional FCHC model. Only the neighborhood of one node is shown. Along the dotted links, connecting to next-nearest neighbors, at most one particle can propagate, with component  $v_4 = 0$ ; along the thick black links, connecting to nearest neighbors, up to two particles can propagate, with components  $v_4 = \pm 1$ .



$b$  "velocity vectors"  $\mathbf{c}_i$  having equal modulus  $c$ , the particle speed.  $\mathbf{c}_i$  has spatial components  $c_{i\alpha}$  ( $\alpha = 1, \dots, D$ ).<sup>1</sup> We require the following for  $\mathbf{c}_i$ :

1. For any  $\mathbf{r}_* \in \mathcal{L}$ , the set of the  $\mathbf{r}_* + \mathbf{c}_i$ 's is the set of nearest neighbors of  $\mathbf{r}_*$ .
2. Any two nodes can be connected via a finite chain of nearest neighbors.
3. For any pair  $(\mathbf{c}_i, \mathbf{c}_j)$  there exists an element in the "crystallographic" group  $\mathcal{G}$  of isometries globally preserving the set of velocity vectors, which maps  $\mathbf{c}_i$  into  $\mathbf{c}_j$ .
4. For any velocity vector  $\mathbf{c}_i$ , we denote by  $\mathcal{G}_i$  the subgroup of  $\mathcal{G}$  which leaves  $\mathbf{c}_i$  invariant and thus leaves its orthogonal hyperplane,  $\Pi_i$ , globally invariant; we assume that (a) there is no non-vanishing vector in  $\Pi_i$  invariant under all the elements of  $\mathcal{G}_i$  and (b) the only linear transformations within the space  $\Pi_i$  commuting with all the elements of  $\mathcal{G}_i$  are proportional to the identity.

Now, we construct the automaton. To each node  $\mathbf{r}_*$  we attach a  $b$ -bit state  $n(\mathbf{r}_*) = \{n_i(\mathbf{r}_*), i = 1, \dots, b\}$ , where the  $n_i$ 's are Boolean variables. The updating of the "Boolean field",  $n(\cdot)$ , involves two successive steps: collision followed by propagation. We choose this particular order for technical convenience; after a large number of iterations, it will become irrelevant which step was first.<sup>2</sup> Propagation is defined as

$$n_i(\mathbf{r}_*) \rightarrow n_i(\mathbf{r}_* - \mathbf{c}_i). \quad (2.1)$$

The spatial shifting by  $\mathbf{c}_i$  is performed on a periodically<sup>3</sup> wrapped around lattice with  $O(L)$  sites in any direction; eventually,  $L \rightarrow \infty$ . Collision is the simultaneous application at each node of nondeterministic transition rules from an in-state  $s = \{s_i, i = 1, \dots, b\}$  to an out-state  $s' = \{s'_i, i = 1, \dots, b\}$ . Each transition is assigned a probability  $A(s \rightarrow s') \geq 0$ , normalized to one ( $\sum_s A(s \rightarrow s') = 1 \forall s$ ), and depending only on  $s$  and  $s'$  and not on the node. The following additional assumptions are made.

5. Conservation laws: the only collections of  $b$  real numbers  $a_i$  such that

$$\sum_i (s'_i - s_i) A(s \rightarrow s') a_i = 0, \quad \forall s, s', \quad (2.2)$$

<sup>1</sup>In this paper, Greek and Roman indices refer respectively to components and velocity labels. Summation over repeated Greek indices, but not Roman ones, is implicit.

<sup>2</sup>For deterministic lattice gases, such as HPP, it is possible to bring out the reversibility of the updating rule by defining the state of the automaton at half-integer times, with particles located at the middle of links connecting nearest-neighbor nodes; updating then comprises half a propagation, followed by collision, followed by another half propagation [22].

<sup>3</sup>Other boundary conditions at the lattice edge can also be used—for example, "wind-tunnel" conditions [25,26,28].

are linear combinations of 1 (for all  $i$ ) and of  $c_{i1}, \dots, c_{iD}$ , i.e.  $a_i$  is related to mass and momentum conservation.

6. Invariance under all isometries preserving the velocity set:

$$A(g(s) \rightarrow g(s')) = A(s \rightarrow s'), \quad \forall g \in \mathcal{G}, \quad \forall s, s'. \quad (2.3)$$

7. Semi-detailed balance:

$$\sum_s A(s \rightarrow s') = 1, \quad \forall s'. \quad (2.4)$$

Various comments are now in order. Semi-detailed balance, also used in discrete velocity Boltzmann models [17], means that if before collision all states have equal probabilities, they stay so after collision. It is trivially satisfied when the collision rule is deterministic and one-to-one. There exists also a stronger assumption, detailed balance (that is  $A(s \rightarrow s') = A(s' \rightarrow s)$ ), which will not be needed here. The HPP, FHP, and FCHP lattice gases satisfy the above assumptions (1) through (4). The proofs are given in Appendix A. The other assumptions (5) through (7) hold by construction with the exception of the chiral versions of FHP. The latter do not satisfy (6) because the collision rules are not invariant under the mirror-symmetries with respect to velocity vectors. Full  $\mathcal{G}$ -invariance holds for the velocity set of the pseudo-four-dimensional model, which is the same as for the FCHC model; however, the spatial structure is only invariant under the smaller group of the three-dimensional cubic lattice.

The invariance assumptions introduced above have important consequences for the transformation properties of vectors and tensors. The following definitions will be used. A tensor is said to be  $\mathcal{G}$ -invariant if it is invariant under any isometry in  $\mathcal{G}$ . A set of  $i$ -dependent tensors of order  $p$   $\{T_i = t_{i\alpha_1 \alpha_2 \dots \alpha_p}, i = 1, \dots, b\}$  is said to be  $\mathcal{G}$ -invariant if any isometry in  $\mathcal{G}$  changing  $c_i$  into  $c_j$ , changes  $T_i$  into  $T_j$ . Note that this is stronger than global invariance under the group  $\mathcal{G}$ . The velocity moment of order  $p$  is defined as  $\sum_i c_{i\alpha_1} c_{i\alpha_2} \dots c_{i\alpha_p}$ .

We now list the transformation properties following from  $\mathcal{G}$ -invariance. The proofs are given in Appendix B.

- P1** *Parity-invariance.* The set of velocity vectors is invariant under space-reversal.
- P2** Any set of  $i$ -dependent vectors  $v_{i\alpha}$ , which is  $\mathcal{G}$ -invariant, is of the form  $\lambda c_{i\alpha}$ .
- P3** Any set of  $i$ -dependent tensors  $t_{i\alpha\beta}$ , which is  $\mathcal{G}$ -invariant, is of the form  $\lambda c_{i\alpha} c_{i\beta} + \mu \delta_{\alpha\beta}$ .
- P4** *Isotropy of second-order tensors.* Any  $\mathcal{G}$ -invariant tensor  $t_{\alpha\beta}$  is of the form  $\mu \delta_{\alpha\beta}$ .
- P5** Any  $\mathcal{G}$ -invariant third-order tensor vanishes.

**P6 Velocity moments.** Odd-order velocity moments vanish. The second-order velocity moment is given by

$$\sum_i c_{i\alpha} c_{i\beta} = \frac{bc^2}{D} \delta_{\alpha\beta}. \quad (2.5)$$

There is, in general, no closed form expression for even-order velocity moments beyond second order, with the assumptions made up to this point (see section 6).

### 3. Microdynamics and probabilistic description

#### 3.1 Microdynamical equations

It is possible to give a compact representation of the "microdynamics", describing the application of the updating rules to the Boolean field. This is the cellular automaton analog of Hamilton's equations of motion in classical statistical mechanics. We begin with the HPP lattice gas (section 2.1). Let  $n_i(t_*, \mathbf{r}_*)$ , as defined in section 2.1, denote the HPP Boolean field at the discrete time  $t_*$ . With  $i$  labeling the four cells of an HPP node, the collision rule can be formulated as follows: If the in-state has  $i$  and  $i+2$  empty and  $i+1$  and  $i+3$  occupied, then the opposite holds in the out-state; similarly, if the in-state has  $i+1$  and  $i+3$  empty and  $i$  and  $i+2$  occupied; otherwise, the content of cell  $i$  is left unchanged. Thus, the updating of the Boolean field may be written

$$n_i(t_* + 1, \mathbf{r}_* + \mathbf{c}_i) = (n_i \wedge \neg(n_i \wedge n_{i+2} \wedge \neg n_{i+1} \wedge \neg n_{i+3})) \vee (n_{i+1} \wedge n_{i+3} \wedge \neg n_i \wedge \neg n_{i+2}) \quad (3.1)$$

where the whole r.h.s. is evaluated at  $t_*$  and  $\mathbf{r}_*$ . The symbols  $\wedge$ ,  $\vee$ , and  $\neg$  stand for AND, OR, and NOT respectively. It is known that any Boolean relation can be recoded in arithmetic form ( $\wedge$  becomes multiplication,  $\neg$  becomes one minus the variable, etc.). In this way, we obtain

$$n_i(t_* + 1, \mathbf{r}_* + \mathbf{c}_i) = n_i(t_*, \mathbf{r}_*) + \Delta_i(n). \quad (3.2)$$

The "collision function"  $\Delta_i(n)$ , which can take the values  $\pm 1$  and 0, describes the change in  $n_i(t_*, \mathbf{r}_*)$  due to collisions. For the HPP model, it depends only on  $i$  and on the set of  $n_j$ 's at  $t_*$  and  $\mathbf{r}_*$ , denoted  $n$ ; it is given by

$$\Delta_i(n) = n_{i+1}n_{i+3}(1 - n_i)(1 - n_{i+2}) - n_in_{i+2}(1 - n_{i+1})(1 - n_{i+3}). \quad (3.3)$$

Equation (3.2) (with  $\Delta_i(n)$  given by equation (3.3)) will be called the *microdynamical* HPP equation. It holds for arbitrary  $i$  (modulo four), for arbitrary integer  $t_*$ , and for arbitrary  $\mathbf{r}_* \in \mathcal{L}$  ( $\mathcal{L}$  designates the lattice).

It is easy to extend the microdynamical formalism to other models. For FHP-I (section 2.2), we find that the collision function may be written (it is now defined modulo six)

$$\begin{aligned}
\Delta_i(n) = & \xi_{i,r_*} n_{i+1} n_{i+4} (1 - n_i) (1 - n_{i+2}) (1 - n_{i+3}) (1 - n_{i+5}) \\
& + (1 - \xi_{i,r_*}) n_{i+2} n_{i+5} (1 - n_i) (1 - n_{i+1}) (1 - n_{i+3}) (1 - n_{i+4}) \\
& - n_i n_{i+3} (1 - n_{i+1}) (1 - n_{i+2}) (1 - n_{i+4}) (1 - n_{i+5}) \\
& + n_{i+1} n_{i+3} n_{i+5} (1 - n_i) (1 - n_{i+2}) (1 - n_{i+4}) \\
& - n_i n_{i+2} n_{i+4} (1 - n_{i+1}) (1 - n_{i+3}) (1 - n_{i+5})
\end{aligned} \quad (3.4)$$

Here,  $\xi_{i,r_*}$  denotes a time- and site-dependent Boolean variable which takes the value one when head-on colliding particles are to be rotated counter-clockwise and zero otherwise (remember, that there are two possible outcomes of such collisions). For the theory, the simplest choice is to assign equal probabilities to the two possibilities and to assume independence of all the  $\xi$ 's. In practical implementations, other choices are often more convenient.

We now give the microdynamical equation for the general class of nondeterministic models defined in section 2.4. Propagation is as before. For the collision phase at a given node, it is convenient to sum over all  $2^b$  in-states  $s = \{s_i = 0 \text{ or } 1, i = 1, \dots, b\}$  and  $2^b$  out-states  $s'$ . The nondeterministic transitions are taken care of by the introduction at each time and node and for any pair of states  $(s, s')$  of a Boolean variable  $\xi_{ss'}$  (time and space labels omitted for conciseness). We assume that

$$\langle \xi_{ss'} \rangle = A(s \rightarrow s'), \quad \forall s, s', \quad (3.5)$$

where  $A(s \rightarrow s')$  is the transition probability introduced in section 2.4; the angular brackets denote averaging. We also assume that

$$\sum_{s'} \xi_{ss'} = 1, \quad \forall s. \quad (3.6)$$

Since the  $\xi$ 's are Boolean, equation (3.6) means that, for a given in-state  $s$  and a given realization of  $\xi_{ss'}$ , one and only one out-state  $s'$  is obtained. It is now clear that the microdynamical equation can be written as

$$n_i(t_* + 1, r_* + c_i) = \sum_{s, s'} s'_i \xi_{ss'} \prod_j n_j^{s_j} (1 - n_j)^{(1-s_j)}. \quad (3.7)$$

The factor  $s'_i$  ensures the presence of a particle in the cell  $i$  after the collision; the various factors in the product over the index  $j$  ensure that before the collision the pattern of  $n_j$ 's matches that of  $s_j$ 's. Using equation (3.7) and the identity

$$\sum_s s_i \prod_j n_j^{s_j} (1 - n_j)^{(1-s_j)} = n_i, \quad (3.8)$$

we can rewrite the microdynamical equation in a form that brings out the collision function

$$\begin{aligned}
n_i(t_* + 1, r_* + c_i) &= n_i + \Delta_i(n) \\
\Delta_i(n) &= \sum_{s, s'} (s'_i - s_i) \xi_{ss'} \prod_j n_j^{s_j} (1 - n_j)^{(1-s_j)}.
\end{aligned} \quad (3.9)$$

In the sequel, it will often be useful to have a compact notation. We define the collision operator,

$$C : n_i(\mathbf{r}_*) \mapsto n_i(\mathbf{r}_*) + \Delta_i(n(\mathbf{r}_*)), \quad (3.10)$$

the streaming operator,

$$S : n_i(\mathbf{r}_*) \mapsto n_i(\mathbf{r}_* - \mathbf{c}_i), \quad (3.11)$$

and the evolution operator, the composition of the latter,

$$\mathcal{E} = S \circ C. \quad (3.12)$$

The entire updating can now be written as

$$n(t_* + 1, \cdot) = \mathcal{E}n(t_*, \cdot), \quad (3.13)$$

where the point in the second argument of the  $n$ 's stands for all the space variables.

An interesting property of the microdynamical equation, not shared by the Hamilton equations of ordinary statistical mechanics, is that it remains meaningful for an *infinite* lattice, since the updating of any given node involves only a finite number of neighbors.

### 3.2 Conservation relations

Conservation of mass and momentum *at each node* in the collision process can be expressed by the following relations for the collision function:

$$\sum_i \Delta_i(n) = 0, \quad \forall n \in \{0, 1\}^b, \quad (3.14)$$

$$\sum_i \mathbf{c}_i \Delta_i(n) = 0, \quad \forall n \in \{0, 1\}^b, \quad (3.15)$$

where  $\{0, 1\}^b$  denotes the set of all possible  $b$ -bit words. This implies important conservation relations for the Boolean field:

$$\sum_i n_i(t_* + 1, \mathbf{r}_* + \mathbf{c}_i) = \sum_i n_i(t_*, \mathbf{r}_*), \quad (3.16)$$

$$\sum_i \mathbf{c}_i n_i(t_* + 1, \mathbf{r}_* + \mathbf{c}_i) = \sum_i \mathbf{c}_i n_i(t_*, \mathbf{r}_*). \quad (3.17)$$

### 3.3 The Liouville equation

We now make the transition, traditional in statistical mechanics, from a deterministic to a probabilistic point of view. This can be obscured by the fact that some of our models are already probabilistic. So, let us assume for a while that the evolution operator is deterministic and invertible (as is the case for HPP).

Assuming that we have a finite lattice, we define the phase space,  $\Gamma$ , as the set of all possible assignments  $s(\cdot) = \{s_i(\mathbf{r}_*), i = 1, \dots, b, \mathbf{r}_* \in \mathcal{L}\}$  of the Boolean field  $n_i(\mathbf{r}_*)$ . A particular assignment of the Boolean field will be called a *configuration*. We now consider at time  $t_* = 0$  an *ensemble* of initial conditions, each endowed with a probability  $P(0, s(\cdot)) \geq 0$ , such that

$$\sum_{s(\cdot) \in \Gamma} P(0, s(\cdot)) = 1. \quad (3.18)$$

We let each configuration in the ensemble evolve according to the automaton updating rule, i.e., with the evolution operator  $\mathcal{E}$  of equation (3.13). The latter being, here, invertible, conservation of probability is expressed as

$$P(t_* + 1, s(\cdot)) = P(t_*, \mathcal{E}^{-1}s(\cdot)). \quad (3.19)$$

This equation is clearly the analog of the Liouville equation of statistical mechanics, and will be given the same name. Alternatively, the Liouville equation can be written

$$P(t_* + 1, Ss(\cdot)) = P(t_*, C^{-1}s(\cdot)). \quad (3.20)$$

To derive this, we have used equation (3.12) and put the streaming operator in the l.h.s., a form which will be more convenient subsequently.

In the *nondeterministic* case, we must enlarge the probability space to include not only the phase space of initial conditions, but the space of all possible choices of the Boolean variables  $\xi(ss')$ , which at each time and each node select the unique transition from a given in-state  $s$  (see section 3.1). Since the  $\xi$ 's are independently chosen at each time, the entire Boolean field  $n(t_*, \cdot)$  is a Markov process (with deterministic rules, this process is degenerate). What we will continue to call the Liouville equation is actually the Chapman-Kolmogorov equation for this Markov process, namely

$$P(t_* + 1, Ss'(\cdot)) = \sum_{s(\cdot) \in \Gamma} \prod_{\mathbf{r}_* \in \mathcal{L}} A(s(\mathbf{r}_*) \rightarrow s'(\mathbf{r}_*)) P(t_*, s(\cdot)). \quad (3.21)$$

This equation just expresses that the probability at  $t_* + 1$  of a given (propagated) configuration  $s'(\cdot)$  is the sum of the probabilities at  $t_*$  of all possible original configurations  $s(\cdot)$  times the transition probability. The latter is a product, because we assumed that the  $\xi$ 's are chosen independently at each node. In the deterministic case,  $A(s(\mathbf{r}_*) \rightarrow s'(\mathbf{r}_*))$  selects the unique configuration  $C^{-1}s'(\cdot)$ , so that equation (3.20) is recovered.



### 3.4 Mean quantities

Having introduced a probabilistic description, we now turn to mean quantities. For an "observable"  $q(n(t_*,.))$ , which depends on the Boolean field at a single time, the mean is given by ensemble averaging over  $P(t_*, s(.))$

$$\langle q(n(t_*,.)) \rangle = \sum_{s(.)\in\Gamma} q(s(.))P(t_*, s(.)). \quad (3.22)$$

An important role will be played in the sequel by the following mean quantities: the *mean population*

$$N_i(t_*, \mathbf{r}_*) = \langle n_i(t_*, \mathbf{r}_*) \rangle, \quad (3.23)$$

the *density*, and the *mass current* (mean momentum)

$$\rho(t_*, \mathbf{r}_*) = \sum_i N_i(t_*, \mathbf{r}_*), \quad \mathbf{j}(t_*, \mathbf{r}_*) = \sum_i \mathbf{c}_i N_i(t_*, \mathbf{r}_*). \quad (3.24)$$

Note that these are mean quantities per node, not per unit area or volume. The *density per cell* is defined as  $d = \rho/b$ . Finally, the *mean velocity*  $\mathbf{u}$  is defined by

$$\mathbf{j}(t_*, \mathbf{r}_*) = \rho(t_*, \mathbf{r}_*) \mathbf{u}(t_*, \mathbf{r}_*). \quad (3.25)$$

Note that under duality (exchange of particles and holes),  $\rho$  changes into  $b - \rho$ ,  $d$  into  $1 - d$ ,  $\mathbf{j}$  into  $-\mathbf{j}$ , and  $\mathbf{u}$  into the "mean hole-velocity"  $\mathbf{u}_H = -\mathbf{u}d/(1 - d)$ .

Averaging of the microdynamical conservation relations 3.16 and 3.17 leads to conservation relations for the mean populations

$$\sum_i N_i(t_* + 1, \mathbf{r}_* + \mathbf{c}_i) = \sum_i N_i(t_*, \mathbf{r}_*), \quad (3.26)$$

$$\sum_i \mathbf{c}_i N_i(t_* + 1, \mathbf{r}_* + \mathbf{c}_i) = \sum_i \mathbf{c}_i N_i(t_*, \mathbf{r}_*). \quad (3.27)$$

## 4. Equilibrium solutions

It has been shown by Hardy, Pomeau, and de Pazzis [22] that the HPP model has very simple statistical equilibrium solutions (which they call invariant states) in which the Boolean variables at all the cells are independent. Such equilibrium solutions are the lattice gas equivalent of Maxwell states in classical statistical mechanics and are therefore crucial for deriving hydrodynamics. There are similar results for the general class of nondeterministic models introduced in section 2.4, which are now discussed.

### 4.1 Steady solutions of the Liouville equation

We are interested in equilibrium solutions, that is, steady-state solutions of the Liouville equation (3.21) for a finite, periodically wrapped around lattice. Collisions on the lattice are purely local (their impact parameter is zero). This suggests the existence of equilibrium solutions with no single-time spatial correlations. The lattice properties being translation-invariant, the distribution should be the same at each node. Thus, we are looking for equilibrium solutions of the form

$$P(s(\cdot)) = \prod_{\mathbf{r}_*} p(s(\mathbf{r}_*)), \quad (4.1)$$

where  $p(s)$ , the probability of a given state, is node-independent. Maximization of the entropy (see Appendix F) suggests that  $p(s)$  should be completely factorized over all cells, that is, of the form

$$p(s) = \prod_i N_i^{s_i} (1 - N_i)^{(1-s_i)}. \quad (4.2)$$

Note that  $N_i^{s_i} (1 - N_i)^{(1-s_i)}$  is the probability of a Boolean variable with mean  $N_i$ .

Now, we must check that there are indeed solutions of the form that we have been guessing. Substitution of  $P(s(\cdot))$  given by equation (4.1) with  $p(s)$  given by equation (4.2) into the Liouville equation (3.21) leads to

$$\prod_j N_j^{s'_j} (1 - N_j)^{(1-s'_j)} = \sum_s A(s \rightarrow s') \prod_j N_j^{s_j} (1 - N_j)^{(1-s_j)}, \quad \forall s', \quad (4.3)$$

where  $N_i$  is the mean population of cell  $i$ , independent of the node and of the time.

Equation (4.3) is a set  $2^b$  (the number of different states) equations for  $b$  unknowns. The fact that it actually possesses solutions is nontrivial. Furthermore, these solutions can be completely described. Indeed, we have the following lemma.

**Lemma 1.** *The following statements are equivalent:*

1. The  $N_i$ 's are a solution of equation (4.3).
2. The  $N_i$ 's are a solution of the set of  $b$  equations

$$\sum_{ss'} (s'_i - s_i) A(s \rightarrow s') \prod_j N_j^{s_j} (1 - N_j)^{(1-s_j)} = 0, \quad \forall i. \quad (4.4)$$

3. The  $N_i$ 's are given by the Fermi-Dirac distribution

$$N_i = \frac{1}{1 + \exp(h + \mathbf{q} \cdot \mathbf{c}_i)}, \quad (4.5)$$

where  $h$  is an arbitrary real number and  $\mathbf{q}$  is an arbitrary  $D$ -dimensional vector.

The proof of the equivalence is given in Appendix C; it makes use of semi-detailed balance and the absence of spurious invariants. The most important consequence of the lemma is the *Universality Theorem*. Nonde-terministic lattice gas models satisfying semi-detailed balance and having no spurious invariants admit universal equilibrium solutions, completely factorized over all nodes and all cells, with mean populations given by the Fermi-Dirac distribution (4.5), dependent only on the density  $\rho$  and the mass current  $\mathbf{j} = \rho\mathbf{u}$ , and independent of the transition probabilities  $A(s \rightarrow s')$ .

The proof follows from the observation that the Lagrange multipliers  $h$  and  $\mathbf{q}$  of the Fermi-Dirac distribution can be calculated in terms of the density and the mass current through the relations

$$\rho = \sum_i N_i = \sum_i \frac{1}{1 + \exp(h + \mathbf{q} \cdot \mathbf{c}_i)}, \quad (4.6)$$

$$\rho\mathbf{u} = \sum_i N_i \mathbf{c}_i = \sum_i \mathbf{c}_i \frac{1}{1 + \exp(h + \mathbf{q} \cdot \mathbf{c}_i)}. \quad (4.7)$$

For the HPP model, this set of equations is reducible to a cubic polynomial equation, so that explicit solutions are known [22]. For the FHP model, explicit solutions are known only for special cases [61].

It is not particularly surprising for models that have a built-in exclusion principle (not more than one particle per cell) to obtain a Fermi-Dirac distribution at equilibrium. Note that the factorized equilibrium solutions remain meaningful on an infinite lattice. There is no proof at the moment that the only equilibrium solutions which are relevant in the limit of infinite lattices are of the above form, namely completely factorized (which then *implies* the Fermi-Dirac distribution). There is strong numerical evidence, for those models that have been simulated, that the Fermi-Dirac is the only relevant one [8,25,27].

## 4.2 Low-speed equilibria

In the "real world", equilibrium distributions with different mean velocities are simply related by a Galilean transformation. Galilean invariance does not hold at the microscopic level for a lattice gas; therefore, there is no simple relation between the equilibria with vanishing and nonvanishing mean velocity. For subsequent derivations of fluid dynamical equations, we will only need equilibria with low speeds, that is with  $u = |\mathbf{u}| \ll c$ , the particle speed. Such equilibria can be calculated perturbatively in powers of  $u$ .

We write the equilibrium distribution as

$$N_i = f_F D(h(\rho, \mathbf{u}) + \mathbf{q}(\rho, \mathbf{u}) \cdot \mathbf{c}_i), \quad (4.8)$$

where we have used the Fermi-Dirac function

$$f_F D(x) = \frac{1}{1 + e^x}. \quad (4.9)$$

We observe that

$$\mathbf{u} = 0 \Rightarrow N_i = \frac{\rho}{b} = d. \quad (4.10)$$

Indeed, by assumption (3) of section 2.4, there exists an isometry of the lattice exchanging any two velocity vectors  $\mathbf{c}_i$  and  $\mathbf{c}_j$ ; the vector  $\mathbf{u} = 0$  being also trivially invariant, the mean population  $N_i$  is independent of  $i$ . Thus,  $f_{FD}(\mathbf{h}(\rho, 0)) = d$  and  $\mathbf{q}(\rho, 0) = 0$ .

Furthermore, it follows from parity-invariance ( $\mathbf{u} \rightarrow -\mathbf{u}$ ,  $\mathbf{c}_i \rightarrow -\mathbf{c}_i$ ) that

$$h(\rho, -\mathbf{u}) = h(\rho, \mathbf{u}), \quad \mathbf{q}(\rho, -\mathbf{u}) = -\mathbf{q}(\rho, \mathbf{u}). \quad (4.11)$$

We now expand  $h$  and  $\mathbf{q}$  in powers of  $\mathbf{u}$

$$\begin{aligned} h(\rho, \mathbf{u}) &= h_0 + h_2 u^2 + O(u^4) \\ q_\alpha(\rho, \mathbf{u}) &= q_1 u_\alpha + O(u^3), \end{aligned} \quad (4.12)$$

where  $h_0$ ,  $h_2$ , and  $q_1$  depend on  $\rho$ . The fact that  $h_2$  and  $q_1$  are scalars rather than second-order tensors is a consequence of the isotropy of second-order tensors (property P4 of section 2.4). We substitute equation (4.12) into equation (4.8) and expand the mean populations in powers of  $\mathbf{u}$

$$N_i = f_{FD} + q_1 f'_F D \mathbf{u} \cdot \mathbf{c}_i + h_2 f'_F D u^2 + \frac{1}{2} q_1^2 f''_F D (\mathbf{u} \cdot \mathbf{c}_i)^2 + O(u^3). \quad (4.13)$$

Here,  $f_{FD}$ ,  $f'_F D$ , and  $f''_F D$  are the values at  $h_0$  of the Fermi-Dirac function and its first and second derivatives. From equation (4.13), we calculate the density  $\rho = \sum_i N_i$  and the mass current  $\rho \mathbf{u} = \sum_i \mathbf{c}_i N_i$ , using the velocity moment relations (P6 of section 2.4). Identification gives  $h_0$ ,  $h_2$ , and  $q_1$  in terms of  $\rho$ . This is then used to calculate the equilibrium mean population up to second order in  $\mathbf{u}$ ; we obtain

$$N_i^{\text{eq}}(\rho, \mathbf{u}) = \frac{\rho}{b} + \frac{\rho D}{c^2 b} \mathbf{c}_{i\alpha} u_\alpha + \rho G(\rho) Q_{i\alpha\beta} u_\alpha u_\beta + O(u^3) \quad (4.14)$$

where

$$G(\rho) = \frac{D^2}{2c^4 b} \frac{b-2\rho}{b-\rho} \quad \text{and} \quad Q_{i\alpha\beta} = \mathbf{c}_{i\alpha} \mathbf{c}_{i\beta} - \frac{c^2}{D} \delta_{\alpha\beta}. \quad (4.15)$$

In equation (4.14), the superscript "eq" stresses that the mean population are evaluated at equilibrium.

Note that the coefficient  $G(\rho)$  of the quadratic term vanishes for  $\rho = b/2$ , that is, when the density of particles and holes are the same. This result, which holds more generally for the coefficients of any even power of  $\mathbf{u}$ , follows by duality:  $N_i^{\text{eq}}$  goes into  $1 - N_i^{\text{eq}}$  and  $\mathbf{u}$  into  $-\mathbf{u}$  at  $\rho = b/2$ . It does not matter whether or not the collision rules are duality-invariant, as long as they satisfy semi-detailed balance, since the equilibrium is then universal.

## 5. Macroynamical equations

In the "real world", fluid dynamics may be viewed as the gluing of *local* thermodynamic equilibria with slowly varying parameters [62,63]. Lattice gases also admit equilibrium solutions.<sup>4</sup> These have continuously adjustable parameters, the mean values of the conserved quantities, namely mass and momentum. On a very large lattice, we can set up local equilibria with density and mass current slowly changing in space and time. From the conservation relations, we will derive by a multi-scale technique *macroynamical* equations, that is, PDEs for the large scale and long-time behavior of density and mass current.

We consider a lattice gas satisfying all the assumptions of section 2.4. We denote by  $\rho(\mathbf{r}_*)$  and  $\mathbf{u}(\mathbf{r}_*)$  the density and (mean) velocity<sup>5</sup> at lattice node  $\mathbf{r}_*$ . We assume that these quantities are changing on a spatial scale  $\epsilon^{-1}$  (in units of lattice constant). This requires that the lattice size  $L$  be itself at least  $O(\epsilon^{-1})$ . Eventually, we let  $\epsilon \rightarrow 0$ . The spatial change is assumed to be sufficiently regular to allow interpolations for the purpose of calculating derivatives.<sup>6</sup> When time and space are treated as continuous, they are denoted  $t$  and  $\mathbf{r}$ . We further assume that the density is  $O(1)$  and that the velocity is small compared to the particle speed  $c$ .<sup>7</sup> We expect the following phenomena:

1. relaxation to local equilibrium on time scale  $\epsilon^0$ ,
2. density perturbations propagating as sound waves on time scale  $\epsilon^{-1}$ ,
3. diffusive (and possibly advective) effects on time scale  $\epsilon^{-2}$ .

We thus use a three-time formalism:  $t_*$  (discrete),  $t_1 = \epsilon t_*$ , and  $t_2 = \epsilon^2 t_*$ , the latter two being treated as continuous variables. We use two space variables:  $\mathbf{r}_*$  (discrete) and  $\mathbf{r}_1 = \epsilon \mathbf{r}_*$  (continuous).

Let us denote by  $N_i^{(0)}(\mathbf{r}_*)$  the mean equilibrium populations based on the local value of  $\rho$  and  $\mathbf{u}$ . They are given by equation (4.14). The actual mean populations  $N_i(t, \mathbf{r})$  will be close to the equilibrium values and may be expanded in powers of  $\epsilon$ :

$$N_i = N_i^{(0)}(t, \mathbf{r}) + \epsilon N_i^{(1)}(t, \mathbf{r}) + O(\epsilon^2). \quad (5.1)$$

The corrections should not contribute to the local values of density and mean momentum; thus,

$$\sum_i N_i^{(1)}(t, \mathbf{r}) = 0 \quad \text{and} \quad \sum_i \mathbf{c}_i N_i^{(1)}(t, \mathbf{r}) = 0. \quad (5.2)$$

<sup>4</sup>The qualification "thermodynamic" is not so appropriate since there is no relevant energy variable.

<sup>5</sup>Henceforth, we will just write "velocity", since this *mean velocity* changes in space.

<sup>6</sup>The interpolations can be done via the Fourier representation if the lattice is periodic.

<sup>7</sup>Eventually, we will assume the velocity to be  $O(\epsilon)$ , but at this point it is more convenient to keep  $\epsilon$  and  $u$  as independent expansion parameters.

We now start from the exact conservation relations (3.26) and (3.27) and expand both the  $N_i$ 's and the finite differences in powers of  $\epsilon$ . Note that all finite differences must be expanded to second order; otherwise, the viscous terms are not correctly captured. Time and space derivatives will be denoted  $\partial_t$  and  $\partial_r = \{\partial_\alpha, \alpha = 1, \dots, D\}$ . For the multi-scale formalism, we make the substitutions

$$\partial_t \rightarrow \epsilon \partial_{t_1} + \epsilon^2 \partial_{t_2} \quad \text{and} \quad \partial_r \rightarrow \epsilon \partial_{r_1}. \quad (5.3)$$

The components of  $\partial_{r_1}$  will be denoted  $\partial_{1\alpha}$ .

To leading order,  $O(\epsilon)$ , we obtain

$$\partial_{t_1} \sum_i N_i^{(0)} + \partial_{1\beta} \sum_i c_{i\beta} N_i^{(0)} = 0, \quad (5.4)$$

and

$$\partial_{t_1} \sum_i c_{i\alpha} N_i^{(0)} + \partial_{1\beta} \sum_i c_{i\alpha} c_{i\beta} N_i^{(0)} = 0. \quad (5.5)$$

We now substitute the equilibrium values (4.14) for the  $N_i^{(0)}$ 's and use the velocity moment relations P6 of section 2.4. We obtain the "macrodynamical Euler equations"

$$\partial_{t_1} \rho + \partial_{1\beta} (\rho u_\beta) = 0, \quad (5.6)$$

and

$$\partial_{t_1} (\rho u_\alpha) + \partial_{1\beta} P_{\alpha\beta} = 0. \quad (5.7)$$

$P_{\alpha\beta}$  is the momentum-flux tensor,<sup>8</sup>

$$\begin{aligned} P_{\alpha\beta} &\equiv \sum_i c_{i\alpha} c_{i\beta} N_i^{eq} \\ &= \frac{c^2}{D} \rho \delta_{\alpha\beta} + \rho G(\rho) T_{\alpha\beta\gamma\delta} u_\gamma u_\delta + O(u^4), \end{aligned} \quad (5.8)$$

with

$$T_{\alpha\beta\gamma\delta} = \sum_i c_{i\alpha} c_{i\beta} Q_{i\gamma\delta}, \quad (5.9)$$

and  $G(\rho)$  and  $Q_{i\gamma\delta}$  given by equation (4.15) of section 4. Note that the correction term in the r.h.s. of equation (5.8) is  $O(u^4)$  rather than  $O(u^3)$ ; indeed, it follows from the parity-invariance of the lattice gas that first-order spatial derivative terms do not contain odd powers of  $u$ .

We now proceed to the next order,  $O(\epsilon^2)$ . We expand equations (3.26) and (3.27) to second order; collecting all  $O(\epsilon^2)$  terms, we obtain

$$\partial_{t_2} \sum_i N_i^{(0)} + \frac{1}{2} \partial_{t_1} \partial_{t_1} \sum_i N_i^{(0)} + \partial_{t_1} \partial_{1\beta} \sum_i c_{i\beta} N_i^{(0)}$$

<sup>8</sup> Actually, this is only the leading order approximation to the momentum-flux.



$$+ \frac{1}{2} \partial_{1\beta} \partial_{1\gamma} \sum_i c_{i\beta} c_{i\gamma} N_i^{(0)} + \partial_{t_1} \sum_i N_i^{(1)} + \partial_{1\beta} \sum_i c_{i\beta} N_i^{(1)} = 0, \quad (5.10)$$

and

$$\begin{aligned} & \partial_{t_2} \sum_i c_{i\alpha} N_i^{(0)} + \frac{1}{2} \partial_{t_1} \partial_{t_1} \sum_i c_{i\alpha} N_i^{(0)} + \partial_{t_1} \partial_{1\beta} \sum_i c_{i\alpha} c_{i\beta} N_i^{(0)} \\ & + \frac{1}{2} \partial_{1\beta} \partial_{1\gamma} \sum_i c_{i\alpha} c_{i\beta} c_{i\gamma} N_i^{(0)} + \partial_{t_1} \sum_i c_{i\alpha} N_i^{(1)} \\ & + \partial_{1\beta} \sum_i c_{i\alpha} c_{i\beta} N_i^{(1)} = 0. \end{aligned} \quad (5.11)$$

By equation (5.2),  $\sum_i N_i^{(1)} = 0$  and  $\sum_i c_{i\alpha} N_i^{(1)} = 0$ . For the  $N_i^{(0)}$ 's, we substitute their low-speed equilibrium form (4.14), leaving out  $O(u^2)$  terms. Re-expressing derivatives of  $\rho$  and  $\rho u$  with respect to  $t_1$  in terms of space derivatives, using equations (5.6) and (5.7), we obtain

$$\partial_{t_2} \rho = 0 \quad (5.12)$$

and

$$\partial_{t_2} (\rho u_\alpha) + \partial_{1\beta} \left( \sum_i c_{i\alpha} c_{i\beta} N_i^{(1)} + \frac{D}{2c^2 b} T_{\alpha\beta\gamma\delta} \partial_{1\gamma} (\rho u_\delta) \right) = O(u^2). \quad (5.13)$$

Equation (5.12) tells us that there is no mass diffusion (there is a single species of particles). Equation (5.13) describes the momentum diffusion over long ( $O(\epsilon^{-2})$ ) time-scales. It has two contributions. The term involving  $T_{\alpha\beta\gamma\delta}$  comes from particle propagation and we will comment on it later.

The other term in equation (5.13) involves the deviations  $N_i^{(1)}$  from the equilibrium mean populations.  $N_i^{(1)}$  vanishes when the equilibrium is uniform. It must therefore be a linear combination of gradients (with respect to  $\mathbf{r}_1$ ) of  $\rho$  and  $\rho u$ . Linear response theory is needed to calculate the coefficients. At this point, we will only make use of symmetry arguments to reduce the number of coefficients. We assume that  $\mathbf{u}$  is small, so that to leading order equilibria are invariant under the isometry group  $\mathcal{G}$  of the lattice (see section 2.4). Since the gradient of  $\rho$  is a vector and the gradient of  $\rho u$  is a second-order tensor, properties **P2** and **P3** of section 2.4 allow us to write

$$N_i^{(1)} = \sigma c_{i\alpha} \partial_{1\alpha} \rho + (\psi c_{i\alpha} c_{i\beta} + \chi \delta_{\alpha\beta}) \partial_{1\alpha} (\rho u_\beta). \quad (5.14)$$

By equation (5.2), we have  $\sigma = 0$  and  $c^2 \psi + D\chi = 0$ . Note that  $\psi$  should depend on  $\rho$ , but not on  $\mathbf{u}$ , since it is evaluated at  $\mathbf{u} = 0$ . Substituting the expression for  $N_i^{(1)}$  into equation (5.13), we obtain

$$\partial_{t_1} (\rho u_\alpha) + \partial_{1\beta} \left[ \left( \psi(\rho) + \frac{D}{2c^2 b} \right) T_{\alpha\beta\gamma\delta} \partial_{1\gamma} (\rho u_\delta) \right] = O(u^2). \quad (5.15)$$

In the sequel, it will be more convenient to collapse the set of four equations, governing the evolution of  $\rho$  and  $\rho u$  on  $O(\epsilon^{-1})$  and  $O(\epsilon^{-2})$  time-scales, into a pair of equations, written in terms of the original variables  $t$  and  $\mathbf{r}$  (in their continuous version). We thus obtain the *macrodynamical equations*

$$\begin{aligned} \partial_t \rho &+ \partial_\beta (\rho u_\beta) = 0, \\ \partial_t (\rho u_\alpha) &+ \partial_\beta \left( \rho G(\rho) T_{\alpha\beta\gamma\delta} u_\gamma u_\delta + \frac{\epsilon^2}{D} \rho \delta_{\alpha\beta} \right) \\ &+ \partial_\beta \left[ \left( \psi(\rho) + \frac{D}{2c^2b} \right) T_{\alpha\beta\gamma\delta} \partial_\gamma (\rho u_\delta) \right] \\ &= O(\epsilon u^3) + O(\epsilon^2 u^2) + O(\epsilon^3 u). \end{aligned} \quad (5.16)$$

The equivalence of equations (5.16) and (5.17) to (5.6), (5.7), (5.12), and (5.15) follows by equation (5.3). Note that equation (16) is the standard density equation of fluid mechanics and that equation (5.17) already has a strong resemblance to the Navier-Stokes equations.

## 6. Recovering isotropy

The macrodynamical equations (5.16) and (5.17) are not fully isotropic. The presence of a lattice with discrete rotational symmetries is still felt through the tensor

$$T_{\alpha\beta\gamma\delta} = \sum_i c_{i\alpha} c_{i\beta} Q_{i\gamma\delta} = \sum_i c_{i\alpha} c_{i\beta} \left( c_{i\gamma} c_{i\delta} - \frac{c^2}{D} \delta_{\gamma\delta} \right), \quad (6.1)$$

appearing in both the nonlinear and diffusive terms of (5.17). Furthermore, the higher-order terms in the r.h.s. of equation (5.17) have no reason to be isotropic. This should not worry us since they will eventually turn out to be irrelevant. Contrary to translational discreteness, rotational discreteness cannot go away under the macroscopic limit; the latter involves large scales but not in any way "large angles", since the group of rotations is compact.

We have seen in section 2.4 that tensors up to third order having the same invariance group  $\mathcal{G}$  as the discrete velocity set are isotropic. Not so for tensors of fourth order such as  $T_{\alpha\beta\gamma\delta}$ . Indeed, for the HPP model (section 2.1), explicit calculation of the momentum-flux tensor, given by equation (5.8), is quite straightforward. The result is

$$\begin{aligned} P_{11} &= \\ \rho G(\rho)(u_1^2 - u_2^2) + \frac{\rho}{2} + O(u^4), \quad P_{22} &= \rho G(\rho)(u_2^2 - u_1^2) + \frac{\rho}{2} + O(u^4), \end{aligned} \quad (6.2)$$

$$P_{12} = P_{21} = 0, \quad (6.3)$$

with

$$G(\rho) = \frac{2 - \rho}{4 - \rho}. \quad (6.4)$$

The only second-order tensors quadratic in the velocity being  $u_\alpha u_\beta$  and  $u \cdot u \delta_{\alpha\beta}$ , the tensor  $P_{\alpha\beta}$  is not isotropic.

In order to eventually obtain the Navier-Stokes equations, the tensor  $T_{\alpha\beta\gamma\delta}$  given by equation (6.1) must be isotropic, that is, *invariant under the full orthogonal group*. This tensor is pairwise symmetrical in  $(\alpha, \beta)$  and  $(\gamma, \delta)$ ; from equation (6.1), it follows that it satisfies

$$\sum_{\gamma} T_{\alpha\beta\gamma\gamma} = 0, \quad \sum_{\alpha\beta} T_{\alpha\beta\alpha\beta} = bc^4 \left(1 - \frac{1}{D}\right). \quad (6.5)$$

When the tensor  $T_{\alpha\beta\gamma\delta}$  is isotropic, these properties uniquely constrain it to be of the following form:

$$T_{\alpha\beta\gamma\delta} = \frac{bc^4}{D(D+2)} \left( \delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma} - \frac{2}{D} \delta_{\alpha\beta} \delta_{\gamma\delta} \right). \quad (6.6)$$

For general group-theoretical material concerning the isotropy of tensors with discrete symmetries in the context of lattice gases, we refer the reader to reference 39. Crucial observations for obtaining the two- and three-dimensional Navier-Stokes equations are the isotropy of pairwise symmetrical tensors for the triangular FHP lattice in two dimensions and the face-centered-hypercubic (FCHC) lattice in four dimensions, and thus also for the pseudo-four-dimensional three-dimensional model. We give now elementary proofs of these results.

In two dimensions, it is convenient to consider  $T_{\alpha\beta\gamma\delta}$  as a linear map from the space  $E$  of two-by-two real symmetrical matrices into itself:

$$T: A_{\alpha\beta} \mapsto T_{\alpha\beta\gamma\delta} A_{\gamma\delta}. \quad (6.7)$$

A basis of the space  $E$  is formed by the matrices  $P_1$ ,  $P_2$ , and  $P_3$ , associated with the orthogonal projections onto the  $x_1$ -axis and onto two other directions at  $2\pi/3$  and  $4\pi/3$ . In this representation, an arbitrary  $E$ -matrix may be written as

$$A = \chi_1 P_1 + \chi_2 P_2 + \chi_3 P_3, \quad (6.8)$$

and  $T$  becomes a three-by-three matrix  $T_{ab}$ , ( $a, b = 1, 2, 3$ ). The key observation is that the hexagonal group (rotations by multiples of  $\pi/3$ ) becomes the permutation group of  $P_1$ ,  $P_2$ , and  $P_3$ . Thus,  $T_{ab}$  is invariant under arbitrary permutations of the coordinates, i.e., is of the form

$$T_{ab} = \phi \text{diag}_{ab}(1, 1, 1) + \chi 1_{ab}, \quad (6.9)$$

where  $\text{diag}_{ab}(1, 1, 1)$  is the diagonal matrix with entries one,  $1_{ab}$  is the matrix with all entries equal to one, and  $\phi$  and  $\chi$  are arbitrary scalars. From equation (6.8), we have

$$\text{tr}(A) = \chi_1 + \chi_2 + \chi_3, \quad (6.10)$$

where  $\text{tr}$  denotes the trace. We also note that

$$P_1 + P_2 + P_3 = (3/2)I, \quad (6.11)$$

where  $I$  is the identity (check it for the unit vectors of the  $x_1$  and  $x_2$  axis). Using equations (6.10) and (6.11), we can rewrite equation (6.9) as

$$T: A \mapsto \phi A + \frac{3}{2}\chi \operatorname{tr}(A)I. \quad (6.12)$$

Reverting to tensor notations, this becomes

$$T_{\alpha\beta\gamma\delta} = \frac{\phi}{2}(\delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}) + \frac{3\chi}{2}\delta_{\alpha\beta}\delta_{\gamma\delta}, \quad (6.13)$$

which is obviously isotropic.

We turn to the four-dimensional case, using the FCHC model of section 2.3. Invariance under permutations of coordinates and reversal of any coordinate implies that the most general possible form for  $T_{\alpha\beta\gamma\delta}$  is

$$T_{\alpha\beta\gamma\delta} = \phi\delta_{\alpha\beta}\delta_{\gamma\delta} + \chi(\delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}) + \psi\delta_{\alpha\beta}\delta_{\gamma\delta}. \quad (6.14)$$

The  $\chi$  and  $\psi$  terms are already isotropic. The vanishing of  $\phi$  is a consequence of the invariance of the velocity set under the symmetry  $\Sigma$  with respect to the hyperplane  $x_1 + x_2 + x_3 + x_4 = 0$ , that is,

$$x_\alpha \mapsto x_\alpha - \sigma, \quad \sigma = \frac{1}{2} \sum_\alpha x_\alpha. \quad (6.15)$$

Indeed, consider the vector  $v_\alpha = (2, 0, 0, 0)$ . Contracting the  $\phi$  term four times with  $v_\alpha$ , we obtain  $16\phi$ ; the image of  $v_\alpha$  under  $\Sigma$  is  $w_\alpha = (1, -1, -1, -1)$ , which contracted four times with the  $\phi$  term gives  $4\phi$ . Thus, invariance requires  $\phi = 0$ , which proves isotropy.

We return to the general  $D$ -dimensional case, assuming isotropy. Substituting equation (6.6) into the macrodynamical momentum equation (5.17), we obtain

$$\begin{aligned} & \partial_t(\rho u_\alpha) + \partial_\beta(\rho g(\rho)u_\alpha u_\beta) + \partial_\alpha\left(c_s^2\rho\left(1 - g(\rho)\frac{u^2}{c^2}\right)\right) \\ &= \partial_\beta\left[(\nu_c(\rho) + \nu_p)\left(\partial_\alpha(\rho u_\beta) + \partial_\beta(\rho u_\alpha) - \frac{2}{D}\delta_{\alpha\beta}\partial_\gamma(\rho u_\gamma)\right)\right] \\ &+ O(\epsilon u^3) + O(\epsilon^2 u^2) + O(\epsilon^3 u), \end{aligned} \quad (6.16)$$

with

$$\begin{aligned} g(\rho) &= \frac{D}{D+2} \frac{b-2\rho}{b-\rho}, \quad c_s^2 = \frac{c^2}{D}, \\ \nu_c(\rho) &= -\frac{bc^4}{D(D+2)}\psi(\rho), \quad \nu_p = -\frac{c^2}{2(D+2)}. \end{aligned} \quad (6.17)$$

Note that  $g(\rho)$  appearing in equation (6.17) is not the same as  $G(\rho)$  introduced in equation (4.15). Note also that  $\psi(\rho)$ , which was introduced in section 5, is still to be determined (see section 8).

We have now recovered macroscopic isotropy; equation (6.16) is very closely related to the fluid dynamical momentum (Navier-Stokes) equations. We postpone all further remarks to the next section.

## 7. Fluid dynamical regimes

Let us rewrite the macrodynamical equations for mass and momentum, derived in the previous sections in a compact form which brings out their similarities with the equations of fluid dynamics:

$$\partial_t \rho + \partial_\beta (\rho u_\beta) = 0, \quad (7.1)$$

$$\partial_t (\rho u_\alpha) + \partial_\beta P_{\alpha\beta} = \partial_\beta S_{\alpha\beta} + O(\epsilon u^3) + O(\epsilon^2 u^2) + O(\epsilon^3 u). \quad (7.2)$$

The momentum-flux tensor  $P_{\alpha\beta}$  and the viscous stress tensor  $S_{\alpha\beta}$  are given by

$$P_{\alpha\beta} = c_s^2 \rho \left( 1 - g(\rho) \frac{u^2}{c^2} \right) \delta_{\alpha\beta} + \rho g(\rho) u_\alpha u_\beta, \quad (7.3)$$

and

$$S_{\alpha\beta} = \nu(\rho) \left( \partial_\alpha (\rho u_\beta) + \partial_\beta (\rho u_\alpha) - \frac{2}{D} \delta_{\alpha\beta} \partial_\gamma (\rho u_\gamma) \right) \\ \nu(\rho) = \nu_c(\rho) + \nu_p, \quad (7.4)$$

where  $g(\rho)$ ,  $c_s^2$ ,  $\nu_c$ , and  $\nu_p$  are defined in equation (6.17). Their values for the FHP-I and FCHC models are given below:

$$g(\rho) = \frac{3-\rho}{6-\rho}, \quad c_s^2 = \frac{1}{2}, \quad \nu_c(\rho) = -\frac{3}{4}\psi(\rho), \quad \nu_p = -\frac{1}{8}, \quad \text{for FHP-I} \\ g(\rho) = \frac{4}{3} \frac{12-\rho}{24-\rho}, \quad c_s^2 = \frac{1}{2}, \quad \nu_c(\rho) = -4\psi(\rho), \quad \nu_p = -\frac{1}{6}, \quad \text{for FCHC.} \quad (7.5)$$

Various remarks are now in order. When the velocity  $\mathbf{u}$  is very small, the momentum-flux tensor reduces to a diagonal pressure term  $p\delta_{\alpha\beta}$  with the pressure given by the "isothermal" relation

$$p = c_s^2 \rho. \quad (7.6)$$

From this, we infer that the speed of sound should be  $c_s$ , namely  $1/\sqrt{2}$  for FHP-I and FCHC.

The momentum-flux tensor in the "real world" is  $P_{\alpha\beta} = p\delta_{\alpha\beta} + \rho u_\alpha u_\beta$ . This form is a consequence of Galilean invariance, which allows one to relate thermodynamic equilibria with vanishing and nonvanishing mean velocities. The lattice gas momentum-flux tensor (7.3) with nonvanishing velocity differs by an additive term in the pressure and a multiplicative density-dependent factor  $g(\rho)$  in the advection term. We will see later in this section how Galilean invariance can nevertheless be recovered.

Equation (7.4) is the stress-strain relation for a Newtonian fluid having kinematic viscosity  $\nu_c + \nu_p$  and vanishing bulk viscosity [64]. The traceless

character of  $S_{\alpha\beta}$  (which implies this vanishing of the bulk viscosity) comes from the traceless character of  $Q_{i\alpha\beta}$ , defined by equation (4.15); this result would be upset by the presence of rest particles such as exist in the models FHP-II and III (see Appendix E). The kinematic viscosity has two contributions. One is the "collision viscosity"  $\nu_c$ , not yet determined, which depends on the details of the collisions and is positive (see section 8). The other one is the "propagation viscosity"  $\nu_p$ , which is negative and does not involve the collisions. The presence of such a negative propagation viscosity is an effect of the lattice discreteness [42].

The general strategy by which standard fluid dynamical equations are derived from equations (7.1) and (7.2) is to rescale the space, time, and velocity variables in such a way as to make undesirable terms irrelevant as  $\epsilon \rightarrow 0$ . Three different regimes will be considered in the following subsections. They correspond respectively to sound propagation, sound propagation with slow damping, and incompressible (Navier-Stokes) fluid dynamics.

### 7.1 Sound propagation

Consider a weak perturbation of the equilibrium solution with density  $\rho_0$  and velocity zero. We write

$$\rho = \rho_0 + \rho'. \quad (7.7)$$

In a suitable limit, we expect that the only relevant terms in equations (7.1) and (7.2) will be<sup>9</sup>

$$\begin{aligned} \partial_t \rho' + \rho_0 \nabla \cdot \mathbf{u} &= 0 \\ \rho_0 \partial_t \mathbf{u} + c_s^2 \nabla \rho' &= 0. \end{aligned} \quad (7.8)$$

Formally, this regime is obtained by setting

$$\mathbf{r} = \epsilon^{-1} \mathbf{r}_1, \quad t = \epsilon^{-1} t_1, \quad \rho' = \epsilon^a \rho'_1, \quad \mathbf{u} = \epsilon^a \mathbf{U}, \quad a > 0. \quad (7.9)$$

It is then straightforward to check that the leading order terms take the form of equations (7.8) (in the rescaled variables). Eliminating  $\mathbf{u}$  in equation (7.8), we obtain the scalar wave equation

$$\frac{\partial^2}{\partial t^2} \rho' - c_s^2 \nabla^2 \rho' = 0. \quad (7.10)$$

In other words, density and velocity perturbations with amplitudes  $o(1)$  on temporal and spatial scales  $O(\epsilon)$  propagate as sound waves with speed  $c_s$ .<sup>10</sup> Since the present regime of undamped sound waves involves only tensors of second order, it also applies to the HPP model.

<sup>9</sup>From here on, we use vector notation whenever possible.

<sup>10</sup>We have used here the Landau  $O()$  and  $o()$  notation.



## 7.2 Damped sound

Another regime includes the viscous damping term, so that instead of equation (7.8), we should have

$$\begin{aligned}\partial_t \rho' + \rho_0 \nabla \cdot \mathbf{u} &= 0 \\ \rho_0 \partial_t \mathbf{u} + c_s^2 \nabla \rho' &= \rho_0 \nu (\rho_0) \left( \nabla^2 \mathbf{u} + \frac{D-2}{D} \nabla \nabla \cdot \mathbf{u} \right).\end{aligned}\quad (7.11)$$

To obtain this regime, we proceed as in section 7.1 and include an additional time  $t_2 = \epsilon^2 t$ . Furthermore, in the scaling relation (7.9) we now require  $a > 1$ , that is,  $\mathbf{u}$  and  $\rho'$  should be  $o(\epsilon)$ ; otherwise, the nonlinear term also becomes relevant. Note that the damping is now on a time scale  $O(\epsilon^{-2})$ . Since propagation and damping are on time scales involving different powers of  $\epsilon$ , it is not possible to describe them in a single equation without mixing orders.

## 7.3 Incompressible fluid dynamics: the Navier-Stokes equations

It is known that many features of low Mach number<sup>11</sup> flows in an ordinary gas can be described by the incompressible Navier-Stokes equation

$$\begin{aligned}\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} &= -\nabla p + \nu \nabla^2 \mathbf{u} \\ \nabla \cdot \mathbf{u} &= 0.\end{aligned}\quad (7.12)$$

In the “real world”, the incompressible Navier-Stokes equation can be derived from the full compressible equations, using a Mach number expansion. There are some fine points in this expansion for which we refer the interested reader to reference 65. Ignoring these, the essential observation is that, to leading order, density variations become irrelevant everywhere except in the pressure term; the latter becomes slaved to the nonlinear term by the incompressibility constraint.

Just the same kind of expansion (with the same difficulties) can be applied to lattice gas dynamics. We start from equations (7.1) and (7.2) and freeze the density by setting it equal to the constant and uniform value  $\rho_0$  everywhere except in the pressure term, where we keep the density fluctuations. We also ignore all higher-order terms  $O(\epsilon^3 u)$ , etc. This produces the following set of equations:

$$\begin{aligned}\rho_0 \partial_t \mathbf{u} + \rho_0 g(\rho_0) \mathbf{u} \cdot \nabla \mathbf{u} &= -c_s^2 \nabla (p' - p(0)g(p_0) \frac{u^2}{c^2}) + \rho_0 \nu (\rho_0) \nabla^2 \mathbf{u} \\ \nabla \cdot \mathbf{u} &= 0.\end{aligned}\quad (7.13)$$

<sup>11</sup>The Mach number is the ratio of a characteristic flow velocity to the speed of sound.

The resulting equations (7.13) differ from equation (7.2) only by the presence of the factor  $g(\rho_0)$  in front of the advection term  $\mathbf{u} \cdot \nabla \mathbf{u}$ . As it stands, equation (7.13) is not Galilean invariant. This, of course, reflects the lack of Galilean invariance at the lattice level. Similarly, the vanishing of  $g(\rho_0)$  when the density per cell  $d = \rho_0/b$  is equal to  $1/2$ , i.e., for equal mean numbers of particles and holes, reflects a duality-invariance of the lattice gas without counterpart in the "real world" (see end of section 4.2). However, as soon as  $d < 1/2$ , it is straightforward to reduce equation (7.13) to the true Navier-Stokes equations (7.12); it suffices to rescale time and viscosity:

$$t \rightarrow \frac{t}{g(\rho_0)}, \quad \nu \rightarrow g(\rho_0)\nu. \quad (7.14)$$

Now we show that there is actually a rescaling of variables which reduces the macrodynamical equations to the incompressible Navier-Stokes equations. We set

$$\mathbf{r} = \epsilon^{-1}\mathbf{r}_1, \quad t = \frac{1}{g(\rho_0)}\epsilon^{-2}T, \quad \mathbf{u} = \epsilon\mathbf{U},$$

$$(p' - p(0))g(\rho_0)\frac{u^2}{c_s^2} = \frac{\rho_0 g(\rho_0)}{c_s^2}\epsilon^2 P', \quad \nu = g(\rho_0)\nu'. \quad (7.15)$$

Thus, all the relevant terms are  $O(\epsilon^2)$  in equation (7.1) and  $O(\epsilon^3)$  in equation (7.2). The higher-order terms in the r.h.s. of equation (7.2) are  $O(\epsilon^4)$  or smaller. In this way, we obtain to leading order ( $\nabla_1$  denotes the gradient with respect to  $\mathbf{r}_1$ )

$$\partial_T \mathbf{U} + \mathbf{U} \cdot \nabla_1 \mathbf{U} = -\nabla_1 P' + \nu' \nabla_1^2 \mathbf{U}$$

$$\nabla_1 \cdot \mathbf{U} = 0, \quad (7.16)$$

which are exactly the incompressible Navier-Stokes equations.

Various comments are now made. The expansion leading to equation (7.16) is a large-scale and low Mach number expansion (the former is here inversely proportional to the latter). It also follows from the scaling relations (7.15) that the Reynolds number is kept fixed. It is not possible within our framework to have an asymptotic regime leading to nonlinear compressible equations at finite Mach number. Indeed, the speed of sound is here a *finite* fraction of the particle speed, and it is essential that the macroscopic velocity be small compared to particle speed, so as not to be contaminated by higher-order nonlinearities. It is noteworthy that models can be constructed having many rest particles (zero-velocity) with arbitrarily low speed of sound.

In a pure Navier-Stokes context, the non-Galilean invariance at the microscopic level is not a serious difficulty; as we have seen, Galilean invariance is recovered macroscopically, just by rescaling the time variable. However, when the models discussed here are generalized to include, for example,

multi-phase flow or buoyancy effects, a more serious problem may arise because the advection term of scalar quantities, such as chemical concentrations or temperature, involves usually a factor  $g(\rho)$  different from that of the nonlinear advection term in the Navier-Stokes equations. Various solutions to this problem have been proposed [48,66].

There is a variant of our formalism, leading also to the incompressible Navier-Stokes equations, but in terms of the *mass current*  $\mathbf{j} = \rho\mathbf{u}$  rather than the velocity  $\mathbf{u}$ . The analog of equation (7.13) (without rescaling) is then

$$\partial_t \mathbf{j} + \frac{g(\rho_0)}{\rho_0} \mathbf{j} \cdot \nabla \mathbf{j} = -c_s^2 \nabla \rho' + \nu(\rho_0) \nabla^2 \mathbf{j}$$

$$\nabla \cdot \mathbf{j} = 0. \quad (7.17)$$

Since  $\mathbf{j}$  and  $g(\rho_0)/\rho_0$  change sign under duality, equation (7.17) brings out duality-invariance.<sup>12</sup> A more decisive advantage of the  $\mathbf{j}$ -representation is that it gives a better approximation to the *steady state* Navier-Stokes equations when the Mach number is only moderately small. This is because in the steady state the continuity equation implies exactly  $\nabla \cdot \mathbf{j} = 0$ .

In three dimensions, when we use the pseudo-four-dimensional FCHC model, there are three independent space variables  $\mathbf{r} = (x_1, x_2, x_3)$ , but four velocity components:

$$\mathbf{U}_f = (\mathbf{U}, U_4) = (U_1, U_2, U_3, U_4). \quad (7.18)$$

The four-velocity  $\mathbf{U}_f$  satisfies the four-dimensional Navier-Stokes equations with no  $x_4$ -dependence. Thus, the three-velocity  $\mathbf{U}$  satisfies the three-dimensional Navier-Stokes equations (7.16),<sup>13</sup> while  $U_4$  satisfies (note that the pressure term drops out)

$$\partial_T U_4 + \mathbf{U} \cdot \nabla_1 U_4 = \nu' \nabla_1^2 U_4. \quad (7.19)$$

This is the equation for a *passive scalar* with unit Schmidt number (ratio of viscosity to diffusivity).

Finally, we refer the reader to Appendix D for the inclusion of body forces in the Navier-Stokes equations.

<sup>12</sup>In the  $\mathbf{u}$ -representation, duality-invariance is broken because we have decided to work with the velocity of *particles* rather than with that of *holes*.

<sup>13</sup>Since the velocity set of the pseudo-four-dimensional model is the same as in four dimensions, isotropy is ensured for all fourth-order tensors depending only on the velocity set. Thus, the nonlinear term has the correct isotropic form. The viscous term is isotropic within the Boltzmann approximation (see section 8.2); otherwise, deviations from isotropy are expected to be small [2].

## 8. The viscosity

All the macroscopic equations derived in section 7 have a universal form which does not depend on the details of collisions. The kinematic shear viscosity  $\nu$ , which we will henceforth call the viscosity, does not possess this universality. Transport coefficients such as the viscosity characterize the linear response of equilibrium solutions to small externally imposed perturbations. It is known in statistical mechanics that the relaxation (or dissipation) of external perturbations is connected to the fluctuations at equilibrium via *fluctuation-dissipation* relations. Such relations have a counterpart for lattice gases. Two quite different approaches are known. In section 8.1, following a suggestion already made in [23], we present the “noisy” hydrodynamics viewpoint, in the spirit of Landau and Lifschitz [67,68]. Another approach, in the spirit of Kubo [69] and Green [70], using a Liouville equation formalism, may be found in reference 43. In section 8.2, we introduce the lattice analog of the Boltzmann approximation, which allows an explicit calculation of the viscosity. In section 8.3, we discuss some implications for the Reynolds numbers of incompressible flows simulated on lattice gases.

### 8.1 Fluctuation-dissipation relation and “noisy” hydrodynamics

We first explain the basic ideas in words. Spontaneous fluctuations at equilibrium involve modes of all possible scales. The fluctuations of very large scales should have their dynamics governed by the macroscopic equations derived in sections 5 through 7. Such fluctuations are also expected to be very weak, so that *linear* hydrodynamics should apply. Large-scale spontaneous fluctuations are constantly regenerated, and in a random manner; this regeneration is provided by a random force (noise) term which can be identified and expressed in terms of the fluctuating microscopic variables. If this random force has a short correlation-time (i.e., small compared to the life-time of the large-scale fluctuations under investigation), then each large-scale mode  $v$  has its dynamics governed by a Langevin equation.<sup>14</sup> It follows that the variance  $\langle v^2 \rangle$  can be expressed in terms of the damping coefficient  $\gamma$  (related to the viscosity) and of the time-correlation function of the random force. Alternatively, the variance  $\langle v^2 \rangle$  can be calculated from the known one-time equilibrium properties. Identification gives the viscosity in terms of equilibrium time-correlation functions. This is the general program that we now carry out for the special case of lattice gases. We restrict ourselves to equilibrium solutions with zero mean velocity.

We will use in this section the following notation. The density  $\rho$  and the mass current  $j$  are no longer given by their expressions (3.24) in terms of the mean populations; instead, they are defined in terms of the fluctuating Boolean field

<sup>14</sup>For the case of lattice gases, we will actually obtain a finite difference equation.

$$\rho(t_*, \mathbf{r}_*) = \sum_i n_i(t_*, \mathbf{r}_*), \quad \mathbf{j}(t_*, \mathbf{r}_*) = \sum_i \mathbf{c}_i n_i(t_*, \mathbf{r}_*). \quad (8.1)$$

We denote by  $\tilde{n}_i$  the fluctuating part of the Boolean field, defined by

$$n_i(t_*, \mathbf{r}_*) = d + \tilde{n}_i(t_*, \mathbf{r}_*), \quad (8.2)$$

where  $d$  is the density per cell.

We introduce *meso-averaged* fields by taking *spatial* averages over a distance  $\epsilon^{-1}$ .<sup>15</sup> These will be denoted by angular brackets with the subscript *ma*. The meso-averages of  $n_i$ ,  $\rho$ , and  $\mathbf{j}$  are denoted  $\bar{n}_i$ ,  $\bar{\rho}$ , and  $\bar{\mathbf{j}}$  respectively. Locally, the equilibrium relation (4.14) should hold approximately for the meso-averaged populations. We thus write

$$\bar{n}_i = \frac{\bar{\rho}}{b} + \frac{D}{c^2 b} \bar{\mathbf{j}} \cdot \mathbf{c}_i + \delta_i + \bar{n}_i^{(1)}(t_*, \mathbf{r}_*). \quad (8.3)$$

$\delta_i$  represents the (still unknown) input from non-hydrodynamic fluctuations;  $\bar{n}_i^{(1)}$  is the contribution analogous to  $\epsilon N_i^{(1)}$  in equation (5.1), arising from the gradients of meso-averages. Note that in equation (8.3) we dropped contributions nonlinear in the mass current; indeed, we should be able to determine the viscosity from just linear hydrodynamics.<sup>16</sup>

We now derive the equations for noisy hydrodynamics. As usual, we start from the microscopic conservation relations (3.16) and (3.17) and we take their meso-averages:

$$\sum_i [\bar{n}_i(t_* + 1, \mathbf{r}_* + \mathbf{c}_i) - \bar{n}_i(t_*, \mathbf{r}_*)] = 0, \quad (8.4)$$

$$\sum_i \mathbf{c}_i [\bar{n}_i(t_* + 1, \mathbf{r}_* + \mathbf{c}_i) - \bar{n}_i(t_*, \mathbf{r}_*)] = 0. \quad (8.5)$$

Substituting equation (8.3) into equation (8.5), we obtain

$$\begin{aligned} & \frac{1}{b} \sum_i \mathbf{c}_i [\bar{\rho}(t_* + 1, \mathbf{r}_* + \mathbf{c}_i) - \bar{\rho}(t_*, \mathbf{r}_*)] + \frac{D}{c^2 b} \sum_i \mathbf{c}_i \mathbf{c}_i [\bar{\mathbf{j}}(t_* + 1, \mathbf{r}_* + \mathbf{c}_i) - \bar{\mathbf{j}}(t_*, \mathbf{r}_*)] \\ & + \sum_i \mathbf{c}_i [\bar{n}_i^{(1)}(t_* + 1, \mathbf{r}_* + \mathbf{c}_i) - \bar{n}_i^{(1)}(t_*, \mathbf{r}_*)] = \mathbf{f}(t_*, \mathbf{r}_*), \end{aligned} \quad (8.6)$$

where

$$\mathbf{f}(t_*, \mathbf{r}_*) = - \sum_i \mathbf{c}_i [\delta_i(t_* + 1, \mathbf{r}_* + \mathbf{c}_i) - \delta_i(t_*, \mathbf{r}_*)] \quad (8.7)$$

is the random force. Using equations (8.1) through (8.5), we can also write (to leading order in gradients)

<sup>15</sup>More precisely, by dropping spatial Fourier components with wavenumber  $k > \epsilon$ .

<sup>16</sup>This is not exactly true in two dimensions as we will see below.

$$\mathbf{f}(t_*, \mathbf{r}_*) = \left\langle \frac{1}{c^2 b} \sum_{ij} (c^2 \mathbf{c}_i + D \mathbf{c}_i \cdot \mathbf{c}_j \mathbf{c}_i) [\tilde{n}_j(t_* + 1, \mathbf{r}_* + \mathbf{c}_i) - \tilde{n}_j(t_* + 1, \mathbf{r}_* + \mathbf{c}_j)] \right\rangle_{ma} \quad (8.8)$$

The l.h.s. of equation (8.6) is expanded in powers of gradients (i.e., of  $\epsilon$ ), as we did in section 5. However, we keep finite differences rather than derivatives in time because of the presence of the rapidly varying random force. Since we only want to identify the shear viscosity (the bulk viscosity is zero), it suffices to extract the solenoidal part of the hydrodynamical equation. For this and other reasons, it is better to work in Fourier space. We define the (spatial) Fourier transform of the fluctuating Boolean field by

$$\tilde{n}_i(t_*, \mathbf{r}_*) = \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}_*} \hat{n}(t_*, \mathbf{k}), \quad (8.9)$$

where the components of  $\mathbf{k}$  are multiples of  $2\pi$  divided by the lattice periodicities in the various directions. We similarly define  $\hat{\mathbf{j}}$  and  $\hat{\mathbf{f}}$ , the Fourier transforms of the mass current and the random force. Their solenoidal parts, projection on the hyperplane perpendicular to  $\mathbf{k}$ , are denoted  $\hat{\mathbf{j}}_{\perp}$  and  $\hat{\mathbf{f}}_{\perp}$ .

To leading order in  $k$ , we obtain from equation (8.8) using equation (2.5)

$$\hat{\mathbf{f}}_{\perp}(t_*, \mathbf{k}) = - \sum_j i\mathbf{k} \cdot \mathbf{c}_j \left( \mathbf{c}_j - \frac{\mathbf{c}_j \cdot \mathbf{k} \mathbf{k}}{k^2} \right) \hat{n}_j(t_* + 1, \mathbf{k}). \quad (8.10)$$

The meso-averaging is just the restriction that  $k < \epsilon$ . Fourier transforming equation (8.6) and taking the solenoidal part, we obtain for small  $k$

$$\hat{\mathbf{j}}_{\perp}(t_* + 1, \mathbf{k}) - \hat{\mathbf{j}}_{\perp}(t_*, \mathbf{k}) + \nu k^2 \hat{\mathbf{j}}_{\perp}(t_*, \mathbf{k}) = \hat{\mathbf{f}}_{\perp}(t_*, \mathbf{k}). \quad (8.11)$$

This is our discrete Langevin equation. Note that  $\nu$  is the (total) viscosity  $\nu = \nu_e + \nu_p$ . In principle, we must expand to second order in  $k$  to obtain the viscous terms, but we could as well have written the l.h.s of equation (8.11) a priori, since we want to use equation (8.11) to *determine* the viscosity. It is straightforward to solve the linear finite-difference equation (8.11). From the solution, we calculate the variance of  $\hat{\mathbf{j}}_{\perp}$  and obtain, when the viscous damping time  $1/(\nu k^2)$  is large compared to the correlation time of the random force

$$\langle |\hat{\mathbf{j}}_{\perp}(t_*, \mathbf{k})|^2 \rangle = \frac{1}{2\nu k^2} \sum_{t_*=-\infty}^{t_*=+\infty} \langle \hat{\mathbf{f}}_{\perp}(t_*, \mathbf{k}) \cdot \hat{\mathbf{f}}_{\perp}^*(t_*, \mathbf{k}) \rangle \quad (8.12)$$

where the asterisk denotes complex conjugation. The variance of  $\hat{\mathbf{j}}_{\perp}$  can also be calculated directly using equation (8.1) and

$$\begin{aligned}\langle \tilde{n}_i(t_*, \rho_*) \tilde{n}_j(t_*, 0) \rangle &= \langle \tilde{n}_i^2 \rangle \delta_{ij} \delta_{\rho_*} \\ \langle \tilde{n}_i^2 \rangle &= \langle n_i^2 \rangle - \langle n_i \rangle^2 = d - d^2,\end{aligned}\quad (8.13)$$

where  $\delta_{\rho_*}$  denotes a Kronecker delta in the spatial separation  $\rho_*$ . We obtain

$$\left\langle |\hat{j}_\perp(t_*, \mathbf{k})|^2 \right\rangle = \frac{1}{V} b c^2 d (1 - d) \frac{D - 1}{D}, \quad (8.14)$$

where  $V$  denotes the total number of lattice points in the periodicity volume. Thus, the l.h.s. of equation (8.12) is  $\mathbf{k}$ -independent. We evaluate the r.h.s of equation (8.12) in the limit  $k \rightarrow 0$ , using equation (8.10). We skip some intermediate steps in which we (i) use the stationariness of the fluctuations at equilibrium, (ii) use the isotropy of second- and fourth-order symmetrical tensors, (iii) interchange the  $\mathbf{k} \rightarrow 0$  limit and the infinite summation over  $t_*$ .<sup>17</sup> Identifying the two expressions (8.12) and (8.14), we obtain for the viscosity

$$\begin{aligned}\nu &= \frac{D}{2(D-1)(D+2)} \frac{1}{b c^2} \frac{1}{d(1-d)} \frac{1}{V} \\ &\quad \sum_{t_*=-\infty}^{t_*=+\infty} \sum_{i,j,\alpha,\beta} Q_{i\alpha\beta} Q_{j\alpha\beta} \langle \hat{n}_i(t_*, 0) \hat{n}_j^*(0, 0) \rangle \\ &= \frac{D}{2(D-1)(D+2)} \frac{1}{b c^2} \frac{1}{d(1-d)} \sum_{t_*=-\infty}^{t_*=+\infty} \\ &\quad \sum_{\rho_* \in \mathcal{L}} \sum_{i,j,\alpha,\beta} Q_{i\alpha\beta} Q_{j\alpha\beta} \langle \tilde{n}_i(t_*, \rho_*) \tilde{n}_j(0, 0) \rangle\end{aligned}\quad (8.15)$$

with

$$Q_{i\alpha\beta} = c_{i\alpha} c_{i\beta} - \frac{c^2}{D} \delta_{\alpha\beta}. \quad (8.16)$$

This completes the fluctuation-dissipation calculation of the viscosity. A consequence of the Fourier-space representation (the upper half of equation (8.15)) is the positivity of the viscosity; indeed, the viscosity is, within a positive factor, the time-summation of the autocorrelation of  $\sum_i Q_{i\alpha\beta} \hat{n}_i(t_*, 0)$ .

Several comments are now in order. It is easily checked that the  $t_* = 0$  contribution to the viscosity (lower part of equation (8.15) is  $c^2/(2(D+2))$ , that is, just the opposite of the "propagation viscosity"  $\nu_p$  introduced in section 7. The viscosity is the sum of the collision viscosity  $\nu_c$  and  $\nu_p$ . Using the identity

$$\sum_{t_*=-\infty}^{t_*=+\infty} Z(t_*) = 2 \sum_{t_*=0}^{t_*=+\infty} Z(t_*) - Z(0), \quad (8.17)$$

<sup>17</sup>This is equivalent to assuming that the viscosity is finite, see below.



(for an even function  $Z(t_*)$ ), we find that  $\nu_c$  has a representation similar to (8.15) (lower part), with an additional factor of 2 and the summation over  $t_*$  extending only from 0 to  $\infty$ . We thereby recover an expression derived in reference 43, using a discrete variant of the Green-Kubo formalism. It is reassuring to have two completely different derivations of the viscosity, since we consider our fluctuation-dissipation derivation somewhat delicate.

It is of interest that the fluctuation-dissipation derivation gives directly the (total) viscosity. This suggests that the splitting into collision and propagation viscosities is an artifact of our multi-scale formalism.

There is no closed form representation of the correlation function  $\langle \tilde{n}_i(t_*, \rho_*) \tilde{n}_j(0, 0) \rangle$ , except for short times. However, (8.15) is a good starting point for a Monte-Carlo calculation of the viscosity [43].

In our derivation, we have dropped all contributions from *nonlinear* terms in the mass current  $j$ . Is this justified? If we reinstate the nonlinear terms, we obtain, for the solenoidal part of the meso-averaged mass current, the Navier-Stokes equations (7.17) of section 8 with the additional random force given in the Fourier representation by equation (8.10). On macroscopic scales, this force may be considered as  $\delta$ -correlated in time. Its spectrum follows, for small  $k$ , a  $k^{D+1}$  power-law.<sup>18</sup> The Navier-Stokes equations with this kind of power-law forcing is one of the few problems in nonlinear statistical fluid mechanics which can be systematically analyzed by renormalization group methods [71,72]. For  $D > 2$ , the nonlinear term is irrelevant for small  $k$  so that our calculation of the viscosity is legitimate. At the "crossover" dimension  $D = 2$ , the nonlinear term becomes "marginal"; it produces a renormalization of the viscosity which is then logarithmically scale-dependent. Thus, in the limit of infinite scale-separation, the viscosity becomes infinite in two dimensions. This is an instance of the known divergence of transport coefficients in two-dimensional statistical mechanics [68,73]. Alternatively, the divergence of the viscosity in two dimensions can be viewed as due to the presence of a "long-time-tail", proportional to  $t_*^{-D/2}$ , in the correlation function appearing in equation (8.15). Attempts have been made to observe long-time-tails and scale-dependence of the viscosity in Monte-Carlo simulations of lattice gas models [8,23,43,44]. This is not easy because (i) the effects show up only at very long times (or large scales) and may then be hidden by Monte-Carlo noise (insufficient averaging), and (ii) the effects should get weaker as the number  $b$  of cells per node increases (see end of section 8.2).

Finally, the noisy hydrodynamics formalism can be used to estimate to what extent the microscopic noise contaminates the hydrodynamic macroscopic signal. Estimates, assuming the signal to be meso-averaged in space and time, have been made in the context of fully developed incompressible two- and three-dimensional turbulence.<sup>19</sup> It has been found that in two dimensions noise is relevant only at scales less than the dissipation scale,

<sup>18</sup>A factor  $k^2$  comes from the average squared Fourier amplitude and another factor  $k^{D-1}$  from the  $D$ -dimensional volume element.

<sup>19</sup>Note that in the incompressible case, only solenoidal noise is relevant.

while in three dimensions this happens only far out in the dissipation range [74].

## 8.2 The Lattice Boltzmann approximation

Explicit calculation of transport coefficients can be done for lattice gases, using the Boltzmann approximation. In this approximation, one assumes that *particles entering a collision process have no prior correlations*. The microdynamical formalism of section 3.1 is particularly well suited for deriving what we will call the *lattice Boltzmann equation*. We take the ensemble average of equation (3.9). The Boolean variables  $n_i$  become the mean populations  $N_i$ . The average of the collision function  $\Delta_i$  can be completely factorized, thanks to the Boltzmann approximation. We obtain

$$N_i(t_* + 1, \mathbf{r}_* + \mathbf{c}_i) = N_i(t_*, \mathbf{r}_*) + \Delta_i^{\text{boltz}}$$

$$\Delta_i^{\text{boltz}} = \sum_{s,s'} (s'_i - s_i) A(s \rightarrow s') \prod_j N_j^{s_j} (1 - N_j)^{(1-s_j)}. \quad (8.18)$$

Here, all the  $N_j$ 's are evaluated at  $t_*$  and  $\mathbf{r}_*$ . The  $A(s \rightarrow s')$ 's, the transition probabilities introduced in section 2.4, are the averages of the Boolean transition variables  $\xi_{ss'}$ . Note that the (Boltzmann) *collision function*  $\Delta_i^{\text{boltz}}$  vanishes at equilibrium.

The Boltzmann approximation in ordinary gases is associated with low density situations, when the mean-free path is so large that particles entering a collision come mostly from distant uncorrelated regions. The Boltzmann approximation for a lattice gas appears to have a very broad validity, not particularly restricted to low densities.<sup>20</sup> We will come back to the matter at the end of this section.

Our lattice Boltzmann equation (8.18) is a *finite difference* equation. There is a differential version of it, obtained by Taylor-expanding the finite differences to first order, namely

$$\partial_t N_i + \mathbf{c}_i \cdot \nabla N_i = \Delta_i^{\text{boltz}} \quad (8.19)$$

where  $\Delta_i^{\text{boltz}}$  is defined as in equation (8.18). Boltzmann equations of the form (8.19) have been extensively studied as discrete velocity approximations to the ordinary Boltzmann equation [15-17,19]. The (differential) Boltzmann formalism has been applied to various lattice gas models [35,39]. This formalism correctly captures all hydrodynamic phenomena involving only first-order derivatives. Indeed, for these, we have seen that only the equilibrium solutions matter, and the latter are completely factorized. Diffusive phenomena involve second-order derivatives. Hence, the *propagation viscosities* (see section 7), which are an effect of lattice-discreteness, are not

<sup>20</sup> Even at low densities, the Boltzmann approximation may not be valid. Indeed, without effectively changing the dynamics, we can reduce the density by arbitrary large factors by having the particles initially located on a sub-lattice with some large periodicity; these are, however, pathologically unstable configurations.

captured by the (differential) Boltzmann equation. At low densities, where collision viscosities dominate over propagation viscosities, the discrepancy is irrelevant.

We do not intend to engage in extended discussions of the consequences of the lattice Boltzmann equation because most of the derivation of the hydrodynamical equations is independent of this approximation. There are, however, two important results which follow from the lattice Boltzmann equation. The first concerns the irreversible approach to equilibrium. It is derived by adapting an H-theorem formalism to the fully discrete context (see Appendix F by Hénion).

The second result is an explicit derivation of the viscosity. From the Boltzmann equation, this is usually done by a Chapman-Enskog formalism [75,76] (see also Gatignol's monography, [17]). This formalism is easily adapted to the lattice Boltzmann equation [77]. With the general multi-scale formalism of sections 5 through 7, we have already covered a substantial fraction of the ground. Furthermore, an alternative derivation which stays completely at the microscopic level is presented in this volume by Hénion, who also discusses consequences of his explicit viscosity-formula [42]. We will therefore be brief.

The problem of the viscosity amounts to finding the coefficient  $\psi$  relating the gradient of the mass current  $\rho u$  to the first-order perturbation  $N_i^{(1)}$  of the mean population, through (see equation (5.14) of section 5)

$$\begin{aligned} N_i^{(1)} &= \psi Q_{i\alpha\beta} \partial_{1\alpha} (\rho u_\beta) \\ Q_{i\alpha\beta} &= c_{i\alpha} c_{i\beta} - \frac{c_i^2}{D} \delta_{\alpha\beta}. \end{aligned} \quad (8.20)$$

We start from equation (5.1) with  $N_i^{(0)}$  given by equation (4.14). We substitute into the lattice Boltzmann equation (8.18) and identify the terms  $O(\epsilon)$ . For this, we Taylor-expand finite differences to first order, use equations (5.6) and (5.7) to express time-derivatives in terms of space-derivatives, and ignore all terms beyond the linear ones in the velocity. We obtain

$$\frac{D}{bc^2} Q_{i\alpha\beta} \partial_{1\alpha} (\rho u_\beta) = \sum_j A_{ij} N_j^{(1)}. \quad (8.21)$$

Here,

$$A_{ij} = \left[ \frac{\partial \Delta_i^{\text{Boltz}}}{\partial N_j} \right]_{N_i = \rho/b} \quad (8.22)$$

is the *linearized collision matrix*, evaluated at the zero-velocity equilibrium, which can be expressed in compact form as [42]

$$\begin{aligned} A_{ij} &= -\frac{1}{2} \sum_{ss'} (s_i - s'_i) A(s \rightarrow s') d^{p-1} (1-d)^{b-p-1} (s_j - s'_j), \\ p &= \sum_i s_i. \end{aligned} \quad (8.23)$$

We eliminate  $N_i^{(1)}$  between equations (8.20) and (8.21), to obtain

$$\left[ \frac{D}{bc^2} Q_{i\alpha\beta} - \psi \sum_j A_{ij} Q_{j\alpha\beta} \right] \partial_{1\alpha} (\rho u_\beta) = 0. \quad (8.24)$$

This should hold for arbitrary gradients of the mass current. Thus, the quantity between square brackets vanishes. This means that, for any  $(\alpha, \beta)$ ,  $Q_{i\alpha\beta}$ , considered as a vector with components labeled by  $i$ , is an eigenvector of the linearized collision matrix with eigenvalue  $D/(bc^2\psi)$ ; a direct proof of this may be derived from the  $\mathcal{G}$ -invariance. From equation (8.24), we can easily calculate  $\psi$ ; the simplest method is to multiply the vanishing square bracket by  $Q_{i\alpha\beta}$  and sum over  $i$ ,  $\alpha$ , and  $\beta$ . If, in addition, we assume the isotropy of fourth-order tensors, we can use equation (6.17) to obtain a closed-form expression for the collision viscosity

$$\nu_c = - \frac{c^2}{D + 2 \sum_{ij\alpha\beta} Q_{i\alpha\beta} A_{ij} Q_{j\alpha\beta}}. \quad (8.25)$$

In Appendix E, we give explicit formulae calculated from equation (8.25) for the viscosities of the FHP models (including those with rest particles which require minor amendements of our formalism).

We finally address the question of the validity of the lattice Boltzmann equation. Comparisons of the viscosities obtained from simulations [25,29,31,33] or Monte-Carlo calculations [77] with the predictions of the lattice Boltzmann approximation suggest that the validity of the latter is not limited to low densities. We know that equilibrium solutions are factorized and that transport coefficients can be calculated with arbitrarily weak macroscopic gradients. However, this cannot be the basis for the validity of the Boltzmann approximation: a weak *macroscopic* gradient implies that the probability of changing the state of a given node from its equilibrium value is small; but when such a change takes place, it produces a strong *microscopic* perturbation in its environment. Otherwise, there would be no (weak) divergence of the viscosity in two dimensions; indeed, the Boltzmann approximation does not capture noise-induced renormalization effects (see end of section 8.1). A more likely explanation of the success of the lattice Boltzmann approximation may be that it is the leading order in some kind of  $1/b$  expansion, where  $b$  is the number of velocity cells at each node. At the moment, we can only support this by the following heuristic argument. Deviations from Boltzmann require correlations between particles entering a collision. The latter arise from previous collisions;<sup>21</sup> when  $b$  is large, the weight pertaining to such events ought to be small.

### 8.3 The Reynolds number

Knowing the kinematic shear viscosity in terms of the density and the collision rules, we can calculate the Reynolds number associated to a large-scale flow.

<sup>21</sup>Collisions produce correlations whenever the particles are not exactly at equilibrium.

A natural unit of length is the lattice constant (distance of adjacent nodes), which has been taken equal to one for the two-dimensional HPP and FHP models. The four-dimensional FCHC model has a lattice constant of  $\sqrt{2}$ , but its three-dimensional projected version, the pseudo-four-dimensional FCHC model, resides on a cubic lattice which has also unit lattice constant. The time necessary for microscopic information to propagate from one node to its connecting neighbors defines a natural unit of time. We then have a natural unit of velocity: the speed necessary to travel the lattice constant (or the projected lattice constant for the pseudo-four-dimensional model) in a unit time. In these units, the characteristic scale and velocity of the flow will be denoted by  $\ell_0$  and  $u_0$ .

The standard definition of the Reynolds number is

$$R = \frac{\text{characteristic scale} \times \text{characteristic velocity}}{\text{kinematic shear viscosity}}. \quad (8.26)$$

In deriving the Navier-Stokes equations in section 7.3, we rescaled space, time, velocity, pressure, and viscosity (cf. equation (7.15)). The rescaling of space (by  $\epsilon$ ) and of velocity (by  $\epsilon^{-1}$ ) cancel in the numerator of equation (8.26). The rescaled viscosity is  $\nu'(\rho_0) = \nu(\rho_0)/g(\rho_0)$ . Hence, the Reynolds number is

$$R = \ell_0 u_0 \frac{g(\rho_0)}{\nu(\rho_0)}. \quad (8.27)$$

In order to operate in an incompressible regime, the velocity  $u_0$  should be small compared to the speed of sound  $c_s$ . The latter is model-dependent:  $c_s = 1/\sqrt{2}$  for FHP-I and FCHC,  $c_s = \sqrt{3/7}$  for FHP-II and FHP-III (see section 7 and Appendix E). Let us therefore re-express the Reynolds number in terms of the Mach number

$$M = \frac{u_0}{c_s}. \quad (8.28)$$

We obtain

$$R = M \ell_0 R_*(\rho_0), \quad (8.29)$$

where

$$R_*(\rho_0) = \frac{c_s g(\rho_0)}{\nu(\rho_0)} \quad (8.30)$$

contains all the *local* information.

In flow simulations using lattice gases, it is of interest to operate at the density which maximizes  $R_*$ . Let us work this out for the simplest case of FHP-I. For the viscosity, we use the lattice Boltzmann value given in Appendix E. We have

$$g(\rho_0) = \frac{1}{2} \frac{1-2d}{1-d}, \quad \nu(\rho_0) = \frac{1}{12d(1-d)^3} - \frac{1}{8}, \quad d = \frac{\rho_0}{6}. \quad (8.31)$$

Here,  $d$  is the mean density per cell. Substituting in equation (8.30), we find that

$$R_*^{\max} = \max R_* = 0.387, \quad \text{for } d = d_{\max} = 0.187. \quad (8.32)$$

Results for FHP-II and FHP-III are given in Appendix E. Note that a gain of about a factor 6 is achieved in going from FHP-I to FHP-III, because the latter includes many more collisions. For the pseudo-four-dimensional FCHC model there is work in progress on the optimization of collisions. It is already known that  $R_*^{\max}$  is at least 6.4 [78].

High Reynolds number incompressible turbulent flows have a whole range of scales. The smallest effectively excited scale is called the dissipation scale and denoted  $\ell_d$ . It is then of interest to find how many lattice constants are contained in  $\ell_d$ , since this will determine how effective lattice gases are in simulating high Reynolds number flows [1,36]. For this, let  $\ell_0$  denote the integral scale of the flow. Between  $\ell_0$ ,  $\ell_d$ , and the Reynolds number  $R$ , there is the following relation

$$\frac{\ell_d}{\ell_0} = CR^{-m}. \quad (8.33)$$

$m = 1/2$  in two dimensions and  $m = 3/4$  in three dimensions;  $C$  is a dimensionless constant not given by theory. In two dimensions, equation (8.33) is a consequence of the Batchelor-Kraichnan [79,80] phenomenological theory of the enstrophy cascade, which is well supported by numerical simulations [81]. In three dimensions, equation (8.33) follows from the Kolmogorov [82] phenomenological theory of the energy cascade, which is well supported<sup>22</sup> by experimental data [83]. Using equations (8.29) and (8.33) and assuming that  $R_*$  has its maximum value  $R_*^{\max}$ , we obtain

$$\ell_d = C (MR_*^{\max})^{-\frac{1}{2}} \ell_0^{\frac{1}{2}} = C (MR_*^{\max})^{-1} R^{\frac{1}{2}} \quad \text{in 2-D}, \quad (8.34)$$

and

$$\ell_d = C (MR_*^{\max})^{-\frac{3}{4}} \ell_0^{\frac{1}{4}} = C (MR_*^{\max})^{-1} R^{\frac{1}{4}} \quad \text{in 3-D}. \quad (8.35)$$

In all cases, we see that  $\ell_d \rightarrow \infty$  as  $R \rightarrow \infty$ , but more slowly in three than in two dimensions. We are thus assured that at high Reynolds numbers the separation of scale between the lattice constant and  $\ell_d$  necessary for hydrodynamic behavior is satisfied. Having it too well satisfied may however be a mixed blessing, as stressed in reference 36. Indeed, in hydrodynamic simulations using lattice gases, it is not desirable to have too much irrelevant microscopic information. We note that  $\ell_0$  appears in equations (8.34) and (8.35) with a larger exponent in the two-dimensional case; thus, the above mentioned problem is most severe for large lattices in two dimensions.

<sup>22</sup>Small intermittency corrections which would slightly increase the exponent  $m$  cannot be ruled out.



The highest Reynolds number which can be simulated by lattice gas methods in three dimensions can be estimated as follows. We take  $M = 0.3$ , a Mach number at which compressibility effects can be safely ignored [84]; we take the maximum known value  $R_*^{\max} = 6.4$  for the FCHC model, and we take  $\ell_0 = 10^3$ , a fairly large value which implies a memory requirement of at least 24 gigabits; from equation (8.29), we find that the maximum Reynolds number is about two thousand. It is of interest both in two and three dimensions to try to decrease the viscosity, thereby increasing  $R_*^{\max}$ . Note that it is not correct to infer from dimensional analysis that necessarily  $R_*^{\max}$  must be  $O(1)$ .  $R_*^{\max}$  is very much a function of the *complexity* of collisions. For example, by going from FHP-I to FCHC (which can also be projected down to two dimensions),  $R_*^{\max}$  increases more than sixteen times.

## 9. Conclusion

In statistical mechanics, there are many instances where two models, microscopically quite different, have the same large-scale properties. For example, the Ising model and a real Ferromagnet have presumably the same large-scale critical behavior. Similarly, the lattice gases studied in this paper, such as FHP and FCHC, are macroscopically indistinguishable from real fluids. This provides us with an attractive alternative to the traditional simulations of fluid mechanics. In lattice gas simulations, we just manipulate bits representing occupation of microscopic cells. The physical interpretation need not be in terms of particles moving and colliding. The idea can clearly be extended to include processes such as chemical reactions or multi-phase flow [53-57]. An open question is whether there are cellular automata implementations of processes which in the real world do not have a discrete microscopic origin, such as propagation of e.m. waves. More generally, what are the PDEs which can be *efficiently* implemented on cellular automata? We emphasize *efficiently*, because there are always brute force implementations: replace derivatives by finite differences on a regular grid and use finite floating point truncations of the continuous fields. The result may be viewed as a cellular automaton, but one in which there is no "bit democracy", insofar as there is a rigid hierarchical order between the bits.

Our derivation of hydrodynamics from the microdynamics leaves room for improvement. A key assumption made in section 4.1 may be formulated as follows. Among the invariant measures of the microdynamical equations, only the completely factorized ones (which play the role here of the micro-canonical ensemble) are relevant in the limit of large lattices. On a finite lattice with deterministic and invertible updating rules, we expect that there are many other invariant measures. Indeed, phase space is a finite set and updating is a permutation of this set; it is thus unlikely that there should be a closed orbit going through all points. So, we do not expect the discrete equivalent of an ergodic theorem. Anyway, ergodic results should be irrelevant. On the one hand, on an  $L \times L$  lattice with  $b$  bits per node, its



takes  $2^b L^2$  updates to visit all configurations (if they are accessible). On the other hand, we know (from simulations) that local equilibrium is achieved in a few updates and global equilibrium is achieved on a diffusive time scale (approximately  $L^2$ ). We believe that, on large lattices, the factorized equilibrium distributions constitute some kind of "fixed point" to which there is rapid convergence of the iterated Boolean map defined by the microdynamical equations of section 3.1. Understanding this process should clarify the mechanism of irreversibility in lattice gases and, eventually, in real gases.

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### Appendix A. Basic symmetries of HPP, FHP, and FCHC models

We show that the models HPP, FHP, and FCHC, introduced in section 2, satisfy the symmetry assumptions (1) through (4) of section 2.4. Assumptions (1) and (2) are obvious for all three models. Let us consider (3) and (4) successively for the three models.

#### HPP

Let us take the  $x_1$  axis in the direction of the vector  $c_1$ . The isometry group  $\mathcal{G}$  of the velocity set is generated by permutations of the  $x_1$  and  $x_2$  coordinates and reversals of any of them. Clearly, any two vectors  $c_i$  and  $c_j$  can be exchanged by some isometry, so that assumption (3) holds. Consider a particular vector, say,  $c_1$ . The subgroup  $\mathcal{G}_1$ , leaving  $c_1$  invariant reduces to the identity and reversal of  $x_2$ ; this implies parts (a) and (b) of assumption (4).

#### FHP

Let us take the  $x_1$  axis in the direction of  $c_1$ . The isometry group  $\mathcal{G}$  is now generated by rotations of  $\pi/3$  and reversal of the  $x_2$  coordinate. Assumption (3) is obvious. The subgroup  $\mathcal{G}_1$  reduces again to the identity and the reversal of  $x_2$ , so that (4) follows.

## FCHC

The FCHC lattice was defined in section 2.3 with explicit reference to coordinates  $x_1, x_2, x_3$ , and  $x_4$ . In this coordinate system, the velocity set is formed of

$$\begin{aligned} &(\pm 1, \pm 1, 0, 0), \quad (\pm 1, 0, \pm 1, 0), \quad (\pm 1, 0, 0, \pm 1) \\ &(0, \pm 1, \pm 1, 0), \quad (0, \pm 1, 0, \pm 1), \quad (0, 0, \pm 1, \pm 1). \end{aligned} \quad (\text{A.1})$$

By the orthonormal change of variables

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}, \quad (\text{A.2})$$

the velocity set becomes

$$\begin{aligned} &(\pm\sqrt{2}, 0, 0, 0), \quad (0, \pm\sqrt{2}, 0, 0), \quad (0, 0, \pm\sqrt{2}, 0), \quad (0, 0, 0, \pm\sqrt{2}), \\ &(\pm\frac{1}{\sqrt{2}}, \pm\frac{1}{\sqrt{2}}, \pm\frac{1}{\sqrt{2}}, \pm\frac{1}{\sqrt{2}}). \end{aligned} \quad (\text{A.3})$$

The isometry group  $\mathcal{G}$  is generated by permutations and reversals of the  $x_\alpha$  coordinates and by the symmetry with respect to the hyperplane  $x_1 + x_2 + x_3 + x_4 = 0$ , which is conveniently written in terms of  $y_\alpha$  coordinates as

$$\Sigma: (y_1, y_2, y_3, y_4) \mapsto (-y_3, y_2, -y_1, y_4). \quad (\text{A.4})$$

Assumption (3) is obvious in any of the coordinate systems. As for assumption (4), let us consider the subgroup  $\mathcal{G}_1$  leaving invariant, say, the vector with  $y_\alpha$  coordinates  $(0, 0, 0, 1/\sqrt{2})$ . The restriction of  $\mathcal{G}_1$  to the hyperplane  $y_4 = 0$  is generated by the identity, permutations, and reversals of  $y_1, y_2$ , and  $y_3$ . Assumptions (a) and (b) follow readily.

## Appendix B. Symmetry-related properties

Using assumptions (1) through (4) of section 2.4, we prove properties **P1** through **P6**.

**P1 Parity-invariance.** The set of velocity vectors is invariant under space-reversal.

Indeed, on a Bravais lattice, vectors connecting neighboring nodes come in opposite pairs.

**P2** Any set of  $i$ -dependent vectors  $v_{i\alpha}$ , which is  $\mathcal{G}$ -invariant, is of the form  $\lambda c_{i\alpha}$ .

We write  $\mathbf{v}_i$  as the sum of its projection on  $\mathbf{c}_i$  and of a vector perpendicular to  $\mathbf{c}_i$ . This decomposition being  $\mathcal{G}$ -invariant, the latter vector vanishes by (4a).

**P3** Any set of  $i$ -dependent tensors  $t_{i\alpha\beta}$ , which is  $\mathcal{G}$ -invariant, is of the form  $\lambda c_{i\alpha} c_{i\beta} + \mu \delta_{\alpha\beta}$ .

To the tensors  $t_{i\alpha\beta}$ , we associate the linear operators  $T_i : x_\alpha \mapsto t_{i\alpha\beta} x_\beta$ .  $\mathcal{G}$ -invariance means that the  $T_i$ 's commute with any lattice isometry leaving  $c_i$  invariant. We now write the  $\mathcal{G}$ -invariant decomposition

$$T_i = P_i T_i P_i + (I - P_i) T_i P_i + P_i T_i (I - P_i) + (I - P_i) T_i (I - P_i), \quad (\text{B.1})$$

where  $I$  is the identity in  $\mathbb{R}^D$  and  $P_i$  is the orthogonal projection on  $c_i$ . The second operator in equation (B.1), applied to an arbitrary vector  $w$ , gives

$$(I - P_i) T_i P_i w = \frac{w \cdot c_i}{c^2} (I - P_i) T_i c_i. \quad (\text{B.2})$$

The vectors  $(I - P_i) T_i c_i$  are  $\mathcal{G}$ -invariant and orthogonal to  $c_i$ , and thus vanish by (4a). The third operator in B.1 vanishes for similar reasons (use the  $\mathcal{G}$ -invariance of the transposed of the  $T_i$ 's). The fourth operator in B.1 is, by (4b) proportional to  $I_i$ , the identity in the subspace orthogonal to  $c_i$ . Since  $I = I_i + P_i$ , the proof is completed.

We mention that we obtained **P3** by trying to formalize a result used by Hénon [42] in deriving a closed-form viscosity formula.

**P4** *Isotropy of second-order tensors.* Any  $\mathcal{G}$ -invariant tensor  $t_{\alpha\beta}$  is of the form  $\mu \delta_{\alpha\beta}$ .

This is a special case of **P3**, when there is no  $i$ -dependence.

**P5** Any  $\mathcal{G}$ -invariant third-order tensor vanishes.

This follows from **P1** (parity invariance).

**P6** *Velocity moments.* Odd-order velocity moments vanish. The second-order velocity moment is given by

$$\sum_i c_{i\alpha} c_{i\beta} = \frac{bc^2}{D} \delta_{\alpha\beta}. \quad (\text{B.3})$$

The vanishing of odd-order moments is a consequence of **P1**. Equation (B.3) follows from **P4** and the identity

$$\sum_i c_{i\alpha} c_{i\alpha} = bc^2. \quad (\text{B.4})$$

### Appendix C. Equilibrium solutions

We prove the

**Lemma 1.** *The following statements are equivalent:*

1. *The  $N_i$ 's are a solution of*

$$\prod_j N_j^{s'_j} (1 - N_j)^{(1-s'_j)} = \sum_s A(s \rightarrow s') \prod_j N_j^{s_j} (1 - N_j)^{(1-s_j)}, \quad \forall s'. \quad (C.1)$$

2. *The  $N_i$ 's are a solution of the set of  $b$  equations*

$$\Delta_i(N) \equiv \sum_{s, s'} (s'_i - s_i) A(s \rightarrow s') \prod_j N_j^{s_j} (1 - N_j)^{(1-s_j)} = 0, \quad \forall i. \quad (C.2)$$

3. *The  $N_i$ 's are given by the Fermi-Dirac distribution*

$$N_i = \frac{1}{1 + \exp(h + \mathbf{q} \cdot \mathbf{c}_i)}, \quad (C.3)$$

where  $h$  is an arbitrary real number and  $\mathbf{q}$  is an arbitrary  $D$ -dimensional vector.

**Proof:** (1) implies (2).

We multiply equation (C.1) by  $s'_i$  and sum over all states  $s'$  to obtain

$$\sum_{s'} s'_i \prod_j N_j^{s'_j} (1 - N_j)^{(1-s'_j)} = \sum_{s, s'} s'_i A(s \rightarrow s') \prod_j N_j^{s_j} (1 - N_j)^{(1-s_j)}. \quad (C.4)$$

In the l.h.s. of equation (C.4), we change the dummy variable  $s'$  into  $s$  and decorate it with a factor  $A(s \rightarrow s')$ , summed over  $s'$ , which is one by normalization of probability. Transferring everything into the r.h.s., we obtain equation (C.2). Note that the l.h.s of equation (C.2) resembles the "collision function"  $\Delta_i$  of section 3.1 (equation (3.9)), but is evaluated with the mean populations instead of the Boolean populations  $n_i$ . The relation  $\Delta_i = 0$  expresses that there is no change in the mean populations under collisions. ■

**Proof:** (2) implies (3).

We define

$$\tilde{N}_i \equiv \frac{N_i}{1 - N_i}, \quad (C.5)$$

$$\Pi \equiv \prod_j (1 - N_j). \quad (\text{C.6})$$

Equation (C.2) may be written

$$\Delta_i / \Pi = \sum_{ss'} (s'_i - s_i) A(s \rightarrow s') \prod_j \tilde{N}_j^{s_j} = 0. \quad (\text{C.7})$$

We now make use of a trick employed in proving H-Theorems in discrete velocity models (see [17], p. 29). We multiply equation (C.7) by  $\log \tilde{N}_i$ , sum over  $i$ , and use

$$\sum_i (s'_i - s_i) \log \tilde{N}_i = \log \frac{\prod_j \tilde{N}_j^{s'_j}}{\prod_j \tilde{N}_j^{s_j}}, \quad (\text{C.8})$$

to obtain

$$\sum_{ss'} A(s \rightarrow s') \log \left( \frac{\prod_j \tilde{N}_j^{s'_j}}{\prod_j \tilde{N}_j^{s_j}} \right) \prod_j \tilde{N}_j^{s_j} = 0. \quad (\text{C.9})$$

Semi-detailed balance ( $\sum_s A(s \rightarrow s') = \sum_{s'} A(s \rightarrow s') = 1$ ) implies that

$$\sum_{ss'} A(s \rightarrow s') \left( \prod_j \tilde{N}_j^{s_j} - \prod_j \tilde{N}_j^{s'_j} \right) = 0. \quad (\text{C.10})$$

Combining equations (C.9) and (C.10), we obtain

$$\sum_{ss'} A(s \rightarrow s') \left[ \log \left( \frac{\prod_j \tilde{N}_j^{s'_j}}{\prod_j \tilde{N}_j^{s_j}} \right) \prod_j \tilde{N}_j^{s_j} + \prod_j \tilde{N}_j^{s_j} - \prod_j \tilde{N}_j^{s'_j} \right] = 0. \quad (\text{C.11})$$

We make use of the relation ( $x > 0, y > 0$ )

$$y \log \frac{x}{y} + y - x = - \int_x^y \log \frac{t}{x} dt \leq 0, \quad (\text{C.12})$$

equality being achieved only when  $x = y$ . The l.h.s. of equation (C.11) is a linear combination of expressions of the form (C.12) with nonnegative weights  $A(s \rightarrow s')$ . For it to vanish, we must have

$$\prod_j \tilde{N}_j^{s_j} = \prod_j \tilde{N}_j^{s'_j}, \quad \text{whenever } A(s \rightarrow s') \neq 0. \quad (\text{C.13})$$

This is equivalent to

$$\sum_i \log(\tilde{N}_i) (s'_i - s_i) A(s \rightarrow s') = 0 \quad \forall s, s'. \quad (\text{C.14})$$

Equation (C.13) means that  $\log \tilde{N}_i$  is a collision invariant. We now use assumption (5) of section 2.4, concerning the absence of spurious invariants, to conclude that

$$\log \tilde{N}_i = -(\mathbf{h} + \mathbf{q} \cdot \mathbf{c}_i), \quad (\text{C.15})$$

which is the most general collision invariant (a linear combination of the mass invariant and of the  $D$  momentum invariants). Reverting to the mean populations  $N_i = \tilde{N}_i / (1 + \tilde{N}_i)$ , we obtain (C.3).

**Proof:** (3) implies (1).

Equation (C.3) implies

$$\sum_j \log(\tilde{N}_j) (s_j - s'_j) = 0, \quad \text{whenever } A(s \rightarrow s') \neq 0. \quad (\text{C.16})$$

This implies

$$\sum_s A(s \rightarrow s') \left( \prod_j \tilde{N}_j^{(s_j - s'_j)} - 1 \right) = 0. \quad (\text{C.17})$$

Using semi-detailed balance, this may be written as

$$1 = \sum_s A(s \rightarrow s') \frac{\prod_j \tilde{N}_j^{s_j}}{\prod_j \tilde{N}_j^{s'_j}}. \quad (\text{C.18})$$

Reverting to the  $N_j$ 's, we obtain equation (C.1). This completes the proof of the equivalence lemma. ■

#### Appendix D. Inclusion of body-forces

Using the same notation as in section 7.3, we wish to obtain a Navier-Stokes equation with a body-force  $\mathbf{f}$ , that is

$$\partial_T \mathbf{U} + \mathbf{U} \cdot \nabla_1 \mathbf{U} = -\nabla_1 P' + \nu' \nabla_1^2 \mathbf{U} + \mathbf{f} \\ \nabla_1 \cdot \mathbf{U} = 0. \quad (\text{D.1})$$

The force  $\mathbf{f}$  may depend on space and time and can be velocity-independent (case I; e.g. gravity) or linear in the velocity  $\mathbf{U}$  (case II; e.g. Coriolis force). The idea is to introduce a bias in the transition rules so as to give a net momentum input. Since all the terms in the Navier-Stokes momentum equation are  $O(\epsilon^3)$  and the hydrodynamic velocity is  $O(\epsilon)$  (before rescaling), the bias should be  $O(\epsilon^3)$  for case I and  $O(\epsilon^2)$  for case II.

We give now the modified form of the microdynamical equation (3.9) appropriate for body-forces. We introduce, in addition to the Boolean (transition) variables  $\xi_{ss'}$  of section 3.1, the Boolean variables  $\xi'_{ss'}$  such that

$$\langle \xi'_{ss'} \rangle = B(s \rightarrow s'). \quad (\text{D.2})$$

The  $B(s \rightarrow s')$ 's are a set of transition probabilities associated to the body-force; they satisfy normalization

$$\sum_{s'} B(s \rightarrow s') = 1, \quad (\text{D.3})$$

and mass conservation

$$\sum_i (s'_i - s_i) B(s \rightarrow s') = 0, \quad \forall s, s'. \quad (\text{D.4})$$

They do not satisfy momentum conservation, semi-detailed balance and  $\mathcal{G}$ -invariance. The  $\xi'_{ss'}$ 's are chosen independently at each discrete time and node and the  $B(s \rightarrow s')$ 's may depend on space and time; further constraints will be given below. We also need a Boolean variable  $\zeta$  which acts as a *switch*: when  $\zeta = 0$  the force is off and the usual transition rules apply. The mean of  $\zeta$  is given by

$$\langle \zeta \rangle = \rho_0 g(\rho_0) \epsilon^n$$

$$n = 3 \quad \text{case I}, \quad n = 2 \quad \text{case II}. \quad (\text{D.5})$$

This will take care of the scaling factors arising from the change of variables (7.15). The modified microdynamical equation is now

$$n_i(t_* + 1, \mathbf{r}_* + \mathbf{c}_i) = n_i + \Delta_i(n)$$

$$\Delta_i(n) =$$

$$\sum_{s, s'} (s'_i - s_i) ((1 - \zeta) \xi_{ss'} + \zeta \xi'_{ss'}) \prod_j n_j^{s_j} (1 - n_j)^{(1-s_j)}. \quad (\text{D.6})$$

Let us evaluate the body-force resulting from the insufficient additional  $\xi'$  term. For this, we multiply by  $\mathbf{c}_i$  and average over the equilibrium distribution; deviations from equilibrium arising from hydrodynamic gradients are irrelevant. We ignore the  $\zeta$ -factor since it just provides the scaling factor.

We begin with case I. The average is then evaluated over the zero-velocity equilibrium distribution with density per cell  $d$ ; we obtain

$$\mathbf{f} = \sum_{s, s', i} \mathbf{c}_i (s'_i - s_i) B(s \rightarrow s') \left( \frac{d}{1-d} \right)^p (1-d)^b, \quad p = \sum_j s_j \quad (\text{D.7})$$

where  $b$  is the number of cells per node. Equation (D.7) is the additional constraint on the  $B(s \rightarrow s')$ 's for case I. If  $\mathbf{f}$  is space- and/or time-dependent, so are the  $B(s \rightarrow s')$ 's. It is easy to check that for any given vector  $\mathbf{f}$ , there exist Boolean transition variables  $\xi'_{ss'}$  of mean  $B(s \rightarrow s')$  satisfying equation (D.7). When  $\mathbf{f}$  is in the direction of a particular velocity vector, say  $\mathbf{c}_{i_0}$ , we can flip particles with velocity  $-\mathbf{c}_{i_0}$  into particles with velocity  $\mathbf{c}_{i_0}$  whenever this is possible, while leaving all other particles unchanged. This is done with a probability dependent on the amplitude of the force. Other directions of the force are handled by superposition.

We turn to case II. We wish to obtain a force of the form



$$f_{\alpha} = C_{\alpha\beta} U_{\beta} \quad (\text{D.8})$$

where  $C_{\alpha\beta}$  is a  $D$ -dimensional matrix. When the velocity  $\mathbf{U}$  vanishes, the body-force should also vanish; this requires

$$\sum_{s,s',i} \mathbf{c}_i (s'_i - s_i) B(s \rightarrow s') \left( \frac{d}{1-d} \right)^p (1-d)^b = 0, \quad p = \sum_j s_j. \quad (\text{D.9})$$

With nonvanishing velocity, we must use the corresponding equilibrium populations given to relevant order by (cf. equation (4.14))

$$N_i = d + \frac{dD}{c^2} \mathbf{c}_{i\alpha} u_{\alpha}. \quad (\text{D.10})$$

Here, we have used the unscaled velocity  $\mathbf{u}$ . Below, however, we will use  $\mathbf{U}$  since the scaling factor is taken care of by the Boolean switch  $\zeta$ . Using (D.10) in (D.6), we find that the average momentum imparted by  $\xi'_{ss'}$  transitions is to leading order linear in  $\mathbf{U}$ . Identifying with equation (D.8), we find that the  $B(s \rightarrow s')$ 's must satisfy the following constraints

$$C_{\alpha\beta} = \frac{D}{c^2} (1-d)^{b-1} \sum_{s,s',i} \mathbf{c}_{i\alpha} (s'_i - s_i) B(s \rightarrow s') \left( \frac{d}{1-d} \right)^p \sum_j s_j c_{j\beta},$$

$$p = \sum_j s_j. \quad (\text{D.11})$$

Equations (D.9) and (D.11) are the additional constraints on the  $B(s \rightarrow s')$ 's for case II.

As an illustration, consider the case of the pseudo-four-dimensional FCHC model with a Coriolis force  $2\mathbf{\Omega} \wedge \mathbf{U}$ , where  $\mathbf{\Omega}$  is in the  $x_3$ -direction. A possible implementation for the  $\xi'_{ss'}$  transitions is through rotation by  $\pi/2$  around the  $x_3$ -axis of those particles having their velocity perpendicular to this axis (with a probability dependent on  $\mathbf{\Omega}$ ).

## Appendix E. Catalog of results for FHP models

The purpose of this appendix is to summarize all known analytic results for the FHP models, including the models II and III which have rest particles. Adapting the theory to cases with at most one rest particle is quite straightforward if one includes the rest-particle velocity, namely vector zero. Our derivations made extensive use of properties P1 to P6 of section 2.4. With rest particles, P1, P2, P4, and P5 are unchanged. In P3,  $\lambda$  and  $\mu$  have usually different values for moving and rest particles. P6 becomes

$$\sum_i \mathbf{c}_{i\alpha} \mathbf{c}_{i\beta} = \frac{(b-1)c^2}{D} \delta_{\alpha\beta}, \quad (\text{E.1})$$

	FHP-I	FHP-II	FHP-III
$\rho_0$	$6d$	$7d$	$7d$
$c_s$	$\frac{1}{\sqrt{2}}$	$\sqrt{\frac{3}{7}}$	$\sqrt{\frac{3}{7}}$
$g$	$\frac{1}{2} \frac{1-2d}{1-d}$	$\frac{7}{12} \frac{1-2d}{1-d}$	$\frac{7}{12} \frac{1-2d}{1-d}$
$\nu$	$\frac{1}{12} \frac{1}{d(1-d)^3} - \frac{1}{8}$	$\frac{1}{28} \frac{1}{d(1-d)^3} \frac{1}{1-4d/7} - \frac{1}{8}$	$\frac{1}{28} \frac{1}{d(1-d)} \frac{1}{1-8d(1-d)/7} - \frac{1}{8}$
$\zeta$	0	$\frac{1}{98} \frac{1}{d(1-d)^4} - \frac{1}{28}$	$\frac{1}{98} \frac{1}{d(1-d)} \frac{1}{1-2d(1-d)} - \frac{1}{28}$
$R_*^{\max}$	0.387	1.08	2.22
$d_{\max}$	0.187	0.179	0.285

Table 1: Analytic results for three FHP models

where  $b$  is still the number of bits, so that  $b - 1$  is the number of particles moving with speed  $c$ .

In Table 1 below, we give results in terms of the mean density per cell  $d$  for the following quantities: the mean density  $\rho_0$ , the coefficient  $g(\rho_0)$  rescaling the nonlinear term in the Navier-Stokes equation (see for example equation (7.13)), the kinematic shear viscosity  $\nu$ , the kinematic bulk viscosity  $\zeta$ , the maximum value  $R_*^{\max}$  of the coefficient  $R_*$  appearing in the Reynolds number (see equation (8.29)), and  $d_{\max}$ , the density at which the Reynolds number is maximum. The viscosities  $\nu$  and  $\zeta$  are calculated within the lattice Boltzmann approximation (see section 8.2).  $\rho_0\zeta$  is the dynamic bulk viscosity; when it does not vanish, as is the case with rest particles, equation (7.11) becomes

$$\partial_t \rho' + \rho_0 \nabla \cdot \mathbf{u} = 0$$

$$\rho_0 \partial_t \mathbf{u} + c_s^2 \nabla \rho' = \rho_0 \nu \left( \nabla^2 \mathbf{u} + \frac{D-2}{D} \nabla \nabla \cdot \mathbf{u} \right) + \rho_0 \zeta \nabla \nabla \cdot \mathbf{u}. \quad (\text{E.2})$$

## Appendix F. An H-theorem for lattice gases<sup>23</sup>

### F.1 Notation and basic equations

We number from 1 to  $b$  the cells at a given node ( $b$  is the number of different velocity vectors). It is not necessary that the velocity moduli are equal. Also, it will not be necessary to specify any symmetry for the lattice or for the collision rules. Finally, we will not make use of the conservation of the

<sup>23</sup>by M. Hénon, Observatoire de Nice.

number of particles or of the momentum, so that the proof is applicable to lattices where these conservation laws are violated.

We write  $s_i = 1$  if particle  $i$  is present in the *input state*, 0 if it is absent. An input state is thus defined by  $s = (s_1, \dots, s_b)$ . The number of distinct input states is  $2^b$ .

We call  $P(s)$  the probability of an input state  $s$ . We have

$$\sum_s P(s) = 1. \quad (\text{F.1})$$

We call  $N_i$  the probability that particle  $i$  is present. We have

$$N_i = \sum_s s_i P(s), \quad 1 - N_i = \sum_s (1 - s_i) P(s). \quad (\text{F.2})$$

We define in the same way  $s'_i$ ,  $s' = (s'_1, \dots, s'_b)$ ,  $P'(s')$ ,  $N'_i$  for the *output state*.

We call  $A(s \rightarrow s')$  the probability that an input state  $s$  is changed into an output state  $s'$  by the collision. We have

$$P'(s') = \sum_s P(s) A(s \rightarrow s'). \quad (\text{F.3})$$

We have, of course,

$$\sum_{s'} A(s \rightarrow s') = 1, \quad (\text{F.4})$$

where the sum is over all output states. We will assume that the collision rules obey *semi-detailed balance*, i.e., that we have also

$$\sum_s A(s \rightarrow s') = 1. \quad (\text{F.5})$$

## F.2 Local theorem

**Lemma 1.** *If  $f(x)$  is a convex function ( $d^2 f/dx^2 > 0$ ), then*

$$\sum_{s'} f[P'(s')] \leq \sum_s f[P(s)]. \quad (\text{F.6})$$

**Proof:** From general properties of convex functions, we have

$$f \left[ \frac{\sum_s q(s) P(s)}{\sum_s q(s)} \right] \leq \frac{\sum_s q(s) f[P(s)]}{\sum_s q(s)}, \quad (\text{F.7})$$

where the  $q(s)$  are arbitrary positive or zero coefficients. Taking  $q(s) = A(s \rightarrow s')$ , with  $s'$  given, and using equations (F.3) and (F.5), we obtain

$$f[P'(s')] \leq \sum_s A(s, s') f[P(s)]. \quad (\text{F.8})$$

Summing over  $s'$  and using equation (F.4), we obtain equation (F.6). ■

**Lemma 2.** *The following inequality holds:*

$$\sum_{s'} P'(s') \ln P'(s') \leq \sum_s P(s) \ln P(s). \quad (\text{F.9})$$

**Proof:** We apply Lemma 1 with  $f(x) = x \ln x$ . ■

**Lemma 3.** *The following inequality holds:*

$$\sum_s P(s) \ln P(s) \geq \sum_{i=1}^b [N_i \ln N_i + (1 - N_i) \ln(1 - N_i)]. \quad (\text{F.10})$$

*The equality holds if and only if*

$$P(s_1, \dots, s_b) = \prod_{i=1}^b N_i^{s_i} (1 - N_i)^{1-s_i}. \quad (\text{F.11})$$

**Proof:**<sup>24</sup> The right-hand side of equation (F.10) can be written, using equation (F.2):

$$\sum_{i=1}^b \sum_s [s_i P(s) \ln N_i + (1 - s_i) P(s) \ln(1 - N_i)], \quad (\text{F.12})$$

or

$$\sum_s P(s) \ln \left[ \prod_{i=1}^b N_i^{s_i} (1 - N_i)^{1-s_i} \right]. \quad (\text{F.13})$$

Therefore, equation (F.10) can also be written

$$\sum_s P(s) \ln \left[ \frac{\prod_{i=1}^b N_i^{s_i} (1 - N_i)^{1-s_i}}{P(s)} \right] \leq 0. \quad (\text{F.14})$$

We have, for any  $x$ :

$$\ln x \leq x - 1, \quad (\text{F.15})$$

where the equality holds only if  $x = 1$ . Therefore,

$$\ln \left[ \frac{\prod_{i=1}^b N_i^{s_i} (1 - N_i)^{1-s_i}}{P(s)} \right] \leq \frac{\prod_{i=1}^b N_i^{s_i} (1 - N_i)^{1-s_i}}{P(s)} - 1. \quad (\text{F.16})$$

Multiplying this by  $P(s)$  and summing over  $s$ , we obtain the desired result. ■

The relation (F.11) corresponds to the Boltzmann approximation (independence of input particles).

<sup>24</sup>inspired by reference 85.

### Local H-theorem

If the collision rules satisfy semi-detailed balance, and in the Boltzmann approximation, the following inequality holds:

$$\begin{aligned} & \sum_{i=1}^b [N'_i \ln N'_i + (1 - N'_i) \ln(1 - N'_i)] \\ & \leq \sum_{i=1}^b [N_i \ln N_i + (1 - N_i) \ln(1 - N_i)]. \end{aligned} \quad (\text{F.17})$$

**Proof:** From Lemma 3, we have

$$\sum_s P(s) \ln P(s) = \sum_{i=1}^b [N_i \ln N_i + (1 - N_i) \ln(1 - N_i)]. \quad (\text{F.18})$$

Combining with Lemma 2:

$$\sum_{s'} P'(s') \ln P'(s') \leq \sum_{i=1}^b [N_i \ln N_i + (1 - N_i) \ln(1 - N_i)]. \quad (\text{F.19})$$

Finally, applying Lemma 3 to the  $N'_i$ 's and the  $P'$ 's, we obtain equation (F.17). ■

We remark that both conditions of the theorem are necessary; one can easily find counterexamples if one or the other is not satisfied. Consider, for instance, a node of the HPP lattice with probabilities before collision:  $P(1,0,1,0) = 1/2$ ,  $P(0,1,0,0) = 1/2$ . We have:  $N_1 = 1/2$ ,  $N_2 = 1/2$ ,  $N_3 = 1/2$ ,  $N_4 = 0$ ; the Boltzmann approximation is not satisfied. We take the usual HPP collision rules. The probabilities after collision are then  $P'(0,1,0,1) = 1/2$ ,  $P'(0,1,0,0) = 1/2$ . From this, we deduce  $N'_1 = 0$ ,  $N'_2 = 1$ ,  $N'_3 = 0$ ,  $N'_4 = 1/2$ , and it can be immediately verified that the left-hand member of equation (F.17) is larger than the right-hand member.

Similarly, let us modify the collision rules and keep only one kind of collision:  $(1,0,1,0)$  gives  $(0,1,0,1)$ , but not conversely. Semi-detailed balance is not satisfied. Take for instance  $N_1 = N_2 = N_3 = N_4 = 1/2$ . We assume that the Boltzmann approximation holds; therefore,  $P(s) = 1/16$  for all  $s$ . We deduce  $P'(1,0,1,0) = 0$ ;  $P'(0,1,0,1) = 2/16$ ;  $P'(s') = 1/16$  for the other  $s'$ ;  $N'_1 = N'_3 = 7/16$ ,  $N'_2 = N'_4 = 9/16$ ; and here again the inequality (F.17) is violated.

### F.3 Global theorem

First we sum equation (F.17) over all lattice nodes. We obtain a sum over all cells at all lattice nodes; their total number will be denoted by  $r$ :

$$\sum_{j=1}^r [N'^{(j)} \ln N'^{(j)} + (1 - N'^{(j)}) \ln(1 - N'^{(j)})]$$

$$\leq \sum_{j=1}^r [N^{(j)} \ln N^{(j)} + (1 - N^{(j)}) \ln(1 - N^{(j)})]. \quad (\text{F.20})$$

Next we remark that this sum is invariant under propagation. We can therefore extend the theorem to an arbitrary number of time steps, and we obtain (with the same hypotheses as for the local theorem):

### Global H-theorem

The function

$$\sum_{j=1}^r [N^{(j)} \ln N^{(j)} + (1 - N^{(j)}) \ln(1 - N^{(j)})] \quad (\text{F.21})$$

is non-increasing as the lattice gas evolves.

### Appendix F.1 Interpretation in terms of information theory

Consider a probability distribution over  $\nu$  possible cases:  $p_1, \dots, p_\nu$ . The associated information is

$$\log_2 \nu + \sum_{i=1}^{\nu} p_i \log_2 p_i. \quad (\text{F.22})$$

This information has a minimal value 0 if all cases have the same probability:  $p_1 = \dots = p_\nu = 1/\nu$ . It has a maximal value  $\log_2 \nu$  if one of the  $p_i$  is 1 while the others are 0, i.e., for a deterministic choice between the  $\nu$  cases.

We come back to lattices.  $P(s)$  represents a probability distribution on  $2^b$  cases, and therefore an information

$$b + \sum_s P(s) \log_2 P(s). \quad (\text{F.23})$$

Thus, Lemma 2 expresses the following property: if semi-detailed balance is satisfied, then the information contained in the  $P$  can only remain constant or decrease in a collision.

From the  $P$ 's, we can compute the  $N_i$ 's by the formulas (F.2), but the converse is not generally true; in other words, the  $P$ 's contain more information than the  $N_i$ 's. Lemma 3 expresses this fact.

In the particular case of the Boltzmann approximation, the particles are considered as independent, and therefore, the  $P$ 's contain no more information than the  $N_i$ 's. We have then the equality in equation (F.10).

The proof of the local H-theorem can therefore be interpreted as follows: (i) initially the  $N_i$ 's are given; this represents a given information; (ii) we compute the corresponding  $P$ 's in the Boltzmann approximation; the information does not change; (iii) we compute the collision and obtain the  $P''$ 's; the information decreases or stays constant; (iv) we compute the  $N''$ 's from the  $P''$ 's; here again, the information decreases or stays constant.

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