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Global Invariants and Equilibrium States in Lattice Gases

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It is now well known that, in addition to the physical conserved quantities, lattice gases also have other unphysical ones related to the discretization of their phase space. From an abstract point of view a lattice gas can be considered like a full discrete Markov process L and these spurious conserved quantities yield the existence of a nonspatially homogeneous equilibrium state for L^k. We show that a particular set of these conserved quantities is of special interest: Its elements will be called regular. These regular invariants are simply built from the local ones and their projection on each node is always a locally conserved quantity. Moreover, for most models they are one-to-one related to the Gibbs states of L^k which remain factorized. It turns out that all the classical known spurious invariants are regular and one can exhibit simple conditions to build models with only regular invariants. For the latter it is then justified to determine the transport coefficients of the locally conserved densities with the Green–Kubo procedure.

KEY WORDS: Lattice gases; cellular automata; global invariants; invariants in discrete stochastic processes; equilibrium states in lattice gases.

INTRODUCTION

One can think of a lattice gas cellular automaton (LGCA) as a finite isolated collection of particles with a finite set of velocities which move at integer times from nodes to nodes on a finite regular lattice. The collisions occur at the nodes of the lattice and locally conserve some quantities such as mass, momentum, or energy which appear as linear functions of the microscopic state of the node. These quantities are called local linear invariants; their averages are conserved densities whose evolution equations described the macroscopic dynamics of the LGCA under proper

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limits. In this paper, from an abstract point of view we will consider a lattice gas as a full discrete Markov process $\boldsymbol{L}$, and thus we use integral notations, since they allow a wide variety of lattice gases to be described under the same formalism. Besides, they are close to the usual notations of continuous statistical theories. All the models considered here are supposed to obey semi-detailed balance.

One of the best known example of such system is the FHP[1] model, which provides a tool to simulate 2D incompressible Navier–Stokes equations. The most powerful method to investigate the hydrodynamics of LGCA consists of adapting the standard linear response theory of classical nonequilibrium statistical mechanics[2] to these full discrete systems, as is shown in ref. 3. This theory leads to the construction of a Green's correlation function which determines the local average of the conserved densities (i.e., of the local invariants) at any time as a linear functional of the thermodynamic variables in an initial local equilibrium state: The evolution is described by the Liouville equation of the lattice gas. One then assumes that this initial state relaxes to a global spatially homogeneous equilibrium state which is used to evaluate the Green's function. This final homogeneous state is completely defined by the initial assigned values of conserved densities, since the system is isolated.

Let us then call *global linear* 1-*invariant* any linear function $\Phi(\cdot)$ defined on the whole phase space of the LGCA and such that the density $\boldsymbol{k}\exp(\Phi(\mathbf{n}))$ is a Gibbs equilibrium distribution for the system (i.e., a factorized fixed point of $\boldsymbol{L}$), $\boldsymbol{k}$ being a normalization constant and $\mathbf{n}$ a point in phase space. Since Φ is linear, $\Phi(\mathbf{n})$ appears as a sum over all the nodes α: $\sum_\alpha \langle \phi(\alpha), \mathbf{n}(\alpha)\rangle$, where $\phi(\alpha)$ is the projection of Φ at node α. A global linear 1-invariant Φ is then spatially homogeneous if and only if $\phi(\alpha)$ is constant over the nodes. One can then show that the only global homogeneous 1-invariants are those whose projection on each node is a (constant) local invariant (in fact, for models which obey semi-detailed balance: see Section 2). Then, if there are, for example, r independent local invariants, there are also only r independent global homogeneous 1-invariants and thus we need r thermodynamic intensive variables in order to determine the homogeneous Gibbs states of the system. Let us note that this implies that any *spurious* global 1-invariant is not homogeneous.

Now, if for a given LGCA, any global linear 1-invariant is homogeneous, it will only admit homogeneous equilibrium states (this is, for example, the case for the FHP model; see Section 6); under these conditions the Green's correlation function can be inverted in Fourier space and one obtains the expressions for the transport coefficients after taking the proper limits via the Green–Kubo procedure.

Conversely, if the LGCA admits nonhomogeneous global 1-invariants, it will admit nonhomogeneous equilibrium states and thus there is no reason that an initial nonequilibrium state relaxes to a homogeneous equilibrium one: This is, for example, the case of most models on the square lattice, such as the HPP model[4-6] and the 8- and 9-bit models,[7-10] and of many one-dimensional models[11-13] where spurious global 1-invariants occur. There is then a set of additional thermodynamic variables. On the one hand, this leads to a modification of the Green's function in order to take the inhomogeneity into account and on the other hand, which is the most important point, this new correlation function canot be inverted without further hypothesis and the Green–Kubo procedure breaks down.

However, there is an important case where it is nevertheless possible to complete the Green–Kubo procedure in spite of the existence of spurious nonhomogeneous global 1-invariants: This case occurs if any global 1-invariant is such that its projection on each node remains a local invariant (not necessarily constant). We will say that such a global 1-invariant is *regular*. In the linear response theory one is then led to evaluate the Green's function with a nonhomogeneous equilibrium distribution (see Section 5), which can now be inverted in Fourier space. But the spatial variations of the conserved densities arising from the inhomogeneity of the final equilibrium state yield a modification of the transport equations as shown in refs. 10 and 17. Thus, it is essential to know if the global 1-invariants of a LGCA are regular or not.

One part of the program of this paper will then be to exhibit conditions for easily testing if the global 1-invariants of a given LGCA are regular. With these conditions, it turns out that most of the known models have precisely only regular global 1-invariants and it is not surprising that all the spurious 1-invariants discovered so far are regular. Moreover, we will show that these regular 1-invariants can be simply determined from the local ones by requiring that they are invariant under the free propagation operator. This agrees with similar results obtained by Levermore and d'Humières.[14] Furthermore, we will show in the examples that all the geometric invariants mentioned in the literature (the line invariants[15] of the HPP model, the geometric staggered invariants of the 8- and 9-bit models,[10] etc.) all have the same status: They are regular 1-invariants in the sense of the previous definition and they are all defined and computable from Proposition 5 of Section 2. Thus, for most models, one can systematically find these global conserved quantities including the spurious ones either analytically (see examples in Section 6) or numerically following the procedures proposed by Zanetti[16] or d'Humières *et al.*[11]

In Section 1, after introducing the notations, we give in Proposition 1 a characterization of the fixed points of $\boldsymbol{L}$, and therefore a model whose any fixed point is invariant under the free propagation operator will be called *regular*. This characterization of the fixed points leads us in Section 2 to give a first general but natural definition of the global linear 1-invariants. These are defined as the linear fixed points for the generalized process obtained by extending $\boldsymbol{L}$ to the whole set of integrable functions in phase space. We show in Proposition 4 that this general definition is equivalent to the previous one. We then close this section by giving in Proposition 5 a practical characterization of the regular 1-invariants. In Section 3 we show one of the main results of this paper, i.e., that the global linear 1-invariants of a regular model are regular. We then give practical conditions in order to ascertain if a stochastic model is regular. In Proposition 13 of Section 5 we extend the class of models which have only regular global 1-invariants to these which admit what we call a *regular configuration*. The latter class includes most models used for simulating hydrodynamics.

Another part of our program will be to show that all the types of *dynamic invariants* mentioned in the literature (the staggered invariants,[15–18] the chessboard invariants,[15] etc.) also all have the same status: they are the global linear invariants, but for iterated processes $\boldsymbol{L}^p$. We call these global invariants *p-invariants*. In Section 4, similarly to the 1-invariants, we define the p-invariants as the "linear fixed points" of $\boldsymbol{L}^p$. It turns out that this definition is simply a generalization of what d'Humières *et al.* have called[11] *global linear invariants with a time period p*. We then extend the notion of regular invariants to the p-invariants through Definition 6 and we show in Proposition 13 that these regular invariants are univocally related to the Gibb's equilibrium distribution of $\boldsymbol{L}^p$ which remain factorized at any time. An interesting result is then given in Proposition 7, which states that the p-invariants of a model which obeys the testing conditions of Section 3 are all regular.

Finally, in the examples of Section 6 we take advantage of the characterizations of the regular invariants given in Propositions 5 and 8 to determine analytically the global 1-, 2-, and 3-invariants of some known models. We effectively show that the known spurious dynamic invariants (for example, the three staggered momenta of the FHP model discovered by McNamara and Zanetti[16–18] fall in the class of regular p-invariants introduced here.

1. NOTATIONS

Since we want to derive results which are valid for various models as well as for multispeed lattice gases with or without rest particles,[19] with static energy levels,[20–22] or which "photons,"[23] we will introduce some general notation. Almost everywhere in this paper we will not need to specify the details of the microscopic world and thus we will consider a "lattice" gas to be given by two finite sets: $\mathscr{E}$, the space of states, with N elements; and $\mathscr{L}$, the set of nodes, with L elements. A configuration is then a field $\mathbf{n}$ on $\mathscr{L}$ of elements of $\mathscr{E}$. The set of configurations will be called $\mathscr{W}$: it is the phase space for the considered model. Its microscopic evolution is then described by giving an invertible map $\mathscr{S}$ on $\mathscr{W}$, called the free propagation operator, and a set of global transition probabilities $\{\mathscr{A}(\mathbf{n} \to \mathbf{n}')\}$ from $\mathscr{W}^2$ to $[0, 1]$ that characterizes the "collision" process. We will further clarify the structure of these objects when needed. In order to keep close to the usual notations for stochastic processes, we will use integral notations, but all the integrals will be taken the counting measure. The $\{\mathscr{A}\}$ obey the following relations:

$$\forall \mathbf{n}: \quad \int_{\mathscr{W}} \mathscr{A}(\mathbf{n} \to \mathbf{n}')\, d\mathbf{n}' = 1; \qquad \int_{\mathscr{W}} \mathscr{A}(\mathbf{n}' \to \mathbf{n})\, d\mathbf{n}' = 1$$

The first relation simply expresses that $\{\mathscr{A}(\mathbf{n} \to \cdot)\}$ are probabilities and the second is the semi-detailed balance hypothesis. Let us then note that deterministic models are described when the range of $\{\mathscr{A}(\mathbf{n} \to \mathbf{n}')\}$ is $\{0, 1\}$; the previous relations are then equivalent to the existence of an invertible operator $\mathscr{C}$ (the so-called microscopic collision operator) on $\mathscr{W}$ such that for all $\mathbf{n}$: $\mathscr{A}(\mathbf{n} \to \mathscr{C}(\mathbf{n})) = 1$. We denote $\mathscr{D}(\mathscr{W})$ the set of densities on $\mathscr{W}$ and we consider the Markov process $\boldsymbol{L}$:

$$f \in \mathscr{D}(\mathscr{W}) \to \boldsymbol{L}(f): \qquad \boldsymbol{L}(f)(\mathbf{n}) = \int_{\mathscr{W}} f(\mathbf{n}')\, \mathscr{A}(\mathbf{n}' \to \mathscr{S}^{-1}(\mathbf{n}))\, d\mathbf{n}' \tag{1}$$

The relation

$$f_{p+1}(\mathbf{n}) = \int_{\mathscr{W}} f_p(\mathbf{n}')\, \mathscr{A}(\mathbf{n}' \to \mathscr{S}^{-1}(\mathbf{n}))\, d\mathbf{n}' \tag{2}$$

on sequences (f_p) on $\mathscr{D}(\mathscr{W})$ is the Liouville equation of the lattice gas.[24] In the deterministic case, relation (1) simply reduces to $\boldsymbol{L}(f)(\mathbf{n}) = f(\mathscr{C}^{-1}\mathscr{S}^{-1}(\mathbf{n}))$. A stationary solution of (2) is thus a constant sequence $f_p = f$ where f is a fixed point of $\mathscr{L}$.

The information function $\boldsymbol{H}$ on $\mathscr{D}(\mathscr{W})$ is defined by

$$\boldsymbol{H}(f) = \int_{\mathscr{W}} f(\mathbf{n})\, \mathrm{Log}(f(\mathbf{n}))\, d\mathbf{n}$$

From the semi-detailed balance and the convexity of $x \,\mathrm{Log}\, x$, it follows that $\boldsymbol{H}(\boldsymbol{L}(f)) \leqslant \boldsymbol{H}(f)$ for all f. Moreover, since $x \,\mathrm{Log}\, x$ is strictly convex on $[0, 1]$, we have the equivalence (see Appendix A):

$$\boldsymbol{H}(\boldsymbol{L}(f)) = \boldsymbol{H}(f) \Leftrightarrow \forall \mathbf{n}, \mathbf{n}', \mathbf{n}'' \in \mathscr{W}^3 \quad \mathscr{A}(\mathbf{n} \to \mathbf{n}')\, \mathscr{A}(\mathbf{n}'' \to \mathbf{n}')[f(\mathbf{n}) - f(\mathbf{n}'')] = 0$$

Thus, one can show the following proposition, whose proof is given in Appendix A:

Proposition 1. A density f is a fixed point of L if and only if it satisfies

$$\forall \mathbf{n}, \mathbf{n}' \in \mathscr{W}^2 \quad \mathscr{A}(\mathbf{n} \to \mathbf{n}')[f(\mathbf{n}) - f(\mathscr{S}(\mathbf{n}'))] = 0$$

Let us then introduce a decomposition of $\mathscr{W}$ in disjoint subsets that are similar to the orbits for a deterministic dynamical system. For that purpose we will say that two configurations $\mathbf{n}, \mathbf{m}$ define a "link" $\{\mathbf{n}, \mathbf{m}\}$ if we have $\mathscr{A}(\mathbf{n} \to \mathscr{S}^{-1}(\mathbf{m})) \neq 0$ or $\mathscr{A}(\mathbf{m} \to \mathscr{S}^{-1}(\mathbf{n})) \neq 0$. We then will say that two configurations $\mathbf{n}, \mathbf{m}$ are connected if there exists a sequence $\mathbf{n}_0 = \mathbf{n}, \mathbf{n}_1, ..., \mathbf{n}_p = \mathbf{m}$ of configurations (with $p \geqslant 1$) such that each pair $\{\mathbf{n}_i, \mathbf{n}_{i+1}\}$ is a link. One can verify that the relation "to be connected" on $\mathscr{W}$ is an equivalence relation. The corresponding classes are thus called 1-*paths* for the Markov process L. For a deterministic model these 1-paths are actually the orbits of the associated dynamical system. The fixed points of L are then also characterized by the following result.

Proposition 2. A density $f \in \mathscr{D}(\mathscr{W})$ is a fixed point of L if and only if it is constant on each 1-path.

We will say that a 1-path is *regular* if it is invariant under $\mathscr{S}$ and hence we adopt the following definition:

Definition 1. A model will be called *regular* if every 1-path of this model is regular.

Let us then note that, following Proposition 2, this definition is equivalent to the property that every fixed point of L is invariant under $\mathscr{S}$. Thus, regular models are of particular interest from a physical point of view since one would reasonably expect this last property. Moreover, we will see in Section 3 that the global invariants of regular models are regular, as stated in the Introduction. Unfortunately, in general any model is not regular. Let us observe that in order to have a regular deterministic model, the operators $\mathscr{C}$ and $\mathscr{S}$ must satisfy the following property:

$$\forall \mathbf{n} \in \mathscr{W}, \quad \exists k \in \mathbb{N} / \mathscr{C}(\mathscr{S}\mathscr{C})^k(\mathbf{n}) = \mathbf{n}$$

where $\mathscr{C}$ is the microscopic collision operator introduced previously. For instance, a deterministic model where $\mathscr{C}^2$ is the identity map on $\mathscr{W}$ (which is usually true) is regular if and only if $\mathbf{n}$ and $\mathscr{C}(\mathbf{n})$ are on the same orbit, for any configuration $\mathbf{n}$.

For nondeterministic models we will show in Section 3 that one can exhibit a class of regular models by assuming simple conditions on transition probabilities.

2. GLOBAL LINEAR INVARIANTS AND FIXED POINTS OF L

In the following we will need further information on $\mathscr{S}$ and $\mathscr{E}$. In order to illustrate the notations that will be used, let us consider the case of the HPP[4–6] model (see Section 6) on the periodic 2D square lattice. The state of a node α is described (with the usual notations) by four Boolean variables: $\mathbf{n}(\alpha) = (x_1, x_2, x_3, x_4)$. For each $j = 1,..., 4$ the condition $x_j = 1$ will stand for the presence of a particle with velocity $\mathbf{c}_j$ at the considered node, and $x_j = 0$ for its absence. The free propagation operator $\mathscr{S}$ is then defined by giving four permutations p_j of $\mathscr{L}$: $p_j(\alpha) = \alpha - \mathbf{c}_j$ such that we have

$$\forall \mathbf{n} \in \mathscr{W}, \forall \alpha \in \mathscr{L}, \qquad \mathscr{S}(\mathbf{n})(\alpha) = (\mathbf{n}_1(p_1(\alpha)), \mathbf{n}_2(p_2(\alpha)), \mathbf{n}_3(p_3(\alpha)), \mathbf{n}_4(p_4(\alpha)))$$

Thus, in the sequel we will consider $\mathscr{E}$ to be the Cartesian product $\mathscr{E}^1 \times \mathscr{E}^2 \times \cdots \times \mathscr{E}^b$ of b finite sets or *channels* and that the free propagation operator $\mathscr{S}$ is prescribed by setting b permutations of $\mathscr{L}$: $p_1, p_2,..., p_b$ such that

$$\forall \mathbf{n} \in \mathscr{W}, \qquad \forall \alpha \in \mathscr{L}, \quad \mathscr{S}(\mathbf{n})(\alpha) = (\mathbf{n}_1(p_1(\alpha)), \mathbf{n}_2(p_2(\alpha)),..., \mathbf{n}_b(p_b(\alpha))) \quad (3)$$

where each $\mathbf{n}_j(\alpha)$ belongs to $\mathscr{E}^j$. This notation takes into account not only pure kinetic models like the HPP model, but also most of the LGA models.

Let us then observe that if a given $\mathscr{E}^j$ has exactly two elements (i.e., if there is at most one particle in this channel), it can be identified with the set $\{0, 1\}$. This is the case for the usual HPP or FHP models. But from both theoretical and practical points of view one can allow for more than two states in a given channel $\mathscr{E}^j$. This can be, for example, the case of models with rest particles or with energy levels. Hence, if the number of states n_j of a channel $\mathscr{E}^j$ is not a power of two and if we want a Boolean representation of this channel (for computational commodity) we are led to constrain this representation. One can then note that any finite set of n_j elements can always be identified with the Boolean manifold:

$$\left\{(x_1, x_2,..., x_{n_j}) \in \{0, 1\}^{n_j} \Big/ \sum_{i=1}^{n_j} x_i = 1\right\} \quad (4)$$

Thus, for the following we will then assume that each $\mathscr{E}^j$ is defined by the relation (4). This notation generalizes that introduced in previous works[20–22] and allows most models used in the literature to be described. One of the advantages of this representation is to avoid taking care of the exclusion principle. Let us note that a configuration is then represented by a Boolean vector in $\mathbb{R}^{NL}$ which always has exactly bL components equal to 1 and the others equal to 0. The configuration $\mathbf{n}_0$ defined by the following relation will be called "empty":

$$[\mathbf{n}_0]_i^j(\alpha) = \delta_{i1} \qquad \text{for all} \quad \alpha, i, j$$

The space state $\mathscr{E}$ is then a subset of $\mathbb{R}^N$, while $\mathscr{W}$ is a subset of $\mathbb{R}^{NL}$, once an order has been chosen on $\mathscr{L}$. If Φ is a vector in $\mathbb{R}^{NL}$, we will denote $\Phi(\alpha)$ the αth projection of Φ on $\mathbb{R}^N$. The components of Φ [resp. of $\Phi(\alpha)$] will be denoted by $\Phi_i^j(\alpha)$ (resp. Φ_i^j), where α varies from 1 to L and stands for the nodes, while $i = 1,..., n_j$ stands for the components on $\mathbb{R}^{n_j}$ with $j = 1,..., b$. We denote by $\langle \cdot, \cdot \rangle$ the canonical scalar product on both $\mathbb{R}^N$ and $\mathbb{R}^{NL}$. If Φ is a vector in $\mathbb{R}^{NL}$ we will also denote Φ the linear form associated by the relation $\Phi(\mathbf{n}) = \langle \Phi, \mathbf{n} \rangle$. The free propagation operator $\mathscr{S}$ on $\mathscr{W}$ as given by the relation (3) induces a linear transformation on $\mathbb{R}^{NL}$, also denoted $\mathscr{S}$, which is defined for each Φ in $\mathbb{R}^{NL}$ by

$$\mathscr{S} \cdot \Phi(\alpha) = (\Phi^1(p_1(\alpha)), \Phi^2(p_2(\alpha)),..., \Phi^b(p_b(\alpha)))$$

where each Φ^j belongs to $\mathbb{R}^{nj}$. One can then observe that $\mathscr{S}$ is an orthogonal map, i.e., $\mathscr{S}^{-1} = \mathscr{S}^t$, or equivalently

$$\forall \Phi, \Psi \in \mathbb{R}^{NL} \times \mathbb{R}^{NL}, \quad \langle \mathscr{S}\Phi, \mathscr{S}\Psi \rangle = \langle \Phi, \Psi \rangle$$

We then assume that the global transition probabilities are constructed from a set of node-independent local transition probabilities: $a(X \to X')$ from $\mathscr{E} \times \mathscr{E}$ to [0, 1], such that

$$\mathscr{A}(\mathbf{n}' \to \mathbf{n}) = \prod_{\alpha \in \mathscr{L}} a(\mathbf{n}(\alpha) \to \mathbf{n}'(\alpha))$$

We also assume that they satisfy similar relations to the global ones:

$$\forall X \quad \int_{\mathscr{E}} a(X \to X')\, dX' = 1; \quad \int_{\mathscr{E}} a(X' \to X)\, dX' = 1$$

Hence, we have considered that all the nodes are equivalent for the collision process. Thus, if $\mathscr{L}$ is a regular lattice, the subsequent results on global invariants will stand for periodic lattices without boundaries.

We then define, as usual,[11,24] a local linear invariant as follows.

Definition 2. A *local linear invariant* is a vector ϕ of $\mathbb{R}^N$ that satisfies

$$\forall X, Y \in \mathscr{E} \times \mathscr{E}, \qquad a(X \to Y)\langle \phi, X - Y \rangle = 0$$

The scalar product is taken in $\mathbb{R}^N$. The local linear invariants constitute a linear subspace of $\mathbb{R}^N$, denoted $\mathscr{K}_{\text{loc}}$. Now, since Proposition 1 gives a characterization of the fixed points of $\boldsymbol{L}$, we adopt the following definition of the global linear invariants for the process $\boldsymbol{L}$:

Definition 3. A vector Φ of $\mathbb{R}^{NL}$ will be called a *global linear 1-invariant* if it satisfies the relation

$$\forall \mathbf{n}, \mathbf{n}' \in \mathscr{W}^2, \quad \mathscr{A}(\mathbf{n} \to \mathbf{n}')\langle \Phi, \mathbf{n} - \mathscr{S}(\mathbf{n}') \rangle = 0$$

The scalar product is taken in $\mathbb{R}^{NL}$. The global linear 1-invariants constitute then a linear subspace of $\mathbb{R}^{NL}$, denoted $\mathscr{K}^1_{gl}$. This definition agrees with the definition of d'Humières *et al.*[11] for deterministic LGCA and corresponds to what they have called *global linear invariant with a time period* 1. In general, although Φ is a global invariant, there is no reason for $\Phi(\alpha)$ to be a local invariant. Thus we introduce the following definition:

Definition 4. A global 1-invariant will be called *regular* if its projection on each node is a local invariant.

At each local invariant there is associated a global one Φ defined by $\Phi(\alpha) = \phi$ for each node α. Conversely we have the following result:

Proposition 3. The only global 1-invariants such that $\Phi(\alpha) = \phi =$ const at each node are regular: We will call them *homogeneous* global 1-invariants.

This result is an obvious consequence of Lemma 2 given at the end of this section. Thus $\mathscr{K}_{\text{loc}}$ is embedded in $\mathscr{K}^1_{gl}$ and the dimension of $\mathscr{K}^1_{gl}$ is always greater than or equal to that of $\mathscr{K}_{\text{loc}}$.

One readily sees that the linear form associated with each global invariant is constant on every 1-path. Thus, one deduces from Proposition 2 that, if $\Phi_1, \Phi_2, ..., \Phi_p$ are p independent global invariants, every density f on $\mathscr{W}$ that satisfies

$$\forall \mathbf{n} \in \mathscr{W}, \quad f(\mathbf{n}) = g(\Phi_1(\mathbf{n}), \Phi_2(\mathbf{n}), ..., \Phi_p(\mathbf{n})) \tag{5}$$

(where g is a positive function on $\mathbb{R}^p$) is a fixed point of $\boldsymbol{L}$. The converse is, in general, wrong. Hence we deduce the following proposition, which shows that the previous definition of the global 1-invariants and that given in the Introduction are equivalent:

Proposition 4. A vector Φ of $\mathbb{R}^{NL}$ is a linear global 1-invariant if and only if there exists a constant k such that the density f, defined for any configuration $\mathbf{n}$ in $\mathscr{W}$ by $f(\mathbf{n}) = k\exp(\Phi(\mathbf{n}))$ (where k is a normalization constant), is a fixed point of $\boldsymbol{L}$.

This last proposition is general and holds even if the transition probabilities are not factorized through the nodes. Let us note that in general there may exist nonhomogeneous global linear invariants and hence non-spatially-homogeneous fixed points of $\boldsymbol{L}$.

Our description of the phase space introduces through Definitions 2 and 3 some unphysical invariants associated with the constraints $\sum_{i=1}^{n_j} x_i = 1$ on each $\mathscr{E}^j$ (see, for example, ref. 20). More exactly, let us call $I(j)$ the vector of $\mathbb{R}^N$ defined by $[I(j)]_i^r = \delta_{jr}$ (there are exactly b such vectors), $I(j, \alpha)$ the vector of $\mathbb{R}^{NL}$ defined by $[I(j, \alpha)](\beta) = \delta_{\alpha\beta} I(j)$, and $\mathscr{K}'_{gl}$ the subspace generated by the $I(j, \alpha)$, its dimension being bL. If Ψ is a vector of $\mathscr{K}'_{gl}$, one then deduces from relation (4) that the scalar product $\langle \Psi, \mathbf{n} \rangle$ is a constant independent of the configuration $\mathbf{n}$. Hence $\mathscr{K}'_{gl}$ is a subspace of $\mathscr{K}^1_{gl}$, but these invariants do not affect the dynamics of the LGA, since the associated linear forms keep constant values on the whole phase space.

We will then call $\mathscr{K}^{d,1}_{gl}$ the subspace of $\mathscr{K}^1_{gl}$ *orthogonal* to $\mathscr{K}'_{gl}$ and its elements the global *dynamical* 1-invariants of the automaton. Thus, every stationary density given by (5) is in fact only a function of the dynamical invariants and the complete determination of the linear 1-invariants of a given model reduces to the determination of the dynamical ones. In the same way we will divide $\mathscr{K}_{\text{loc}}$ into $\mathscr{K}^d_{\text{loc}}$ and $\mathscr{K}'_{\text{loc}}$, where $\mathscr{K}'_{\text{loc}}$ is generated by the vectors $I(j)$. For a pure kinetic model where each $\mathscr{E}^j$ has two elements, there is then a one-to-one relation between the whole set of global dynamical linear invariants and the whole set of global linear invariants in the usual representation, since there are no more constraints on the entries (see the examples in Section 6). We will then need the following lemma:

Lemma 1. If Φ is a vector orthogonal to $\mathscr{K}'_{gl}$ and if we have $\langle \Phi, \mathbf{m}_i \rangle = \text{Cste}$ for a given configuration $\mathbf{m}_0$ and for the $(NL\text{-}bL)$ configurations $\mathbf{m}_i$ obtained by successively permuting in $\mathbf{m}_0$ a one and a zero node after node and on each $\mathscr{E}^i$, then $\Phi = 0$ and $\text{Cste} = 0$.

Proof. Let $\{\mathbf{m}_i,\ i = 1,..., NL - bL\}$ be the set of the configurations obtained by successively permuting in $\mathbf{m}_0$ a one and a zero node after node and on each $\mathscr{E}^j$: each $\mathbf{m}_i$ differs from $\mathbf{m}_0$ on at most one node and at this node on only one of the $\mathscr{E}^j$. If Ψ is a vector in $\mathscr{K}'_{gl}$, we then have $\langle \Psi, \mathbf{m}_i - \mathbf{m}_0 \rangle = 0$ for each $i \geqslant 1$. Then the set $\{\mathbf{m}_i - \mathbf{m}_0\}$ is a basis of the subspace orthogonal to $\mathscr{K}'_{gl}$ in $\mathbb{R}^{NL}$. But we then have $\langle \Phi, \mathbf{m}_i - \mathbf{m}_0 \rangle = 0$ for any *configuration* $\mathbf{m}_i$, which implies that Φ is in $\mathscr{K}'_{gl}$. Thus, since Φ is also orthogonal to $\mathscr{K}'_{gl}$, we have $\Phi = 0$ and Cste $= 0$.

This lemma applies in particular to the global dynamical 1-invariants. One can then observe that $\mathscr{K}'_{gl}$ is globally invariant under $\mathscr{S}$, while its elements are obviously regular. Hence the subspace of $\mathbb{R}^{NL}$ orthogonal to $\mathscr{K}'_{gl}$ (and which contains the dynamical global 1-invariants) is globally invariant under $\mathscr{S}$. But unfortunately without any further hypothesis one cannot state that the whole set $\mathscr{K}^1_{gl}$ is globally invariant under $\mathscr{S}$, although one would reasonably expect it. The following proposition provides then quite a remarkable connection between the regular dynamical 1-invariants and the 1-invariants which are $\mathscr{S}$-invariant:

Proposition 5. A global dynamical 1-invariant Φ is regular if and only if it satisfies

$$\mathscr{S}\Phi = \Phi$$

In order to prove this proposition, Lemma 2 shows that any global 1-invariant which satisfies the condition $\mathscr{S}\Phi = \Phi$ is regular, so that this condition is sufficient. Conversely, if Φ is a regular dynamical 1-invariant, then the density $f(\mathbf{n}) = \boldsymbol{k} \exp(\Phi(\mathbf{n}))$ is a fixed point of $\boldsymbol{L}$. From Definitions 1 and 2 and since Φ is regular, we deduce that $\exp(\Phi(\mathbf{n})) = \exp(\mathscr{S}\Phi(\mathbf{n}))$ and thus $\langle \Phi, \mathbf{n} \rangle = \langle \mathscr{S}\Phi, \mathbf{n} \rangle$ for any configuration $\mathbf{n}$. Now, since $\mathscr{S}$ is an orthogonal transformation, the fector $\mathscr{S}\Phi - \Phi$ remains in the subspace of $\mathbb{R}^{NL}$ orthogonal to $\mathscr{K}'_{gl}$. We then deduce from Lemma 1 that $\mathscr{S}\Phi = \Phi$.

Lemma 2. Let Φ be a vector in $\mathbb{R}^{NL}$. If

$$\forall \mathbf{n}, \mathbf{n}' \in \mathscr{W}^2, \quad \mathscr{A}(\mathbf{n} \to \mathbf{n}') \langle \Phi, \mathbf{n} - \mathbf{n}' \rangle = 0$$

then for every node α, $\Phi(\alpha)$ is in $\mathscr{K}_{\text{loc}}$.

To prove this lemma, it is sufficient to sum the equality over all configurations $\mathbf{n}, \mathbf{n}'$ such that $\mathbf{n}(\alpha) = X$ and $\mathbf{n}'(\alpha) = Y$, where α is a fixed node and X, Y fixed elements in $\mathscr{E}$.

Hence, the dynamical regular 1-invariants are the elements of the following subspace:

$$\mathscr{K}^{s,1}_{gl} = \{\Phi \in \mathbb{R}^{NL} / \mathscr{S}\Phi = \Phi \text{ and } \forall \alpha \in \mathscr{L}, \ \Phi(\alpha) \in \mathscr{K}^d_{\text{loc}}\} \qquad (6)$$

This subspace will then play an essential part in the study of the dynamical properties of any LGCA, and it is of particular importance for a given model to know if $\mathscr{K}^{d,1}_{gl}$ is equal to $\mathscr{K}^{s,1}_{gl}$. In fact, as we will see, this is true for most models, including the regular ones.

3. GLOBAL LINEAR 1-INVARIANTS IN REGULAR MODELS

We have seen before that the complete determination of $\mathscr{K}^{1}_{gl}$ reduces to the determination of $\mathscr{K}^{d,1}_{gl}$ which always contains $\mathscr{K}^{s,1}_{gl}$.

For regular models one can then prove the following proposition, which is one of the main results of this section:

Proposition 6. All the linear 1-invariants of a regular model are regular and the dynamical ones are characterized by the following identity:

$$\mathscr{K}^{d,1}_{gl} = \mathscr{K}^{s,1}_{gl} \tag{7}$$

This result is quite remarkable, since it yields a complete determination of the global linear 1-invariants and it also implies that they are independent of the details of the collision process as soon as the model is regular. This last point was the background hypothesis in the method proposed in ref. 16. The main arguments to prove (7) will be the $\mathscr{S}$-invariance of the 1-paths and the fact that the global linear invariants are constant on every 1-path (see Appendix B).

However, if the set of paths is only globally invariant under $\mathscr{S}$, one obtains a weaker result, that is, $\mathscr{K}^{d,1}_{gl}$ (and consequently the whole set $\mathscr{K}^{1}_{gl}$) is globally invariant under $\mathscr{S}$ (see also Appendix B).

We will show in Section 5 that this proposition can be still extended to a larger class of models, including most of the lattice gases used for describing hydrodynamics (see Proposition 13).

Moreover, this characterization of the global invariants for the process $\boldsymbol{L}$ can be generalized, at least for a class of stochastic regular models, to any process $\boldsymbol{L}^k$, as is shown in Section 4.

A natural question which then immediately comes in mind is: Is it possible to decide whether or not a model is regular without having previously determined its invariants? In order to answer this question, we will consider the class of models where the global transition probabilities obey the three properties:

(P1) $\forall \mathbf{n}, \mathbf{m} \in \mathscr{W}^2,\ \mathscr{A}(\mathbf{n} \to \mathbf{m}) \neq 0 \Rightarrow \mathscr{A}(\mathbf{m} \to \mathbf{n}) \neq 0$

(P2) $\mathscr{A}(\mathbf{m} \to \mathbf{n}) \neq 0,\ \mathscr{A}(\mathbf{r} \to \mathbf{n}) \neq 0,\ \mathbf{m} \neq \mathbf{r} \Rightarrow \mathscr{A}(\mathbf{m} \to \mathbf{r}) \neq 0$

(P3) $\mathbf{n} \neq \mathbf{m} \Rightarrow \mathscr{A}(\mathbf{n} \to \mathbf{m}) < 1$

Properties (P1) and (P2) express a kind of microreversibility which is satisfied by all usual LGAs [for deterministic models (P2) is true, since $\mathscr{C}$ is invertible, while (P(1) just imposes that $\mathscr{C}^2$ is the identity map on $\mathscr{W}$, which is usually the case for deterministic LGA].

Property (P3) expresses the stochasticity of the nontrivial collisions. Let us note that it is always possible to modify a given model in order to have (P3) without changing its local invariants or its symmetries. Let us also note that, for deterministic models, (P3) is uninteresting since it leads to only trivial collisions.

The following proposition provides then an answer to the previous question:

Proposition 7. Any model which satisfies the three properties (P1)–(P3) is regular.

This result is rather remarkable since it only involves the collision process and not the propagation operator itself nor the topological details of the paths. The main argument to prove this comes from the fact that the phase space is finite, which leads us to establish that for every initial density f_0 we have (see Appendix C)

$$\forall \varepsilon > 0, \exists N \in \mathbb{N}; p \geqslant N \Rightarrow \forall \mathbf{n} \in \mathscr{W}: |f_{p+1}(\mathscr{S}(\mathbf{n})) - f_p(\mathbf{n})| \leqslant \varepsilon \tag{8}$$

The proof is achieved by setting f_0 as a fixed point of $\boldsymbol{L}$. We then have $f_p = f_0$ for any order p. By applying (8) to the corresponding sequence (f_p) we then finally obtained that f_0 is invariant under $\mathscr{S}$. Hence, models which obey (P1)–(P3) are regular.

Relation (8) simply expresses that the effect of the collisions fades as time goes on, and thus the process tends to be only propagative.

Also notice that (8) yields the following relation for any finite integer k:

$$\forall \varepsilon > 0, \exists N \in \mathbb{N}; p \geqslant N \Rightarrow \forall \mathbf{n} \in \mathscr{W}: |f_{p+k}(\mathscr{S}^k(\mathbf{n})) - f_p(\mathbf{n})| \leqslant k\varepsilon$$

and thus for these models, the fixed points of $\boldsymbol{L}^k$ are invariant under $\mathscr{S}^k$. We do not know if this remains true or not for all regular models.

4. GENERALIZATION TO L^k

In order to apply to the process $\boldsymbol{L}^k$ the same treatment as to $\boldsymbol{L}$, let us define the transition probabilities of order k, $\mathscr{A}^k$, by

$$\mathscr{A}^k(\mathbf{n} \to \mathbf{n}') = \int_{\mathscr{W}^{k-1}} \mathscr{A}(\mathbf{n} \to \mathscr{S}^{-1}(\mathbf{n}_1))\, \mathscr{A}(\mathbf{n}_1 \to \mathscr{S}^{-1}(\mathbf{n}_2)) \cdots \mathscr{A}(\mathbf{n}_{k-1} \to \mathbf{n}')$$
$$\times\, d\mathbf{n}_1\, d\mathbf{n}_2 \cdots d\mathbf{n}_{k-1}$$

with the convention $\mathscr{A}^1(\mathbf{n} \to \mathbf{n}') = \mathscr{A}(\mathbf{n} \to \mathbf{n}')$. The $\{\mathscr{A}^k(\mathbf{n} \to \cdot)\}$ are probabilities on $\mathscr{W}$ and they also obey a semi-detailed balance. We have

$$\boldsymbol{L}^k(f)(\mathbf{n}) = \int_{\mathscr{W}} f(\mathbf{n}')\, \mathscr{A}^k(\mathbf{n}' \to \mathscr{S}^{-1}(\mathbf{n}))\, d\mathbf{n}'$$

Let us then note that L^k is expressed with the transition probabilities of order k by replacing in the definition (1) of L, $\mathscr{A}$ by $\mathscr{A}^k$. Thus, in the same way as for L, we can associate to L^k a set of paths and a set of global linear invariants $\mathscr{K}^k_{gl}$. The first will be called k-paths and the second, global linear k-invariants. We then have the following definition:

Definition 5. A vector Φ of $\mathbb{R}^{NL}$ will be called *global linear k-invariant* for $k \geqslant 1$ if it satisfies the relation

$$\forall \mathbf{n}, \mathbf{n}' \in \mathscr{W}^2, \qquad \mathscr{A}^k(\mathbf{n} \to \mathbf{n}') \langle \Phi, \mathbf{n} - \mathscr{S}(\mathbf{n}')) \rangle = 0$$

In the deterministic case these k-invariants are exactly what d'Humières *et al.*[11] have called *global linear invariant with a time period k.*

Moreover, as for L, a density f will be a fixed point of L^k if and only if it is constant on each k-path. Hence, from Definition 5 one can see that the linear form associated with any global k-invariant is constant on every k-path. Thus, if $\Phi_1, \Phi_2,..., \Phi_p$ are p independent global k-invariants, every density f on $\mathscr{W}$ which satisfies

$$\forall \mathbf{n} \in \mathscr{W}, \quad f(\mathbf{n}) = g(\Phi_1(\mathbf{n}), \Phi_2(\mathbf{n}),..., \Phi_p(\mathbf{n})) \tag{9}$$

(where g is a positive function on $\mathbb{R}^p$) is a fixed point of L^k. Any 1-invariant is obviously a global linear k-invariant and thus $\mathscr{K}'_{gl}$ is included in $\mathscr{K}^k_{gl}$ for any k. We then denote by $\mathscr{K}^{d,k}_{gl}$ the subspace of $\mathscr{K}^k_{gl}$ *orthogonal* to $\mathscr{K}'_{gl}$; its elements will be called the global *dynamical* k-invariants of the automaton. Thus, every stationary density given by (9) is in fact only a function of the dynamical k-invariants and the complete determination of the k-invariants reduces to the determination of $\mathscr{K}^{d,k}_{gl}$.

Note that any fixed point of L^k ($k \geqslant 1$) is also a fixed point of L^{ik} for any integer i. The same is true for the global linear k-invariants. Thus, a linear global k-invariant which is not a global invariant for any other process L^r with $r < k$ will be called a *specific* k-invariant. We then generalize the concept of regular invariant to the k-invariants through the following definition:

Definition 6. A global k-invariant will be called *regular* if at each node α the projections $\Phi(\alpha)$, $\mathscr{S}\Phi(\alpha)$,..., $\mathscr{S}^{k-1}\Phi(\alpha)$ are local invariants.

The regular k-invariants will play, like the regular 1-invariants for the process L, an important role in the application of the linear response theory to L^k. Indeed, as we will see in the next section (at least for a wide class of models) they univocally define the fixed points of L^k which remain factorized at any time (see Proposition 13). Any element of $\mathscr{K}'_{gl}$ is obviously a regular k-invariant, while the regular dynamical k-invariants are characterized by the following proposition:

Proposition 8. A regular dynamical k-invariant Φ necessarily satisfies

$$\mathscr{S}^k\Phi = \Phi$$

We will prove this result in the next section. Thus, the regular dynamical k-invariants are the elements of the following subspace:

$$\mathscr{K}_{gl}^{s,k} = \{\Phi \in \mathbb{R}^{NL}/\mathscr{S}^k\Phi = \Phi \text{ and } \forall\alpha \in \mathscr{L},\ \Phi(\alpha), \mathscr{S}\Phi(\alpha),..., \mathscr{S}^{k-1}\Phi(\alpha) \in \mathscr{K}_{\text{loc}}^{d}\} \tag{10}$$

This set always contains $\mathscr{K}_{gl}^{s,1}$ and it is simply a generalization of this last set. A regular k-invariant which is also an r-invariant with $r < k$ is obviously a regular r-invariant, and moreover, from Proposition 8, if r and k are two prime integers, then it is simply a (regular) 1-invariant. Conversely, if k is a prime integer, any regular k-invariant which is not a 1-invariant is necessarily a specific k-invariant. The following proposition then provides quite a remarkable result:

Proposition 9. The global linear k-invariants of a model which obeys the three properties (P1)–(P3) are regular and its dynamical ones are characterized by the identity

$$\mathscr{K}_{gl}^{d,k} = \mathscr{K}_{gl}^{s,k} \tag{11}$$

The proof is given in Appendix D, but since it is a little lengthy, we have limited it to the case $k = 2$. As later illustrated on the examples in Section 6, the subspace $\mathscr{K}_{gl}^{s,k}$ contains, according to the model and the values of k, the so-called dynamic staggered invariants[15–17] and also the line and chessboard invariants.[15] Thus, they all have the same status: they are regular k-invariants (usually $k = 2$). Hence we suspect that Proposition 9 holds for all regular models, but this remains a conjecture. Nevertheless, at least for models which obey (P1)–(P3) one is then theoretically able to determine all the linear invariants at any order: Moreover, if Φ is a global k-invariant, then $\{\Phi, \mathscr{S}\Phi,..., \mathscr{S}^{k-1}\Phi\}$ are also l-invariants but not necessarily independent, even if Φ is a specific k-invariant (see, for example, the 2-invariants of the HPP models).

At each permutation p on the nodes $\mathscr{L}$ we can associate a permutation on $\mathscr{W}$ defined by $p(\mathbf{n})(\alpha) = \mathbf{n}(p(\alpha))$. The factorization of the global transition probabilities into local ones imposes the invariance of these global transition probabilities under any permutation of $\mathscr{L}$. Hence the transition probabilities of any order k are invariant under each permutation p of $\mathscr{L}$ which commutes with each p_i in the definition of $\mathscr{S}$, i.e.,

$\mathscr{A}^k(\mathbf{n} \to \mathbf{n}') = \mathscr{A}^k(p(\mathbf{n}) \to p(\mathbf{n}'))$. Thus, the set of k-paths, for any k, is globally invariant under the group of the permutations which commute with each p_i. Consequently, since p induces an orthogonal transformation on $\mathbb{R}^{NL}$ defined by $p(\Phi)(\alpha) = \Phi(p(\alpha))$, the sets $\mathscr{K}^k_{gl}$, $\mathscr{K}^{d,k}_{gl}$, $\mathscr{K}'_{gl}$, $\mathscr{K}^{s,k}_{gl}$ are also globally invariant under the group of the permutations which commute with each p_i. For usual lattice gases on regular periodic lattices this implies that these sets are invariant under the translation group of the lattice. This translation invariance has been largely investigated in ref. 11, where it is the basic ingredient of the method proposed by the authors in order to determine the global linear invariants.

Let us conclude this section with some general remarks:

1. The fixed points of $\boldsymbol{L}^k$ cannot be distinguished from those of $\boldsymbol{L}$ with an entropy criterion.

2. If f_0 is a fixed point of $\boldsymbol{L}^k$, then $f_1, f_2,..., f_{k-1}$ are also fixed points of $\boldsymbol{L}^k$ and the density $(f_0 + f_1 + \cdots + f_{k-1})/k$ is then a fixed point of $\boldsymbol{L}$. Moreover, if f_0 is specific to $\boldsymbol{L}^k$ (i.e., it is not a fixed point of another process $\boldsymbol{L}^r$ with $r < k$), then $f_0, f_1,..., f_{k-1}$ are k different and specific fixed points of $\boldsymbol{L}^k$.

3. For a model which obeys (P1)–(P3) one deduces from (8) that if some fixed point of $\boldsymbol{L}^k$ is invariant under $\mathscr{S}$, then it is simply a fixed point of $\boldsymbol{L}$. So, if k and l are two prime integers, the only common fixed points of $\boldsymbol{L}^k$ and $\boldsymbol{L}^l$ are fixed points of $\boldsymbol{L}$. The same holds of course for the global linear invariants. However, this last result is always true for deterministic models, since $\mathscr{S}\mathscr{C}$ is invertible.

5. GIBBS DENSITIES FOR $\boldsymbol{L}^k$

The notations are those introduced in Section 2. We will denote by $\mathbf{E}$ the set of vectors $\phi \in \mathbb{R}^N$ such that each ϕ^j_i is in $]0, 1[$ with $\sum_{i=1}^{n_j} \phi^j_i = 1$ for all j. At each density on $\mathscr{W}$ we can associate a *mean population* vector field $\mathbf{N} \in \bar{\mathbf{E}}^L$ defined by

$$\forall i, j, \alpha, \quad N^j_i(\alpha) = \int_{\mathscr{W}} n^j_i(\alpha)\, f(\mathbf{n})\, d\mathbf{n}$$

If $\mathbf{N} \in \mathbf{E}^L$, we will denote by $\mathrm{Log}(\mathbf{N})$ the vector in $\mathbb{R}^{NL}$ whose components are $\mathrm{Log}(N^j_i(\alpha))$. A density f on $\mathscr{W}$ will be called *factorized* if it is factorized over all states and nodes. Thus it is given by

$$f(\mathbf{n}) = \prod_{\alpha} \cdot \prod_{j=1}^{b} \cdot \prod_{i=1}^{n_j} \cdot [N^j_i(\alpha)]^{n^j_i(\alpha)} \tag{12}$$

where $\mathbf{N}$ is its mean population field. It will be called homogeneous if $\mathbf{N}(\alpha)$ is constant over the nodes. Hence any strictly positive [i.e., $f(\mathbf{n}) > 0$ for all n] factorized density f can always be written under the following form:

$$f(\mathbf{n}) = \exp(\langle \mathrm{Log}(\mathbf{N}), \mathbf{n} \rangle) \tag{13}$$

where $\mathbf{N}$ is its mean population field.

The following proposition characterizes the factorized fixed points of $\boldsymbol{L}^k$:

Proposition 10. A (strictly positive) factorized density f is a fixed point of $\boldsymbol{L}^k$ if and only if there exists a global linear k-invariant $\boldsymbol{\Phi}$ and a constant $\boldsymbol{k}$ such that

$$\forall \mathbf{n} \in \mathscr{W}, \quad f(\mathbf{n}) = \boldsymbol{k} \exp(\langle \boldsymbol{\Phi}, \mathbf{n} \rangle) \tag{14}$$

The proposition is a direct consequence of relation (13) and of the characterization of the fixed points. Moreover, since it is known from information theory that the information of a factorized density is lower than that of any other with the same mean population field, the factorized fixed points of $\boldsymbol{L}^k$ appear as the Gibbs microcanonical distribution for this process. We will call them *global k-equilibrium distributions.* The homogeneous ones which are usually considered are then those associated with homogeneous global invariants: they are factorized fixed points for all processes $\boldsymbol{L}^k$. In relation (14) the couple $(\boldsymbol{k}, \boldsymbol{\Phi})$ is unique when $\boldsymbol{\Phi}$ is a dynamical k-invariant. One then deduces from (13) and (14) that a (strictly positive) factorized density is a global k-equilibrium distribution if and only if the vector $\mathrm{Log}(\mathbf{N})$ is a global linear k-invariant. These k-equilibrium distributions are one-to-one related to the mean values of the global k-invariants, as stated in the following proposition:

Proposition 10 bis. Let $\mathbf{N}$ be a vector in $\mathbf{E}^L$ (i.e., a strictly positive mean population field). There then exists a unique field $\mathbf{N}_{\mathrm{eq}}$ in $\mathbf{E}^L$ which satisfies

$$\forall \boldsymbol{\Phi} \in \mathscr{K}^k_{gl}, \quad \langle \boldsymbol{\Phi}, \mathbf{N} \rangle = \langle \boldsymbol{\Phi}, \mathbf{N}_{\mathrm{eq}} \rangle$$

and such that the distribution $f(\mathbf{n}) = \exp(\langle \mathrm{Log}(\mathbf{N}_{\mathrm{eq}}), \mathbf{n} \rangle)$ is a global k-equilibrium distribution.

A proof of this result, based on asymptotic properties of algebroid functions, is given in ref. 25, but a direct proof for LGAs which only uses the convexity of the information function is proposed in ref. 28. In other words, this proposition states that there is a one-to-one correspondence between the mean values of the global conserved quantities and the thermodynamic variables of the LGCA.

It is easy to prove the existence of fixed points which are not just functions of the global linear invariants and hence, in general, there exist fixed points which are not equilibrium distributions.

If f is factorized, we always have the following identity:

$$\int_{\mathscr{W}} [L(f)(\mathscr{S}\mathbf{n}) - f(\mathbf{n})]\, \mathbf{n}(\alpha)\, d\mathbf{n}$$

$$= \int_{\mathscr{E}\times\mathscr{E}} a(X \to Y)(Y - X) \prod_{j=1}^{b} \cdot \prod_{i=1}^{n_j} \cdot [N_i^j(\alpha)]^{X_i^j}\, dX\, dY \qquad (15)$$

The rhs of (15), which is similar to the Boltzmann collision integral, only depends on $\mathbf{N}(\alpha)$ and it will be denoted $\delta(\mathbf{N}(\alpha))$. If $\mathbf{N}$ is a vector in $\mathbf{E}$, the following propositions which characterize the homogeneous factorized fixed points of $\boldsymbol{L}$ are then equivalent:

$$\begin{aligned} &\text{(a)}\quad \delta(\mathbf{N}) = 0 \\ &\text{(b)}\quad \mathrm{Log}(\mathbf{N}) \in \mathscr{K}_{\mathrm{loc}} \\ &\text{(c)}\quad \langle \delta(\mathbf{N}), \mathrm{Log}(\mathbf{N}) \rangle = 0 \\ &\text{(d)}\quad f(\mathbf{n}) = \prod_{\alpha} \cdot \prod_{j=1}^{n} \cdot \prod_{i=1}^{n_j} \cdot [N_i^j]^{n_i^j(\alpha)} \quad \text{is a fixed point of } \boldsymbol{L} \end{aligned} \qquad (16)$$

The result is based on the semi-detailed balance hypothesis and hence it holds for any model. A proof can be deduced from ref. 25 with only slight modifications (see Appendix E). This is a generalization of similar equivalences[24] for models with a single speed. For a regular model the following characterization of the 1-equilibrium distributions holds:

Proposition 11. Let $\boldsymbol{L}$ be the Markov operator of a regular model. Then a factorized strictly positive density f is a fixed point of $\boldsymbol{L}$ if and only the vector $\mathbf{N}$ satisfies

$$\mathscr{S}\mathbf{N} = \mathbf{N} \qquad (17)$$

$$\mathrm{Log}(\mathbf{N}(\alpha)) \in \mathscr{K}_{\mathrm{loc}}, \quad \forall \alpha \qquad (18)$$

Indeed, from (13) any factorized density which obeys (17) and (18) obviously satisfies the condition of Proposition 1. Conversely, if f is a factorized fixed point of a regular model, we deduce from Propositions 10 and 6 that (18) is true, so that relations (15) and (16) yield (17).

Let us then note that if a factorized density satisfies (18), then the density $L(f)$ is also factorized and its mean population field is $\mathscr{S}\mathbf{N}$. Similarly, if Φ is a regular dynamical k-invariant, then the density $f(\mathbf{n}) = k\exp(\langle \Phi, \mathbf{n}\rangle)$ (where k is a normalization constant) is a k-equilibrium distribution. But since Φ is regular, the successive powers $L^i(f)$ are factorized and we have

$$L^k(f)(\mathbf{n}) = k\exp(\langle \mathscr{S}^k\Phi, \mathbf{n}\rangle)$$

Hence we deduce that $\mathscr{S}^k\Phi = \Phi$, which proves Proposition 8.

Thus, for a model which obeys (P1)–(P3), its global k-equilibrium distributions *remain factorized* (i.e., k-equilibrium) at any time.

In order to point out another class of models which obey Proposition 11 and hence Proposition 6, let us introduce the following definitions.

If a configuration $\mathbf{n}$ satisfies $\mathscr{S}(\mathbf{n}) = \mathbf{n}$ and $\mathscr{A}(\mathbf{n} \to \mathbf{n}) = 1$ we will say that it is stationary (this implies that the 1-path which contains $\mathbf{n}$ is reduced to $\mathbf{n}$). We will then say that a stationary configuration $\mathbf{n}$ is regular if any other configuration $\mathbf{n}'$, such that $\mathbf{n}'$ differs from $\mathbf{n}$ on at most one node and at this node on at most one of the $\mathscr{E}^j$, satisfies $\mathscr{A}(\mathbf{n}' \to \mathbf{n}') = 1$.

For the usual LGA models where all the particles have the same mass if the local collisions conserve mass and momentum (and energy for models with massless particles[20–22]), the empty configuration is regular. The same is true for models with particles of different masses if the partial masses[26] are conserved: Most models used to describe hydrodynamics fall in this category.

Interesting results concerning the global linear invariants of models which admit a regular configuration come from the following proposition:

Proposition 12. Let L be the Markov operator of a model which has a regular configuration. And let f be a strictly positive factorized density with a mean population field $\mathbf{N}$. Then the density $L(f)$ is also factorized if and only if

$$\forall\alpha, \quad \mathrm{Log}(\mathbf{N}(\alpha)) \in \mathscr{K}_{\mathrm{loc}}$$

For these conditions, the mean population field of $L(f)$ is $\mathscr{S}\mathbf{N}$.

When f is factorized as noted previously, condition (18) is obviously sufficient for $L(f)$ also to be factorized. This proposition states that the converse is true if the model admits a regular configuration. A proof is given in Appendix *E*. As a corollary, one deduces that Proposition 11 and therefore Proposition 6 hold for models which have a regular configuration. Thus we have the following result:

Proposition 13. Let L be the Markov operator of a model which has a regular configuration; then:

(i) A factorized strictly positive density f is a fixed point of $\boldsymbol{L}$ if and only the vector $\mathbf{N}$ satisfies relations (17) and (18).

(ii) All the linear 1-invariants of this model are regular and the dynamical ones are characterized by the identity (7):

$$\mathscr{K}_{gl}^{d,1} = \mathscr{K}_{gl}^{s,1}$$

(iii) More generally, a k-equilibrium distribution is factorized at any time if and only if the vector Log(N) is a regular k-invariant. It then satisfies $\mathscr{S}^k\mathbf{N} = \mathbf{N}$.

Indeed, (i) and (iii) are direct consequences of Proposition 12 and (i) obviously implies (ii). Moreover, one can prove (see also Appendix E) that each global dynamical k-invariant of such a model is invariant under $\mathscr{S}^k$ (but unfortunately not necessarily regular). Hence, for these models the k-equilibrium distributions are invariant under $\mathscr{S}^k$ [this last result and points (i) and (ii) of Proposition 13 also hold under the weaker condition obtained by substituting into the definition of a regular configuration the condition $\mathscr{A}(\mathbf{n}' \to \mathbf{n}') \neq 0$ with $\mathscr{A}(\mathbf{n}' \to \mathbf{n}') = 1$]. Unfortunately, since in general the partition of the phase space induced by the global linear 1-invariants does not coincide with the 1-paths (it only contains them), these models are not necessarily regular.

We conclude this section with a remark on the connection between the nonhomogeneous global 1-invariants in a regular model and its Green's correlation function. Let $(\phi^1,..., \phi^r)$ be a basis of the local invariants, and let $(\Phi^1,..., \Phi^r,..., \Phi^{r+s})$ be a basis for the global linear 1-invariants; since the model is regular, we then have for each Φ^j and each node α

$$\Phi^j(\alpha) = \sum_{i=1}^{r} a_i^j(\alpha)\phi^i$$

Hence, in such a system any 1-equilibrium distribution, characterized by the thermodynamic variables $(\lambda_1,..., \lambda_r,..., \lambda_{r+s})$ associated to all the previous global 1-invariants, can always be rewritten under the form $\boldsymbol{k}\exp[\sum_\alpha \sum_{i=1}^r \chi_i(\alpha)\langle\phi^i, \mathbf{n}(\alpha)\rangle]$, where the $\chi_i(\alpha)$ are given by $\chi_i(\alpha) = \sum_{j=1}^{r+s} a_i^j(\alpha)\lambda_j$. In this last expression the thermodynamic variables associated to the nonhomogeneous conserved quantities are hidden and spatial variations are introduced in the remaining ones. One is then led to evaluate the Green's function with this nonhomogeneous equilibrium distribution which can nevertheless be inverted in Fourier space: The usual Green–Kubo procedure can then be performed. But the spatial variations of the conserved densities coming from the inhomogeneity of the final equilibrium state yields a modification of the transport equations as shown in refs. 10 and 17.

6. EXAMPLES

In this section we will illustrate the previous results by determining the global linear invariants for some known LGA models on the square and hexagonal 2D lattices. We will illustrate in detail the case of the HPP model, which can be considered as a paradigm. In the usual models there is at most one particle with a given velocity $\mathbf{c}_j$ at a given node; thus, in our representation of the phase space the corresponding $\mathscr{E}^j$ has only two elements, (0, 1) and (1, 0), and it can be identified with the set $\{0, 1\}$. In doing this identification we recover the usual notations for the LGCA. For example, with a pure kinetic model where each $\mathscr{E}^j$ has two elements this identification maps the whole set of global dynamical linear invariants with the whole set of global linear invariants in the usual representation, since there are no longer constraints on the coordinates.

6.1. Global Invariants for HPP Models

6.1.1. Global 1-Invariants for the Process *L*. The HPP model is the simplest 2D model, introduced by Hardy *et al.*,[4-6] where four kinds of moving particles are considered on a periodic square lattice $\mathscr{L}$, with q lines and p columns. Each node is identified with the vector $a\mathbf{i}+b\mathbf{j}$ ($p \geqslant a \geqslant 1$, $q \geqslant b \geqslant 1$), where $\mathbf{i}$ and $\mathbf{j}$ are two orthogonal unit vectors. The space of states $\mathscr{E}$ is the Cartesian product $\mathscr{E}^1 \times \mathscr{E}^2 \times \mathscr{E}^3 \times \mathscr{E}^4$ of four identical Boolean manifolds:

$$\mathscr{E}^2 = \mathscr{E}^2 = \mathscr{E}^3 = \mathscr{E}^4 = \{(x_1, x_2) \in \{0, 1\}^2 / x_1 + x_2 = 1\} = \{(1, 0), (0, 1)\}$$

For each $\mathscr{E}^j$ the state (0, 1) will stand for the presence of a particle of velocity $\mathbf{c}_j$ at the considered node, and the state (1, 0) for its absence. Here $\mathbf{c}_1 = \mathbf{i}$, $\mathbf{c}_2 = \mathbf{j}$, $\mathbf{c}_3 = -\mathbf{i}$, $\mathbf{c}_4 = -\mathbf{j}$. The particles all have the same mass m, the iteration time being the unit of time. The free propagation operator $\mathscr{S}$ is defined as in Section 2 by giving four permutations p_j of $\mathscr{L}$:

$$p_j(a\mathbf{i} + b\mathbf{j}) = (a\mathbf{i} + b\mathbf{j}) - \mathbf{c}_j$$

In this relation two vectors $(a\mathbf{i} + b\mathbf{j})$ and $(a'\mathbf{i} + b'\mathbf{j})$ are identified if $(a - a')$ is a multiple of p while $(b - b')$ is a multiple of q. If $(X_1, X_2, X_3, X_4, X_5, X_6, X_7, X_8)$ is the state of the node α, the total mass $m(\alpha)$ and the total momentum $\mathbf{p}(\alpha)$ are given by

$$m(\alpha) = m(X_2 + X_4 + X_6 + X_8) = 4m - m(X_1 + X_3 + X_5 + X_7)$$

$$\mathbf{p}(\alpha) = m(X_2\mathbf{c}_1 + X_4\mathbf{c}_2 + X_6\mathbf{c}_3 + X_8\mathbf{c}_4) = -m(X_1\mathbf{c}_1 + X_3\mathbf{c}_2 + X_5\mathbf{c}_3 + X_7\mathbf{c}_4)$$

The set $\mathscr{K}'_{\text{loc}}$ is then generated by the four following vectors of $\mathbb{R}^8$: (1, 1, 0, 0, 0, 0, 0, 0), (0, 0, 1, 1, 0, 0, 0, 0), (0, 0, 0, 0, 1, 1, 0, 0), (0, 0, 0, 0, 0, 0, 1, 1).

Thus, since the local dynamical invariants are orthogonal to $\mathscr{K}'_{\text{loc}}$, they are included in the following subspace of $\mathbb{R}^8$:

$$\{(-x_1, x_1, -x_2, x_2, -x_3, x_3, -x_4, x_4); (x_1, x_2, x_3, x_4) \in \mathbb{R}^4\}$$

Now if we identify this subspace with $\mathbb{R}^4$ and each $\mathscr{E}^j$ with $\{0, 1\}$ [by mapping (0, 1) onto 1 and (1, 0) onto 0], we recover the usual notation for the HPP model, and thus the usual local invariants are precisely the local dynamical invariants in our notation. Thus, in order to simplify the notation, we will use this identification.

In the HPP model, the local collisions preserve the total mass and the total momentum at each node and thus the set $\mathscr{K}^d_{\text{loc}}$ is generated by the three vectors of $\mathbb{R}^4$:

$$\mathbf{I}_1 = (1, 1, 1, 1), \qquad \mathbf{I}_2 = (1, 0, -1, 0), \qquad \mathbf{I}_3 = (0, 1, 0, -1)$$

One can observe that the empty configuration is regular and thus the set of all global dynamical 1-invariants is simply given by Proposition 13. Let then Φ be a global dynamical invariant. Its projection $\Phi(\alpha)$ at each node is identified with the vector $(\Phi_1(\alpha), \Phi_2(\alpha), \Phi_3(\alpha), \Phi_4(\alpha))$ of $\mathbb{R}^4$, and so there exists a field $((\lambda^1(\alpha), \lambda^2(\alpha), \lambda^3(\alpha))$ of real numbers such that

$$\forall \alpha: \quad \Phi(\alpha) = \lambda^1(\alpha)\mathbf{I}_1 + \lambda^2(\alpha)\mathbf{I}_2 + \lambda^3(\alpha)\mathbf{I}_3 \tag{19}$$

We now have to determine the $\lambda^i(\alpha)$ in order to satisfy $\mathscr{S}\Phi = \Phi$.

This can be done analytically and after some algebra one finds that the following conditions are necessary and sufficient:

$$\begin{aligned} \forall \alpha, &\quad \lambda^1(\alpha) = \lambda^1 \\ \forall \alpha, a, &\quad \lambda^2(\alpha) = \lambda^2(\alpha + a\mathbf{i}) = \lambda^2(L_\alpha) \\ \forall \alpha, b, &\quad \lambda^3(\alpha) = \lambda^3(\alpha + b\mathbf{j}) = \lambda^3(C_\alpha) \end{aligned}$$

where L_α (resp. C_α) is the line (resp. the column) with contains α. Hence there are $(p+q)+1$ independent global dynamical invariants for the process $\boldsymbol{L}$. One of them corresponds to the conservation of the total mass and the other, which was already found by HPP, corresponds to the conservation of the x (resp. y) component of the momentum along the lines (resp. the columns).

6.1.2. Global 2-Invariants for L^2. In order to determine all the global dynamical invariants of L^2 we now assume that the collision rules are chosen such that the model satisfies (P1)–(P3) and thus Proposition 9 holds. We then start with relation (19), and we have to determine the field $((\lambda^1(\alpha), \lambda^2(\alpha), \lambda^3(\alpha))$ such that $\mathscr{S}^2\Phi = \Phi$ and $\mathscr{S}\Phi(\alpha)$ is in $\mathscr{K}^d_{\text{loc}}$. One then observes that $\mathscr{S}^2$is deduced from $\mathscr{S}$ by replacing each permutation p_j by p_j^2. One can then divide the lattice $\mathscr{L}$ into four subsets, $\mathscr{L}_0$, $\mathscr{L}_1$, $\mathscr{L}_2$, and $\mathscr{L}_3$, with $\mathscr{L}_0 = \{2a\mathbf{i} + 2b\mathbf{j}\}$, $\mathscr{L}_1 = \{(2a+1)\mathbf{i} + (2b+1)\mathbf{j}\}$, $\mathscr{L}_2 = \{(2a+1)\mathbf{i} + 2b\mathbf{j}\}$, and $\mathscr{L}_3 = \{2a\mathbf{i} + (2b+1)\mathbf{j}\}$, each of them being invariant under any p_j^2. Thus, from the previous results we deduce that if a given node α belongs to $\mathscr{L}_i$, we then have

$$\lambda^1(\alpha) = \lambda^1_i$$
$$\lambda^2(\alpha) = \lambda^2_i(L_\alpha)$$
$$\lambda^3(\alpha) = \lambda^3_i(C_\alpha)$$

where L_α (resp. C_α) is the line (resp. the column) which contains α. Then the condition $\mathscr{S}\Phi(\alpha) \in \mathscr{K}^d_{\text{loc}}$ only imposes that $\lambda^1_0 = \lambda^1_1$, $\lambda^1_2 = \lambda^1_3$. Note that there is no coupling between the mass and the momentum coefficients.

Now the number of independent coefficients depends on the parity of p and q. Indeed, if the number of lines (resp. of columns) is odd, then $\mathscr{L}_0 = \mathscr{L}_2$ and $\mathscr{L}_1 = \mathscr{L}_3$ (resp. $\mathscr{L}_0 = \mathscr{L}_3$ and $\mathscr{L}_1 = \mathscr{L}_2$); thus, all the λ^1_i are equal, and to a given line (resp. a given column) there is associated only one λ^2 (resp. one λ^3). Thus, there are at most $2(p+q)+2$ independent global dynamical linear 2-invariants: $(p+q)+1$ of them can be chosen as the linear invariants associated with the process L mentioned in the previous section; the others are specific to L^2. These supplementary invariants are necessarily nonhomogeneous, and their existence depends on the parity of p and q:

1. If p and q are even, one of them is a mass invariant and corresponds to the following conserved quantity:

$$\sum_{\alpha \in \mathscr{L}} (-1)^{\alpha \cdot (\mathbf{i}+\mathbf{j})} m(\alpha) \tag{20}$$

This states that the total mass of the particles which lie on $\mathscr{L}_0 \cup \mathscr{L}_1$ (or on $\mathscr{L}_2 \cup \mathscr{L}_3$) is conserved on even times, and thus it can be viewed as a "chessboard invariant" as defined in ref. 15. The other $(p+q)$ invariants correspond to conservation of the x (resp. y) component of the momentum, staggered along lines (resp. columns).

2. If p (resp. q) is odd, (20) is no longer a conserved quantity. There are then q (resp. p) specific 2-invariants which correspond to the

conservation of the y (resp. x) component of the momentum, staggered along columns (resp. lines).

3. If p and q are odd, there are no specific 2-invariants.

Let us then note that (20) is also conserved by any process $\boldsymbol{L}^{2k}$ since any fixed point of $\boldsymbol{L}^2$ is obviously a fixed point of $\boldsymbol{L}^{2k}$. In other words, it keeps a constant value on any configuration obtained after an even number of iterations of the automaton. Thus, some authors have denoted this conserved quantity on even "times" k by

$$(-1)^k \sum_{\alpha \in \mathscr{L}} (-1)^{\alpha \cdot (\mathbf{i}+\mathbf{j})} m(\alpha)$$

This kind of conserved quantity has been called a dynamic staggered (global) invariant. In fact, these dynamic staggered invariants always appear as linear 2-invariants; they are one-to-one related to the Gibbs distribution of $\boldsymbol{L}^2$. If we denote by Φ the staggered mass 2-invariant, one observes that, although Φ is a specific 2-invariant, Φ and $\mathscr{S}\Phi$ are not independent, since $\mathscr{S}\Phi = -\Phi$.

6.1.3. Global 3-Invariants for $\boldsymbol{L}^3$. The analysis is similar to the case of the 2-invariants. We again start with relation (19), and we have to determine the field $((\lambda^1(\alpha), \lambda^2(\alpha), \lambda^3(\alpha))$ such that $\mathscr{S}^2\Phi = \Phi$ and that $\mathscr{S}\Phi(\alpha)$ and $\mathscr{S}^{-1}\Phi(\alpha)$ are in $\mathscr{K}^d_{\text{loc}}$. We divide the lattice into nine subsets, each invariant under any p_j^3. Under the condition $\mathscr{S}^3\Phi = \Phi$ the field $\{\lambda^i(\alpha)\}$ depends at most on $3(p+q)+9$ independent values: There are nine mass coefficients and $3(p+q)$ momentum coefficients. The remaining conditions reduce to five the maximum number of independent mass coefficients and to $(p+q)+4$ the maximum number of momentum coefficients. There is no coupling between these two classes. Since we know that $\mathscr{K}^{s,k}_{gl}$ always contains $\mathscr{K}^{s,l}_{gl}$ there are then at most eight specific independent 3-invariants which are not 1-invariants or 2-invariants: four of them are mass invariants, the other are momentum invariants. Once we know this, it is very simple to exhibit them. Indeed, let us consider the following subsets:

$$\mathscr{L}_4 = \{a\mathbf{i} + b\mathbf{j} / (a-b) \equiv 0\ (3)\}$$

$$\mathscr{L}_5 = \{a\mathbf{i} + b\mathbf{j} / (a-b) \equiv 1\ (3)\}$$

$$\mathscr{L}_6 = \{a\mathbf{i} + b\mathbf{j} / (a-b) \equiv 2\ (3)\}$$

$$\mathscr{L}_7 = \{a\mathbf{i} + b\mathbf{j} / (a+b) \equiv 0\ (3)\}$$

$$\mathscr{L}_8 = \{a\mathbf{i} + b\mathbf{j} / (a+b) \equiv 1\ (3)\}$$

$$\mathscr{L}_9 = \{a\mathbf{i} + b\mathbf{j} / (a+b) \equiv 2\ (3)\}$$

The following quantities are then 3-invariants (one can also deduce them from symmetry conditions):

$$\sum_{\alpha \in \mathscr{L}_i} m(\alpha), \qquad i = 4,..., 9$$

$$\sum_{\alpha \in \mathscr{L}_i} \mathbf{p}(\alpha) \cdot (\mathbf{i} + \mathbf{j}), \qquad i = 4,..., 6$$

$$\sum_{\alpha \in \mathscr{L}_i} \mathbf{p}(\alpha) \cdot (\mathbf{i} - \mathbf{j}), \qquad i = 7,..., 9$$

Only eight of them can be specific, since the total mass and momentum on the whole lattice are conserved at any order.

Hence, if p or q is not a multiple of 3, all the $\mathscr{L}_i$ are merged into $\mathscr{L}$ and there are no specific 3-invariants (all the mentioned quantities are equal and 1-invariants) conversely if p and q are multiples of three, these quantities are independent, and there are effectively eight specific 3-invariants.

6.2. Global Invariants for 9-Bit Models on the Square Lattice

This model was initially introduced by d'Humières and Lallemand[8] in order to make fourth-order tensors isotropic. It is an extension of the HPP model obtained by adding four kinds of moving particles with speed $\sqrt{2}$ and one rest particle. Thus, we will simply extend the notations of the previous section: $\mathscr{E}^1$, $\mathscr{E}^2$, $\mathscr{E}^3$, $\mathscr{E}^4$ will represent the particles with speed 1, $\mathscr{E}^5$, $\mathscr{E}^6$, $\mathscr{E}^7$, $\mathscr{E}^8$ those with speed $\sqrt{2}$, and $\mathscr{E}^9$ the rest particle. We will set $\mathbf{c}_5 = \mathbf{i} + \mathbf{j}$, $\mathbf{c}_6 = -\mathbf{i} + \mathbf{j}$, $\mathbf{c}_7 = \mathbf{i} - \mathbf{j}$, and $\mathbf{c}_8 = \mathbf{i} - \mathbf{j}$. The total mass $m(\alpha)$, the total momentum $\mathbf{p}(\alpha)$, and the total energy $e(\alpha)$ are

$$m(\alpha) = m(X_2 + X_4 + X_6 + X_8 + X_{10} + X_{12} + X_{14} + X_{16} + X_{18})$$

$$\mathbf{p}(\alpha) = m(X_1 \mathbf{c}_1 + X_4 \mathbf{c}_2 + X_6 \mathbf{c}_3 + X_8 \mathbf{c}_4 + X_{10} \mathbf{c}_5 + X_{12} \mathbf{c}_6 + X_{14} \mathbf{c}_7 + X_{16} \mathbf{c}_8)$$

$$2e(\alpha) = m[(X_2 + X_4 + X_6 + X_8) + 2(X_{10} + X_{12} + X_{14} + X_{16})]$$

Now we identify each $\mathscr{E}^j$ with $\{0, 1\}$ [by mapping (0, 1) onto 1 and (1, 0) onto 0]. We assume that the local collisions preserve the total mass, the total momentum, and the total kinetic energy at each node and thus the set $\mathscr{K}^d_{\text{loc}}$ is (after identification) generated by the four vectors of $\mathbb{R}^9$:

$$\mathbf{I}_1 = (1, 1, 1, 1, 1, 1, 1, ,1, 1)$$

$$\mathbf{I}_2 = (1, 0, -1, 0, 1, -1, -1, 1, 0)$$

$$\mathbf{I}_3 = (0, 1, 0, -1, 1, 1, -1, -1, 0)$$

$$\mathbf{I}^4 = (1, 1, 1, 1, 2, 2, 2, 2, 0)$$

The empty configuration is regular and thus the set of all global dynamical invariants is simply given by Proposition 13. Let then Φ be a global dynamical invariant; its projection $\Phi(\alpha)$ at each node is identified with a vector of $\mathbb{R}^9$ and there then exists a field $((\lambda^1(\alpha), \lambda^2(\alpha), \lambda^3(\alpha), \lambda^4(\alpha))$ of real numbers such that

$$\forall\alpha: \quad \Phi(\alpha) = \lambda^1(\alpha)\mathbf{I}_1 + \lambda^2(\alpha)\mathbf{I}^2 + \lambda^3(\alpha)\mathbf{I}_3 + \lambda^4(\alpha)\mathbf{I}_4$$

We now have to determine the $\lambda^i(\alpha)$ in order to satisfy $\mathscr{S}\Phi = \Phi$. After some algebra one finds that $\lambda^2(\alpha) = \lambda^2$ and $\lambda^3(\alpha) = \lambda^3$ are constant on the whole lattice, while the $\lambda^1(\alpha)$ and $\lambda^4(\alpha)$ are constant if p or q is odd and they depend on three parameters when p and q are even. Thus, in this last case, in addition to the four homogeneous invariants, there is a nonhomogeneous global 1-invariant which is a geometric staggered invariant and corresponds to the conservation of the following quantity:

$$\sum_{\alpha \in \mathscr{L}} (-1)^{\alpha \cdot (\mathbf{i}+\mathbf{j})}[m(\alpha) - 2e(\alpha)]$$

One can also look for the global 2-invariants as in the case of the HPP model. They are all determined by Proposition 9, provided we assume properties (P1)–(P3). The analysis shows that there are then only two possible specific 2-invariants associated to the following quanties:

$$\mathbf{p}_1 = \sum_{\alpha \in \mathscr{L}} (-1)^{\alpha \cdot \mathbf{i}}\mathbf{p}(\alpha) \cdot \mathbf{i}$$

$$\mathbf{p}_2 = \sum_{\alpha \in \mathscr{L}} (-1)^{\alpha \cdot \mathbf{j}}\mathbf{p}(\alpha) \cdot \mathbf{j}$$

where are dynamic staggered momenta; $\mathbf{p}^1$ (resp. $\mathbf{p}_2$) is defined if the number of columns (resp. the number of lines) is even.

6.3. Global Invariants for Some Model on the Hexagonbal Lattice

The first model that we examine is a 12-bit extension of the FHP model obtained by adding six moving particles with mass m_2 and speed $\sqrt{3}$ to the initial six particles with mass m_1 and speed 1. In addition to the total mass and the total momentum, the local collisions also preserve the partial mass of each moving species. These models are then comparable to the eight-bit models on the square lattice. They are suitable to describe mass diffusion processes, as shown in refs. 21 and 26, where some examples are given in detail. The notations are similar to those of Section 6.1: Each node is identified with the vector $a\mathbf{e}_1 + b\mathbf{e}_2$ ($p \geqslant a \geqslant 1$, $q \geqslant b \geqslant 1$), where $\mathbf{e}_1 = \mathbf{i}$ and $\mathbf{e}_2 = (\mathbf{i} + \sqrt{3}\mathbf{j})/2$. The velocities of particles with speed 1 are $\mathbf{c}_1,..., \mathbf{c}_6$ and of those with speed $\sqrt{3}$ are $\mathbf{c}_7,..., \mathbf{c}_{12}$. The first set (resp. the second) is obtained by successively rotating $\mathbf{e}_1$ (resp. $\mathbf{e}_1 + \mathbf{e}_2$) by $\pi/3$. One can observe that the empty configuration is again regular and thus the global 1-invariants are deduced from Proposition 13. If we set $m_1 = 2m_2$, we can choose local collisions such that they preserve the two partial masses and the total momentum at each node without other spurious local invariants. Hence the set $\mathscr{K}^d_{\text{loc}}$ is (after identification) generated by the four vectors of $\mathbb{R}^{12}$:

$$\mathbf{I}_1 = (1, 1, 1, 1, 1, 1; 0, 0, 0, 0, 0, 0)$$

$$\mathbf{I}_2 = (0, 0, 0, 0, 0, 0; 1, 1, 1, 1, 1, 1)$$

$$\mathbf{I}_3 = (2, 1, -1, -2, -1, 1; 1, 0, -1, -1, 0, 1)$$

$$\mathbf{I}_4 = (0, 3, 3, 0, -3, -3; 1, 2, 1, -1, -2, -1)$$

where $\mathbf{I}_1$ (resp. $\mathbf{I}_2$) correspond to the mass of the slow (resp. the fast) particles and $\mathbf{I}_3$ and $\mathbf{I}_4$ to the components of the momentum.

The analysis is then similar to the previous cases; we divide the lattice into the three following subsets:

$$\begin{aligned} \mathscr{L}_0 &= \{a\mathbf{e}_1 + b\mathbf{e}^2/(a-b) \equiv 0\ (3)\} \\ \mathscr{L}_1 &= \{a\mathbf{e}_1 + b\mathbf{e}_2/(a-b) \equiv 1\ (3)\} \\ \mathscr{L}_2 &= \{a\mathbf{e}_1 + b\mathbf{e}_2/(a-b) \equiv 2\ (3)\} \end{aligned} \tag{21}$$

After some algebra, one finds that all the global linear dynamical 1-invariants are generated by the three homogeneous invariants associated to $\mathbf{I}_1$, $\mathbf{I}_3$, and $\mathbf{I}_4$ and by three others associated to the conservation of the fast particles on the subsets (21):

$$\sum_{\alpha \in \mathscr{L}_i} m_2(\alpha), \qquad i = 0, 1, 2 \tag{22}$$

Hence, if p or q is not a multiple of 3, all the $\mathscr{L}_i$ are merged into $\mathscr{L}$ and there are only four independent global dynamical invariants, which are homogeneous [in fact, the quantities defined by (22) are all equal to the total mass of fast particles on the whole lattice]. Conversely, if p and q are multiples of three, (22) defines three independent quantities and there are effectively six 1-invariants: two nonhomogeneous ones, which correspond to the conservation of the mass of fast particles on each $\mathscr{L}_i$, and the four homogeneous ones. In particular this implies that there is no nonhomogeneous global 1-invariant in the FHP model. A simple analysis shows that the only global 2-invariants of the FHP model (given by Proposition 9) are the three homogeneous 1-invariants and, depending on the parity of p and q, the three following (now well known) dynamical staggered momenta[16–18]:

$$\mathbf{p}_i = \sum_{\alpha \in \mathscr{L}} (-1)^{\alpha \cdot \mathbf{c}^i} \mathbf{p}(\alpha) \cdot \mathbf{c}^i$$

where $(\mathbf{c}^i, \mathbf{c}^{i+1})$ is for each i the dual basis of $(\mathbf{c}_i, \mathbf{c}_{i+1})$. However, these staggered 2-invariants disappear in the 12-bit model, in which there are no specific 2-invariants.

Some variants of these models are models with temperature, which are simply obtained by setting $m_1 = m_2$ and adding static energy levels (see refs. 20–22 for details and examples). The local collisions can be set such that they preserve the total mass, the total momentum, and the total energy at each node without spurious local invariants. The empty configuration is regular and thus the set of all global dynamical invariants is again given by Proposition 13. The analysis shows that in addition to the four homogeneous global invariants, if and only if p and q are multiples of three, these models admit two supplementary independent nonhomogeneous invariants associated to the conservation of the following quantities:

$$\sum_{\alpha \in \mathscr{L}_i} [m(\alpha) - 2e(\alpha)], \qquad i = 0, 1, 2 \tag{23}$$

where the subsets $\mathscr{L}_i$ are given by (21). Note the similarity with the 9-bit model.

Other models with temperature can be built by adding particles with higher speed.[27] One of the simplest is constructed by adding six moving particles with speed 2 (the velocity set is generated by rotating $2\mathbf{e}_1$) and a rest particle. All particles have the same mass and the local collisions can be set such that they preserve the total mass, the total momentum, and the total kinetic energy. The addition of particles with speed 2 breaks the conservation of the quantities (23) and in this 19-bit model the only global 1-invariants are the homogeneous ones. If instead of adding particles with speed 2 we had added particles with speed 3, the nonhomogeneous invariants would not vanish. Nevertheless, in numerical simulations, since the system evolves in fact on only one particular 1-path, the preparation of the initial state will be crucial in order to obtain dynamics not affected by (23).

7. CONCLUSION

In this study we have pointed out the important part played by the regular global invariants. But in order to obtain LGCA models which produce the same hydrodynamics as real fluids one needs the global k-invariants to be all homogeneous, which guarantees that any k-equilibrium distribution is a fixed point of $\boldsymbol{L}$. The first step is to be sure that the global k-invariants are regular, which is provided, for example, by Proposition 9. The second is to guarantee the absence of any specific regular k-invariants for $k > 1$. This seems to be achieved by suitable choice of the periods and of the velocity set, but may require further improvement. Lastly we have to eliminate the nonhomogeneous 1-invariants, whose existence seems to be related to the choice of the lattice.

APPENDIX A

Proof of Proposition 1. We can write

$$\begin{aligned} &\boldsymbol{H}(\boldsymbol{L}(f)) - \boldsymbol{H}(f) \\ &= \int_{\mathscr{W}} \left\{ \left[\int_{\mathscr{W}} f_p(\mathbf{n}')\, \mathscr{A}(\mathbf{n}' \to \mathscr{S}^{-1}(\mathbf{n}))\, d\mathbf{n}' \right] \right. \\ &\quad \times \operatorname{Log}\left(\left[\int_{\mathscr{W}} f_p(\mathbf{n}')\, \mathscr{A}(\mathbf{n}' \to \mathscr{S}^{-1}(\mathbf{n}))\, d\mathbf{n}' \right] \right) \\ &\quad \left. - \left[\int_{\mathscr{W}} \operatorname{Log}(f(\mathbf{n}'))\, f(\mathbf{n}')\, \mathscr{A}(\mathbf{n}' \to \mathscr{S}^{-1}(\mathbf{n}))\, d\mathbf{n}' \right] \right\} d\mathbf{n} \end{aligned}$$

From the convexity of $x \operatorname{Log} x$ and the semi-detailed balance, we deduce that the term between the $\{\cdot\}$ in the integral is negative, thus we have $\boldsymbol{H}(\boldsymbol{L}(f)) \leqslant \boldsymbol{H}(f)$ for all f. Moreover, $\boldsymbol{H}(\boldsymbol{L}(f)) = \boldsymbol{H}(f)$ imposes that this term is zero for all $\mathbf{n}$. But $x \operatorname{Log} x$ is strictly convex, that is,

$$\begin{aligned} &\sum_i \alpha_i x_i \operatorname{Log}(x_i) - \left(\sum_i \alpha_i x_i \right) \operatorname{Log}\left(\sum_i \alpha_i x_i \right) = 0 \\ &\qquad \Rightarrow \forall i, j: \quad x_i = x_j \quad \left(\text{with } \alpha_i > 0; \sum_i \alpha_i = 1 \right) \end{aligned}$$

We then deduce [by replacing $\mathscr{S}^{-1}(\mathbf{n})$ by $\mathbf{n}$ in the above expression] that

$$\forall \mathbf{n}, \mathbf{n}', \mathbf{n}'' \in \mathscr{W}^3, \quad \mathscr{A}(\mathbf{n} \to \mathbf{n}')\, \mathscr{A}(\mathbf{n}'' \to \mathbf{n}')[f(\mathbf{n}) - f(\mathbf{n}'')] = 0 \qquad \text{(A1)}$$

Conversely, if (A1) stands, a direct evaluation of $\boldsymbol{H}(\boldsymbol{L}(f))-\boldsymbol{H}(f)$ gives 0. Thus, one can show that a density f is a fixed point of $\boldsymbol{L}$ if and only if it satisfies

$$\forall \mathbf{n}, \mathbf{n}' \in \mathscr{W}^2, \quad \mathscr{A}(\mathbf{n} \to \mathbf{n}')[f(\mathbf{n}) - f(\mathscr{S}(\mathbf{n}'))] = 0 \tag{A2}$$

Proof. If (A2) is true, a direct evaluation of $\boldsymbol{L}(f)(\mathbf{n})$ shows that f is a fixed point of $\boldsymbol{L}$. Conversely, if f is a fixed point of $\boldsymbol{L}$, we have $\boldsymbol{H}(\boldsymbol{L}(f)) = \boldsymbol{H}(f)$, which yields relation (A1). Using then relation (1), since f is a fixed point of $\boldsymbol{L}$, an integration of (A1) over $\mathbf{n}''$ finally yields (A2).

APPENDIX B

Proof of Proposition 6. We have pointed out in Section 3 that if the set of 1-paths is only globally invariant under $\mathscr{S}$, one obtains a weaker result, that is, $\mathscr{K}_{gl}^{d,1}$ is globally invariant under $\mathscr{S}$. Let us first show this.

Let Φ be a global invariant; then from Definition 3

$$\forall \mathbf{n}, \mathbf{n}' \in \mathscr{W}^2, \quad \mathscr{A}(\mathbf{n} \to \mathscr{S}^{-1}(\mathbf{n}'))\langle \Phi, \mathbf{n} - \mathbf{n}' \rangle = 0$$

If $\mathscr{A}(\mathbf{n} \to \mathscr{S}^{-1}(\mathbf{n}')) = 0$, then $\mathscr{A}(\mathbf{n} \to \mathscr{S}^{-1}(\mathbf{n}'))\langle \mathscr{S}\Phi, \mathbf{n} - \mathbf{n}')\rangle = 0$. If not, then $\mathbf{n}$ and $\mathbf{n}'$ are in the same 1-path, but since the 1-paths are globally invariant under $\mathscr{S}$, $\mathscr{S}^{-1}(\mathbf{n})$ and $\mathscr{S}^{-1}(\mathbf{n}')$ are also in the same path.

But since Φ is constant on a 1-path, $\langle \Phi, \mathscr{S}^{-1}(\mathbf{n}) - \mathscr{S}^{-1}(\mathbf{n}') \rangle = 0$ and since $\mathscr{S}$ is orthogonal, we finally have

$$\forall \mathbf{n}, \mathbf{n}' \in \mathscr{W}^2, \quad \mathscr{A}(\mathbf{n} \to \mathscr{S}^{-1}(\mathbf{n}'))\langle \mathscr{S}\Phi, \mathbf{n} - \mathbf{n}' \rangle = 0$$

Thus, $\mathscr{S}\Phi$ is a global invariant and then $\mathscr{K}_{gl}^{1}$ is globally invariant under $\mathscr{S}$. But $\mathscr{S}$ is an orthogonal linear map, and since $\mathscr{K}_{gl}^{d,1}$ is orthogonal to $\mathscr{K}'_{gl}$, then $\mathscr{K}_{gl}^{d,1}$ is also globally invariant under $\mathscr{S}$ as announced. This result suggests that for nonregular models, the set of global linear invariants would be larger than $\mathscr{K}_{gl}^{s,1}$.

Recall that we have denoted

$$\mathscr{K}_{gl}^{s,1} = \{\Phi \in \mathbb{R}^{NL} / \mathscr{S}\Phi = \Phi \text{ and } \forall \alpha \in \mathscr{L}, \Phi(\alpha) \in \mathscr{K}_{\mathrm{loc}}^{d}\}$$

For regular models we prove that relation (7) of Proposition 6 holds:

$$\mathscr{K}_{gl}^{d,1} = \mathscr{K}_{gl}^{s,1}$$

But $\mathscr{K}_{gl}^{s,1}$ is always obviously included in $\mathscr{K}_{gl}^{d,1}$ and hence we have just to prove that $\mathscr{K}_{gl}^{d,1}$ is included in $\mathscr{K}_{gl}^{s,1}$.

Thus, let Φ be a global dynamical 1-invariant of a regular model.

Since the 1-paths are $\mathscr{S}$-invariant and since Φ is constant on a given 1-path, we have

$$\forall \mathbf{n} \in \mathscr{W}, \quad \langle \Phi, \mathbf{n} \rangle = \langle \Phi, \mathscr{S}^{-1}\mathbf{n} \rangle$$

or equivalently

$$\forall \mathbf{n} \in \mathscr{W}, \quad \langle \Phi - \mathscr{S}\Phi, \mathbf{n} \rangle = 0 \tag{B1}$$

And, since the 1-paths are $\mathscr{S}$-invariant, we know from the previous result that $\Phi - \mathscr{S}\Phi$ is in $\mathscr{K}^{d,1}_{gl}$. By applying Lemma 1 of Section 2 to (B1), we then deduce that $\Phi - \mathscr{S}\Phi = 0$. We have now just to verify that the αth projection of Φ is in $\mathscr{K}^{d}_{\text{loc}}$. The definition of $\mathscr{K}^{d,1}_{gl}$ and $\mathscr{K}'_{\text{loc}}$ implies that in any case $\Phi(\alpha)$ is orthogonal to $\mathscr{K}'_{\text{loc}}$. From the definition of global linear invariants and since $\Phi = \mathscr{S}\Phi$ we then have

$$\forall \mathbf{n}, \mathbf{n}' \in \mathscr{W}^2, \qquad \mathscr{A}(\mathbf{n} \to \mathbf{n}')\langle \Phi, \mathbf{n} - \mathbf{n}' \rangle = 0$$

We then achieve the proof of (7) by using Lemma 2 of Section 2.

In order to achieve the proof of Proposition 6, it remains to show that the linear 1-invariants are all regular. Any linear 1-invariant is by definition the sum of two orthogonal vectors, one in $\mathscr{K}^{d,1}_{gl}$, the other in $\mathscr{K}'_{gl}$. Because of relation (7) the first is regular and the second is obviously regular from its definition, hence their sum is also regular.

APPENDIX C

Proof of Proposition 7. Let us recall properties (P1)–(P3):

(P1) $\forall \mathbf{n}, \mathbf{m} \in \mathscr{W}^2$, $\mathscr{A}(\mathbf{n} \to \mathbf{m}) \neq 0 \Rightarrow \mathscr{A}(\mathbf{m} \to \mathbf{n}) \neq 0$

(P2) $\mathscr{A}(\mathbf{m} \to \mathbf{n}) \neq 0$, $\mathscr{A}(\mathbf{r} \to \mathbf{n}) \neq 0$, $\mathbf{m} \neq \mathbf{r} \Rightarrow \mathscr{A}(\mathbf{m} \to \mathbf{r}) \neq 0$

(P3) $\mathbf{n} \neq \mathbf{m} \Rightarrow \mathscr{A}(\mathbf{n} \to \mathbf{m}) < 1$

Proposition 7 states that any model which satisfies the three properties (P1)–(P3) is regular, the main argument being the fact that the phase space is finite.

In order to prove the previous result, we just have to establish the relation (8) of Section 3. That is: for every initial density f_0 we have

$$\forall \varepsilon > 0, \exists N \in \mathbb{N}, \quad p \geqslant N \Rightarrow \forall \mathbf{n} \in \mathscr{W}: |f_{p+1}(\mathscr{S}(\mathbf{n})) - f_p(\mathbf{n})| \leqslant \varepsilon$$

Proof. Let us consider a model which obeys (P1)–(P3). At each configuration $\mathbf{n}$, we associate a number $m(\mathbf{n})$ defined by

$$m(\mathbf{n}) = 1, \qquad \text{if} \quad \mathscr{A}(\mathbf{n} \to \mathbf{n}) = 1$$

$$\text{Inf}\{\mathscr{A}(\mathbf{m} \to \mathbf{n})\, \mathscr{A}(\mathbf{r} \to \mathbf{n})\}, \qquad \text{if} \quad \mathscr{A}(\mathbf{n} \to \mathbf{n}) \neq 1$$

The Inf is taken over all configurations $\mathbf{m}$ and $\mathbf{r}$ such that $\mathbf{m} \neq \mathbf{r}$ and $\mathscr{A}(\mathbf{m} \to \mathbf{n}) \neq 0$, $\mathscr{A}(\mathbf{r} \to \mathbf{n}) \neq 0$. We then define m as $m = \text{Inf}\{\mathbf{n} \in \mathscr{W}, m(\mathbf{n})\}$. *Since $\mathscr{W}$ is finite*, m is strictly positive. Let us then consider the sequence (X_p) associated to a given f_0 by

$$X_p = X(f_p) = \int_{\mathscr{W}} f_p^2(\mathbf{n})\, d\mathbf{n}$$

This sequence is well defined *since $\mathscr{W}$ is finite*, and due to the convexity of x^2 this sequence is decreasing and thus converging. Hence, for any given $\varepsilon > 0$ there exists an integer N such that for any $p \geqslant N$ we have $0 \leqslant X_p - X_{p+1} \leqslant \varepsilon$. From the semi-detailed balance and since $\mathscr{S}$ preserves the measure, one can write

$$X_p - X_{p+1} = \int_{\mathscr{W}} \left\{ \left[\int_{\mathscr{W}} f_p^2(\mathbf{n}') \mathscr{A}(\mathbf{n}' \to \mathscr{S}^{-1}(\mathbf{n}))\, d\mathbf{n}' \right] - \left[\int_{\mathscr{W}} f_p(\mathbf{n}')\, \mathscr{A}(\mathbf{n}' \to \mathscr{S}^{-1}(\mathbf{n}))\, d\mathbf{n}' \right]^2 \right\} d\mathbf{n}$$

But since x^2 is convex, the number under the first integral is always positive for each $\mathbf{n}$. Thus for $p \geqslant N$ we have

$$0 \leqslant \left[\int_{\mathscr{W}} f_p^2(\mathbf{n}')\, \mathscr{A}(\mathbf{n}' \to \mathscr{S}^{-1}(\mathbf{n}))\, d\mathbf{n}' \right] - \left[\int_{\mathscr{W}} f_p(\mathbf{n}')\, \mathscr{A}(\mathbf{n}' \to \mathscr{S}^{-1}(\mathbf{n}))\, d\mathbf{n}' \right]^2 \leqslant \varepsilon$$

If we now multiply the first term in the middle of this inequality by $1 = \int_{\mathscr{W}} \mathscr{A}(\mathbf{n}'' \to \mathscr{S}^{-1}(\mathbf{n}))\, d\mathbf{n}''$, it yields after rearrangement

$$0 \leqslant \frac{1}{2} \int_{\mathscr{W}^2} [f_p(\mathbf{n}') - f_p(\mathbf{n}'')]^2\, \mathscr{A}(\mathbf{n}' \to \mathscr{S}^{-1}(\mathbf{n}))\, \mathscr{A}(\mathbf{n}'' \to \mathscr{S}^{-1}(\mathbf{n}))\, d\mathbf{n}'\, d\mathbf{n}''] \leqslant \varepsilon$$

Hence we deduce that for any $\mathbf{n}$, if $\mathscr{A}(\mathbf{m} \to \mathscr{S}^{-1}(\mathbf{n})) \neq 0$ and $\mathscr{A}(\mathbf{r} \to \mathscr{S}^{-1}(\mathbf{n})) \neq 0$, then for $p \geqslant N$ we have

$$|f_p(\mathbf{m}) - f_p(\mathbf{r})| \leqslant \left(\frac{\varepsilon}{m} \right)^{1/2}$$

But since $\mathscr{S}$ is a bijection, we finally deduce that for each initial density f_0 and for each $\varepsilon > 0$ there exists an integer N such that for any configuration $\mathbf{n}$ and any $p \geqslant N$ we have

$$\mathscr{A}(\mathbf{m} \to \mathbf{n}) \neq 0,\ \mathscr{A}(\mathbf{r} \to \mathbf{n}) \neq 0 \Rightarrow |f_p(\mathbf{m}) - f_p(\mathbf{r})| \leqslant \left(\frac{\varepsilon}{m} \right)^{1/2} \tag{C1}$$

We then consider any given $\mathbf{n}$ in $\mathscr{W}$. If $\mathscr{A}(\mathbf{n} \to \mathbf{n}) = 1$, then (8) is obvious; let us then assume that $\mathscr{A}(\mathbf{n} \to \mathbf{n}) \neq 1$. From property (P3) and semi-detailed balance, we deduce that there exist at least two configurations $\mathbf{m} \neq \mathbf{r}$ such that $\mathscr{A}(\mathbf{m} \to \mathbf{n}) \neq 0$ and $\mathscr{A}(\mathbf{r} \to \mathbf{n}) \neq 0$. From (P2), we then have $\mathscr{A}(\mathbf{m} \to \mathbf{r}) \neq 0$ and from (P1), $\mathscr{A}(\mathbf{n} \to \mathbf{r}) \neq 0$. We then apply (C1) to $\mathbf{r}$ and we deduce

$$\forall \varepsilon > 0, \quad \exists N, \qquad p \geqslant N, \quad \mathscr{A}(\mathbf{m} \to \mathbf{n}) \neq 0 \Rightarrow |f_p(\mathbf{m}) - f_p(\mathbf{n})| \leqslant \varepsilon$$

But we have

$$f_{p+1}(s(\mathbf{n})) = \int_{\mathscr{W}} [f_p(\mathbf{n}') - f_p(\mathbf{n})] \, \mathscr{A}(\mathbf{n}' \to \mathbf{n}) \, d\mathbf{n}' + f_p(\mathbf{n})$$

The last two relations finally yield (8).

A useful simplification in the presentation of this proof has been suggested to me by D. d'Humières.

APPENDIX D

Proof of Proposition 9. Here, we show the following characterization of $\mathscr{K}_{gl}^{d,k}$ for models which obey (P1)–(P3):

$$\mathscr{K}_{gl}^{d,k} = \mathscr{K}_{gl}^{s,k}$$

where $\mathscr{K}_{gl}^{d,k}$ is the set of the global linear dynamical k-invariants of $\boldsymbol{L}^k$ and where we have denoted

$$\mathscr{K}_{gl}^{s,k} = \{\Phi \in \mathbb{R}^{NL} / \mathscr{S}^k \Phi = \Phi \text{ and } \forall \alpha \in \mathscr{L}, \Phi(\alpha), \mathscr{S}\Phi(\alpha), ..., \mathscr{S}^{k-1}\Phi(\alpha) \in \mathscr{K}_{\text{loc}}^{d}\}$$

Similarly to the case $k = 1$, we just have to show that $\mathscr{K}_{gl}^{d,k}$ is included in $\mathscr{K}_{gl}^{s,k}$.

Thus, let us consider a model which obeys (P1)–(P3). We have seen in Section 3 that the fixed points of $\boldsymbol{L}^k$ are then invariant under $\mathscr{S}^k$. So we deduce that each k-path of $\mathscr{L}^k$ is invariant under $\mathscr{S}^k$. Now a demonstration similar to that proposed in Appendix B for the elements of $\mathscr{K}_{gl}^{d,1}$ shows that if Φ is in $\mathscr{K}_{gl}^{d,k}$, then $\mathscr{S}^k \Phi = \Phi$. It now just remains to see that $\mathscr{S}^i \Phi(\alpha)$ is in $\mathscr{K}_{\text{loc}}^{d}$ for any node α and $i = 1, ..., k-1$. This is a little lengthy and thus we limit it here to the case $k = 2$.

Let Φ be a nonzero elements of $\mathscr{K}_{gl}^{d,2}$. We will first prove that $\mathscr{S}\Phi(\alpha)$ is in $\mathscr{K}_{\text{loc}}^{d}$ for all α.

Let us consider the density $g_0(\mathbf{n}) = \boldsymbol{k} \exp[\Phi(\mathbf{n})]$ (where $\boldsymbol{k}$ is a normalization constant) which is a fixed point for $\boldsymbol{L}^2$. We then set $g_1 = \boldsymbol{L} g_0$. The sequence (g_n) defined by $g_n = \boldsymbol{L}^n g_0$ is then reduced to $g_{2p} = g_0$ and

$g_{2p+1}=g_1$. By applying relation (8) of Section 3 to (g_n), one then deduces that

$$\forall \mathbf{n} \in \mathscr{W}, \quad g_1(\mathscr{S}\mathbf{n}) = g_0(\mathbf{n})$$

that is,

$$\int_{\mathscr{W}} g_0(\mathbf{n}')\, \mathscr{A}(\mathbf{n}' \to \mathbf{n})\, d\mathbf{n}' = g_0(\mathbf{n}) \tag{D1}$$

But since Φ is a linear global 2-invariant, we have from Definition 5 of the linear invariant of $\boldsymbol{L}^k$

$$\forall \mathbf{n}, \mathbf{n}', \mathbf{n}_1 \in \mathscr{W}^3, \quad \mathscr{A}(\mathbf{n}' \to \mathscr{S}^{-1}(\mathbf{n}_1))\, \mathscr{A}(\mathbf{n}_1 \to \mathscr{S}^{-1}(\mathbf{n}))[g_0(\mathbf{n}) - g_0(\mathbf{n}')] = 0 \tag{D2}$$

We then sum (D2) over all $\mathbf{n}'$ in $\mathscr{W}$ and by using (D1) this yields

$$\forall \mathbf{n}, \mathbf{n}_1 \in \mathscr{W}^2, \quad \mathscr{A}(\mathbf{n}_1 \to \mathscr{S}^{-1}(\mathbf{n}))[g_0(\mathbf{n}) - g_0(\mathscr{S}^{-1}\mathbf{n}_1)] = 0$$

or equivalently

$$\forall \mathbf{n}, \mathbf{n}_1 \in \mathscr{W}^2, \qquad \mathscr{A}(\mathscr{S}^{-1}(\mathbf{n}_1) \to \mathscr{S}^{-1}(\mathbf{n}))[g_0(\mathbf{n}) - g_0(\mathscr{S}^{-2}\mathbf{n}_1)] = 0$$

But g_0 is invariant under $\mathscr{S}^2$, and this last relation yields

$$\forall \mathbf{n}, \mathbf{n}_1 \in \mathscr{W}^2, \quad \mathscr{A}(\mathscr{S}^{-1}(\mathbf{n}_1) \to \mathscr{S}^{-1}(\mathbf{n}))[g_0(\mathbf{n}) - g_0(\mathbf{n}_1)] = 0$$

Now, $\exp(\cdots)$ is a bijection on $\mathbb{R}$ and thus this last relation can be replaced by

$$\forall \mathbf{n}, \mathbf{n}_1 \in \mathscr{W}^2, \quad \mathscr{A}(\mathscr{S}^{-1}(\mathbf{n}_1) \to \mathscr{S}^{-1}(\mathbf{n}))\langle \Phi, \mathbf{n} - \mathbf{n}_1 \rangle = 0$$

From Lemma 2 of Section 2, this implies that $\mathscr{S}^{-1}\Phi(\alpha)$ and consequently $\mathscr{S}\Phi(\alpha)$ are in $\mathscr{K}^d_{\text{loc}}$ for any α. It remains to show that $\Phi(\alpha)$ is also in $\mathscr{K}^d_{\text{loc}}$. Let us then consider again relation (D2), but writing it under the following form:

$$\forall \mathbf{n}, \mathbf{n}', \mathbf{n}_1 \in \mathscr{W}^3, \qquad \mathscr{A}(\mathrm{n}' \to \mathscr{S}^{-1}(\mathbf{n}_1))\, \mathscr{A}(\mathbf{n}_1 \to \mathbf{n})[g_0(\mathscr{S}\mathrm{n}) - g_0(\mathbf{n}')] = 0$$

But since $\mathscr{S}\Phi(\alpha)$ is in $\mathscr{K}^d_{\text{loc}}$, we have $\mathscr{A}(\mathbf{n}_1 \to \mathbf{n})[g_0(\mathscr{S}\mathbf{n}) - g_0(\mathscr{S}\mathbf{n}_1)] = 0$. We now sum over all $\mathbf{n}$ in $\mathscr{W}$ and by use of (D1) this yields, after replacing $\mathbf{n}'$ by $\mathscr{S}^{-1}(\mathbf{n}')$,

$$\forall \mathbf{n}', \mathbf{n}_1 \in \mathscr{W}^2, \quad \mathscr{A}(\mathscr{S}^{-1}(\mathbf{n}') \to \mathscr{S}^{-1}(\mathbf{n}_1))[g_0(\mathscr{S}\mathbf{n}_1) - g_0(\mathscr{S}^{-1}\mathbf{n}')] = 0$$

Since g_0 is $\mathscr{S}^2$-invariant, we obtain

$$\forall \mathbf{n}', \mathbf{n}_1 \in \mathscr{W}^2, \quad \mathscr{A}(\mathbf{n}' \to \mathbf{n}_1)[g_0(\mathbf{n}_1) - g_0(\mathbf{n}')] = 0$$

Applying again Lemma 2 of Section 2, we finally deduce that $\Phi(\alpha)$ is in $\mathscr{K}^d_{\text{loc}}$ for any α, which then yields the proof of the relation (11) for the case $k=2$.

In the general case, the machinery of the proof is identical : one has to show successively that $\mathscr{S}^{k-1}\Phi(\alpha)$, and then $\mathscr{S}^{k-2}\Phi(\alpha)$– and then down to $\Phi(\alpha)$ are in $\mathscr{K}^d_{\text{loc}}$ for any α. This is achieved by recurrence on the order once it has been shown for $\mathscr{S}^{k-1}\Phi(\alpha)$.

In order to achieve the proof of Proposition 9, it remains to show that the linear k-invariants are all regular; the argument is in fact the same as in Appendix B. Any linear linear k-invariant is by definition the sum of two orthogonal vectors, one in $\mathscr{K}^{d,k}_{gl}$, the other in $\mathscr{K}'_{gl}$. Because of relation (11) the first one is regular while the second is obviously regular from its definition and that of $\mathscr{S}$, hence their sum is also regular.

APPENDIX E

We first establish the equivalences in relation (16):

(a) $\delta(\mathbf{N}) = 0$

(b) $\text{Log}(\mathbf{N}) \in \mathscr{K}_{\text{loc}}$

(c) $\langle \delta(\mathbf{N}), \text{Log}(\mathbf{N}) \rangle = 0$

(d) $f(\mathbf{n}) = \prod_{\alpha} \cdot \prod_{j=1}^{b} \cdot \prod_{i=1}^{n} \cdot [N^j_i]^{\mathbf{n}^j_i(\alpha)}$ is a fixed point of $\boldsymbol{L}$

where $\mathbf{N}$ is a vector in $]0, 1[^N$. We have obviously (b) $\Rightarrow$ (d) $\Rightarrow$ (a) $\Rightarrow$ (c). Indeed, if (b) is true, then relations (17) and (18) are verified since $\mathbf{N}$ is constant over the nodes and thus f is a fixed point of $\boldsymbol{L}$. Thus, from (15) we have $\delta(\mathbf{N}) = 0$ and hence $\langle \delta(\mathbf{N}), \text{Log}(\mathbf{N}) \rangle = 0$. It now just remains to see that (c) $\Rightarrow$ (b).

Thus, if X and Y are two elements in $\mathscr{E}$, we set

$$x(X) = \prod_{j=1}^{b} \cdot \prod_{i=1}^{n_j} \cdot [N^j_i]^{X^j_i} \qquad \text{and} \qquad y(Y) = \prod_{j=1}^{b} \cdot \prod_{i=1}^{n_j} \cdot [N^j_i]^{Y^j_i}$$

The expression $\langle \delta(N), \text{Log}(N) \rangle = 0$ can be rewritten in the form

$$\int_{\mathscr{E} \times \mathscr{E}} a(X \to Y)\, x(X) \, \text{Log}\left(\frac{y(Y)}{x(X)}\right) dX\, dY = 0 \tag{E1}$$

But from semi-detailed balance we have

$$1=\int_{\mathscr{E}} x(X)\,dX=\int_{\mathscr{E}\times\mathscr{E}} a(X\to Y)\,x(X)\,dX\,dY$$

$$=\int_{\mathscr{E}} y(Y)\,dY=\int_{\mathscr{E}\times\mathscr{E}} a(X\to Y)\,y(Y)\,dX\,dY$$

Thus, (E1) yields

$$\int_{\mathscr{E}\times\mathscr{E}} a(X\to Y)\,x(X)\left[\operatorname{Log}\left(\frac{y(Y)}{x(X)}\right)+1-\frac{y(Y)}{x(X)}\right]dX\,dY=0$$

But the function $\operatorname{Log}(u)+1-u$ is $\leqslant 0$ for any $u>0$ and it is 0 is and only if $u=1$. Thus, the previous equality implies that for all X and Y we must have $a(X\to Y)[y(Y)-x(X)]=0$. But it is equivalent to

$$\forall X,\ Y\in\mathscr{E}\times\mathscr{E},\quad a(X\to Y)\{\operatorname{Log}[y(Y)]-\operatorname{Log}[x(X)]\}=0$$

Or by evaluating $\operatorname{Log}(y)$ and $\operatorname{Log}(x(X))$

$$\forall X,\ Y\in\mathscr{E}\times\mathscr{E},\quad a(X\to Y)\langle \operatorname{Log}(\mathbf{N}),\ Y-X\rangle=0$$

Thus, $\operatorname{Log}(\mathbf{N})$ is in $\mathscr{K}_{\text{loc}}$ and finally (c) $\Rightarrow$ (b).

Proof of Proposition 12. Let us consider a model which admits a regular configuration, say $\mathbf{m}_0$. Let $\{\mathbf{m}_i\}$, $i\geqslant 1$, be the set of configurations which differ from $\mathbf{m}_0$ on at most one node and one $\mathscr{E}^j$. It is composed of $(NL-bL)$ configurations obtained (see Lemma 1, Section 2) by successively permuting in $\mathbf{m}_0$ a one and a zero node after node and on each $\mathscr{E}^j$. We prove that if the densities f and $\boldsymbol{L}(f)$ are both factorized, then the following relations hold:

$$\mathscr{S}\mathbf{N}=\mathbf{N}^* \tag{E2}$$

$$\operatorname{Log}(\mathbf{N}(\alpha))\in\mathscr{K}_{\text{loc}},\qquad \forall\alpha \tag{E3}$$

where $\mathbf{N}$ and $\mathbf{N}^*$ are the mean population fields of resp. f and $\boldsymbol{L}(f)$. Now let us project the vectors $\operatorname{Log}(\mathbf{N})$ and $\operatorname{Log}(\mathbf{N}^*)$ on $\mathscr{K}'_{gl}$ such that $\operatorname{Log}(\mathbf{N})=\Phi'+\Phi$, $\operatorname{Log}(\mathbf{N}^*)=\Psi'+\Psi$, where Φ' and Ψ' are in $\mathscr{K}'_{gl}$ while Φ and Ψ are in its orthogonal. Since Φ' and Ψ' are constant on the whole phase space, there exists two constants $\boldsymbol{k}$ and $\boldsymbol{k}^*$ such that the densities f and $\boldsymbol{L}(f)$ are given by

$$\forall\mathbf{n},\quad f(\mathbf{n})=\exp(\langle \operatorname{Log}(\mathbf{N}),\mathbf{n}\rangle\rangle)=\boldsymbol{k}\exp(\langle\Phi,\mathbf{n}\rangle) \tag{E4}$$

$$\forall\mathbf{n},\quad \boldsymbol{L}(f)(\mathbf{n})=\exp(\langle \operatorname{Log}(\mathbf{N}^*,\mathbf{n}\rangle)=\boldsymbol{k}^*\exp(\langle\Psi,\mathbf{n}\rangle) \tag{E5}$$

Let us then observe that the set $\{\mathbf{m}_i\}$, $i \geqslant 0$, is globally invariant under $\mathscr{S}$. This set is composed of configurations which are collisionally invariant. Let then $\mathbf{m}_i$ be such a configuration; in these conditions $\mathscr{S}^{-1}(\mathbf{m}_i)$ has the same property and thus $\mathscr{A}(\mathbf{m}' \to \mathscr{S}^{-1}(\mathbf{m}_i))$ is nonzero if and only if $\mathbf{m}' = \mathscr{S}^{-1}(\mathbf{m}_i)$. Then, from the definition (1) of $\boldsymbol{L}$ and from (E4) we will necessarily have for this configuration $\mathbf{m}_i$

$$\boldsymbol{L}(f)(\mathbf{m}_i) = \boldsymbol{k} \exp(\langle \mathscr{S}\Phi, \mathbf{m}_i \rangle)$$

and hence from (E5)

$$\boldsymbol{k} \exp(\langle \mathscr{S}\Phi, \mathbf{m}_i \rangle) = \boldsymbol{k}^* \exp(\langle \Psi, \mathbf{m}_i \rangle) \tag{E6}$$

This last relation then yields

$$\forall i \geqslant 0, \quad \langle \mathscr{S}\Phi - \Psi, \mathbf{m}_i \rangle = \mathrm{Log}\left(\frac{\boldsymbol{k}}{\boldsymbol{k}^*}\right) \tag{E7}$$

But, since $\mathscr{S}$ is an orthogonal map, $\mathscr{S}\Phi$ remains, like Φ, in the subspace orthogonal to $\mathscr{K}'_{gl}$. By applying Lemma 1 of Section 2 to (E7), we then deduce that $\Psi = \mathscr{S}\Phi$ and $\boldsymbol{k} = \boldsymbol{k}^*$. Replacing these equalities in (E5) yields $\forall \mathbf{n}$, $\boldsymbol{L}(f)(\mathbf{n}) = \mathbf{k} \exp(\langle \mathscr{S}\Phi, \mathbf{n} \rangle)$. Now the lhs of identity (15) is obviously equal to zero, which gives, considering the definition of the mean population, $\mathscr{S}\mathrm{N} = \mathrm{N}^*$, and so (E2) is proven. Now, since in the identity (15) the lhs is zero, the rhs is also zero. This yields for any node α, $\delta(N(\alpha)) = 0$, and finally (E3) results from the equivalences (16).

Let us now prove that any dynamical k-invariant of such a model is $\mathscr{S}^k$-invariant. Let us then observe that in fact the set $\{\mathbf{m}_i\}$, $i \geqslant 0$, is globally invariant under $\mathscr{S}^k$. Thus, if $\mathbf{m}_i$ is such a configuration, we will have

$$\mathscr{A}^k(\mathbf{m}_i \to \mathscr{S}^{k-1}\mathbf{m}_i) \neq 0$$

Hence, from the definition of the global k-invariant and if Φ is a dynamical one, we obtain

$$\langle \Phi, \mathbf{m}_i - \mathscr{S}^k\mathbf{m}_i \rangle = 0 \qquad \text{or} \qquad \langle \Phi - \mathscr{S}^{-k}\Phi, \mathbf{m}_i \rangle = 0$$

The proof is then completed, as previously, by applying Lemma 1 of Section 2.

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