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Exact Stability Results in Stochastic Lattice Gas Cellular Automata

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In this paper we consider a lattice gas as a discrete Markov process, with a Markov operator $\mathfrak{L}$ acting on the phase space of the lattice gas cellular automata. We are interested in the asymptotic properties of the sequences of densities in both Liouville and Boltzmann descriptions. We show that under appropriate hypotheses, in both descriptions, the sequence of densities are asymptotically periodic. It is then possible, by introducing a slight modification in the transition process, to avoid the existence of cycles and to ensure the stability of the stationary densities. We point out the particular part played by the regular global linear invariants that define the asymptotic Gibbs states in a one-to-one way for most models.

KEY WORDS: Lattice gases; cellular automata; discrete stochastic processes; asymptotic properties of lattice Boltzmann equation.

INTRODUCTION

This paper is the continuation of the work presented in ref. 1. We are interested here in the long-time-scale behavior of lattice gases in both Boltzmann and Liouville descriptions, still within the context of discrete Markov processes. In the Liouville description, a lattice gas cellular automaton (LGCA) is idealized as a fully discrete Markov process. The corresponding Markov operator will be denoted by $\mathfrak{L}$ and we will study the asymptotic behavior of density sequences: $f_{n+1} = \mathfrak{L}(f_n)$. We will always consider that the Markov kernel obeys a semi-detailed balance; this hypothesis is standard for having an H-theorem.

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In ref. 1 we investigated the global linear invariants of LGCA and showed that the so-called "regular" ones are of particular interest for the dynamics.

In this paper, for LGCA on periodic lattices:

1. We exhibit the existence of cycles for the Liouville equation. If the transition probabilities obey suitable properties, we prove that these cycles are the attractors of the system and that any sequence of densities evolves toward a limit cycle.
2. We present exact stability results in Boltzmann's description. We exhibit the existence of cycles for the Boltzmann equation and show that for most models these cycles are asymptotically stable and are the (strictly positive) attractors of the system.
3. In order to avoid the occurrence of these cycles, the transition process must be modified by adding more stochasticity. We investigate here a simple modification that consists in randomly selecting, at each time step and after the collision stage, between performing a displacement or a new collision stage. For such a modified LGCA we will show that the attractors are now stationary densities in both descriptions. Unfortunately, the diffusive hydrodynamics is affected. For instance, in the FHP model, a self-diffusion term appears in the continuity equation.

The paper is organized as follows.

Section 1 is devoted to a presentation of the main results. After introducing the notations we recall the results of ref. 1 that will be required here. The results of the present study are presented in Section 1.4.

In Section 2 we are interested in usual stochastic LGCA for which collision and propagation steps alternate. The fixed points of $\mathfrak{L}^k$ where $k \geqslant 1$ is an integer, will be characterized. Under restrictive properties, denoted by (P1)–(P4), we prove that for any initial condition f_0, the sequence $f_{n+1} = \mathfrak{L}(f_n)$ is asymptotically periodic, the actual period of the limiting sequence being an integer factor of the period T of the free propagation operator.

In Section 3 we study the solutions of the so-called "Boltzmann equation". The phase space of an LGCA is embedded in a finite-dimensional linear vector space. Thus, at each density f we can associate a factorized density, denoted by Fact(f), which has the same mean population per velocity channel as f. The Boltzmann hypothesis for LGCA consists in assuming that "particles" which enter a "collision" have no prior correlations. From a statistical point of view, the dynamics of the LGCA is then modeled by the operator $[\mathrm{Fact} \circ \mathfrak{L}]$ and we are interested in the asymptotic behavior of sequences $f_{n+1} = [\mathrm{Fact} \circ \mathfrak{L}](f_n)$, where f_0 is itself a factorized density. This yields a recurrence relation on the corresponding mean populations usually called the "Boltzmann equation" of the LGCA [see relation (8)]. This equation must be regarded as a discrete dynamical system on the mean populations. We are first led to determine all the possible attractors: as in the Liouville approach, we also expect to obtain limit cycles. We then begin by studying the fixed points of $[\mathrm{Fact} \circ \mathfrak{L}]^k$, where k is the integer period of the cycle. For a wide class of models, these cycles are only related to a particular subset of the linear fixed points of $\mathfrak{L}^k$, called regular k-invariants. These regular k-invariants are directly connected to the local invariants and can be entirely determined. Therefore, for these models, we can obtain all possible cycles of the "Boltzmann equation", their period being always an integer factor of the period T. We will then prove that these cycles are conditionally asymptotically stable. Moreover, any sequence of mean populations which stays in a compact subset of $]0,1[$ is asymptotically periodic: the previous cycles are the attractors of this dynamical system.

In Section 4 we then examine a possible modification of the transition process which yields, always with the previous properties P(i), the convergence of any sequence (f_n) to a fixed point of $\mathfrak{L}$. The necessity of modifying the transition process in order to reach more stochasticity is not new. In earlier works[5, 9, 10] some authors proposed to modify the streaming process by inserting a stochastic stirring updating. Here, the modification consists in introducing an independent random variable—say $\Xi \in \{0, 1\}$—which will govern the free propagation stage. After the collision step, and on the whole lattice, we will perform the propagation if $\Xi = 0$ or another collision if $\Xi = 1$. The local collisional invariants and the Gibbs states of $\mathfrak{L}$ are not modified. We then also avoid periodic behavior in the Boltzmann equation: for a wide class of models, the fixed points of $\mathrm{Fact} \circ \mathfrak{L}$ (i.e., the Gibbs states of $\mathfrak{L}$) are now the only (strictly positive) attractors and they are all conditionally asymptotically stable. Moreover, any sequence of mean populations which stays in a compact subset of $]0,1[$ is then convergent. Unfortunately, as mentioned previously, the diffusive hydrodynamics is modified: A self-diffusion mass current appears in the FHP model.

1. PRESENTATION

1.1. Notations. The Liouville Equation

One can think of a lattice gas cellular automaton (LGCA) as a finite collection of particles, moving at integer times from nodes to nodes on a periodic, regular D-dimensional lattice $\mathscr{L}$, generated by the D vectors $(\mathbf{e}_1, \ldots, \mathbf{e}_D)$. At any time the velocity of each particle is selected from a finite set of b possible velocities $(\mathbf{c}_1,..., \mathbf{c}_b)$, each $\mathbf{c}_j$ being an integer combination of the $\mathbf{e}_i$.

Although it is rather straightforward to generalize all the subsequent results to models with an arbitrary number of particles per velocity channel, for simplicity we will restrict ourselves to models obeying the so-called exclusion principle: at most one particle with a given velocity on a given node. The state of a node at a given time is then described by a Boolean vector $\mathbf{X} = (X_1,..., X_b)$ which belongs to the set $\mathbf{E} = \{0, 1\}^b$. That is, $X_j = 1$ stands for the presence of a particle with velocity $\mathbf{c}_j$ and $X_j = 0$ for its absence. The configuration of the whole lattice at time t is a Boolean field $\mathbf{n}(., t)$ of $\mathbf{W} = \mathbf{E}^{\mathscr{L}}$. This system evolves by performing at each time t the two following steps:

1. *Collision step*: The input state $\mathbf{X} = \mathbf{n}(\alpha, t)$ of each node α is changed into a state $\mathbf{Y} = \mathbf{m}(\alpha, t)$ according to a node- and time-independent transition probability $a(\mathbf{X} \to \mathbf{Y})$.

2. *Propagation step*: After having performed the collision step on the whole lattice, each particle moves according to its velocity. Hence the component n_j of the output state $\mathbf{n}(\alpha, t+1)$ of a node α at time $t+1$ is set to $m_j(\alpha - \mathbf{c}_j, t)$.

The most popular example of such system is the FHP[2], model which provides a tool to simulate 2D incompressible Navier–Stokes equations.

The set $\mathbf{W}$ is embedded into $[\mathbb{R}^b]^{\mathscr{L}}$. The shift operator $\mathfrak{S}$ from $[\mathbb{R}^b]^{\mathscr{L}}$ to $[\mathbb{R}^b]^{\mathscr{L}}$ is defined by

$$\Phi \in [\mathbb{R}^b]^{\mathscr{L}} \to \mathfrak{S}\Phi / \forall \alpha \in \mathscr{L} : [\mathfrak{S}\Phi](\alpha) = (\Phi_1(\alpha - \mathbf{c}_1),..., \Phi_b(\alpha - \mathbf{c}_b))$$

This operator is an orthogonal linear map on $[\mathbb{R}^b]^{\mathscr{L}}$ for the scalar product defined by

$$\langle \Phi, \Psi \rangle = \sum_{\alpha \in \mathscr{L}} \sum_{j=1}^{b} \Phi_j(\alpha)\, \Psi_j(\alpha)$$

The global transition probability $\mathscr{A}(\mathbf{n} \to \mathbf{n}')$ from a configuration $\mathbf{n}$ to a configuration $\mathbf{n}'$ is the product

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

The local transition probabilities are such that

$$\forall \mathbf{X} \in E, \qquad \sum_{\mathbf{Y} \in \mathbf{E}} a(\mathbf{X} \to \mathbf{Y}) = 1$$

The hydrodynamic properties of these discrete systems are usually investigated via the standard methods of classical statistical mechanics,[3] The system is then considered as a Markov process on $\mathbf{W}$. Let p_0 be an initial probability measure on $\mathbf{W}$; then the probability $p_{t+1}(\mathbf{n})$ for finding the system in the configuration $\mathbf{n}$ at time $t+1$ is related to the probability measure p_t at time t through the relation

$$p_{t+1}(\mathbf{n}) = \sum_{\mathbf{m} \in \mathbf{W}} \mathscr{A}(\mathbf{m} \to \mathfrak{S}^{-1}\mathbf{n})\, p_t(\mathbf{m}) \tag{1}$$

This relation defines a Markov operator $\mathfrak{L}$ on the set of all real-valued functions on $\mathbf{W}$:

$$f \to \mathfrak{L}(f)/\mathfrak{L}(f)(\mathbf{n}) = \sum_{\mathbf{m} \in \mathbf{W}} \mathscr{K}(\mathbf{m}, \mathbf{n}) f(\mathbf{m}) \tag{2a}$$

where the Markov kernel is given by

$$\mathscr{K}(\mathbf{m}, \mathbf{n}) = \mathscr{A}(\mathbf{m} \to \mathfrak{S}^{-1}\mathbf{n}) \tag{2b}$$

The statistical evolution of the LGCA is described by the following recurrence relation:

$$p_{t+1} = \mathfrak{L}(p_t) = \mathfrak{L}^{t+1}(p_0) \tag{3}$$

Relation (1) is usually referred as the Liouville equation of the LGCA; it is the Chapman–Kolmogorov equation of the process. For the following we will reserve the notation p for a density (i.e., a probability) and f for a general real-valued function on $\mathbf{W}$.

1.2. The Boltzmann Equation

If p is a density on $\mathbf{W}$, we will denote $\mathbf{N} \in ([0, 1]^b)^{\mathscr{L}}$ the associated field of mean populations. That is

$$\mathbf{N} = \sum_{\mathbf{n} \in \mathbf{W}} \mathbf{n}\, p(\mathbf{n}) \tag{4}$$

The Boltzmann hypothesis in lattice gases consists in assuming that particles which enter a collision have no prior correlations. Hence the density p^{in} of input states is fully factorized through the nodes and the velocity channels. It is then uniquely defined by its mean population field $\mathbf{N}$:

$$p^{\text{in}}(\mathbf{n}) = \prod_{\alpha \in \mathscr{L}} \prod_{j=1}^{b} [N_j(\alpha)]^{n_j(\alpha)} [1 - N_j(\alpha)]^{1 - n_j(\alpha)} \tag{5a}$$

For the following, if $\mathbf{V}$ is a vector in $\mathbb{R}^b$ (or in $[\mathbb{R}^b]^{\mathscr{L}}$), we will denote by $\bar{\mathbf{V}}$ the vector of $\mathbb{R}^b$ (resp. $[\mathbb{R}^b]^{\mathscr{L}}$) whose components are $V_j/(1-V_j)$ [resp. $V_j(\alpha)/[1-V_j(\alpha)]$]. Let us notice that a strictly positive factorized density [i.e., $p(\mathbf{n})>0$, $\forall \mathbf{n}\in\mathbf{W}$] given by (5a) can also be written as

$$p^{\text{in}}(\mathbf{n}) = \mathfrak{k}\exp(\langle \Phi, \mathbf{n}\rangle), \qquad \mathfrak{k}>0 \tag{5b}$$

where Φ is a vector of $[\mathbb{R}^b]^{\mathscr{L}}$ whose components are $\operatorname{Log}(\bar{N}_j(\alpha))$ and $\mathfrak{k}=p^{\text{in}}(\mathbf{0})$, with $\mathbf{0}$ being the empty configuration.

If p_t is factorized, the mean population fields $\mathbf{N}(t)$ and $\mathbf{N}(t+1)$ of the two densities p_t and $\mathfrak{L}(p_t)$ are then related through

$$\mathbf{N}_j(\alpha+\mathbf{c}_j, t+1) - \mathbf{N}_j(\alpha, t) = \delta_j[\mathbf{N}(\alpha, t)], \qquad j=1,..., b \tag{6a}$$

where for each $\mathbf{U}$ in $\mathbb{R}^b$, $\delta[\mathbf{U}]$ is the following polynomial vector of $\mathbb{R}^b$:

$$\delta_j[\mathbf{U}] = \sum_{\mathbf{X},\mathbf{Y}\in\mathbf{E}\times\mathbf{E}} a(\mathbf{X}\to\mathbf{Y})(\mathbf{Y}_j-\mathbf{X}_j) \times \prod_{k=1}^{b} [\mathbf{U}_k]^{(\mathbf{X}_k)}[1-\mathbf{U}_k]^{(1-\mathbf{X}_k)}, \qquad j=1,..., b \tag{6b}$$

The relations (6) are usually referred to as the Boltzmann equation of the LGCA. For brevity we will also write (6) as the following recurrence relation on vectors of $([0, 1]^b)^{\mathscr{L}}$:

$$\mathbf{N}(t+1) = \mathscr{F}(\mathbf{N}(t)) \tag{7}$$

Let us note that in relations (6), the components of δ are polynomial functions in the components of $\mathbf{N}(\alpha)$, so we can extend the action of $\mathscr{F}$ on the whole set $[\mathbb{R}^b]^{\mathscr{L}}$. An other way to look at the Boltzmann equation of a lattice gas is to consider it as a recurrence relation on probability densities on $\mathbf{W}$. Indeed, from a general point of view one can associate to each density p on $\mathbf{W}$ having a mean populations field $\mathbf{N}$ a fully factorized density $\operatorname{Fact}(p)$ given by relations (5). Then, the recurrence relations (6)–(7) on mean populations are equivalent to the following recurrence relation on densities on $\mathbf{W}$:

$$p_{t+1} = \operatorname{Fact}(\mathfrak{L}(p_t)) = [\operatorname{Fact}\circ\mathfrak{L}]^{t+1}(p_0) \tag{8}$$

1.3. The Linear Invariants

In this paper, we are interested in exact results concerning the long-time behavior of density sequences which obey the Liouville equation (3) or the Boltzmann equation (8) when the transition probabilities obey a *semi-detailed* balance. That is

$$\forall \mathbf{X} \in \mathbf{E}, \qquad \sum_{\mathbf{Y} \in \mathbf{E}} a(\mathbf{Y} \to \mathbf{X}) = 1 \tag{9}$$

We are first interested in the fixed points of both operators $\mathfrak{L}^k$ or $[\mathrm{Fact} \circ \mathfrak{L}]^k$. For that purpose, we introduce the Markov kernels of any integer order k by setting

$$\mathscr{K}^k(\mathbf{m}, \mathbf{n}) = \sum_{(\mathbf{n}_1, \ldots, \mathbf{n}_{k-1}) \in \mathbf{W}^{k-1}} \mathscr{K}(\mathbf{m}, \mathbf{n}_1)\, \mathscr{K}(\mathbf{n}_1, \mathbf{n}_2) \cdots \mathscr{K}(\mathbf{n}_{k-1}, \mathbf{n})$$

Thus, $\mathfrak{L}^k$ is expressed with the kernel of order k by replacing in the definition (2) of $\mathfrak{L}$, $\mathscr{K}$ by $\mathscr{K}^k$. The local linear invariant are defined as follows[4].

Definition 1. A *local linear invariant* is a vector ϕ of $\mathbb{R}^b$ such that

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

The local linear invariants constitute a linear subspace of $\mathbb{R}^b$, denoted $\mathbb{K}_{\mathrm{loc}}$. The linear fixed points of $\mathfrak{L}^k$ will be called global linear k-invariants. They are defined as follows.

Definition 2. A *global linear k-invariant* is a vector Φ of $[\mathbb{R}^b]^{\mathscr{L}}$ which verifies

$$\forall \mathbf{m}, \mathbf{n} \in \mathbf{W} \times \mathbf{W}, \qquad \mathscr{K}^k(\mathbf{m}, \mathbf{n}) \langle \Phi, \mathbf{m} - \mathbf{n} \rangle = 0$$

The global linear k-invariants constitute a linear subspace of $[\mathbb{R}^b]^{\mathscr{L}}$ which will be denoted as $\mathbb{K}^k_{\mathrm{gl}}$. A vector Φ of $[\mathbb{R}^b]^{\mathscr{L}}$ is a global linear invariant if and only if the factorized density $p(\mathbf{n}) = \mathfrak{f} \exp(\langle \Phi, \mathbf{n} \rangle)$, where $\mathfrak{f}$ is a normalization constant, is a fixed point of $\mathfrak{L}^k$ (see Proposition 1 in the next section). Thus the global linear invariants are obviously connected to the (time-periodic) cycles in the Boltzmann equation; using properties of the information function, we can prove that any fixed point p of $[\mathrm{Fact} \circ \mathfrak{L}]^k$ is necessarily a factorized fixed point of $\mathfrak{L}^k$. But this fixed point must also be such that the successive iterates $\mathfrak{L}^n(p)$ for any n remain factorized. The Boltzmann equation is not concerned with the whole set of global linear invariants of the Markov operator $\mathfrak{L}$. Nevertheless, among the global linear invariants one can then point out a simple subspace which obeys this later factorization property. This subspace is the set of the global regular k-invariants introduced and studied in ref. 1. They are defined as follows.

Definition 3. A *global regular k-invariant* is a vector Φ of $[\mathbb{R}^b]^{\mathscr{L}}$ such that

$$\mathfrak{S}^k\Phi = \Phi \quad \text{and} \quad \forall\alpha \in \mathscr{L}, \quad \Phi(\alpha), [\mathfrak{S}\Phi](\alpha),..., [\mathfrak{S}^{k-1}\Phi](\alpha) \in \mathbb{K}_{\text{loc}}$$

The global regular k-invariants constitute a linear subspace of $[\mathbb{R}^b]^{\mathscr{L}}$ denoted $\mathbb{K}_{\text{gl}}^{r,k}$. These regular k-invariants are actually global invariants in the sense of Definition 2. This type of global invariant exists in any LGCA model and plays an important part in applying the linear response theory to LGCA. They are easily determined from the local ones and they contain the so-called dynamical invariants mentioned in the literature. The spatially homogeneous global linear invariants [that is, $\Phi(\alpha) = \Phi(\beta)$ for any α, β] are associated with the conservation of a given total quantity which is the sum on the lattice of the same local quantity (such as mass, momentum, energy,...). These are regular k-invariants for any order k. But, in general, there also exist non-homogeneous global regular k-invariants which yield the existence of time-periodic sequences for both the Liouville and Boltzmann "equations".

For a wide class of models, the linear global k-invariants are simply reduced to the regular k-invariants. It is the case for models where the global transition probabilities satisfy the following three properties[1]:

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

(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 or of "microsymmetry" which is satisfied by all usual LGA. Property (P3) [or (P4) given below] expresses the stochasticity of the nontrivial collisions and is only satisfied by nondeterministic models (excepting the case where the collisions are all trivial). Let us note that it is always possible to modify any given model in order to have (P3) [or (P4)] without changing its local invariants or its symmetries.

The linear global k-invariants are also reduced to the regular k-invariants for models which obey the following single property:

(P4) $\forall \mathbf{n} \in \mathbf{W}, \mathscr{A}(\mathbf{n} \to \mathbf{n}) \neq 0$

The proof is very similar to that of the previous case and will not be given here. It is noticeable that (P4) implies (P3) and that in fact it is itself much more restrictive than the other three properties.

1.4. Exact Results on Asymptotic Behavior

In the models defined above the global regular k-invariants give all the possible (strictly positive) cycles with a given period k of the Boltzmann equation. Such a cycle, given by $p_{t+1} = [\text{Fact} \circ \mathfrak{L}]^{t+1}(p_0)$ will necessarily be such that $p_0(\mathbf{n}) = \lambda \exp(\langle \Phi, \mathbf{n} \rangle)$, where Φ is a global k-invariant, and hence a regular k-invariant.

We will prove here that such p_0 is then uniquely determined by the projection of its mean population $\mathbf{N}_0$ on the subspace of the regular k-invariants. In other words, there is a one-to-one mapping between the Gibbs states (in the sense of the entropy) of the LGCA and the (global) macroscopic conserved variables. Due to the exclusion principle, these Gibbs states are Fermi–Dirac distributions. This result is given in Proposition 3 and was already reported in ref. 1, where the proof was not presented. For the present study it turns out that this proof is the key for studying the asymptotic behavior of the LGCA in the Boltzmann description and it is therefore given in Appendix C.

Under the properties (P1)–(P3) or simply (P4) we will also prove that:

1. Concerning the Liouville equation, the sequences $p_{t+1} = \mathfrak{L}(p_t)$ are always asymptotically periodic. The periodic orbits of (3) are all conditionally asymptotically stable. This is reported in Proposition 2.

2. Concerning the Boltzmann equation, the (strictly positive) time-periodic solutions are all conditionally asymptotically stable as reported in Proposition 5.

This asymptotic time periodicity at both the Boltzmann and the Liouville level of description is a spurious effect of the discretization. It is a consequence of the existence of fixed points of $\mathfrak{L}^k$ which are different from those of $\mathfrak{L}$. We then propose a simple modification to the transition process which ensures that, for any integer k, the fixed points of $\mathfrak{L}^k$ are always fixed points of $\mathfrak{L}$. Moreover, the latter are the same as those of the nonmodified process. At the Boltzmann level, if all the global linear invariants are homogeneous, the only asymptotic states are the usual homogeneous Gibbs states. This modification consists in introducing an independent random variable, say $\Xi \in \{0, 1\}$, which will govern the free propagation stage. At each integer time, if $\Xi = 0$, a collision updating followed by a streaming updating is performed, while, if $\Xi = 1$, a collision updating is performed alone.

Under the properties (P1)–(P3) or simply (P4) and for this modified model, we prove that:

3. Concerning the Liouville equation, the sequences $p_{t+1} = \mathfrak{L}(p_t)$ are always *convergent*. The fixed points of (3) are all conditionally asymptotically stable as reported in Proposition 6.

4. Concerning the Boltzmann equation, the *only limiting cycles* have a time period of 1, that is, they are stationary. These are then the factorized fixed points of $\mathfrak{L}$. Moreover, the strictly positive ones are uniquely defined by the mean values of the regular global 1-invariants and they are all conditionally asymptotically stable. These results are given in Proposition 8.

One could object that these properties $(P_i)_{i=1,\dots,4}$ are restrictive and are not satisfied by all LGCA. For instance, in the original FHP model, where nontrivial ternary collisions are embedded with a probability equal to 1, properties (P3) and (P4) are not satisfied, although in ref. 9 this rule is precisely modified in order to satisfy (P3).

Fortunately, one can show that the above results concerning the Boltzmann equation of an LGCA remain true provided that the automaton has a suitable number of configurations which are collision-invariant: that is, the model has what we call a regular configuration. A precise definition is given at the end of Section 3. It turns out that, for models with a regular configuration, the periodic sequences of densities, solutions of the Boltzmann equation, are only related to the regular invariants. In other words, if $p_t = [\mathrm{Fact} \circ \mathfrak{L}]^t (p_0)$ with $p_k = p_0$, then there exists a global regular k-invariant Φ such that $p_0(\mathbf{n}) = \lambda \exp(\langle \Phi, \mathbf{n} \rangle)$; see Proposition 4. As reported in Propositions 6 and 8, the above stability results for the Boltzmann equation are also satisfied by these models. Most LGCA, including all usual models used to simulate hydrodynamics (like the FHP models), have a regular configuration.

2. ASYMPTOTIC PERIODICITY AT LIOUVILLE LEVEL OF DESCRIPTION

We will say that a sequence (U_n) is k-periodic if for any n, $U_{n+k} = U_n$, the actual period being then an integer factor of k. We introduce a decomposition of $\mathbf{W}$ into disjoint subsets that are similar to the orbits for a deterministic dynamical system. For this purpose we will say that two configurations $\mathbf{n}$, $\mathbf{m}$ define a "k-link" if we have $K^k(\mathbf{n}, \mathbf{m}) \neq 0$ or $\mathcal{K}^k(\mathbf{m}, \mathbf{n}) \neq 0$. We then will say that two configurations $\mathbf{n}$, $\mathbf{m}$ are k-connected if there exists a sequence $\mathbf{n}_0 = \mathbf{n}, \mathbf{n}_1, \dots, \mathbf{n}_p = \mathbf{m}$ of configurations (with $p \geqslant 1$) such that each pair $\mathbf{n}_i, \mathbf{n}_{i+1}$ is a k-link. The relation "to be k-connected" on $\mathbf{W}$ is an equivalence relation. The corresponding classes are thus called *k-paths* for the Markov process $\mathfrak{L}$: they are the Markov chains for the process $\mathfrak{L}^k$. If p is an integer factor of k, any k-path which contains a configuration $\mathbf{n}$ is obviously included in the p-path which contains $\mathbf{n}$. The converse is wrong in general. The phase space structure is *a priori* very complicated since, in general, the paths are not cycles. However, for a deterministic model the 1-paths are actually the orbits of the associated dynamical system. For the following we will denote by $|\mathscr{P}|$ the number of elements in a path $\mathscr{P}$. We denote by $\mathscr{D}(\mathbf{W})$ [resp. $\mathscr{R}(\mathbf{W})$] the set of densities (resp. of real functions) on $\mathbf{W}$. The information function $\mathfrak{H}$ on $\mathscr{D}(\mathbf{W})$ is defined by

$$\mathfrak{H}(p) = \sum_{\mathbf{W}} p(\mathbf{n}) \operatorname{Log}(p(\mathbf{n})) \tag{10}$$

From the semi-detailed balance and the convexity of $x \operatorname{Log} x$ we deduce that $\mathfrak{H}(\mathfrak{L}^k(p)) \leqslant \mathfrak{H}(p)$ for all p. Moreover, since $x \operatorname{Log} x$ is strictly convex on $[0,1]$, we have the equivalence[1]:

$$\mathfrak{H}[(\mathfrak{L})^k (p)] = \mathfrak{H}(p)$$
$$\Leftrightarrow \forall \mathbf{n}, \mathbf{n}', \mathbf{n}'' \in \mathbf{W}^3 \mathscr{K}^k(\mathbf{n}', \mathbf{n})\, \mathscr{K}^k(\mathbf{n}'', \mathbf{n})(p(\mathbf{n}') - p(\mathbf{n}'')) = 0 \tag{11a}$$

The fixed points are then precisely characterized by the following proposition[1].

Proposition 1. Let $k \geqslant 1$ be an integer. A *density* p is a fixed point of $(\mathfrak{L})^k$ if and only if it satisfies

$$\forall \mathbf{n}, \mathbf{n}' \in \mathbf{W}^2, \qquad \mathscr{K}^k(\mathbf{n}', \mathbf{n})(p(\mathbf{n}) - p(\mathbf{n}')) = 0 \tag{11b}$$

It is known that for usual Markov process[6] any integrable fixed point, say f, of a Markov operator is such that the standard functions $f^+ = \sup(f, 0)$ and $f^- = \sup(-f, 0)$ are also fixed points. Hence, since $\mathbf{W}$ is finite, we can extend Proposition 1 to any real function f. Thus, relation (11b) gives the characterization of any fixed point of $(\mathfrak{L})^k$, in $\mathscr{R}(\mathbf{W})$. Therefore the global linear k-invariants as introduced in Definition 2 naturally appear as the linear fixed points of $(\mathfrak{L})^k$ (by identifying linear forms and vectors).

As a consequence of this proposition we deduce that a real function f is a fixed point of $(\mathfrak{L})^k$ if and only if it is constant on each k-path. From the definition of the paths, we also deduce that $(\mathfrak{L})^k$preserves the measure of the k-paths. In other words, if $\mathscr{P}^k$ is a k-path, we have

$$\forall f \in \mathscr{R}(\mathbf{W}), \qquad \sum_{\mathbf{n} \in \mathscr{P}_k} f(\mathbf{n}) = \sum_{\mathbf{n} \in \mathscr{P}_k} [(\mathfrak{L})^k f](\mathbf{n})$$

To each real function f on $\mathbf{W}$ and each integer $k \geqslant 1$ we can then naturally associate a fixed point of $(\mathfrak{L})^k$. Let us associate to each real function f on **W** the function $\mathrm{Fix}(k, f)$ defined by

$$\forall \mathbf{n} \in \mathbf{W}, \qquad \mathrm{Fix}(k, f)(\mathbf{n}) = \frac{1}{|\mathscr{P}_k|} \sum_{\mathscr{P}_k} f(\mathbf{n}') \tag{12}$$

where $\mathscr{P}_k$ is the k-path which contains $\mathbf{n}$. From the above remarks, $\mathrm{Fix}(k, f)$ is a fixed point of $(\mathfrak{L})^k$. Moreover, it is the only fixed point of $(\mathfrak{L})^k$such that the mean expectation of any k-path is the one of f. In fact, the operator $\mathrm{Fix}(k, \cdot)$ is an orthogonal[2] projector on the subspace of all fixed points of $(\mathfrak{L})^k$.

We have now all the ingredients to prove the expected asymptotic periodicity. Indeed, let then T be the lowest integer such that $\mathfrak{S}^T$ is the identity map on **W** and let us consider a sequence $f_n = \mathfrak{L}^n(f_0)$ of real functions of $\mathscr{R}(\mathbf{W})$ defined by its initial value f_0. Let us then associate to this sequence a periodic sequence (g_n) defined by the following relation:

$$\begin{cases} g_0 = \mathrm{Fix}(T, f_0), \qquad g_1 = \mathrm{Fix}(T, f_1), \ldots, g_{T-1} = \mathrm{Fix}(T, f_{T-1}) \\ g_{kT+p} = g_p \qquad \text{for any} \quad k \geqslant 0, p < T \end{cases} \tag{13}$$

Each g_n is a fixed point of $(\mathfrak{L})^T$, that is, a cycle for $\mathfrak{L}$.

We then deduce the following proposition, which characterizes the asymptotic (time) periodicity of the sequences (f_n) and the ergodicity of the process.

Proposition 2. We assume that the global transition probabilities $\{\mathscr{A}\}$ obey properties (P1)–(P3) or only property (P4). Let f_0 be a real function on **W** and (g_n) be the sequence associated to (f_n) by relation (13). Then $\mathrm{Lim}_{n \to \infty}(f_n - g_n) = 0$.

Furthermore, the sequence (g_n) satisfies

$$\forall \mathbf{n} \in \mathbf{W}, \qquad g_n(\mathbf{n}) = [\mathfrak{L}^n(g_0)](\mathbf{n}) = g_0[\mathfrak{S}^{-n}(\mathbf{n})] \tag{14}$$

Moreover, the sequence (f_n) is Cesaro convergent to the fixed point of $\mathfrak{L}$: $\mathrm{Fix}(1, f_0)$ on **W**. In other words, we have

$$\lim_{n \to \infty} \left[\frac{1}{n} \sum_{i=1}^{n} f_i \right] = \mathrm{Fix}(1, f_0)$$

The proof is a little lengthy and is given in Appendix A. The main argument is the fact that the phase space is finite. Let us notice that, since **W** is finite, the set of all complex functions on **W** is a finite-dimensional vector space. Therefore, the Cesaro convergence is simply a consequence of

[2] For the usual scalar product $\sum_{\mathbf{W}} f(\mathbf{n})\, g(\mathbf{n})$.

a general ergodic theorem of F. Riesz in Banach spaces. The interesting result is the asymptotic periodicity. On the one hand, it shows that any eigenvalue of $\mathfrak{L}$ with a unit modulus is a Tth root of the unit, hence a fixed point of any $(\mathfrak{L})^k$ is always a fixed point of $(\mathfrak{L})^T$. On the other hand, it also indicates that the subspace composed of all fixed points of $(\mathfrak{L})^T$ is asymptotically stable, while the points themselves are conditionally asymptotically stable [that is, for any f_0 such that $g_0 = \mathrm{Fix}(T, f_0)$, we have $\mathrm{Lim}_{n \to \infty}(f_n - g_n) = 0$].

Let us then observe that relation (14) simply expresses that the effect of the collisions fades away with time. Furthermore, one can prove that the operator $\mathrm{Fix}(T, \cdot)$ is an orthogonal projector on a subset of all fixed points of the collision operator alone. Therefore the process tends to be only propagative and defined by the shift operator alone. One can notice that the effective period of the limiting sequence (g_n) is an integer factor of T which is only determined by f_0. If T is a prime number, this period is either 1 (i.e, the sequence converges to a stationary state) or T itself, which can be a large number when dealing with large lattices. This would obviously be connected to the time averages which can be used to obtain mean quantities. However, we do not know if it is possible to obtain these results, in the nondeterministic case, under weaker conditions than (P1)–(P3) or (P4).

Let us conclude this section with a remark on deterministic cases. Deterministic models are described when the range of $\{\mathscr{A}(\mathbf{n} \to \mathbf{n}')\}$ is $\{0, 1\}$; the relation (9) is then equivalent to the existence of a one-to-one operator $\mathscr{C}$ (the so-called microscopic collisional operator) on $\mathbf{W}$ such that for all $n: \mathscr{A}(\mathbf{n} \to \mathscr{C}(\mathbf{n})) = 1$. The Markov operator $\mathfrak{L}$ is then reduced to the Frobenius–Perron operator associated to $\mathfrak{S}\mathscr{C}$. Let T' be the lowest integer such that $(\mathfrak{S}\mathscr{C})^{T'}$ is the identity map on $\mathbf{W}$. Then, any sequence (f_n) defined by relation (3) is periodic, its period being an integer factor of T'. In these conditions the periodicity and the ergodicity are obvious, but in general, $T' \gg T$.

3. ASYMPTOTIC PERIODICITY AT BOLTZMANN LEVEL

3.1. Properties of the Regular Linear Invariants

From the characterization of the fixed points of $\mathfrak{L}^k$ (Proposition 1) and the definition of the linear k-invariants (Definition 2) it turns out that a (strictly positive) factorized density p is a fixed point of $\mathfrak{L}^k$ if and only if there exist a global linear k-invariant Φ and a constant $\mathfrak{k}$ such that $\forall \mathbf{n} \in \mathbf{W}$, $p(\mathbf{n}) = \mathfrak{k} \exp(\langle \Phi, n \rangle)$. A (strictly positive) factorized density is a fixed point of $\mathfrak{L}^k$ if and only if the vector $\mathrm{Log}(\bar{\mathbf{N}})$ is a global linear

k-invariant. These factorized densities are Gibbs equilibrium distributions for the process $\mathfrak{L}^k$ since they correspond to the minimum of the information function when the macroscopic averages $\langle \Phi, \mathbf{N} \rangle$ of the global linear k-invariants are fixed.

An other important property of the global linear k-invariants is that $\mathfrak{L}^k$ preserves the mean expectation of any global linear k-invariant, i.e., $\forall f \in \mathscr{R}(\mathbf{W})$, $\forall \Phi \in \mathbb{K}^k_{gl}$;

$$\sum_{\mathbf{W}} \langle \Phi, \mathbf{n} \rangle f(\mathbf{n}) = \sum_{\mathbf{W}} \langle \Phi, \mathbf{n} \rangle \, \mathfrak{L}^k(f)(\mathbf{n}) \tag{15}$$

It is not obvious that the set of vectors in $[\mathbb{R}^b]^{\mathscr{L}}$ that satisfies (15) coincides with the whole set of global linear k-invariants. It turns out that it is true for models which satisfy (P1)–(P3) or simply (P4).

At the Boltzmann level the asymptotic periodicity is more complicated to point out since the operator $\text{Fact} \circ \mathfrak{L}$ is not linear. As explained in the introduction, any factorized fixed point p of $\mathfrak{L}^k$ is not in general a fixed point of the "Boltzmann operator" $[\text{Fact} \circ \mathfrak{L}]^k$, but a factorized fixed point p of $\mathfrak{L}^k$ is a fixed point of $[\text{Fact} \circ \mathfrak{L}]^k$ if and only if the successive iterates $\mathfrak{L}^i(p)$ remain factorized. This is a consequence of the decreasing of the information $\mathfrak{H}$ when going from p to $\mathfrak{L}(p)$ and then from $\mathfrak{L}(p)$ to $\text{Fact}(\mathfrak{L}(p))$ (see Appendix B).

Thus, among all the global linear k-invariants of an LGCA, only some of them are relevant for the Boltzmann equation.

It turns out that the vectors which satisfy a relation similar to (15) but for the Boltzmann operator $\text{Fact} \circ \mathfrak{L}$ will define a set of fixed points of $[\text{Fact} \circ \mathfrak{L}]^k$. Let us give a formal definition of these vectors which we will call the Boltzmann k-invariants.

Definition 4. A *Boltzmann k-invariant* is a vector Φ of $[\mathbb{R}^b]^{\mathscr{L}}$ such that

$$\forall p \in \mathscr{D}(\mathbf{W}), \qquad \sum_{\mathbf{W}} \langle \Phi, \mathbf{n} \rangle \, p(\mathbf{n}) = \sum_{\mathbf{W}} \langle \Phi, \mathbf{n} \rangle [\text{Fact} \circ \mathfrak{L}]^k \, (p)(\mathbf{n})$$

They constitute a linear subspace of $[\mathbb{R}^b]^{\mathscr{L}}$ that we will denote as $\mathbb{B}^k$. We will see in the next subsection that, for any LGCA, these vectors are linear k-invariants in the sense of Definition 2. For any such vector Φ the density $p_e(\mathbf{n}) = \mathfrak{k} \exp(\langle \Phi, \mathbf{n} \rangle)$ is a factorized fixed point of $\mathfrak{L}^k$; furthermore, it is also a factorized fixed point of $[\text{Fact} \circ \mathfrak{L}]^k$. We will then prove in Proposition 3 that there is a one-to-one mapping between these fixed points and their associated mean values of the Boltzmann k-invariants. In other words, if $\mathbf{N}$ is a mean population vector in $(]0, 1[^b)^{\mathscr{L}}$, there exists one and only one vector $\mathbf{N}_e$ in $(]0,1[^b)^{\mathscr{L}}$ such that $\mathrm{Log}(\bar{\mathbf{N}}_e)$ is in $\mathbb{B}^k$ and $\langle \Psi, \mathbf{N}\rangle = \langle \Psi, \mathbf{N}_e\rangle$ for any vector Ψ in $\mathbb{B}^k$. This $\mathbf{N}_e$ gives a strict minimum for the information function among all $\mathbf{N}$ satisfying $\langle \Psi, \mathbf{N}\rangle = \langle \Psi, \mathbf{N}_e\rangle$ for any vector Ψ in $\mathbb{B}^k$.

If any fixed point of $[\mathrm{Fact} \circ \mathfrak{L}]^k$ was associated to a Boltzmann k-invariant, this last property would yield a marginal conditional asymptotic stability of any (strictly positive) fixed point of $[\mathrm{Fact} \circ \mathfrak{L}]^k$ and the asymptotic periodicity for the mean populations. Unfortunately, we have not been able to prove this result in general and we suspect that it is wrong. However, any factorized density $p(\mathbf{n}) = \mathfrak{k} \exp(\langle \Phi, \mathbf{n}\rangle)$ where Φ is a *regular k-invariant* (see Definition 3) satisfies the factorization condition and is a fixed point of $[\mathrm{Fact} \circ \mathfrak{L}]^k$. More precisely, if $p_0(\mathbf{n}) = \mathfrak{k} \exp(\langle \Phi, \mathbf{n}\rangle)$, where Φ is a regular k-invariant, then at any time t we will have[3] $p_t(\mathbf{n}) = \mathfrak{k} \exp(\langle \mathfrak{S}^t \Phi, \mathbf{n}\rangle)$. Hence p_t is factorized and the projection $[\mathfrak{S}^t \Phi](\alpha)$ at each node is always a local invariant. We do not enter into details, but these two properties will be crucial when performing a standard linear analysis (i.e., a Green–Kubo-like procedure) in order to obtain asymptotic transport properties for these LGCA.

The regular k-invariants are always Boltzmann k-invariants. It is then possible to exhibit a wide class of models where on the one hand the whole set of Boltzmann k-invariants coincides with the set of regular k-invariants and on the other hand the latter define the strictly positive fixed points of $[\mathrm{Fact} \circ \mathfrak{L}]^k$ in a one-to-one way.

This is, for instance, the case of models which satisfy (P1)–(P3) or simply (P4) and also the case of models which have a *regular* configuration (see the definition below). This latter class encloses most models used to simulate hydrodynamics.

Hence, for all these models when starting with suitable initial conditions the mean populations at the Boltzmann level are asymptotically periodic, the limit cycles being only defined by the mean initial values of the *regular T-invariants.*

In ref. 1 we considered a class of models which admit what we have defined as a "regular" configuration. This class is of particular interest since for these models the (strictly positive) fixed points of $[\mathrm{Fact} \circ \mathfrak{L}]^k$ are only those associated to the regular invariants. We will give here a slightly more general definition. If a configuration $\mathbf{n}$ satisfies $\mathfrak{S}(\mathbf{n}) = \mathbf{n}$ and $\mathscr{A}(\mathbf{n} \to \mathbf{n}) \neq 0$, we will say that it is *stationary.* 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 on at most one velocity channel of this node

[3] This is easily seen, combining the equivalent relations (D1) of Appendix D with relations (6).

satisfies $\mathscr{A}(\mathbf{n}' \to \mathbf{n}') \neq 0$. It turns out that any regular configuration in the sense of ref. 1 is regular within this latter definition.

For usual LGCA models where all the particles have the same mass but different velocities and the local collisions conserve mass and momentum (and energy for models with massless particles), the empty configuration is regular since any configuration $\mathbf{n}$ with only one particle gives rise to a trivial collision, i.e., $\mathscr{A}(\mathbf{n} \to \mathbf{n}) = 1$. The same is true for models with particles with different masses if the partial masses are conserved: Most models used to describe hydrodynamics fall in this category, and in fact most of the LGCA described in the literature.

3.2. Properties of the Boltzmann k-Invariants

Let us observe that the information function of a factorized density with a mean population $\mathbf{N}$ is only a function of $\mathbf{N}$, given by

$$\mathbf{H}(\mathbf{N}) = \langle \mathbf{N}, \mathrm{Log}(\mathbf{N}) \rangle + \langle \mathbf{I} - \mathbf{N}, \mathrm{Log}(\mathbf{I} - \mathbf{N}) \rangle$$

where $\mathbf{I}$ is the vector of $[\mathbb{R}^b]^{\mathscr{L}}$ whose components are all equal to 1. As explained in the previous section, the key for the stability study of a limit cycle at the Boltzmann level is the fact that this cycle gives an absolute minimum of the information function among a set of admissible points. This comes from the following general proposition:

Proposition 3. Let $\mathbb{A}$ be a subspace of $[\mathbb{R}^b]^{\mathscr{L}}$. Let $\mathbf{N}^0$ be a vector in $(]0, 1[^b)^{\mathscr{L}}$. Then there exists a unique field $\mathbf{N}_e$ in $(]0, 1[^b)^{\mathscr{L}}$ which satisfies

$$\forall \Phi \in \mathbb{A}, \qquad \langle \Phi, \mathbf{N}^0 \rangle = \langle \Phi, \mathbf{N}_e \rangle \tag{16a}$$

$$\mathrm{Log}(\bar{\mathbf{N}}_e) \in \mathbb{A} \tag{16b}$$

The density $f_e(\mathbf{n}) = \mathfrak{f} \exp(\langle \mathrm{Log}(\bar{\mathbf{N}}_e), \mathbf{n} \rangle)$ among all the factorized densities whose mean population field satisfies (16a) is the only one which gives the absolute minimum of the information function.

A proof of a similar result for semicontinuous Boltzmann discrete models, based on asymptotic properties of algebroid functions, is given in ref. 7. We give in Appendix C a direct proof for LGCA. This proof, which is constructive, yields the next lemma and finally the expected stability.

If in Proposition 3, $\mathbb{A}$ is the set of the global linear k-invariants, we deduce that for any k there is a one-to-one mapping between the factorized fixed points of $\mathfrak{L}^k$ (i.e., the Gibbs states of the LGCA for the process $\mathfrak{L}^k$) and the mean values of the global linear k-invariants.

In deriving the proof of the previous proposition, the following lemma, which will be one of the main ingredients in the investigation of the asymptotic properties of the Boltzmann equation, can be deduced:

Lemma 1. Let $\mathbb{A}$ be a subspace of $[\mathbb{R}^b]^{\mathscr{L}}$. Let $\mathbf{N}_e$ be a vector in $(]0, 1[^b)^{\mathscr{L}}$ which satisfies $\mathrm{Log}(\bar{\mathbf{N}}_e) \in \mathbb{A}$. Let $\mathbb{F}$ be the set of vectors $\mathbf{N}$ in $(]0, 1[^b)^{\mathscr{L}}$, which satisfy

$$\forall \Phi \in \mathbb{A}, \qquad \langle \Phi, \mathbf{N} \rangle = \langle \Phi, \mathbf{N}_e \rangle$$

And let $\bar{\mathbb{F}}$ be the closure of $\mathbb{F}$. Then there exists a real $a > 0$ such that the set $\mathbb{F}_a$ of all the points $\mathbf{N}$ in $\bar{\mathbb{F}}$ satisfying $\mathbf{H}(\mathbf{N}) - \mathbf{H}(\mathbf{N}_e) < a$ is an open subset of $\mathbb{F}$. For each $0 < \varepsilon < a$, the set of all the points $\mathbf{N}$ in $\bar{\mathbb{F}}$ such that $\mathbf{H}(\mathbf{N}) - \mathbf{H}(\mathbf{N}_e) \leqslant \varepsilon$ is a compact subset of $\mathbb{F}_a$.

This lemma guarantees that for an initial condition $\mathbf{N}^0$ in F_a the whole sequence of mean populations in the Boltzmann equation will stay in a compact subset of $(]0, 1[^b)^{\mathscr{L}}$. This is proven in Appendix C.

It is then easy to show that the Boltzmann k-invariants are actually global linear k-invariants. Let Φ be a Boltzmann k-invariant and let us consider the initial density $f_0(\mathbf{n}) = \mathfrak{k} \exp(\langle \Phi, \mathbf{n} \rangle)$ and let $\mathbf{N}^0$ be its mean population vector. Let us set $f_t = [[\mathrm{Fact} \circ \mathfrak{L}]^k]^t (f_0)$ and let $\mathbf{N}^t$ be the corresponding mean population. The vector $\mathrm{Log}(\bar{\mathbf{N}}^0)$ is equal to Φ and is in $\mathbb{B}^k$. Furthermore, considering the Definition 4 of $\mathbb{B}^k$, we have the relation $\langle \Psi, \mathbf{N}^t \rangle = \langle \Psi, \mathbf{N}^0 \rangle$ for any t and any Ψ in $\mathbb{B}^k$. But, among all the vectors $\mathbf{N}$ which satisfy this last relation $\mathbf{N}^0$ is the only one that corresponds to the absolute minimum of the information function. Let us then observe that the latter decreases between any factorized density p and $\mathrm{Fact}(\mathfrak{L}(p))$; moreover, the relation $\mathfrak{H}(p) = \mathfrak{H}(\mathrm{Fact}(\mathfrak{L}(p)))$ implies that $\mathfrak{L}(p)$ is itself factorized. It follows that for any t, $\mathbf{N}^t = \mathbf{N}^0$ and thus f_0 is a fixed point of $[\mathrm{Fact} \circ \mathfrak{L}]^k$ and then of $\mathfrak{L}^k$. Hence Φ is a global linear k-invariant.

Let us now briefly verify that any regular k-invariant is a Boltzmann k-invariant.

Let k be an integer, Φ be a regular k-invariant, and p be any initial factorized density with $\mathbf{N}^0$ as its mean population vector. Let us set $p_t = [\mathrm{Fact} \circ \mathfrak{L}]^t (p)$ and let $\mathbf{N}^t$ be the corresponding mean population. It follows that

$$\langle \Phi, \mathbf{N}^1 \rangle = \sum_{\mathbf{W}} \langle \Phi, \mathbf{n} \rangle \; \mathfrak{L}(p)(\mathbf{n}) = \sum_{\mathbf{W}^2} \langle \Phi, \mathbf{n} \rangle \; p(\mathbf{n}') \, \mathscr{A}(\mathbf{n}' \to \mathfrak{S}^{-1}(\mathbf{n}))$$

Since $\mathfrak{S}$ is orthogonal the last sum can be rewritten as

$$\sum_{\mathbf{W}^2} \langle \mathfrak{S}^{-1}\Phi, \mathfrak{S}^{-1}\mathbf{n}\rangle\, p(\mathbf{n}')\, \mathscr{A}(\mathbf{n}' \to \mathfrak{S}^{-1}(\mathbf{n}))$$

But since Φ is regular, for any node α, $\mathfrak{S}^{-1}\Phi(\alpha)$ is in $\mathbb{K}_{\text{loc}}$ and we then have

$$a(\mathbf{n}'(\alpha) \to \mathfrak{S}^{-1}(\mathbf{n})(\alpha))\langle \mathfrak{S}^{-1}\Phi(\alpha), \mathbf{n}'(\alpha) - \mathfrak{S}^{-1}(\mathbf{n})(\alpha)\rangle = 0$$

So we deduce that

$$\langle \Phi, \mathbf{N}^1\rangle = \sum_{\mathbf{W}^2} \langle \mathfrak{S}^{-1}\Phi, \mathbf{n}'\rangle\, p(\mathbf{n}')\, \mathscr{A}(\mathbf{n}' \to \mathfrak{S}^{-1}(\mathbf{n})) = \langle \mathfrak{S}^{-1}\Phi, \mathbf{N}^0\rangle$$

But $\mathfrak{S}^{-1}\Phi$ is also a regular k-invariant. Hence, the previous relations yield

$$\langle \Phi, \mathbf{N}^2\rangle = \langle \mathfrak{S}^{-1}\Phi, \mathbf{N}^1\rangle = \langle \mathfrak{S}^{-2}\Phi, \mathbf{N}^0\rangle$$

Finally we will have $\langle \Phi, \mathbf{N}^k\rangle = \langle \mathfrak{S}^{-k}\Phi, \mathbf{N}^0\rangle$. But, $\mathfrak{S}^{-k}\Phi = \Phi$ and it follows that any regular k-invariant is then a Boltzmann k-invariant as noticed in the previous section.

Now, for a wide class of models the global regular k-invariants coincide with the Boltzmann k-invariants as stated in the following proposition, proved in Appendix D:

Proposition 4. If an LGCA model satisfies either properties (P1)–(P3) or simply property (P4) or if it has a regular configuration, then the set $\mathbb{B}^k$ of its Boltzmann k-invariants coincides with the set $\mathbb{K}_{\text{gl}}^{r,k}$ of its regular k-invariants. Let r be the lowest common factor of k and T. A factorized density $p_0(\mathbf{n}) = \mathfrak{k} \exp(\langle \Phi, \mathbf{n}\rangle)(\mathfrak{k} > 0)$ is a fixed point of $[\text{Fact} \circ \mathfrak{L}]^k$ if and only if Φ is a regular k-invariant. It is then a fixed point of $[\text{Fact} \circ \mathfrak{L}]^r$ and of $[\text{Fact} \circ \mathfrak{L}]^T$.

3.3. Stability and Periodicity

We are now in position to study the asymptotic behavior of the mean population at the Boltzmann level. For the models considered in the previous proposition, we entirely know all the possible cycles of the Boltzmann equation. It remains to study their stability and to show that they are the only attractors.

Let us then consider a LGCA which satisfies properties (P1)–(P3) or only property (P4), or which has a regular configuration. Let then T be the lowest integer such that $\mathfrak{S}^T$ is the identity map on $\mathbf{W}$. The following proposition characterizes the stability of the fixed points of $[\mathrm{Fac} \circ \mathfrak{Q}]^k$and the asymptotic periodicity of the solutions of the Boltzmann equation.

Proposition 5. Let $\mathbf{N}_0$ be a mean population vector in $(]0, 1[^b)^{\mathscr{L}}$ and let $\mathbb{F}^{(T)}$ be the set of vectors $\mathbf{N}$ in $(]0, 1[^b)^{\mathscr{L}}$, which satisfies[4]

$$\forall \Phi \in \mathbb{K}_{\mathrm{gl}}^{r,T}, \qquad \langle \Phi, \mathbf{N} \rangle = \langle \Phi, \mathbf{N}_0 \rangle$$

Let $\mathbf{N}_{(T)} \in (]0, 1[^b)^{\mathscr{L}}$ be the unique vector of $\mathbb{F}^{(T)}$ such that $\mathrm{Log}(\bar{\mathbf{N}}_{(T)}) \in \mathbb{K}_{\mathrm{gl}}^{r,T}$ and let $\mathbb{F}_{aT}$ be the open neighborhood of $\mathbf{N}_{(T)}$ in $\mathbb{F}^{(T)}$ defined in Lemma 1. Then, if $\mathbf{N}_0 \in \mathbb{F}_{aT}$, the sequence $\mathbf{N}_n = [\mathscr{F}^T]^n (\mathbf{N}_0)$ converges toward $\mathbf{N}_{(T)}$. Moreover, the sequence $\{\mathscr{F}^t(\mathbf{N}_0)\}$ is asymptotically equivalent to the T-periodic sequence $\{\mathscr{F}^t(\mathbf{N}_{(T)})\}$.

As noted previously, any regular k-invariant is a regular T-invariant. Any (strictly positive) cycle of the Boltzmann equation is a fixed point of $[\mathrm{Fact} \circ \mathfrak{Q}]^T$. From Proposition 4, it is then given by $\mathfrak{f} \exp(\langle \log(\bar{\mathbf{N}}_{(T)}), \mathbf{n} \rangle)$, where $\mathrm{Log}(\bar{\mathbf{N}}_{(T)}) \in \mathbb{K}_{\mathrm{gl}}^{r,T}$. The last proposition, which is proved in Appendix E, shows that this cycle is conditionally asymptotically stable. Let us conclude this section with the following remark, which shows the spurious behavior of the sequence of mean populations.

Let $\mathbf{N}_0$ be a mean population vector in $(]0, 1[^b)^{\mathscr{L}}$ and let us assume that the sequence $\{\mathscr{F}^t(\mathbf{N}_0)\}$ stays in a compact subset of $(]0, 1[^b)^{\mathscr{L}}$. By a simple adaptation of the proof of Proposition 5 it follows that this sequence is necessarily asymptotically periodic with a period which is an integer factor of T. Let $\pi_0 = 1 < \pi_1 < \cdots < \pi_n = T$ be the set of all the distinct integer factors of T. Since any regular k-invariant is a T-invariant, this period will be determined by examining the orthogonal projection of $\mathbf{N}_0$ on each subspace $\mathbb{K}_{\mathrm{gl}}^{r,\pi_i}$. Let j be the lowest integer i such that the projection of $\mathbf{N}_0$ on $\mathbb{K}_{\mathrm{gl}}^{r,\pi_i}$ is equal to its projection on $\mathbb{K}_{\mathrm{gl}}^{r,T}$. The effective period of $\{\mathscr{F}^t(\mathbf{N}_0)\}$ will be π_j. But, *although the minimum of the information correspond* to $\pi_i = 1$ (i.e., a fixed point of $\mathscr{F}$), the value of the information of the sequence $\{\mathscr{F}^t(\mathbf{N}_0)\}$ will not in general tend toward this minimum, since the regular T-invariants do not reduce to the 1-invariants (see ref. 1 for examples). Then, any cycle of the Boltzmann equation is conditionally asymptotically stable; when starting with suitable initial conditions, the mean populations at the Boltzmann level are asymptotically periodic, the limit cycle being only defined by the mean initial values of the *regular T-invariants.*

[4] That is, the vectors which have the same projection on the regular T-invariants.

4. TOWARD MODELS WITHOUT PERIODIC BEHAVIOR

The results of Section 2 indicate that the way to ensure the convergence of the Markov process associated to a LGCA [which obeys (P1)–(P3) or (P4)] is to ensure the merging of the T-paths into the 1-paths.

Actually, a necessary and sufficient condition for sequences $(f_p(\mathbf{n}))_{p \in \mathbb{N}}$ to converge under any initial condition f_0 is that for any couple of configurations $(\mathbf{m}, \mathbf{r})$ in the 1-path which contains $\mathbf{n}$, we have

$$\lim_{p \to +\infty} \mathscr{K}^p(\mathbf{m}, \mathbf{r}) = \frac{1}{|\mathscr{P}|}$$

In other words, the transition matrix, usually defined for Markov chains,[8] that is always bistochastic (because of the semi-detailed balance) must also be regular.

Thus, for given collision rules we are led to modify the transition process. Such modifications have already been proposed by several authors.[5, 9, 10] For instance, in ref. 9 (for the FHP model on the infinite plane), a particle is authorized, under proper conditions, to be moved in a direction different from its velocity; this ensures that the strictly positive translation-invariant fixed points of the resulting Markov process are superpositions of Gibbs states. In ref. 5, four copies of the HPP model are considered and the stirring consists in a stochastic switching of particles lying in different planes, followed by a rigid translation of each planes. This last type of stirring updating was first introduced by Boghosian and Levermore[10] for a one-dimensional LGCA.

One of the simplest possible modifications consists in introducing an independent random variable—say $\Xi \in \{0, 1\}$—which will govern the free propagation stage. After the collision step, and on the whole lattice, we will perform the propagation if $\Xi = 0$ or another collision if $\Xi = 1$. We will denote by ξ the mean expectation of Ξ. This procedure is close to the one proposed in ref. 5, but the stirring updating is replaced here by a collision updating. In ref. 5, for $\Xi = 0$ a stochastic stirring updating is performed before the streaming updating.

We then introduce the Markov kernel

$$\forall \mathbf{n}, \mathbf{m} \in \mathbf{W}^2, \qquad \mathscr{K}(\mathbf{m}, \mathbf{n}) = (1 - \xi)\, \mathscr{A}(\mathbf{m} \to \mathfrak{S}^{-1}(\mathbf{n})) + \xi \mathscr{A}(\mathbf{m} \to \mathbf{n}) \qquad (17)$$

Let us then assume that the considered automaton can be idealized by the Markov process associated to the operator Ω as defined by relation (2a). This new kernel also obeys a semi-detailed balance, and Proposition 1 as well as relations (11) hold. The case $\xi = 0$ has been examined in Section 2.

4.1. Stability Results

At each real function f on $\mathbf{W}$ we then associate a function f^* by the following relation:

$$\forall \mathbf{n} \in \mathbf{W}, \qquad f^*(\mathbf{n}) = \text{Fix}(1, f) = \frac{1}{|\mathscr{P}|} \sum_{\mathscr{P}} f(\mathbf{n}') \tag{18}$$

where $\mathscr{P}$ is the 1-path, as defined in Section 2, which contains $\mathbf{n}$. As in Section 2, we deduce that f^* is a fixed point of $\mathfrak{L}$. The operator Fix(1, $\cdot$) is still a projector on the subspace of the fixed points of $\mathfrak{L}$. It now turns out that the result of Proposition 2 can then be strengthened. The following proposition, proven in Appendix F, holds.

Proposition 6. We suppose that $0 < \xi \leqslant 1$ and that the transitions probabilities $\{\mathscr{A}\}$ satisfy properties (P1)–(P3) or only property (P4). Let f be a density and f^* be the fixed point of $\mathfrak{L}$ associated to f by relation (18). Let (f_n) be the sequence defined by $f_0 = f$ and $f_{n+1} = \mathfrak{L}(f_n)$. Then, (f_n) converges to f^*.

This proposition shows that, under this very simple modification of the transition process, the fixed points of $\mathfrak{L}$ are conditionally asymptotically stable in the following sense. If f^* is a fixed point of $\mathfrak{L}$ and if $f_0 = f^* + df$ is a density such that the mean value of df is zero on each 1-path, then the sequence (f_n) relaxes uniformly to f^* on $\mathbf{W}$. Moreover, this proves that the sequence of *operator* $\mathfrak{L}^n$ *converges to Fix(*$1, \cdot$*)* (since $\mathbf{W}$ is finite on the set of all complex functions defined on $\mathbf{W}$) when n goes to infinity. This proposition also indicates that there are no periodic solutions to the Liouville equation $f_{n+1} = \mathfrak{L}(f_n)$, hence, there are no specific fixed points for iterated processes $\mathfrak{L}^k$: they are all fixed points of $\mathfrak{L}$. The only eigenvalue of $\mathfrak{L}$ with a unit modulus is 1 and the corresponding eigenspace is asymptotically stable.

Another feature of the modified process is that any stationary state and hence any 1-path is invariant under the shift $\mathfrak{S}$ [see relationship (F2)–(F3) of Appendix F].

The global linear 1-invariants are, as in the previous sections, the linear fixed points of $\mathfrak{L}$. They are defined by relation (2). They are all regular and the following proposition holds (without any restriction on the transition probabilities but the semi-detailed balance).

Proposition 7. We suppose that $0 < \xi < 1$. A vector Φ of $[\mathbb{R}^b]^{\mathscr{L}}$ is a linear 1-invariant if and only if it satisfies $\mathfrak{S}\Phi = \Phi$ and $\forall \alpha \in \mathscr{L}$, $\Phi(\alpha) \in \mathbb{K}_{\text{loc}}$.

This proposition is established in Appendix F.

At the Boltzmann level we are still interested in sequences of factorized densities which satisfy the recurrence relation (8):

$$p_{t+1} = \mathrm{Fact}(\mathfrak{L}(p_t)) = [\mathrm{Fact} \circ \mathfrak{L}]^{t+1}(p_0)$$

But the Markov kernel is now given by relation (17). The evolution equation for the mean populations is

$$\begin{aligned} &\mathfrak{S}^{-1}\mathbf{N}(t+1) - \mathbf{N}(t) \\ &\quad = \Delta(\mathbf{N}(t)) + \xi[(\mathfrak{S}^{-1}\mathbf{N}(t) - \mathbf{N}(t)) + (\mathfrak{S}^{-1}\Delta(\mathbf{N}(t)) - \Delta(\mathbf{N}(t)))] \end{aligned} \tag{19}$$

where $\Delta(\mathbf{N}(t))$ is the vector of $[\mathbb{R}^b]^{\mathscr{L}}$ whose components are $\delta_j[\mathbf{N}(\alpha, t)]$ [see relation 6b]. For the case $\xi = 0$ relation (19) is the usual Boltzmann equation. It can still be written as $\mathbf{N}(t+1) = \mathscr{F}(\mathbf{N}(t))$, where $\mathscr{F}$ is a C^∞-function on $(\mathbb{R}^b)^{\mathscr{L}}$. The mean value of any linear 1-invariant is conserved, that is,

$$\forall \Phi \in \mathbb{K}_{\mathrm{gl}}^{r,1}, \quad \forall t \in \mathbb{N}, \qquad \langle \Phi, \mathbf{N}(t) \rangle = \langle \Phi, \mathbf{N}(0) \rangle$$

From proposition 7, a factorized density $p_0(\mathbf{n}) = \mathfrak{k} \exp(\langle \Phi, \mathbf{n} \rangle)$ ($\mathfrak{k} > 0$) is a fixed point of $[\mathrm{Fact} \circ \mathfrak{L}]$ if and only if Φ is a regular 1-invariant or equivalently if and only if it is a factorized fixed point of $\mathfrak{L}$. These factorized fixed points are, for a wide class of models, the only ones which leave the information stationary for the "Boltzmann process" (8); the following lemma (proven in Appendix F) holds.

Lemma 2. The kernel $\mathscr{K}$ is given by relation (17) with $0 < \xi < 1$.

1. If the transition probabilities $\{\mathscr{A}\}$ obey properties (P1)–(P3) or only property (P4), let p be any density; then the equality $\mathfrak{H}(\mathfrak{L}(p)) = \mathfrak{H}(p)$ stands if and only if p is a fixed point of $\mathfrak{L}$.
2. If the model has a regular configuration, let $p(n) = \mathfrak{k} \exp(\langle \Phi, \mathbf{n} \rangle)$ ($\mathfrak{k} > 0$) be any factorized density; then the equality $\mathfrak{H}[\mathrm{Fact}(\mathfrak{L}(p))] = \mathfrak{H}(p)$ stands if and only if p is a factorized fixed point of $\mathfrak{L}$.

As in the study of the asymptotic periodicity, this lemma will provide the tools to show the stability of the (strictly positive) fixed points of $[\mathrm{Fact} \circ \mathfrak{L}]$.

We consider a LGCA which obeys properties (P1)–(P3) or only property (P4), or which has a regular configuration. The kernel $\mathscr{K}$ is given by relation (17) with $0 < \xi < 1$. The following proposition holds.

Proposition 8. Let $\mathbf{N}_0$ be a mean population vector in $(]0,1[^b)^{\mathscr{L}}$ and let $\mathbb{F}$ be the set of vectors $\mathbf{N}$ in $(]0,1[^b)^{\mathscr{L}}$, which satisfies

$$\forall \Phi \in \mathbb{K}_{\rm gl}^{r,1}, \qquad \langle \Phi, \mathbf{N} \rangle = \langle \Phi, \mathbf{N}_0 \rangle \tag{20}$$

Let $\mathbf{N}_{\rm eq} \in (]0,1[^b)^{\mathscr{L}}$ be the unique vector of $\mathbb{F}$ such that $\mathrm{Log}(\bar{\mathbf{N}}_{\rm eq}) \in \mathbb{K}_{\rm gl}^{r,1}$ and let $\mathbb{F}_a$ be the open neighborhood of $\mathbf{N}_{\rm eq}$ in $\mathbb{F}$ defined in Lemma 1. Then, if $\mathbf{N}_0 \in \mathbb{F}_a$, the sequence $\mathbf{N}_n = \mathscr{F}^n(\mathbf{N}_0)$ converges toward $\mathbf{N}_{\rm eq}$.

Conversely, let $\mathbf{N}_{\rm eq}$ be a mean population vector in $(]0,1[^b)^{\mathscr{L}}$ such that the density $p(\mathbf{n}) = p(\mathbf{0}) \exp(\langle \log(\bar{\mathbf{N}}_{\rm eq}, \mathbf{n} \rangle)$ is a fixed point of $[\mathrm{Fact} \circ \mathfrak{L}]$. Let $\mathbb{F}$ be the set of vectors $\mathbf{N}$ in $(]0,1[^b)^{\mathscr{L}}$ which satisfy (20) Then, $\log(\bar{\mathbf{N}}_{\rm eq})$ is in $\mathbb{K}_{\rm gl}^{r,1}$ and there exists an open neighborhood of $\mathbf{N}_{\rm eq}$ in $\mathbb{F}$ such that for each $\mathbf{N}_0$ in this neighborhood, the sequence $\mathbf{N}_n = \mathscr{F}^n(\mathbf{N}_0)$ converges toward $\mathbf{N}_{\rm eq}$.

The proof of this latter proposition is similar to that of Proposition 5 and will not be detailed. It ensures, in these models, the stability of the Gibbs states of $\mathfrak{L}$. Similarly, let $\mathbf{N}_0$ be a mean population vector in $(]0,1[^b)^{\mathscr{L}}$ and let us assume that the sequence $\{\mathscr{F}^t(\mathbf{N}_0)\}$ stays in a compact subset of $(]0,1[^b)^{\mathscr{L}}$. It then follows that it is necessarily convergent to the unique Gibbs state associated to $\mathbf{N}_0$. This equilibrium state now corresponds to the absolute minimum of the information among the densities whose mean populations satisfy (20). Moreover, it is uniquely defined by the averages of the regular 1-invariants. Then, we have avoided the spurious asymptotic periodic behavior at both the Liouville and the Boltzmann level of description.

4.2. Hydrodynamic Equations

Let us now say a few words about the hydrodynamics of these modified LGCA. We considered a six-velocity FHP model. The velocities $(\mathbf{c}_1,..., \mathbf{c}_6)$ all have the same modulus c; they are obtained by successively rotating $\mathbf{c}_1$ through angle $\pi/3$. Starting with the Boltzmann equation (19), we have performed a Chapman–Enskog procedure in order to access the transport equations. The zeroth-order expansion yields the Euler equations. They are exactly the same as those of the nonmodified model provided there is a time rescaling by a factor $(1-\xi)$. That is, after resealing [i.e., $t^* = (1-\xi)t$] we have

$$\frac{\partial \rho}{\partial t^*} + \nabla \cdot (\rho \mathbf{v}) = \mathbf{0}$$

$$\frac{\partial \rho \mathbf{v}}{\partial t^*} + \nabla \cdot \left(\sum_{j=1}^{6} N_j^{\rm eq} \mathbf{c}_j \right) = \mathbf{0}$$

where $\mathbf{N}_j^{\rm eq}$ is the local equilibrium mean population associated to $(\rho, \rho\mathbf{v})$.

The first-order expansion yields Navier–Stokes-like equations for the lattice gas. For the balance of momentum, up to leading order in mean velocities and density gradients, one obtains

$$\frac{\partial \rho \mathbf{v}}{\partial t^*} + \nabla \cdot \left(\sum_{j=1}^{6} N_j^{\text{eq}} \mathbf{c}_j \otimes \mathbf{c}_j \right) = \nabla \cdot (\mu[\nabla \mathbf{v} + {}^t\nabla \mathbf{v} - \text{div}(\mathbf{v})\mathbf{I}] + \lambda \nabla \cdot (\mathbf{v})\mathbf{I})$$

where μ is the shear viscosity, given by $\mu = \mu_{\text{coll}} + (\xi - \frac{1}{2})\rho c^2/4$, μ_{coll} being the usual collisional viscosity of the nonmodified FHP model multiplied by the factor $(1 - \xi)$ and the discretization viscosity $\mu_{\text{dis}} = (\xi - \frac{1}{2})\rho c^2/4$ being eventually positive. There appears a nonzero bulk viscosity λ equal to $\xi \rho c^2/4$.

For the mass balance we obtain

$$\frac{\partial \rho}{\partial t^*} + \nabla \cdot (\rho \mathbf{v}) = \nabla \cdot \left[\frac{\xi}{2} \nabla \cdot \left(\sum_{j=1}^{6} N_j^{\text{eq}} \mathbf{c}_j \otimes \mathbf{c}_j \right) \right]$$

Up to leading order in mean velocities and density gradients we have

$$\frac{\xi}{2} \nabla \cdot \left(\sum_{j=1}^{6} N_j^{\text{eq}} \mathbf{c}_j \otimes \mathbf{c}_j \right) \cong D \nabla \rho$$

where the self diffusion coefficient is $D = \lambda/\rho = \xi c^2/4$.

The presence of a bulk viscosity and of a spurious mass current are due to the modification of the model. Their actual influence on incompressible hydrodynamics needs to be evaluated by direct simulations.

APPENDIX A. PROOF OF PROPOSITION 2

The following lemma is satisfied with any Markov kernel under the semi-detailed balance.

Lemma A1. Let f_0 be a real function on $\mathbf{W}$ and (f_n) be the sequence defined by relation (3). Then we have

$$\forall \varepsilon > 0, \exists N \in \mathbb{N}, \qquad p \geqslant N \qquad \text{and} \qquad \mathscr{K}(\mathbf{m}, \mathbf{n}) \neq 0 \Rightarrow |f_{p+1}(\mathbf{n}) - f_p(\mathbf{m})| \leqslant \varepsilon \tag{A1}$$

Proof. At each configuration $\mathbf{n}$, we associate a number $k(\mathbf{n})$ defined by

$$k(\mathbf{n}) = 1 \qquad \text{if} \quad \mathscr{K}(\mathbf{n}, \mathbf{n}) = 1$$

$$k(\mathbf{n}) = \inf\{\mathscr{K}(\mathbf{m}, \mathbf{n})\, \mathscr{K}(\mathbf{r}, \mathbf{n})\} \qquad \text{if} \quad \mathscr{K}(\mathbf{n}, \mathbf{n}) \neq 1$$

The Inf is taken over all configurations $\mathbf{m}$ and $\mathbf{r}$ such that $\mathbf{m} \neq \mathbf{r}$ and $\mathcal{K}(\mathbf{m}, \mathbf{n}) \neq 0$. We then define k as $k = \inf\{\mathbf{n} \in \mathbf{W}, k(\mathbf{n})\}$. Since $\mathbf{W}$ is finite, k is a strictly positive constant that only depends upon the kernel $\mathcal{K}$. Let $\varepsilon > 0$, be given. Then there exists an integer N such that for any $\mathbf{n}$ and any $p \geqslant N$ the following inequality holds (see Appendix C in ref. 1):

$$\mathcal{K}(\mathbf{m}, \mathbf{n}) \neq 0, \qquad \mathcal{K}(\mathbf{r}, \mathbf{n}) \neq 0 \Rightarrow |f_p(\mathbf{m}) - f_p(\mathbf{r})| \leqslant \left(\frac{2\varepsilon}{k}\right)^{1/2} \tag{A2}$$

We then consider any given $\mathbf{n}$ in $\mathbf{W}$. If $\mathcal{K}(\mathbf{m}, \mathbf{n}) \neq 0$, we have

$$f_{p+1}(\mathbf{n}) - f_p(\mathbf{m}) = \sum_{\mathbf{W}} (f_p(\mathbf{n}') - f_p(\mathbf{m}))\, \mathcal{K}(\mathbf{n}', \mathbf{n})$$

Using (A2), this last relation finally yields (A1). ∎

The next result is the key for the asymptotic periodicity. Contrary to the previous one, it depends upon the transition process.

Lemma A2. We suppose that the transitions probabilities $\{\mathcal{A}\}$ obey (P1)–(P3) or only property (P4). Then, for every initial real function f_0 and any integer k, we have

$$\forall \varepsilon > 0, \exists N \in \mathbb{N}, \qquad p \geqslant N \Rightarrow \forall n \in \mathbf{W} : |f_{p+k}(\mathfrak{S}^k(\mathbf{n})) - f_p(\mathbf{n})| \leqslant \varepsilon \tag{A3}$$

This lemma expresses that the process tends to be only propagative. It is proven in ref. 1 for the case $k = 1$. In the general case one applies k times (A3) for $k = 1$. ∎

Proof of Proposition 2. Let (f_n) be a sequence of real functions on $\mathbf{W}$ defined by (3). Applying Lemma A2 to $k = T$ yields

$$\forall \varepsilon > 0, \exists N' \in \mathbb{N}, \qquad p \geqslant N' \Rightarrow \forall \mathbf{m} \in \mathbf{W} : |f_{p+T}(\mathbf{m}) - f_p(\mathbf{m})| \leqslant \frac{\varepsilon}{T+1} \tag{A4}$$

where N' depends upon ε, f_0, and T. Let $\mathbf{n}$, $\mathbf{m}$ be such that $\mathcal{K}^T(\mathbf{m}, \mathbf{n}) \neq 0$. From the definition of $\mathcal{K}^T$ we then deduce that there exists a finite sequence $\mathbf{n}_0 = \mathbf{m}, \mathbf{n}_1, \ldots, \mathbf{n}_T = \mathbf{n}$ of configurations such for each i, $\mathcal{A}(\mathbf{n}_i \to \mathfrak{S}^{-1}(\mathbf{n}_{i+1})) \neq 0$.

From Lemma A1 we can choose an integer N'' which depends upon ε, f_0, and T such that $p \geqslant N''$ implies $|f_{p+i+1}(\mathbf{n}_{i+1}) - f_{p+i}(\mathbf{n}_i)| \leqslant \varepsilon/(T+1)$ for each $i = 0, \ldots, T-1$.

We then sum these inequalities to obtain $|f_{p+T}(\mathbf{n}) - f_p(\mathbf{m})| \leqslant T\varepsilon/(T+1)$. By setting $N = \sup(N', N'')$ and using (A4), we then deduce

$$\forall \varepsilon > 0, \exists N \in \mathbb{N}, \quad p \geqslant N \quad \text{and} \quad \mathcal{K}^T(\mathbf{m}, \mathbf{n})) \neq 0 \Rightarrow |f_p(\mathbf{m}) - f_p(\mathbf{n})| \leqslant \varepsilon \tag{A5}$$

Since a T-Path is finite and since there is a finite number of T-paths, we then deduce by applying (A5) a finite number of times that

$$\forall \varepsilon > 0, \exists N \in \mathbb{N}, \quad p \geqslant N \Rightarrow \forall \mathbf{n}, \mathbf{m} \in \mathbf{W}^2 : \chi_T(\mathbf{n}, \mathbf{m}) \, |f_p(\mathbf{m}) - f_p(\mathbf{n})| \leqslant \varepsilon \qquad \text{(A6)}$$

where $x_T(\mathbf{n}, \mathbf{m})$ is 1 if $\mathbf{n}$ and $\mathbf{m}$ are in the same T-path, and 0 otherwise.

Let us now consider the sequence (f_{nT}) extracted from (f_n). Let $\mathbf{n}$ be a given configuration, and let $\mathscr{P}_T$ be the T-path which contains $\mathbf{n}$. For any $\mathbf{n}'$ in $\mathscr{P}_T$ we have $\text{Fix}(T, f_0)(\mathbf{n}') = \text{Fix}(T, f_0)(\mathbf{n})$. From the definition of the operator Fix and since $(\mathfrak{L})^T$ preserves the measure of the T-paths we will have, $\forall n \in \mathbb{N}$,

$$\begin{aligned} &|\mathscr{P}_T| (\text{Fix}(T, f_0)(\mathbf{n}) - f_{nT}(\mathbf{n})) \\ &\quad = \sum_{\mathbf{n}' \in \mathscr{P}_T} (\text{Fix}(T, f_0)(\mathbf{n}') - f_{nT}(\mathbf{n})) \\ &\quad = \sum_{\mathbf{n}' \in \mathscr{P}_T} (f_0(\mathbf{n}') - f_{nT}(\mathbf{n})) = \sum_{\mathbf{n}' \in \mathscr{P}_T} (f_{nT}(\mathbf{n}') - f_{nT}(\mathbf{n})) \end{aligned}$$

This last equality and (A6) yield

$$\forall \varepsilon > 0, \exists N \in \mathbb{N}, \qquad n \geqslant N \Rightarrow \forall \mathbf{n} \in \mathbf{W} \, |f_{nT}(\mathbf{n}) - \text{Fix}(T, f_0)(\mathbf{n})| \leqslant \varepsilon \quad \text{(A7)}$$

We finally deduce that the sequence (f_{nT}) converges on $\mathbf{W}$ to $\text{Fix}(T, f_0)$. The same result applied to $f_1, f_2, ..., f_{T-1}$ shows that each sequence (f_{nT+k}), $0 \leqslant k < T$, converges uniformly on $\mathbf{W}$ to $\text{Fix}(T, f_k)$. Since T is finite, and considering the definition of the sequence (g_n), we deduce the convergence of (f_n) to (g_n).

For any integer n, we then have

$$g_{n+1} - \mathfrak{L}(g_n) = g_{n+1} - \mathfrak{L}(f_n) + \mathfrak{L}(f_n - g_n) = g_{n+1} - f_{n+1} + \mathfrak{L}(f_n - g_n)$$

The sequence (f_n) converges to (g_n), so, from the continuity of $\mathfrak{L}$ and since (g_n) is periodic, we then deduce that for any integer n, $g_{n+1} = \mathfrak{L}(g_n)$, which proves that $\text{Fix}(T, \cdot)$ and $\mathfrak{L}$ commute. But each g_n is a fixed point of $(\mathfrak{L})^T$ and lemma A2 finally yields relation (14). The Cesaro convergence is then obvious. ▮

APPENDIX B

Proof of the Factorization Property of the Fixed Points of the Boltzmann Operator.

Let p_0 be a factorized density and let us consider the sequence $p_{n+1} = \text{Fact}[\mathfrak{L}(p_n)]$; (p_n) will be a k-periodic sequence if and only if p_0 is a fixed point of $[\text{Fact} \circ \mathfrak{L}]^k$. It is known from information theory that, for any density p, we always have $\mathfrak{H}(\text{Fact}(p)) \leqslant \mathfrak{H}(p)$, the equality standing if and only if $\text{Fact}(p) = p$. Hence, from Proposition 1, we have

$$\mathfrak{H}(p_{n+1}) = \mathfrak{H}(\text{Fact}[\mathfrak{L}(p_n)]) \leqslant \mathfrak{H}(\mathfrak{L}(p_n)) \leqslant \mathfrak{H}(p_n)$$

Hence, the sequence $(\mathfrak{H}(p_n))$ is then decreasing. But since p_0 is a fixed point of $[\text{Fact} \circ \mathfrak{L}]^k$, $(\mathfrak{H}(p_n))$ is then constant and we will have for each n

$$\mathfrak{H}(p_{n+1}) = \mathfrak{H}(\text{Fact}[\mathfrak{L}(p_n)]) = \mathfrak{H}(\mathfrak{L}(p_n)) = \mathfrak{H}(p_n)$$

We then deduce that $\mathfrak{L}(p_n)$ is itself factorized for each n. Hence we have $p_{n+1} = \mathfrak{L}(p_n)$. This implies that (p_n) is a k-periodic sequence of *factorized* densities which satisfies $p_{n+1} = \mathfrak{L}(p_n)$. The converse is obvious.

APPENDIX C

Proof of the Existence and Uniqueness of Gibbs States for Given Mean Conserved Quantities

1. Let us first prove the uniqueness. Let us suppose that there exist two mean population fields $\mathbf{N}_e$ and $\mathbf{N}^*$, both in the open set $(]0, 1[^b)^{\mathscr{L}}$, which satisfy relations (16). Therefore we will have

$$\langle \log(\bar{\mathbf{N}}_e) - \log(\bar{\mathbf{N}}^*), \mathbf{N}_e - \mathbf{N}^* \rangle = 0$$

This equality yields

$$\prod_{\alpha} \cdot \prod_{j=1}^{b} \cdot \left[\frac{[(\bar{N}_e)_j(\alpha)]}{[(\bar{N}^*)_j(\alpha)]} \right]^{[(N_e)_j(\alpha)] - [(N^*)_j(\alpha)]} = 1$$

But each term of this product is $\geqslant 1$ {the function $x/(1-x)$ is increasing on $]0,1[$}, so the product is equal to 1 if and only if $\mathbf{N}_e = \mathbf{N}^*$.

2. Let us now prove the existence. Let then M be the affine subspace which contains $\mathbf{N}^0$ and defined by relation (16a):

$$M = \{\mathbf{X} \in [\mathbb{R}^b]^{\mathscr{L}}; \forall \Phi \in \mathbb{A} : \langle \Phi, \mathbf{N}^0 \rangle = \langle \Phi, \mathbf{X} \rangle\}$$

Let us denote by $\mathbb{F}$ the convex open set of M: $M \cap (]0, 1[^b)^{\mathscr{L}}$. The set $\mathbb{F}$ is a nonempty sûbset of $(]0, 1[^b)^{\mathscr{L}}$ (since it contains $\mathbf{N}^0$). Its closure, $\bar{\mathbb{F}}$, is $M \cap ([0, 1]^b)^{\mathscr{L}}$ and is a convex polyhedron. The function $\mathbf{H}$ is then defined and continuous on $\bar{\mathbb{F}}$, furthermore, it is a C^∞-function on $\mathbb{F}$. Since $\bar{\mathbb{F}}$ is a compact set in M, the function $\mathbf{H}$ has a minimum on $\bar{\mathbb{F}}$, and this minimum is reached on a point $\mathbf{N}_{\text{inf}} \in \bar{\mathbb{F}}$. Let us set $\mathbf{H}(\mathbf{N}_{\text{inf}}) = \mathbf{H}_{\text{inf}}$.

In order to prove that $\mathbf{N}_{\text{inf}}$ is in the open set $\mathbb{F}$, let us first assume that $\mathbf{N}_{\text{inf}}$ is on the boundary of $\mathbb{F}$. Then at least one of the components of $\mathbf{N}_{\text{inf}}$ is necessarily 0 or 1. Let I_0 (resp. I_1) be the set of the indices j such that the component $(\mathbf{N}_{\text{inf}})_j$ is 0 (resp. 1). Since $\mathbf{N}^0$ is in the open set $\mathbb{F}$, and since $\mathbb{F}$ is convex, the segment $[\mathbf{N}^0, \mathbf{N}_{\text{inf}}]$ is in $\overline{\mathbb{F}}$ and can be parametrized as $\mathbf{N}(x) = x\mathbf{N}^0 + (1-x)\,\mathbf{N}_{\text{inf}}$, with $x \in [0, 1]$. Let us then set, for any x in $[0, 1]$, $h(x) = \mathbf{H}(\mathbf{N}(x))$. The function $h(x)$ is then differentiable on $]0, 1[$, and we will have, $\forall x \in]0, 1[$,

$$\frac{d}{dx} h(x) = \left[\sum_{j \in I_0} \mathbf{N}_j^0 \log\left(\frac{x\mathbf{N}_j^0}{1 - x\mathbf{N}_j^0}\right) + \sum_{j \in I_1} (1 - \mathbf{N}_j^0) \log\left(\frac{x(1 - \mathbf{N}_j^0)}{1 - x(1 - \mathbf{N}_j^0)}\right)\right] + \sum_{j \notin I_0, I_1} (\mathbf{N}^0 - \mathbf{N}_{\text{inf}})_j \log\left(\frac{\mathbf{N}_j(x)}{1 - \mathbf{N}_j(x)}\right)$$

When x goes to 0 the last term has a finite limit, while the bracketted one goes to $-\infty$, since $\{I_0, I_1\}$ is nonempty. Hence there exist a real $0 < a < 1$ and a real $b < 0$ such that $(d/dx)\,h(x) < b$ on $]0, a[$. Therefore $h(a) < h(0) = \mathbf{H}_{\text{inf}}$, which contradicts $\mathbf{N}_{\text{inf}}$ on the boundary of $\mathbb{F}$. Hence $\mathbf{N}_{\text{inf}}$ is in $\mathbb{F}$.

Let then $\nabla\mathbf{H}$ be the gradient of $\mathbf{H}$ considered as a function on $(]0, 1[^b)^{\mathscr{S}}$. Since $\mathbf{H}$ is differentiable on $\mathbb{F}$, the gradient $\nabla\mathbf{H}$ of $\mathbf{H}$, considered as a function on $(]0, 1[^b)^{\mathscr{S}}$ is such that $\langle \nabla\mathbf{H}(\mathbf{N}_{\text{inf}}), \delta\mathbf{N}\rangle = 0$ for any vector $\delta\mathbf{N}$ in the subspace orthogonal to $\mathbb{A}$. Since $\nabla\mathbf{H}(\mathbf{N}_{\text{inf}}) = \log(\bar{\mathbf{N}}_{\text{inf}})$, the vector $\log(\bar{\mathbf{N}}_{\text{inf}})$, is then in $\mathbb{A}$.

Now, if this minimum of information were reached at two distinct points of $\overline{\mathbb{F}}$, these points would be, as we have seen, both in the open set $\mathbb{F}$. Therefore two points would exist which satisfy (16b), which is absurd. Hence $\mathbf{N}_{\text{inf}}$ is the expected point $\mathbf{N}_e$. ▮

Proof of Lemma 1. Let us keep the notations used in the proof of the previous proposition. The set $\mathbb{F}$ considered in this lemma is obviously the same as that considered in the previous proof; it is an open subset of M. Let $\partial\mathbb{F}$ be the boundary of $\mathbb{F}$. It is a compact set in M. Let then $\mathbf{H}'$ be the minimum of $\mathbf{H}$ on $\partial\mathbb{F}$. It is reached on some point of $\partial\mathbb{F}$, and from the previous proof we know that $\mathbf{H}' > \mathbf{H}(\mathbf{N}_e)$. Let us then set $a = \mathbf{H}' - \mathbf{H}(\mathbf{N}_e)$. The set $\mathbb{F}_a$ is then included in $\mathbb{F}$; moreover, since $\mathbf{H}$ is continuous on $\mathbb{F}$, it is an open subset of $\mathbb{F}$.

Let then $0 < \varepsilon < a$ and let $\mathbb{F}_\varepsilon$ be the set of all points N in $\overline{\mathbb{F}}$ such that $\mathbf{H}(\mathbf{N}) - \mathbf{H}(\mathbf{N}_e) < \varepsilon$. It is obviously an open subset of $\mathbb{F}_a$. Furthermore, since $\mathbf{H}$ is continuous the closure $\overline{\mathbb{F}}_\varepsilon$ of $\mathbb{F}_\varepsilon$ is included in the set S of all points $\mathbf{N}$ in $\overline{\mathbb{F}}$ such that $\mathbf{H}(\mathbf{N}) - \mathbf{H}(\mathbf{N}_e) \leqslant \varepsilon$. Again, since $\varepsilon < a$, this last set is in $\mathbb{F}_a$ and thus $\overline{\mathbb{F}}_\varepsilon$ is a compact subset of $\mathbb{F}_a$. It remains to see that $S = \overline{\mathbb{F}}_\varepsilon$. This is achieved by noticing that, for each $\mathbf{N}$ in $S-\{\mathbf{N}_e\}$, the function $\mathbf{H}$ is strictly decreasing on the segment $[\mathbf{N}, \mathbf{N}_e]$. Indeed, the hessian of $\mathbf{H}$ on $(]0,1[^b)^{\mathscr{L}}$ is diagonal on the natural basis and its components are the $1/N_j(\alpha)(1-N_j(\alpha))$; it is then a strictly positive metric. Thus each $\mathbf{N}$ in S is the limit of a sequence of points in $\mathbb{F}_\varepsilon$.

APPENDIX D

Proof of Proposition 4. 1. For models which obey (P1)–(P3) or simply (P4), since any global linear k-invariant is a regular one, the whole set of global linear k-invariants coincide with the boltzmann k-invariants.

2. For models which have a regular configuration we will simply prove that any strictly positive fixed point of $[\mathrm{Fact} \circ \mathfrak{L}]^k$ is associated with a regular k-invariant.

Let then $p(\mathbf{n}) = \mathfrak{k} \exp(\langle \Phi, \mathbf{n} \rangle)(\mathfrak{k} > 0)$ be a factorized density and let us assume that $\mathfrak{H}(p) = \mathfrak{H}(\mathfrak{L}(p))$ and $\mathfrak{L}(p)$ is also factorized.

Let $\mathbf{m}_0$ be a regular configuration. 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 velocity. If L is the number of nodes, it is composed of bL configurations obtained (see ref. 1) by successively permuting in $\mathbf{m}_0$ a one and a zero node after node and on each velocity channel. Let us then suppose that the densities p and $\mathfrak{L}(p)$ are both factorized. We will denote by $\mathbf{N}$ and $\mathbf{N}^*$ the mean population fields of resp. p and $\mathfrak{L}(p)$. Let us then observe that the set $\{\mathbf{m}_i\}$, $i \geqslant 0$, is globally invariant under $\mathfrak{S}$. Let then $\mathbf{m}_k$ be such a configuration. As $\mathscr{A}(\mathbf{m}_k \to \mathbf{m}_k) \neq 0$, the configuration $\mathfrak{S}^{-1}(\mathbf{m}_k)$ has the same property and thus $\mathscr{A}(\mathfrak{S}^{-1}(\mathbf{m}_k) \to \mathfrak{S}^{-1}(\mathbf{m}_k)) \neq 0$. But since $\mathfrak{H}(p) = \mathfrak{H}(\mathfrak{L}(p))$, from relation (11a) we deduce that

$$\mathscr{A}(\mathbf{m}' \to \mathfrak{S}^{-1}(\mathbf{m}_k)) \neq 0 \Rightarrow p(\mathbf{m}') = p(\mathfrak{S}^{-1}(\mathbf{m}_k))$$

This yields, by evaluating $\mathfrak{L}(p)(\mathbf{m}_k)$, $\mathfrak{L}(p)(\mathbf{m}_k) = p(\mathfrak{S}^{-1}(\mathbf{m}_k))$, that is,

$$\prod_{\alpha \in \mathscr{L}} \prod_{j=1}^{b} [N_j^*(\alpha)]^{[(m_k)_j(\alpha)]} [1-N_j^*(\alpha)]^{[1-(m_k)_j(\alpha)]} = \prod_{\alpha \in \mathscr{L}} \prod_{j=1}^{b} [N_j(\alpha-\mathbf{c}_j)]^{[(m_k)_j(\alpha)]} [1-N_j(\alpha-\mathbf{c}_j)]^{[1-(m_k)_j(\alpha)]}$$

But we have also $\mathfrak{L}(p)(\mathbf{m}_0) = p(\mathfrak{S}^{-1}(\mathbf{m}_0)) = p(\mathbf{m}_0)$. Let us fix one couple (j, α). There exists a configuration in $\{\mathbf{m}_i\}$, say $\mathbf{m}_k$, which differs from $\mathbf{m}_0$ only through the component $(m_k)^j(\alpha)$. this yields $p(\mathbf{m}_0)[N_j^*(\alpha) - N_j(\alpha-\mathbf{c}_j)] = 0$.

Hence we have $\mathbf{N}^* = \mathfrak{S}\mathbf{N}$. We then deduce from relation (6a) that $\forall\alpha$, $\delta(\mathbf{N}(\alpha)) = 0$. but for any vector $\mathbf{U}$ in $]0, 1[^b$ and any model with semi-detailed balance the following propositions are equivalent[1, 4]:

$$\delta(\mathbf{U}) = 0 \tag{Dla}$$

$$\log(\bar{\mathbf{U}}) \in \mathbb{K}_{\text{loc}} \tag{Dlb}$$

$$\langle \delta(\mathbf{U}), \log(\bar{\mathbf{U}}) \rangle = 0 \tag{Dlc}$$

Since $\Phi = \log(\bar{\mathbf{N}})$, we then deduce that $\forall\alpha$, $\Phi(\alpha)$ is in $\mathbb{K}_{\text{loc}}$.

Now, if p is a fixed point of $[\text{Fact} \circ \mathfrak{L}]^k$, any $\mathfrak{L}^l(p)$ is then factorized with $\mathfrak{H}(p) = \mathfrak{H}(\mathfrak{L}^l(p)) = \mathfrak{H}([\text{Fact} \circ \mathfrak{L}]^l(p))$. Hence, we can successively apply the previous analysis to show that the mean population field of $[\text{Fact} \circ \mathfrak{L}]^l(p)$ is $\mathfrak{S}^l\mathbf{N}$ and that $\forall\alpha$, $\mathfrak{S}^l\Phi(\alpha)$ is in $\mathbb{K}_{\text{loc}}$. But since $p = [\text{Fact} \circ \mathfrak{L}]^k(p)$ it follows that $\mathfrak{S}^k\Phi = \Phi$. Finally, Φ is a regular k-invariant. Since $\mathfrak{S}^T$ is the identity map, p is also a fixed point of $[\text{Fact} \circ \mathfrak{L}]^T(p)$ and Φ a regular r-invariant (r is the l.c.d. of k and T). ▮

APPENDIX E

Proof of Proposition 5. 1. Let us first observe that the sequence $(\mathbf{N}_n)$ is defined by the recurrence relation $\mathbf{N}_n = [\mathscr{F}^T]^n (\mathbf{N}_0)$. Let p_n be the factorized density whose mean population is $\mathbf{N}_n$. Let us then set $H_n = \mathbf{H}(\mathbf{N}_n) = \mathfrak{H}(p_n)$. We have $H_{n+1} = \mathfrak{H}(p_{n+1}) = \mathfrak{H}([\text{Fact} \circ \mathfrak{L}]^T(p_n))$. We will have $H_{n+1} \leqslant H_n$. Hence, the sequence (H_n) is decreasing and since it is bounded below, it is converging to a limit, say H^*. Moreover, if $\mathbf{H}(\mathbf{N}_0) - \mathbf{H}(\mathbf{N}_{(T)}) < a_T$, we know from Lemma 1 that the whole sequence $(\mathbf{N}_n)$ stays in a compact subset of $(]0, 1[^b)^{\mathscr{L}}$. We can then extract from $(\mathbf{N}_n)$ a sequence $(\mathbf{N}_{n_k})$ that converges to a field $\mathbf{N}^*$ where $\mathbf{N}^*$ is in $(]0, 1[^b)^{\mathscr{L}}$. But $\mathscr{F}$ is continuous and we then deduce that the sequence $(\mathscr{F}^T(\mathbf{N}_{n_k}))$ converges to $\mathscr{F}^T(\mathbf{N}^*)$. But the sequence $(\mathscr{F}^T(\mathbf{N}_{n_k}))$ is also extracted from $(\mathbf{N}_n)$. Hence, we will have: $\mathbf{H}(\mathscr{F}^T(\mathbf{N}^*)) = \mathbf{H}(\mathbf{N}^*) = H^*$. Let then $p^* = \mathfrak{k} \exp(\langle \Phi, \mathbf{n} \rangle)$ be the factorized density associated to $\mathbf{N}^*$. We have the inequalities

$$\begin{aligned} H^* = \mathbf{H}(\mathscr{F}^T(\mathbf{N}^*)) &= \mathfrak{H}([\text{Fact} \circ \mathfrak{L}]^T(p^*)) \\ &\leqslant \cdots \leqslant \mathfrak{H}([\text{Fact} \circ \mathfrak{L}](p^*)) \leqslant \mathfrak{H}(\mathfrak{L}(p^*)) \\ &\leqslant \mathfrak{H}(p^*) = \mathbf{H}(\mathbf{N}^*) = H^* \end{aligned}$$

So we deduce that the successive iterates $\mathfrak{L}(p^*)$, $\mathfrak{L}^2(p^*)$,..., $\mathfrak{L}^T(p^*)$ are all *factorized* and that $\mathfrak{H}(p^*) = \mathfrak{H}(\mathfrak{L}(p^*)) = \cdots = \mathfrak{H}(\mathfrak{L}^T(p^*))$. We then deduce the following:

If the model has a regular configuration, we have then seen in appendix D that, for any t, the mean population field of $[\text{Fact} \circ \mathfrak{L}]^t(p^*)$ is $\mathfrak{S}^t \mathbf{N}^*$ and that $\forall\alpha$, $\mathfrak{S}^t \Phi(\alpha)$ [with $\Phi = \log(\bar{\mathbf{N}}^*)$] is in $\mathbb{K}_{\text{loc}}$. If the model satisfies properties (Pi), the same result comes from the Lemma E1 given below in combination with the equivalences (D1). Hence p^* is a fixed point of $[\text{Fact} \circ \mathfrak{L}]^T$ and from Proposition 4 we deduce that $\log(\bar{\mathbf{N}}^*) = \Phi$ is in $\mathbb{K}_{\text{gl}}^{r,T}$. Since $\mathbb{B}^T = \mathbb{K}_{\text{gl}}^{r,T}$, we have

$$\forall \Psi \in \mathbb{K}_{\text{gl}}^{r,T}, \qquad \langle \Psi, \mathbf{N}_n \rangle = \langle \Psi, \mathbf{N}_0 \rangle \tag{E1}$$

Hence, on going to the limit in this expression and from Proposition 3, we deduce that $\mathbf{N}^*$ is the unique mean population, denoted $\mathbf{N}_{(T)}$ in the proposition, which gives the absolute minimum of the information among the points which satisfy (E1). Hence $\mathbf{H}^*$ is the absolute minimum of the function $\mathbf{H}(\mathbf{N})$, reached inside the open set:

$$F = \{\mathbf{N} \in (]0, 1[)^b)^{\mathscr{L}}; \forall \Phi \in \mathbb{K}_{\text{gl}}^{r,T}, \langle \Phi, \mathbf{N} \rangle = \langle \Phi, \mathbf{N}_0 \rangle\}$$

The end of the proof is then achieved by standard arguments using the strict convexity of $\mathbf{H}$ on the compact subset of F which contains the sequence $(\mathbf{N}_n)$ and $\mathbf{N}^*$. Indeed the Hessian of $\mathbf{H}$ on $(]0, 1[^b)^{\mathscr{L}}$ is diagonal on the natural basis and its components are the $1/N_j(\alpha)(1 - N_j(\alpha))$. Let $m > 0$ be the upper bound of the set of scalars $\{2\mathbf{N}_j(\alpha)(1 - \mathbf{N}_j(\alpha))\}_{j,\alpha}$ when $\mathbf{N}$ belongs to the compact subset of F: $\mathbf{H}(\mathbf{N}) - \mathbf{H}(\mathbf{N}^*) \leqslant \mathbf{H}(\mathbf{N}_0) - \mathbf{H}(\mathbf{N}^*)$ (see Lemma 1). On this subset, the inequality $\mathbf{H}(\mathbf{N}) - \mathbf{H}(\mathbf{N}^*) \leqslant \varepsilon$ implies $\langle \mathbf{N} - \mathbf{N}^*, \mathbf{N} - \mathbf{N}^* \rangle \leqslant m\varepsilon$, which yields the convergence of $(\mathbf{N}_n)$ to $\mathbf{N}^*$ (one writes an order two Taylor expression of the function $\mathbf{H}$, on the segment $[\mathbf{N}^*, \mathbf{N}]$, with an integral rest). Finally, since T is finite and $\mathscr{F}$ continuous the sequence $\{\mathscr{F}^t(\mathbf{N}_0)\}$ tends toward the T-periodic sequence $\{\mathscr{F}^t(\mathbf{N}_{(T)})\}$. ∎

Lemma E1. We suppose that the transition probabilities $\{\mathscr{A}\}$ obey properties (P1)–(P3) or only property (P4). Let f be any density.

1. The equality $\mathfrak{H}(\mathfrak{L}(p)) = \mathfrak{H}(p)$ stands if and only if p satisfies

$$\mathfrak{L}(p) = p \circ \mathfrak{S}^{-1}$$

2. Furthermore, the equality $\mathfrak{H}((\mathfrak{L})^k(p)) = \mathfrak{H}(p)$ stands for a given $k \geqslant 1$ if and only if p satisfies

$$\forall i, 1 \leqslant i \leqslant k, \qquad \mathfrak{L}^i(p) = p \circ \mathfrak{S}^{-i}$$

Proof. 1. If a density f satisfies $\mathfrak{L}(p)=p\circ\mathfrak{S}^{-1}$, then a direct evaluation gives $\mathfrak{H}(\mathfrak{L}(p))=\mathfrak{H}(p)$. Conversely, if $\mathfrak{H}(\mathfrak{L}(p))=\mathfrak{H}(p)$, let us then sum relation (11A) over $\mathbf{n}''$. This yields

$$\forall \mathbf{n}, \mathbf{n}' \in \mathbf{W}^2, \qquad \mathscr{K}(\mathbf{n}', \mathbf{n})(p(\mathbf{n}') - \mathfrak{L}(\mathrm{p})(\mathbf{n})) = 0 \tag{E2}$$

Let $\mathbf{n}$ be a configuration. If we have $\mathscr{A}(\mathfrak{S}^{-1}(\mathbf{n}) \to \mathfrak{S}^{-1}(\mathbf{n})) \neq 0$, relation (E2) then implies that $\mathfrak{L}(p)(\mathbf{n}) = p(\mathfrak{S}^{-1}(\mathbf{n}))$. So point 1 is proven with property (P4).

If we have $\mathscr{A}(\mathfrak{S}^{-1}(\mathbf{n}) \to \mathfrak{S}^{-1}(\mathbf{n})) = 0$, we then use property (P3) and the semi-detailed balance to deduce the existence of at least two configurations $\mathbf{m} \neq \mathbf{r}$ such that

$$\mathscr{A}(\mathbf{m} \to \mathfrak{S}^{-1}(\mathbf{n})) \neq 0, \qquad \mathscr{A}(\mathbf{r} \to \mathfrak{S}^{-1}(\mathbf{n})) \neq 0$$

From (E2) we then know that $\mathfrak{L}(p)(\mathbf{n}) = p(\mathbf{m}) = p(\mathbf{r})$. But from properties (P1) and (P2) we also have

$$\mathscr{A}(\mathbf{m} \to \mathbf{r}) \neq 0, \qquad \mathscr{A}(\mathfrak{S}^{-1}(\mathbf{n}) \to \mathbf{r}) \neq 0$$

By using again (E2), we then obtain $\mathfrak{L}(p)(\mathfrak{S}(\mathbf{r})) = p(\mathbf{m}) = p(\mathfrak{S}^{-1}(\mathbf{n}))$. Thus we deduce that $\mathfrak{L}(p)(\mathbf{n}) = p(\mathfrak{S}^{-1}(\mathbf{n}))$. So point 1 is proven under properties (P1)–(P3).

2. Since the sequence $(\mathfrak{H}((\mathfrak{L})^n(p)))$ is decreasing, the equality $\mathfrak{H}((\mathfrak{L})^k(f)) = \mathfrak{H}(f)$ implies

$$\forall i, 1 \leqslant i < k, \qquad \mathfrak{H}((\mathfrak{L})^k(p)) = \cdots = \mathfrak{H}((\mathfrak{L})^i(p)) = \cdots = \mathfrak{H}(\mathfrak{L}(p)) = \mathfrak{H}(p)$$

We apply successively the previous result and deduce point 2. Conversely, a direct evaluation of $\mathfrak{H}((L)^k(p))$ when $\mathfrak{L}^k(p) = f\circ\mathfrak{S}^{-k}$ gives $\mathfrak{H}(p)$. ∎

APPENDIX F

Proof of Proposition 6. We will begin with the following relation, obtained in the proof of lemma A1:

$$\forall \varepsilon > 0, \exists N \in \mathbb{N}, \qquad p \geqslant N \Rightarrow \forall \mathbf{n} \in \mathbf{W} : \mathscr{K}(\mathbf{m}, \mathbf{n}) \neq 0, \mathscr{K}(\mathbf{r}, \mathbf{n}) \neq 0$$
$$\Rightarrow |f_p(\mathbf{m}) - f_p(\mathbf{r})| \leqslant \varepsilon \tag{F1}$$

Let then $\mathbf{n}$ be a fixed configuration and let us assume that $\mathscr{K}(\mathbf{m}, \mathbf{n}) \neq 0$. If $\mathscr{A}(\mathbf{n} \to \mathbf{n}) \neq 0$ and since now $\xi \neq 0$, we then have $\mathscr{K}(\mathbf{n}, \mathbf{n}) \neq 0$. Hence from the previous implication we deduce that $|f_p(\mathbf{m}) - f_p(\mathbf{n})| \leqslant \varepsilon$. In the opposite case, if $\mathscr{A}(\mathbf{n} \to \mathbf{n}) = 0$, we deduce the existence of two configurations $\mathbf{r} \neq \mathbf{r}'$ such that $\mathscr{A}(\mathbf{r} \to \mathbf{n}) \neq 0$, $\mathscr{A}(\mathbf{r}' \to \mathbf{n}) \neq 0$. Hence we will have $\mathscr{A}(\mathbf{n} \to \mathbf{r}') \neq 0$,

$\mathscr{A}(\mathbf{r} \to \mathbf{r}') \neq 0$ and (F1) implies $|f_p(\mathbf{r}) - f_p(\mathbf{n})| \leqslant \varepsilon$. But since $\mathscr{A}(\mathbf{r} \to \mathbf{n}) \neq 0$ and $\mathscr{K}(\mathbf{m}, \mathbf{n}) \neq 0$ we also deduce from (F1) that $|f_p(\mathbf{r}) - f_p(\mathbf{m})| \leqslant \varepsilon$ and so $|f_p(\mathbf{n}) - f_p(\mathbf{m})| \leqslant 2\varepsilon$. Hence we always have

$$\forall \varepsilon > 0, \exists N \in \mathbb{N}, \qquad p \geqslant N \Rightarrow \forall \mathbf{n} \in \mathscr{W} : \mathscr{K}(\mathbf{m}, \mathbf{n}) \neq 0 \Rightarrow |f_p(\mathbf{m}) - f_p(\mathbf{n})| \leqslant \varepsilon$$

Let us denote by $\mathscr{P}(\mathbf{n})$ the 1-path which contains $\mathbf{n}$. Since $\mathscr{W}$ is finite, there exists a fixed bound M such that

$$\forall \varepsilon > 0, \exists N \in \mathbb{N}, \qquad p \geqslant N \Rightarrow \forall \mathbf{n} \in \mathscr{W}: \mathbf{m} \in \mathscr{P}(\mathbf{n}) \Rightarrow |f_p(\mathbf{m}) - f_p(\mathbf{n})| \leqslant M\varepsilon$$

Summing this last relation over $\mathscr{P}(\mathbf{n})$ finally yields

$$\forall \varepsilon > 0, \exists N \in \mathbb{N}, \qquad p \geqslant N; \qquad \forall \mathbf{n} \in \mathscr{W}, \qquad |f_p(\mathbf{n}) - f^*(\mathbf{n})| \leqslant \varepsilon$$

Then, (f_n) is convergent to f^* on $\mathbf{W}$.

Proof of Proposition 7. Let f be a fixed point of $\mathfrak{L}$. Let us show that

$$\forall n, n' \in \mathscr{W}^2, \qquad \mathscr{A}(n \to n')(f(\mathbf{n}) - f(\mathbf{n}')) = 0 \tag{F2}$$

$$\forall n \in \mathscr{W}, \qquad f(\mathbf{n}) = f(\mathfrak{S}\mathbf{n}) \tag{F3}$$

First, let us assume that f is a *density*. From Proposition 1 we have

$$\mathfrak{L}(f) = f \Rightarrow \forall \mathbf{n}, \mathbf{n}' \in \mathbf{W}^2,$$
$$((1-\xi)\,\mathscr{A}(\mathbf{n}' \to \mathfrak{S}^{-1}(\mathbf{n})) + \xi \mathscr{A}(\mathbf{n}' \to \mathbf{n}))(f(\mathbf{n}') - f(\mathbf{n})) = 0$$

For $\xi \neq 0$, the relation $\mathscr{A}(\mathbf{n}' \to \mathbf{n}) \neq 0$ obviously yields $f(\mathbf{n}) = f(\mathbf{n}')$ and (F2) is proven. Using then (F2) and Definition (2a) we deduce that

$$\begin{aligned} f(n) = \mathfrak{L}(f)(n) &= (1-\xi) \sum_{\mathbf{W}} f(\mathbf{n}')\,\mathscr{A}(\mathbf{n}' \to \mathfrak{S}^{-1}(\mathbf{n})) + \xi \sum_{\mathbf{W}} f(\mathbf{n}')\,\mathscr{A}(\mathbf{n}' \to \mathbf{n}) \\ &= (1-\xi) f(\mathfrak{S}^{-1}(\mathbf{n})) + \xi f(\mathbf{n}) \end{aligned}$$

For $\xi \neq 1$ this yields (F3). Conversely, if (F2) and (F3) hold, then f is obviously a fixed point of $\mathfrak{L}$. Second, if f is any real function, we write $f = f^+ - f^-$. Since $\mathfrak{L}$ is a Markov operator, the positive functions f^+ and f^- are also fixed points of $\mathfrak{L}$. The same holds for their associated densities if they are nonzero. Since relations (F2), (F3) are linear with respect to f, we then deduce that (F2), (F3) are necessary and sufficient for f to be a fixed point of $\mathfrak{L}$. Now, if f is a linear form with respect to $\mathbf{n}$, then its associated vector is obviously a regular 1-invariant.

Proof of Lemma 2. 1. Case of models which satisfy (P1)–(P3) or (P4). When p is such that $\mathfrak{H}(\mathfrak{L}(p)) = \mathfrak{H}(p)$, the sum over $\mathbf{n}''$ of relation (11a) gives for $k=1$

$$\forall \mathbf{n}, \mathbf{n}' \in \mathbf{W}^2, \qquad \mathscr{K}(\mathbf{n}', \mathbf{n})[\mathfrak{L}(p)(\mathbf{n}) - p(\mathbf{n}')] = 0$$

Since $\xi \neq 0$, this yields: $\mathscr{A}(\mathbf{n}' \to \mathbf{n})[\mathfrak{L}(p)(\mathbf{n}) - p(\mathbf{n}')] = 0$

The previous relation implies that $\mathfrak{L}(p)(\mathbf{n}) = p(\mathbf{n})$ for any $\mathbf{n}$ such that $\mathscr{A}(\mathbf{n} \to \mathbf{n}) \neq 0$. Hence p is a fixed point of $\mathfrak{L}$ for any model obeying (P4).

Let us now consider the configurations $\mathbf{n}$ such that $\mathscr{A}(\mathbf{n} \to \mathbf{n}) = 0$. For models obeying (P3) and the semi-detailed balance, there exist at least two different configurations $\mathbf{m}$, $\mathbf{r}$ such that

$$\mathscr{A}(\mathbf{m} \to \mathbf{n}) \neq 0 \qquad \text{and} \qquad \mathscr{A}(\mathbf{r} \to \mathbf{n}) \neq 0$$

When properties (P2) and (P1) hold it follows that $\mathscr{A}(\mathbf{m} \to \mathbf{r}) \neq 0$ and $\mathscr{A}(\mathbf{n} \to \mathbf{r}) \neq 0$. Therefore we will have $\mathfrak{L}(p)(\mathbf{n}) = p(\mathbf{m}) = p(\mathbf{r})$ and $\mathfrak{L}(p)(\mathbf{r}) = p(\mathbf{m}) = p(\mathbf{n})$, then $\mathfrak{L}(p)(\mathbf{n}) = p(\mathbf{n})$. Hence p is a fixed point of $\mathfrak{L}$ for any model obeying (P1)–(P3).

2. Case of models which have a regular configuration. The analysis is similar to that of appendix D. Let $p(\mathbf{n}) = \mathfrak{k} \exp(\langle \Phi, \mathbf{n} \rangle)$ ($\mathfrak{k} > 0$) be a density which satisfies $\mathfrak{H}[\mathrm{Fact}(\mathfrak{L}((p))] = \mathfrak{H}(p)$. We then have $\mathfrak{H}[\mathrm{Fact}(\mathfrak{L}((p))] = \mathfrak{H}(p) = \mathfrak{H}[\mathfrak{L}(p)]$. Hence, $\mathfrak{L}(p)$ is itself factorized. By using the notations of Appendix D and with a similar analysis we prove that $\mathbf{N}^* = (1-\xi)\, \mathfrak{S}\mathbf{N} + \xi \mathbf{N}$, where $\mathbf{N}^*$ (resp. $\mathbf{N}$) is the mean population of $\mathfrak{L}(p)$ (resp. p). We then apply the equivalences (11a) to any configuration $\mathbf{m}_k$ in $\{\mathbf{m}_i\}$, and deduce that $p(\mathfrak{S}^{-1}(\mathbf{m}_k)) = p(\mathbf{m}_k)$, which yields $\mathbf{N} = \mathfrak{S}\mathbf{N}$ and finally $\mathbf{N}^* = \mathbf{N}$. Hence p is a factorized fixed point of $\mathfrak{L}$. ∎

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