

Statistical Mechanics of Surjective Cellular Automata

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Abstract Reversible cellular automata are seen as microscopic physical models, and their states of macroscopic equilibrium are described using invariant probability measures. We establish a connection between the invariance of Gibbs measures and the conservation of additive quantities in surjective cellular automata. Namely, we show that the simplex of shift-invariant Gibbs measures associated to a Hamiltonian is invariant under a surjective cellular automaton if and only if the cellular automaton conserves the Hamiltonian. A special case is the (well-known) invariance of the uniform Bernoulli measure under surjective cellular automata, which corresponds to the conservation of the trivial Hamiltonian. As an application, we obtain results indicating the lack of (non-trivial) Gibbs or Markov invariant measures for “sufficiently chaotic” cellular automata. We discuss the relevance of the randomization property of algebraic cellular automata to the problem of approach to macroscopic equilibrium, and pose several open questions. As an aside, a shift-invariant pre-image of a Gibbs measure under a pre-injective factor map between shifts of finite type turns out to be always a Gibbs measure. We provide a sufficient condition under which the image of a Gibbs measure under a pre-injective factor map is not a Gibbs measure. We point out a potential application of pre-injective factor maps as a tool in the study of phase transitions in statistical mechanical models.

Keywords Cellular automata · Gibbs measures · Conservation laws · Macroscopic equilibrium

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1 Introduction

Reversible cellular automata are deterministic, spatially extended, microscopically reversible dynamical systems. They provide a suitable framework—an alternative to Hamiltonian dynamics—to examine the dynamical foundations of statistical mechanics with simple caricature models. The intuitive structure of cellular automata makes them attractive to mathematicians, and their combinatorial nature makes them amenable to perfect simulations and computational study.

Some reversible cellular automata have long been observed, in simulations, to exhibit “thermodynamic behavior”: starting from a random configuration, they undergo a transient dynamics until they reach a state of macroscopic (statistical) equilibrium. Which of the equilibrium states the system is going to settle in could often be guessed on the basis of few statistics of the initial configuration.

One such example is the *Q2R* cellular automaton [91], which is a deterministic dynamics on top of the Ising model. Like the standard Ising model, a configuration of the *Q2R* model consists of an infinite array of symbols $+$ (representing an upward magnetic *spin*) and $-$ (a downward spin) arranged on the two-dimensional square lattice. The symbols are updated in iterated succession of two updating stages: at the first stage, the symbols on the even sites (the black cells of the chess board) are updated, and at the second stage, the symbols on the odd sites. The updating of a symbol is performed according to a simple rule: a spin is flipped if and only if among the four neighboring spins, there are equal numbers of upward and downward spins. The dynamics is clearly *reversible* (changing the order of the two stages, we could traverse backward in time). It also conserves the Ising energy (i.e., the number of pairs of adjacent spins that are anti-aligned).

Few snapshots from a simulation are shown in Fig. 1. Starting with a random configuration in which the direction of each spin is determined by a biased coin flip, the *Q2R* cellular automaton evolves towards a state of apparent equilibrium that resembles a sample from the Ising model at the corresponding temperature.¹ More sophisticated variants of the *Q2R* model show numerical agreement with the phase diagram of the Ising model, at least away from the critical point [15]. See [87], Chapter 17, for further simulations and an interesting discussion.

Wolfram was first to study cellular automata from the point of view of statistical mechanics [93, 94] (see also [95]). He made a detailed heuristic analysis of the so-called elementary cellular automata (those with two states per site and local rule depending on three neighboring sites in one dimension) using computer simulations. One of Wolfram’s observations (the randomizing property of the *XOR* cellular automaton) was mathematically confirmed by Lind [50], although the same result had also been obtained independently by Miyamoto [58]. Motivated by the problem of foundations of statistical mechanics, Takesue made a similar study of elementary *reversible* cellular automata and investigated their ergodic properties and thermodynamic behavior [83–85]. Recognizing the role of conservation laws in presence or absence of thermodynamic behavior, he also started a systematic study of additive conserved quantities in cellular automata [30, 86].

This article concerns the “states of macroscopic equilibrium” and their connection with conservation laws in a class of cellular automata including the reversible ones.

As in statistical mechanics, we identify the “macroscopic states” of lattice configurations with probability measures on the space of all such configurations. The justification and proper

¹ The *Q2R* model has no temperature parameter. A correspondence can however be made with the temperature at which the Ising model has the same expected energy density.

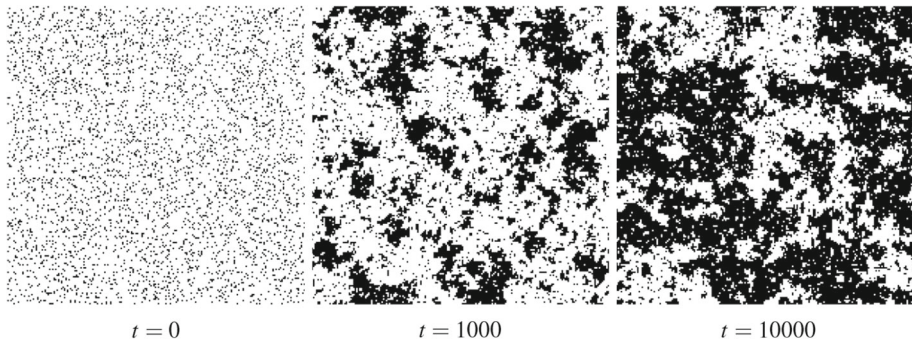


Fig. 1 Simulation of the Q2R cellular automaton on a 200×200 toroidal lattice. *Black* represents an upward spin. The initial configuration is chosen according to a Bernoulli distribution with 1:9 bias. The “macroscopic appearance” of the configuration does not vary significantly after time 10000

interpretation of this formulation is beyond the scope of this article. We content ourselves with recalling two distinct points of view: the *subjective* interpretation (probability measures are meant to describe the partial states of knowledge of an observer; see [36]) and the *frequentist* interpretation (a probability measure represents a class of configurations sharing the same statistics). See [80] for comparison and discussion. If we call tail-measurable observables “macroscopic”, a probability measure that is trivial on the tail events would give a full description of a macroscopic state (see Paragraph (7.8) of [27]). On the other hand, restricting “macroscopic” observables to statistical averages (i.e., averages of local observables over the lattice), one could identify the macroscopic states with probability measures that are shift-invariant and ergodic. The configurations in the ergodic set of a shift-ergodic probability measure (i.e., the generic points in its support; see [66]) may then be considered as “typical” microscopic states for the identified macroscopic state.

The interpretation of “equilibrium” is another unsettling issue that we leave open. Equilibrium statistical mechanics postulates that the equilibrium states (of a lattice model described by interaction energies) are suitably described by Gibbs measures (associated with the interaction energies) [27, 35, 75]. One justification (within the subjective interpretation) is the variational principle that characterizes the shift-invariant Gibbs measures as measures that maximize entropy under a fixed expected energy density constraint. Within a dynamical framework, on the other hand, the system is considered to be in macroscopic equilibrium if its internal fluctuations are not detected by macroscopic observables. One is therefore tempted to identify the equilibrium states of a cellular automaton with (tail-trivial or shift-ergodic) probability measures that are time-invariant. Unfortunately, there are usually an infinity of invariant measures that do not seem to be of physical relevance. For instance, in any cellular automaton, the uniform distribution on the shift and time orbit of a jointly periodic configuration is time-invariant and shift-ergodic, but may hardly be considered a macroscopic equilibrium state. Other conditions such as “smoothness” or “attractiveness” therefore might be needed.

Rather than reversible cellular automata (i.e., those whose trajectories can be traced backward by another cellular automaton), we work with the broader class of surjective cellular automata (i.e., those that act surjectively on the configuration space). Every reversible cellular automaton is surjective, but there are many surjective cellular automata that are not reversible. Surjective cellular automata are nevertheless “almost injective” in that the average amount of information per site they erase in each time step is vanishing. They are precisely

those cellular automata that preserve the uniform Bernoulli measure (cf. Liouville's theorem for Hamiltonian systems). Even if not necessarily physically relevant, they provide a richer source of interesting examples, which could be used in case studies. For instance, most of the known examples of the randomization phenomenon (which, we shall argue, could provide an explanation of approach to equilibrium) are in non-reversible surjective cellular automata.

The invariance of Gibbs measures under surjective cellular automata turns out to be associated with their conservation laws. More precisely, if an additive energy-like quantity, formalized by a Hamiltonian, is conserved by a surjective cellular automaton, the cellular automaton maps the simplex of shift-invariant Gibbs measures corresponding to that Hamiltonian onto itself (Theorem 6). The converse is true in a stronger sense: if a surjective cellular automaton maps a (not necessarily shift-invariant) Gibbs measure for a Hamiltonian to a Gibbs measure for the same Hamiltonian, the Hamiltonian must be conserved by the cellular automaton (Corollary 10). The proof of this correspondence is an immediate consequence of the variational characterization of shift-invariant Gibbs measures and the fact that surjective cellular automata preserve the average entropy per site of shift-invariant probability measures (Theorem 4). An elementary proof of a special case was presented earlier [42].

Note that if a conserved Hamiltonian has a unique Gibbs measure, then that unique Gibbs measure will be invariant under the cellular automaton. This is the case, for example, in one dimension, or when the Hamiltonian does not involve the interaction of more than one site (the Bernoulli case). An important special case is the *trivial* Hamiltonian (all configurations on the same "energy" level) which is obviously conserved by every surjective cellular automaton. The uniform Bernoulli measure is the unique Gibbs measure for the trivial Hamiltonian, and we recover the well-known fact that every surjective cellular automaton preserves the uniform Bernoulli measure on its configuration space (i.e., Corollary 4). If, on the other hand, the simplex of shift-invariant Gibbs measures for a conserved Hamiltonian has more than one element, the cellular automaton does not need to preserve individual Gibbs measures in this simplex (Example 9).

We do not know whether, in general, a surjective cellular automaton maps the non-shift-invariant Gibbs measures for a conserved Hamiltonian to Gibbs measures for the same Hamiltonian, but this is known to be the case for a proper subclass of surjective cellular automata including the reversible ones (Theorem 5), following a result of Ruelle.

The essence of the above-mentioned connection between conservation laws and invariant Gibbs measures comes about in a more abstract setting, concerning the pre-injective factor maps between strongly irreducible shifts of finite type. We show that a shift-invariant pre-image of a (shift-invariant) Gibbs measure under such a factor map is again a Gibbs measure (Corollary 7). We find a simple sufficient condition under which a pre-injective factor map transforms a shift-invariant Gibbs measure into a measure that is not Gibbs (Proposition 9). An example of a surjective cellular automaton is given that eventually transforms every starting Gibbs measure into a non-Gibbs measure (Example 7). As an application in the study of phase transitions in equilibrium statistical mechanics, we demonstrate how the result of Aizenman and Higuchi regarding the structure of the simplex of Gibbs measures for the two-dimensional Ising model could be more transparently formulated using a pre-injective factor map (Example 5).

The correspondence between invariant Gibbs measures and conservation laws allows us to reduce the problem of invariance of Gibbs measures to the problem of conservation of additive quantities. Conservation laws in cellular automata have been studied by many from various points of view (see e.g. [3, 6, 18, 24–26, 30, 62, 68, 74]). For example, simple algorithms have been proposed to find all additive quantities of up to a given interaction range that are conserved by a cellular automaton. Such an algorithm can be readily applied

to find all the full-support Markov measures that are invariant under a surjective cellular automaton (at least in one dimension). We postpone the study of this and similar algorithmic problems to a separate occasion.

A highlight of this article is the use of this correspondence to obtain severe restrictions on the existence of invariant Gibbs measures in two interesting classes of cellular automata with strong chaotic behavior. First, we show that a strongly transitive cellular automaton cannot have any invariant Gibbs measure other than the uniform Bernoulli measure (Corollary 11). The other result concerns the class of one-dimensional reversible cellular automata that are obtained by swapping the role of time and space in positively expansive cellular automata. For such reversible cellular automata, we show that the uniform Bernoulli measure is the unique invariant Markov measure with full support (Corollary 13).

Back to the interpretation of shift-ergodic probability measures as macroscopic states, one might interpret the latter results as an indication of “absence of phase transitions” in the cellular automata in question. Much sharper results have been obtained by others for narrower classes of cellular automata having algebraic structures (see the references in Example 10).

A mathematical description of approach to equilibrium (as observed in the Q2R example) seems to be very difficult in general. The randomization property of algebraic cellular automata (the result of Miyamoto and Lind and its extensions; see Example 13) however provides a partial explanation of approach to equilibrium in such cellular automata. Finding “physically interesting” cellular automata with similar randomization property is an outstanding open problem.

The structure of the paper is as follows. Section 2 is dedicated to the development of the setting and background material. Given the interdisciplinary nature of the subject, we try to be as self-contained as possible. Basic results regarding the pre-injective factor maps between shifts of finite type as well as two degressing applications appear in Sect. 3. In Sect. 4, we apply the results of the previous section on cellular automata. Conservation laws in cellular automata are discussed in Sect. 4.1. Proving the absence of non-trivial conservation laws in two classes of chaotic cellular automata in Sect. 4.3, we obtain results regarding the rigidity of invariant measures for these two classes. Section 4.4 contains a discussion of the problem of approach to equilibrium.

2 Background

2.1 Observables, Probabilities, and Dynamical Systems

Let \mathcal{X} be a compact metric space. By an *observable* we mean a Borel measurable function $f: \mathcal{X} \rightarrow \mathbb{R}$. The set of continuous observables on \mathcal{X} will be denoted by $C(\mathcal{X})$. This is a Banach space with the uniform norm. The default topology on $C(\mathcal{X})$ is the topology of the uniform norm. The set of Borel probability measures on \mathcal{X} will be denoted by $\mathcal{P}(\mathcal{X})$. The expectation operator of a Borel probability measure $\pi \in \mathcal{P}(\mathcal{X})$ is a positive linear (and hence continuous) functional on $C(\mathcal{X})$. Conversely, the Riesz representation theorem states that every normalized positive linear functional on $C(\mathcal{X})$ is the expectation operator of a unique probability measure on \mathcal{X} . Therefore, the Borel probability measures can equivalently be identified as normalized positive linear functionals on $C(\mathcal{X})$. We assume that $\mathcal{P}(\mathcal{X})$ is topologized with the weak topology. This is the weakest topology with respect to which, for every observable $f \in C(\mathcal{X})$, the mapping $\pi \mapsto \pi(f)$ is continuous. The space $\mathcal{P}(\mathcal{X})$ under the weak topology is compact and metrizable. If δ_x denotes the Dirac measure concentrated

at $x \in \mathcal{X}$, the map $x \mapsto \delta_x$ is an embedding of \mathcal{X} into $\mathcal{P}(\mathcal{X})$. The Dirac measures are precisely the extreme elements of the convex set $\mathcal{P}(\mathcal{X})$, and by the Krein–Milman theorem, $\mathcal{P}(\mathcal{X})$ is the closed convex hull of the Dirac measures.

Let \mathcal{X} and \mathcal{Y} be compact metric spaces and $\Phi: \mathcal{X} \rightarrow \mathcal{Y}$ a continuous mapping. We denote the induced mapping $\mathcal{P}(\mathcal{X}) \rightarrow \mathcal{P}(\mathcal{Y})$ by the same symbol Φ ; hence $(\Phi\pi)(E) \triangleq \pi(\Phi^{-1}E)$. The dual map $C(\mathcal{Y}) \rightarrow C(\mathcal{X})$ is denoted by Φ^* ; that is, $(\Phi^*f)(x) \triangleq f(\Phi x)$. The following lemma is well-known.

Lemma 1 *Let \mathcal{X} and \mathcal{Y} be compact metric spaces and $\Phi: \mathcal{X} \rightarrow \mathcal{Y}$ a continuous map.*

- (a) $\Phi: \mathcal{X} \rightarrow \mathcal{Y}$ is one-to-one if and only if $\Phi^*: C(\mathcal{Y}) \rightarrow C(\mathcal{X})$ is onto, which in turn holds if and only if $\Phi: \mathcal{P}(\mathcal{X}) \rightarrow \mathcal{P}(\mathcal{Y})$ is one-to-one.
- (b) $\Phi: \mathcal{X} \rightarrow \mathcal{Y}$ is onto if and only if $\Phi^*: C(\mathcal{Y}) \rightarrow C(\mathcal{X})$ is one-to-one, which in turn holds if and only if $\Phi: \mathcal{P}(\mathcal{X}) \rightarrow \mathcal{P}(\mathcal{Y})$ is onto.

Proof (a) Suppose that $\Phi: \mathcal{X} \rightarrow \mathcal{Y}$ is one-to-one. Let $g \in C(\mathcal{X})$ be arbitrary. Define $\mathcal{Y}_0 \triangleq \Phi\mathcal{X}$. Then $g \circ \Phi^{-1}: \mathcal{Y}_0 \rightarrow \mathbb{R}$ is a continuous real-valued function on a closed subset of a compact metric space. Hence, by the Tietze extension theorem, it has an extension $f: \mathcal{Y} \rightarrow \mathbb{R}$. We have $f \circ \Phi = g \circ \Phi^{-1} \circ \Phi = g$. Therefore, $\Phi^*: C(\mathcal{Y}) \rightarrow C(\mathcal{X})$ is onto.

The other implications are trivial.

- (b) Suppose that $\Phi: \mathcal{X} \rightarrow \mathcal{Y}$ is not onto. Let $\mathcal{Y}_0 \triangleq \Phi\mathcal{X}$ and pick an arbitrary $y \in \mathcal{Y} \setminus \mathcal{Y}_0$. Using the Tietze extension theorem, we can find $f, f' \in C(\mathcal{Y})$ such that $f|_{\mathcal{Y}_0} = f'|_{\mathcal{Y}_0}$ but $f(y) \neq f'(y)$. Then $f \circ \Phi = f' \circ \Phi$. Hence, $\Phi^*: C(\mathcal{Y}) \rightarrow C(\mathcal{X})$ is not one-to-one. Next, suppose that $\Phi: \mathcal{X} \rightarrow \mathcal{Y}$ is onto. By the Krein–Milman theorem, the set $\mathcal{P}(\mathcal{Y})$ is the closed convex hull of Dirac measures on \mathcal{Y} . Let $\pi = \sum_i \lambda_i \delta_{y_i} \in \mathcal{P}(\mathcal{Y})$ be a convex combination of Dirac measures. Pick $x_i \in \mathcal{X}$ such that $\Phi x_i = y_i$, and define $\nu \triangleq \sum_i \lambda_i \delta_{x_i} \in \mathcal{P}(\mathcal{X})$. Then $\Phi\nu = \pi$. Therefore, $\Phi\mathcal{P}(\mathcal{X})$ is dense in $\mathcal{P}(\mathcal{Y})$. Since $\Phi\mathcal{P}(\mathcal{X})$ is also closed, we obtain that $\Phi\mathcal{P}(\mathcal{X}) = \mathcal{P}(\mathcal{Y})$. That is, $\Phi: \mathcal{P}(\mathcal{X}) \rightarrow \mathcal{P}(\mathcal{Y})$ is onto.

The remaining implication is trivial. □

By a *dynamical system* we shall mean a compact metric space \mathcal{X} together with a continuous action $(i, x) \mapsto \varphi^i x$ of a discrete commutative finitely generated group or semigroup \mathbb{L} on \mathcal{X} . In case of a cellular automaton, \mathbb{L} is the set of non-negative integers \mathbb{N} (or the set of integers \mathbb{Z} if the cellular automaton is reversible). For a d -dimensional shift, \mathbb{L} is the d -dimensional hyper-cubic lattice \mathbb{Z}^d . Every dynamical system (\mathcal{X}, φ) has at least one invariant measure, that is, a probability measure $\pi \in \mathcal{P}(\mathcal{X})$ such that $\varphi^i \pi = \pi$ for every $i \in \mathbb{L}$. In fact, every non-empty, closed and convex subset of $\mathcal{P}(\mathcal{X})$ that is closed under the application of φ contains an invariant measure. We will denote the set of invariant measures of (\mathcal{X}, φ) by $\mathcal{P}(\mathcal{X}, \varphi)$.

We also define $C(\mathcal{X}, \varphi)$ as the closed linear subspace of $C(\mathcal{X})$ generated by the observables of the form $g \circ \varphi^i - g$ for $g \in C(\mathcal{X})$ and $i \in \mathbb{L}$; that is,

$$C(\mathcal{X}, \varphi) \triangleq \overline{\langle g \circ \varphi^i - g : g \in C(\mathcal{X}) \text{ and } i \in \mathbb{L} \rangle} \tag{1}$$

(see [75], Sects. 4.7–4.8). Then $\mathcal{P}(\mathcal{X}, \varphi)$ and $C(\mathcal{X}, \varphi)$ are annihilators of each other:

Lemma 2 (see e.g. [43], Proposition 2.13) *Let (\mathcal{X}, φ) be a dynamical system. Then,*

- (a) $\mathcal{P}(\mathcal{X}, \varphi) = \{\pi \in \mathcal{P}(\mathcal{X}) : \pi(f) = 0 \text{ for every } f \in C(\mathcal{X}, \varphi)\}$.

(b) $C(\mathcal{X}, \varphi) = \{f \in C(\mathcal{X}) : \pi(f) = 0 \text{ for every } \pi \in \mathcal{P}(\mathcal{X}, \varphi)\}$.

Proof (a) A probability measure π on \mathcal{X} is in $\mathcal{P}(\mathcal{X}, \varphi)$ if and only if $\pi(g \circ \varphi^i - g) = 0$ for every $g \in C(\mathcal{X})$ and $i \in \mathbb{L}$. Furthermore, for each π , the set $\{f \in C(\mathcal{X}) : \pi(f) = 0\}$ is a closed linear subspace of $C(\mathcal{X})$. Therefore, the equality in (a) holds.

(b) Let us denote the righthand side of the claimed equality in (b) by D . The set D is closed and linear, and contains all the elements of the form $g \circ \varphi^i - g$ for all $g \in C(\mathcal{X})$ and $i \in \mathbb{L}$. Therefore, $C(\mathcal{X}, \varphi) \subseteq D$. Conversely, let $f \in C(\mathcal{X}) \setminus C(\mathcal{X}, \varphi)$. Then every element $h \in \langle f, C(\mathcal{X}, \varphi) \rangle$ has a unique representation $h = a_h f + u_h$ where $a_h \in \mathbb{R}$ and $u_h \in C(\mathcal{X}, \varphi)$. Define the linear functional $J: \langle f, C(\mathcal{X}, \varphi) \rangle \rightarrow \mathbb{R}$ by $J(h) = J(a_h f + u_h) \triangleq a_h$. Then J is bounded ($\|h\| = \|a_h f + u_h\| \geq a_h \delta = |J(h)| \delta$, where $\delta > 0$ is the distance between f and $C(\mathcal{X}, \varphi)$), and hence, by the Hahn-Banach theorem, has a bounded linear extension \widehat{J} on $C(\mathcal{X})$. According to the Riesz representation theorem, there is a unique signed measure π on \mathcal{X} such that $\pi(h) = \widehat{J}(h)$ for every $h \in C(\mathcal{X})$. Let $\pi = \pi^+ - \pi^-$ be the Hahn decomposition of π . Since $\pi(f) = 1$, either $\pi^+(f) > 0$ or $\pi^-(f) > 0$. If $\pi^+(f) > 0$, define $\pi^* \triangleq \frac{1}{\pi^+(\mathcal{X})} \pi^+$; otherwise $\pi^* \triangleq \frac{1}{\pi^-(\mathcal{X})} \pi^-$. Then π^* is a probability measure with $\pi^*(u) = 0$ for every $u \in C(\mathcal{X}, \varphi)$, which according to part (a), ensures that $\pi^* \in \mathcal{P}(\mathcal{X}, \varphi)$. On the other hand $\pi^*(f) > 0$, and hence $f \notin D$. We conclude that $C(\mathcal{X}, \varphi) = D$. □

If $K(\mathcal{X})$ is a dense subspace of $C(\mathcal{X})$, the subspace $C(\mathcal{X}, \varphi)$ can also be expressed in terms of $K(\mathcal{X})$. Namely, if we define

$$K(\mathcal{X}, \varphi) \triangleq \langle h \circ \varphi^i - h : h \in K(\mathcal{X}) \text{ and } i \in \mathbb{L} \rangle, \tag{2}$$

then $C(\mathcal{X}, \varphi) = \overline{K(\mathcal{X}, \varphi)}$. If D_0 is a finite generating set for the group/semigroup \mathbb{L} , the subspace $K(\mathcal{X}, \varphi)$ may also be expressed as

$$\left\{ \sum_{i \in D_0} (h_i \circ \varphi^i - h_i) : h_i \in K(\mathcal{X}) \right\}. \tag{3}$$

In particular, if $\mathbb{L} = \mathbb{Z}$ or $\mathbb{L} = \mathbb{N}$, then every element of $K(\mathcal{X}, \varphi)$ is of the form $h \circ \varphi - h$ for some $h \in K(\mathcal{X})$.

A morphism between two dynamical systems (\mathcal{X}, φ) and (\mathcal{Y}, ψ) is a continuous map $\Theta: \mathcal{X} \rightarrow \mathcal{Y}$ such that $\Theta \varphi = \psi \Theta$. An epimorphism (i.e., an onto morphism) is also called a *factor map*. If $\Theta: \mathcal{X} \rightarrow \mathcal{Y}$ is a factor map, then (\mathcal{Y}, ψ) is a *factor* of (\mathcal{X}, φ) , and (\mathcal{X}, φ) is an *extension* of (\mathcal{Y}, ψ) . A monomorphism (i.e., a one-to-one morphism) is also known as an *embedding*. If (\mathcal{Y}, ψ) is embedded in (\mathcal{X}, φ) by the inclusion map, (\mathcal{Y}, ψ) is called a *subsystem* of (\mathcal{X}, φ) . A *conjugacy* between dynamical systems is the same as an isomorphism; two systems are said to be conjugate if they are isomorphic.

2.2 Shifts and Cellular Automata

A cellular automaton is a dynamical system on symbolic configurations on a lattice. The configuration space itself has translational symmetry and can be considered as a dynamical system with the shift action. We allow constraints on the local arrangement of symbols to include models with so-called hard interactions, such as the hard-core model (Example 3) or the contour model (Example 2). Such a restricted configuration space is modeled by a (strongly irreducible) shift of finite type.

The sites of the d -dimensional (hypercubic) lattice are indexed by the elements of the group $\mathbb{L} \triangleq \mathbb{Z}^d$. A neighborhood is a non-empty finite set $N \subseteq \mathbb{L}$ and specifies a notion of closeness between the lattice sites. The N -neighborhood of a site $a \in \mathbb{L}$ is the set $N(a) \triangleq a + N = \{a + i : i \in N\}$. Likewise, the N -neighborhood of a set $A \subseteq \mathbb{L}$ is $N(A) \triangleq A + N \triangleq \{a + i : a \in A \text{ and } i \in N\}$. The (symmetric) N -boundary of a set $A \subseteq \mathbb{L}$ is $\partial N(A) \triangleq N(A) \cap N(\mathbb{L} \setminus A)$. For a set $A \subseteq \mathbb{L}$, we denote by $N^{-1}(A) \triangleq A - N$ the set of all sites $b \in \mathbb{L}$ that have an N -neighbor in A .

A configuration is an assignment $x : \mathbb{L} \rightarrow S$ of symbols from a finite set S to the lattice sites. The symbol $x(i)$ assigned to a site $i \in \mathbb{L}$ is also called the state of site i in x . For two configurations $x, y : \mathbb{L} \rightarrow S$, we denote by $\text{diff}(x, y) \triangleq \{i \in \mathbb{L} : x(i) \neq y(i)\}$ the set of sites on which x and y disagree. Two configurations x and y are said to be asymptotic (or tail-equivalent) if $\text{diff}(x, y)$ is finite. If $D \subseteq \mathbb{L}$ is finite, an assignment $p : D \rightarrow S$ is called a pattern on D . If $p : D \rightarrow S$ and $q : E \rightarrow S$ are two patterns (or partial configurations) that agree on $D \cap E$, we denote by $p \vee q$ the pattern (or partial configuration) that agrees with p on D and with q on E .

Let S be a finite set of symbols with at least two elements. The set $S^{\mathbb{L}}$ of all configurations of symbols from S on \mathbb{L} is given the product topology, which is compact and metrizable. The convergence in this topology is equivalent to site-wise eventual agreement. If $D \subseteq \mathbb{L}$ is a finite set and x a configuration (or a partial configuration whose domain includes D), the set

$$[x]_D \triangleq \{y \in S^{\mathbb{L}} : y|_D = x|_D\} \tag{4}$$

is called a cylinder with base D . If $p : D \rightarrow S$ is a pattern, we may write more concisely $[p]$ rather than $[p]_D$. In one dimension (i.e., if $\mathbb{L} = \mathbb{Z}$), we may also use words to specify cylinder sets: if $u = u_0u_1 \cdots u_{n-1} \in S^*$ is a word over the alphabet S and $k \in \mathbb{Z}$, we write $[u]_k$ for the set of configurations $x \in S^{\mathbb{Z}}$ such that $x_{k+i} = u_i$ for each $0 \leq i < n$. The cylinders are clopen (i.e., both open and close) and form a basis for the product topology. The Borel σ -algebra on $S^{\mathbb{L}}$ is denoted by \mathfrak{F} . For $A \subseteq \mathbb{L}$, the sub- σ -algebra of events occurring in A (i.e., the σ -algebra generated by the cylinders whose base is a subset of A) will be denoted by \mathfrak{F}_A .

Given a configuration $x : \mathbb{L} \rightarrow S$ and an element $k \in \mathbb{L}$, we denote by $\sigma^k x$ the configuration obtained by shifting (or translating) x by vector k ; that is, $(\sigma^k x)(i) \triangleq x(k + i)$ for every $i \in \mathbb{L}$. The dynamical system defined by the action of the shift σ on $S^{\mathbb{L}}$ is called the full shift. A closed shift-invariant set $\mathcal{X} \subseteq S^{\mathbb{L}}$ is called a shift space and the subsystem of $(S^{\mathbb{L}}, \sigma)$ obtained by restricting σ to \mathcal{X} is called a shift system. We shall use the same symbol σ for the shift action of all shift systems. This will not lead to confusion, as the domain will always be clear from the context.

A shift space $\mathcal{X} \subseteq S^{\mathbb{L}}$ is uniquely determined by its forbidden patterns, that is, the patterns $p : D \rightarrow S$ such that $[p]_D \cap \mathcal{X} = \emptyset$. Conversely, every set F of patterns defines a shift space by forbidding the occurrence of the elements of F ; that is,

$$\mathcal{X}_F \triangleq S^{\mathbb{L}} \setminus \left(\bigcup_{i \in \mathbb{L}} \bigcup_{p \in F} \sigma^{-i}[p] \right). \tag{5}$$

The set of patterns $p : D \rightarrow S$ that are allowed in \mathcal{X} (i.e., $[p] \cap \mathcal{X} \neq \emptyset$) is denoted by $L(\mathcal{X})$. If $D \subseteq \mathbb{L}$ is finite, we denote by $L_D(\mathcal{X}) \triangleq L(\mathcal{X}) \cap S^D$ the set of patterns on D that are allowed in \mathcal{X} . For every pattern $p \in L_D(\mathcal{X})$, there is a configuration $x \in \mathcal{X}$ such that $p \vee x|_{\mathbb{L} \setminus D} \in \mathcal{X}$. Given a finite set $D \subseteq \mathbb{L}$ and a configuration $x \in \mathcal{X}$, we write $L_D(\mathcal{X} | x)$ the set of patterns $p \in L_D(\mathcal{X})$ such that $p \vee x|_{\mathbb{L} \setminus D} \in \mathcal{X}$.

A shift (\mathcal{X}, σ) (or a shift space \mathcal{X}) is *of finite type*, if \mathcal{X} can be identified by forbidding a finite set of patterns, that is, $\mathcal{X} = \mathcal{X}_F$ for a finite set F . The shifts of finite type have the following gluing property: for every shift of finite type (\mathcal{X}, σ) , there is a neighborhood $0 \in M \subseteq \mathbb{L}$ such that for every two sets $A, B \subseteq \mathbb{L}$ with $M(A) \cap M(B) = \emptyset$ and every two configurations $x, y \in \mathcal{X}$ that agree outside $A \cup B$, there is another configuration $z \in \mathcal{X}$ that agrees with x outside B and with y outside A . A similar gluing property is the *strong irreducibility*: a shift (\mathcal{X}, σ) is *strongly irreducible* if there is a neighborhood $0 \in M \subseteq \mathbb{L}$ such that for every two sets $A, B \subseteq \mathbb{L}$ with $M(A) \cap M(B) = \emptyset$ and every two configurations $x, y \in \mathcal{X}$, there is another configuration $z \in \mathcal{X}$ that agrees with x in A and with y in B . Note that strong irreducibility is a stronger version of topological mixing. A dynamical system (\mathcal{X}, φ) is (topologically) *mixing* if for every two non-empty open sets $U, V \subseteq \mathcal{X}$, $U \cap \varphi^{-t}V \neq \emptyset$ for all but finitely many t . A one-dimensional shift of finite type is strongly irreducible if and only if it is mixing. Our primary interest in this article will be the shifts of finite type that are strongly irreducible, for these are sufficiently broad to encompass the configuration space of most physically interesting lattice models.

The morphisms between shift systems are the same as the sliding block maps. A map $\Theta: \mathcal{X} \rightarrow \mathcal{Y}$ between two shift spaces $\mathcal{X} \subseteq S^{\mathbb{L}}$ and $\mathcal{Y} \subseteq T^{\mathbb{L}}$ is a *sliding block map* if there is a neighborhood $0 \in N \subseteq \mathbb{L}$ (a *neighborhood* for Θ) and a function $\theta: L_N(\mathcal{X}) \rightarrow T$ (a *local rule* for Θ) such that

$$(\Theta x)(i) \triangleq \theta \left((\sigma^i x)|_N \right) \tag{6}$$

for every configuration $x \in \mathcal{X}$ and every site $i \in \mathbb{L}$. Any sliding block map is continuous and commutes with the shift, and hence, is a morphism. Conversely, every morphism between shift systems is a sliding block map. Finite type property and strong irreducibility are both conjugacy invariants. A morphism $\Theta: \mathcal{X} \rightarrow \mathcal{Y}$ between two shifts (\mathcal{X}, σ) and (\mathcal{Y}, σ) is said to be *pre-injective* if for every two distinct asymptotic configuration $x, y \in \mathcal{X}$, the configurations Θx and Θy are distinct.

A *cellular automaton* on a shift space \mathcal{X} is a dynamical system identified by an endomorphism $\Phi: \mathcal{X} \rightarrow \mathcal{X}$ of (\mathcal{X}, σ) . The evolution of a cellular automaton starting from a configuration $x \in \mathcal{X}$ is seen as synchronous updating of the state of different sites in x using the local rule of Φ . A cellular automaton (\mathcal{X}, Φ) is said to be *surjective* (resp., *injective*, *pre-injective*, *bijective*) if Φ is surjective (resp., injective, pre-injective, bijective). If Φ is bijective, the cellular automaton is further said to be *reversible*, for (\mathcal{X}, Φ^{-1}) is also a cellular automaton. In this article, we only work with cellular automata that are defined over strongly irreducible shifts of finite type. It is well-known that for cellular automata over strongly irreducible shifts of finite type, surjectivity and pre-injectivity are equivalent (the *Garden-of-Eden* theorem; see below). In particular, every injective cellular automaton is also surjective, and hence reversible.

Let $\mathcal{X} \subseteq S^{\mathbb{L}}$ be a shift space. A linear combination of characteristic functions of cylinder sets is called a *local observable*. An observable $f: \mathcal{X} \rightarrow \mathbb{R}$ is local if and only if it is \mathfrak{F}_D -measurable for a finite set $D \subseteq \mathbb{L}$. A finite set D with such property is a *base* for f ; the value of f at a configuration x can be evaluated by looking at x “through the window D ”. The set of all local observables on \mathcal{X} , denoted by $K(\mathcal{X})$, is dense in $C(\mathcal{X})$. The set of all local observables on \mathcal{X} with base D is denoted by $K_D(\mathcal{X})$.

Let $D \subseteq \mathbb{L}$ be a non-empty finite set. The *D-block presentation* of a configuration $x: \mathbb{L} \rightarrow S$ is a configuration $x^{[D]}: \mathbb{L} \rightarrow S^D$, where $x^{[D]}(i) \triangleq x|_{i+D}$. If \mathcal{X} is a shift space, the set of *D-block presentations* of the elements of \mathcal{X} is called the *D-block presentation* of \mathcal{X} , and is denoted by $\mathcal{X}^{[D]}$. The shifts (\mathcal{X}, σ) and $(\mathcal{X}^{[D]}, \sigma)$ are conjugate via the map $x \mapsto x^{[D]}$.

More background on shifts and cellular automata (from the view point of dynamical systems) can be found in the books [45,48,49].

2.3 Hamiltonians and Gibbs Measures

We will use the term Hamiltonian in more or less the same sense as in the Ising model or other lattice models from statistical mechanics, except that we do not require it to be interpreted as “energy”. A Hamiltonian formalizes the concept of a local and additive quantity, be it energy, momentum or a quantity with no familiar physical interpretation.

Let \mathcal{X} be an arbitrary set. A *potential difference* on \mathcal{X} is a partial mapping $\Delta : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ such that

- (a) $\Delta(x, x) = 0$ for every $x \in \mathcal{X}$,
- (b) $\Delta(y, x) = -\Delta(x, y)$ whenever $\Delta(x, y)$ exists, and
- (c) $\Delta(x, z) = \Delta(x, y) + \Delta(y, z)$ whenever $\Delta(x, y)$ and $\Delta(y, z)$ both exist.

Let $\mathcal{X} \subseteq S^{\mathbb{L}}$ be a shift space. A potential difference Δ on \mathcal{X} is a (relative) *Hamiltonian* if

- (d) $\Delta(x, y)$ exists precisely when x and y are asymptotic,
- (e) $\Delta(\sigma^a x, \sigma^a y) = \Delta(x, y)$ whenever $\Delta(x, y)$ exists and $a \in \mathbb{L}$, and
- (f) For every finite $D \subseteq \mathbb{L}$, Δ is continuous when restricted to pairs (x, y) with $\text{diff}(x, y) \subseteq D$.

Note that due to the compactness of \mathcal{X} , the latter continuity is uniform among all pairs (x, y) with $\text{diff}(x, y) \subseteq D$. If the condition (f) is strengthened by the following condition, we say that Δ is a *finite-range* Hamiltonian.

- (f') There exists a neighborhood $0 \in M \subseteq \mathbb{L}$ (the *interaction neighborhood* of Δ) such that $\Delta(x, y)$ depends only on the restriction of x and y to $M(\text{diff}(x, y))$.

Hamiltonians in statistical mechanics are usually constructed by assigning interaction energies to different local arrangements of site states. Equivalently, they can be constructed using observables. A local observable $f \in K(\mathcal{X})$ defines a finite-range Hamiltonian Δ_f on \mathcal{X} via

$$\Delta_f(x, y) \triangleq \sum_{i \in \mathbb{L}} [f(\sigma^i y) - f(\sigma^i x)] \tag{7}$$

for every two asymptotic configurations $x, y \in \mathcal{X}$. The value of $f \circ \sigma^i$ is then interpreted as the contribution of site i to the energy-like quantity formalized by Δ_f . The same construction works for non-local observables that are “sufficiently short-ranged” (i.e., whose dependence on faraway sites decays rapidly). The *variation* of an observable $f : \mathcal{X} \rightarrow \mathbb{R}$ relative to a finite set $A \subseteq \mathbb{L}$ is defined as

$$\text{var}_A(f) = \sup_{\substack{x, y \in \mathcal{X} \\ x=y \text{ on } A}} |f(y) - f(x)|, \tag{8}$$

where the supremum is taken over all pairs of configurations x and y in \mathcal{X} that agree on A . A continuous observable f is said to have *summable variations* if

$$\sum_{n=0}^{\infty} |\partial I_n| \text{var}_{I_n}(f) < \infty, \tag{9}$$

where $I_n \triangleq [-n, n]^d$ and $\partial I_n \triangleq I_{n+1} \setminus I_n$. Every observable f that has summable variations defines a Hamiltonian via (7), in which the sum is absolutely convergent. We denote the set of observables with summable variations with $SV(\mathcal{X})$. Note that $K(\mathcal{X}) \subseteq SV(\mathcal{X}) \subseteq C(\mathcal{X})$.

Question 1 Is every Hamiltonian on a strongly irreducible shift of finite type generated by an observable with summable variations via (7)? Is every finite-range Hamiltonian on a strongly irreducible shift of finite type generated by a local observable?

Proposition 1 *Every finite-range Hamiltonian on a full shift is generated by a local observable.*

Proof The idea is to write the Hamiltonian as a telescopic sum (see e.g. [30], or [41], Sect. 5).

Let Δ be a finite-range Hamiltonian with interaction range M . Let \diamond be an arbitrary uniform configuration. Let \leq be the lexicographic order on $\mathbb{L} = \mathbb{Z}^d$, and denote by $\text{succ}(k)$, the successor of site $k \in \mathbb{L}$ in this ordering. For every configuration z that is asymptotic to \diamond , we can write

$$\Delta(\diamond, z) = \sum_{k \in \mathbb{L}} \Delta(z_k, z_{\text{succ}(k)}), \tag{10}$$

where z_k is the configuration that agrees with z on every site $i < k$ and with \diamond on every site $i \geq k$. Note that all but a finite number of terms in the above sum are 0.

For every configuration z , we define $f(z) \triangleq \Delta(z_0, z_{\text{succ}(0)})$ with the same definition for z_k as above. This is clearly a local observable with base M . If z is asymptotic to \diamond , the above telescopic expansion shows that $\Delta(\diamond, z) = \Delta_f(\diamond, z)$. If x and y are arbitrary asymptotic configurations, we have $\Delta(x, y) = \Delta(\hat{x}, \hat{y}) = \Delta(\diamond, \hat{y}) - \Delta(\diamond, \hat{x})$, where \hat{x} and \hat{y} are the configurations that agree, respectively, with x and y on $M^{-1}(M(\text{diff}(x, y)))$ and with \diamond everywhere else. Therefore, we can write $\Delta(x, y) = \Delta(\hat{x}, \hat{y}) = \Delta_f(\hat{x}, \hat{y}) = \Delta_f(x, y)$. \square

Whether the above proposition extends to finite-range Hamiltonians on strongly irreducible shifts of finite type is not known, but in [12], examples of shifts of finite type are given on which not every finite-range Hamiltonian is generated by a local observable. On the other hand, the main result of [11] implies that on a one-dimensional mixing shift of finite type, every finite-range Hamiltonian can be generated by a local observable.

The *trivial* Hamiltonian on \mathcal{X} (i.e., the Hamiltonian Δ for which $\Delta(x, y) = 0$ for all asymptotic $x, y \in \mathcal{X}$) plays a special role as it identifies an important notion of equivalence between observables (see Sect. 2.5).

Another important concept regarding Hamiltonians is that of ground configurations. Let $\mathcal{X} \subseteq S^{\mathbb{L}}$ be a shift space and Δ a Hamiltonian on \mathcal{X} . A *ground* configuration for Δ is a configuration $z \in \mathcal{X}$ such that $\Delta(z, x) \geq 0$ for every configuration $x \in \mathcal{X}$ that is asymptotic to z . The existence of ground configurations is well known. We shall use it later in the proof of Theorem 9.

Proposition 2 *Every Hamiltonian on a shift space of finite type has at least one ground configuration.*

Proof Let \mathcal{X} be a shift space of finite type and Δ a Hamiltonian on \mathcal{X} . Let $I_1 \subseteq I_2 \subseteq \dots$ be a chain of finite subsets of \mathbb{L} that is exhaustive (i.e., $\bigcup_n I_n = \mathbb{L}$). For example, we could take $I_n = [-n, n]^d$ in $\mathbb{L} = \mathbb{Z}^d$. Let $z_0 \in \mathcal{X}$ be an arbitrary configuration, and construct a sequence of configurations $z_1, z_2, \dots, \in \mathcal{X}$ as follows.

For each n , choose $z_n \in \mathcal{X}$ to be a configuration with $\text{diff}(z_0, z_n) \subseteq I_n$ such that $\Delta(z_0, z_n)$ is minimum (i.e., $\Delta(z_0, z_n) \leq \Delta(z_0, x)$ for all $x \in \mathcal{X}$ with $\text{diff}(z_0, x) \subseteq I_n$). The minimum exists because $L_{I_n}(\mathcal{X} \mid z_0)$ is finite. By compactness, there is a subsequence $n_1 < n_2 < \dots$ such that z_{n_i} converges. The limit $z \triangleq \lim_{i \rightarrow \infty} z_{n_i}$ is a ground configuration.

To see this, let $x \in \mathcal{X}$ be asymptotic to z , and choose k such that $I_k \supseteq \text{diff}(z, x)$. Since \mathcal{X} is of finite type, there is a $l \geq k$ such that for every two configuration $u, v \in \mathcal{X}$ that agree

on $I_l \setminus I_k$, there is a configuration $w \in \mathcal{X}$ that agrees with u on I_l and with v outside I_k . In particular, for every sufficiently large i , x (and z) agree with z_{n_i} on $I_l \setminus I_k$, and hence there is a configuration x_{n_i} that agrees with x on I_l and with z_{n_i} outside I_k . Then, $\text{diff}(z_{n_i}, x_{n_i}) = \text{diff}(z, x)$. Since $z_{n_i} \rightarrow z$, we also get $x_{n_i} \rightarrow x$. The continuity property of Δ now implies that $\Delta(z_{n_i}, x_{n_i}) \rightarrow \Delta(z, x)$. On the other hand, $\Delta(z_{n_i}, x_{n_i}) = \Delta(z_0, x_{n_i}) - \Delta(z_0, z_{n_i}) \geq 0$. Therefore, $\Delta(z, x) \geq 0$. \square

Example 1 (Ising model) The *Ising model* is a simple model on the lattice designed to give a statistical explanation of the phenomenon of spontaneous magnetization in ferromagnetic material (see e.g. [27,90]). The configuration space of the d -dimensional Ising model is the full shift $\mathcal{X} \triangleq \{-, +\}^{\mathbb{L}}$, where $\mathbb{L} = \mathbb{Z}^d$, and where having $+$ and $-$ at a site i is interpreted as an upward or downward magnetization of the tiny segment of the material approximated by site i . The state of site i is called the *spin* at site i .

The interaction between spins is modeled by associating an interaction energy -1 to every two adjacent spins that are aligned (i.e., both are upward or both downward) and energy $+1$ to every two adjacent spins that are not aligned. Alternatively, we can specify the energy using the energy observable $f \in K(\mathcal{X})$ defined by

$$f(x) \triangleq \begin{cases} \frac{1}{2}(n^-(x) - n^+(x)) & \text{if } x(0) = +, \\ \frac{1}{2}(n^+(x) - n^-(x)) & \text{if } x(0) = -, \end{cases} \tag{11}$$

where $n^+(x)$ and $n^-(x)$ are, respectively, the number of upward and downward spins adjacent to site 0. This defines a Hamiltonian Δ_f . The two uniform configurations (all sites $+$ and all sites $-$) are ground configurations for Δ_f , although Δ_f has many other ground configurations. \circ

Example 2 (Contour model) The *contour model* was originally used to study phase transition in the Ising model. Each site of two-dimensional lattice $\mathbb{L} = \mathbb{Z}^2$ may take a state from the set

$$T \triangleq \{ \square, \blacksquare, \blacksquare, \square, \square, \square, \square, \blacksquare \} \tag{12}$$

Not all configurations are allowed. The allowed configurations are those in which the state of adjacent sites match in the obvious fashion. For example, \square can be placed on the right side of \blacksquare but not on top of it, and \square can be placed on the left side of \square but not on its right side. The allowed configurations depict decorations of the lattice formed by closed or bi-infinite paths (see Fig. 2b). These paths are referred to as *contours*.

The space of allowed configurations $\mathcal{Y} \subseteq T^{\mathbb{Z}}$ is a shift space of finite type. It is also easy to verify that (\mathcal{Y}, σ) is strongly irreducible. Define the local observable $g \in K(\mathcal{Y})$, where

$$g(x) \triangleq \begin{cases} 0 & \text{if } x(0) = \square, \\ 1 & \text{if } x(0) \in \{ \blacksquare, \blacksquare, \square, \square, \square, \square \}, \\ 2 & \text{if } x(0) = \blacksquare. \end{cases} \tag{13}$$

The Hamiltonian Δ_g simply compares the length of the contours in two asymptotic configurations. The uniform configuration in which every site is in state \square is a ground configuration for Δ_g . Any configuration with a single bi-infinite horizontal (or vertical) contour is also a ground configuration for Δ_g . \circ

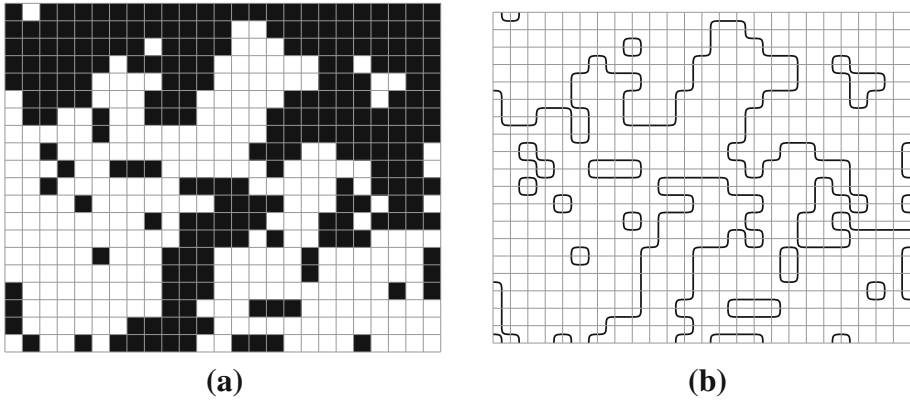


Fig. 2 A configuration of the Ising model (a) and its corresponding contour configuration (b). *Black* represents an upward spin

Example 3 (Hard-core gas) Let $0 \subseteq W \subseteq \mathbb{L}$ be a neighborhood, and define a shift space $\mathcal{X} \subseteq \{0, 1\}^{\mathbb{L}}$ consisting of all configurations x for which $W(i) \cap W(j) = \emptyset$ for every distinct $i, j \in \mathbb{L}$ with $x(i) = x(j) = 1$. This is the configuration space of the *hard-core gas* model. A site having state 1 is interpreted as containing a particle, whereas a site in state 0 is thought of to be empty. It is assumed that each particle occupies a volume W and that the volume of different particles cannot overlap. The one-dimensional version of the hard-core shift with volume $W = \{0, 1\}$ is also known as the *golden mean* shift.

The hard-core shift is clearly of finite type. It is also strongly irreducible. In fact, \mathcal{X} has a stronger irreducibility property: for every two asymptotic configurations $x, y \in \mathcal{X}$, there is a sequence $x = x_0, x_1, \dots, x_n = y$ of configurations in \mathcal{X} such that $\text{diff}(x_i, x_{i+1})$ is singleton. In particular, Proposition 1 can be adapted to cover the Hamiltonians on \mathcal{X} .

Let $h(x) \triangleq 1$ if $x(0) = 1$ and $h(x) \triangleq 0$ otherwise. The Hamiltonian Δ_h compares the number of particles on two asymptotic configurations. The empty configuration is the unique ground configuration for Δ_h . ○

Gibbs measures are a class of probability measures identified by Hamiltonians. Let \mathcal{X} be a shift space. A *Gibbs measure* for a finite-range Hamiltonian Δ is a probability measure $\pi \in \mathcal{P}(\mathcal{X})$ satisfying

$$\pi([y]_E) = e^{-\Delta(x,y)} \pi([x]_E) \tag{14}$$

for every two asymptotic configurations $x, y \in \mathcal{X}$ and all sufficiently large E . (If M is the interaction neighborhood of Δ , the above equality will hold for every $E \supseteq M(\text{diff}(x, y))$.) More generally, if Δ is an arbitrary Hamiltonian on \mathcal{X} , a probability measure $\pi \in \mathcal{P}(\mathcal{X})$ is said to be a Gibbs measure for Δ if

$$\lim_{E \nearrow \mathbb{L}} \frac{\pi([y]_E)}{\pi([x]_E)} = e^{-\Delta(x,y)} \tag{15}$$

for every configuration $x \in \mathcal{X}$ that is in the support of π and every configurations $y \in \mathcal{X}$ that is asymptotic to x . The limit is taken along the directed family of finite subsets of \mathbb{L} with inclusion.² The above limit is in fact uniform among all pairs of configurations x, y

² The original definition of a Gibbs measure given by Dobrushin, Lanford and Ruelle is via conditional probabilities (see e.g. [27]). The definition given here can be shown to be equivalent to the original definition using the martingale convergence theorem. See Appendix.

in the support of π whose disagreements $\text{diff}(x, y)$ are included in a finite set $D \subseteq \mathbb{L}$ (see Appendix). Note also that if \mathcal{X} is strongly irreducible, every Gibbs measure on \mathcal{X} has full support, and therefore, the relation (15) must hold for every two asymptotic $x, y \in \mathcal{X}$. The set of Gibbs measures for a Hamiltonian Δ , denoted by $\mathcal{G}_\Delta(\mathcal{X})$, is non-empty, closed and convex. According to the Krein–Milman theorem, the set $\mathcal{G}_\Delta(\mathcal{X})$ coincides with the closed convex hull of its extremal elements. The extremal elements of $\mathcal{G}_\Delta(\mathcal{X})$ are mutually singular. The subset $\mathcal{G}_\Delta(\mathcal{X}, \sigma)$ of shift-invariant elements of $\mathcal{G}_\Delta(\mathcal{X})$ is also non-empty (using convexity and compactness), closed and convex, and hence equal to the closed convex hull of its extremal elements. The extremal elements of $\mathcal{G}_\Delta(\mathcal{X}, \sigma)$ are precisely its ergodic elements, and hence again mutually singular.

The Gibbs measures associated to finite-range Hamiltonians have the Markov property. A measure π on a shift space $\mathcal{X} \subseteq S^\mathbb{L}$ is called a *Markov measure* if there is a neighborhood $0 \in M \subseteq \mathbb{L}$ such that for every two finite sets $D, E \subseteq \mathbb{L}$ with $M(D) \subseteq E$ and every pattern $p : E \rightarrow S$ with $\pi([p]_{E \setminus D}) > 0$ it holds

$$\pi([p]_D \mid [p]_{E \setminus D}) = \pi([p]_D \mid [p]_{M(D) \setminus D}) . \tag{16}$$

The data contained in the conditional probabilities $\pi([p]_D \mid [p]_{M(D) \setminus D})$ for all choices of D, E and p is called the *specification* of the Markov measure π . The specification of a Gibbs measure associated to a finite-range Hamiltonian is *positive* (i.e., all the conditional distributions are positive) and *shift-invariant*. Conversely, every positive shift-invariant Markovian specification is the specification of a Gibbs measure. In fact, Eq. (14) identifies a one-to-one correspondence between finite-range Hamiltonians and the positive shift-invariant Markovian specifications.

The uniform Bernoulli measure on a full shift $\mathcal{X} \subseteq S^\mathbb{L}$ is the unique Gibbs measure for the trivial Hamiltonian on \mathcal{X} . More generally, the shift-invariant Gibbs measures on a strongly irreducible shift of finite type associated to the trivial Hamiltonian are precisely the measures that maximize the entropy (see below).

We shall call a Gibbs measure *regular* if its corresponding Hamiltonian is generated by an observable with summable variations.

2.4 Entropy, Pressure, and the Variational Principle

Statistical mechanics attempts to explain the macroscopic behaviour of a physical system by statistical analysis of its microscopic details. In the subjective interpretation (see [36]), the probabilities reflect the partial knowledge of an observer. A suitable choice for a probability distribution over the possible microscopic states of a system is therefore one which, in light of the available partial observations, is least presumptive.

The standard approach to pick the least presumptive probability distribution is by maximizing entropy. The characterization of the uniform probability distribution over a finite set as the probability distribution that maximizes entropy is widely known. Maximizing entropy subject to partial observations leads to Boltzmann distribution. The infinite systems based on lattice configurations have a similar (though more technical) picture. Below, we give a minimum review necessary for our discussion. Details and more information can be found in the original monographs and textbooks [27,35,44,75,78]. The equilibrium statistical mechanics, which can be built upon the maximum entropy postulate, has been enormously successful in predicting the absence or presence of phase transitions, and in describing the qualitative features of the phases; see [27].

Let $\mathcal{X} \subseteq S^{\mathbb{L}}$ be a shift space and $\pi \in \mathcal{P}(\mathcal{X})$ a probability measure on \mathcal{X} . The *entropy* of a finite set $A \subseteq \mathbb{L}$ of sites under π is

$$H_{\pi}(A) \triangleq - \sum_{p \in L_A(\mathcal{X})} \pi([p]_A) \log \pi([p]_A). \tag{17}$$

(By convention, $0 \log 0 \triangleq 0$.) This is the same as the Shannon entropy of the random variable \mathbf{x}_A in the probability space (\mathcal{X}, π) , where \mathbf{x}_A is the projection $x \mapsto x|_A$. Let us recall few basic properties of the entropy. The entropy $H(\mathbf{x})$ of a random variable \mathbf{x} is non-negative. If \mathbf{x} takes its values in a finite set of cardinality n , then $H(\mathbf{x}) \leq \log n$. The entropy is sub-additive, meaning that $H((\mathbf{x}, \mathbf{y})) \leq H(\mathbf{x}) + H(\mathbf{y})$ for every two random variables \mathbf{x} and \mathbf{y} . If $\mathbf{y} = f(\mathbf{x})$ depends deterministically on \mathbf{x} , we have $H(f(\mathbf{x})) \leq H(\mathbf{x})$.

Let $I_n \triangleq [-n, n]^d \subseteq \mathbb{L}$ be the centered $(2n + 1) \times (2n + 1) \times \dots \times (2n + 1)$ box in the lattice. If π is shift-invariant, the sub-additivity of $A \mapsto H_{\pi}(A)$ ensures that the limit

$$h_{\pi}(\mathcal{X}, \sigma) \triangleq \lim_{n \rightarrow \infty} \frac{H_{\pi}(I_n)}{|I_n|} = \inf_{n \geq 0} \frac{H_{\pi}(I_n)}{|I_n|} \tag{18}$$

exists (Fekete’s lemma). The limit value $h_{\pi}(\mathcal{X}, \sigma)$ is the average entropy per site of π over \mathcal{X} . It is also referred to as the (*Kolmogorov-Sinai*) *entropy* of the dynamical system (\mathcal{X}, σ) under π (see [92], Theorem 4.17).

The entropy functional $\pi \mapsto h_{\pi}(\mathcal{X}, \sigma)$ is non-negative and affine. Although it is not continuous, it is upper semi-continuous.

Proposition 3 (Upper Semi-continuity) *If $\lim_{i \rightarrow \infty} \pi_i = \pi$, then $\limsup_{i \rightarrow \infty} h_{\pi_i}(\mathcal{X}, \sigma) \leq h_{\pi}(\mathcal{X}, \sigma)$.*

Proof The pointwise infimum of a family of continuous functions is upper semi-continuous. □

The entropy functional is also bounded. Due to the compactness of $\mathcal{P}(\mathcal{X}, \sigma)$ and the upper semi-continuity of $\pi \mapsto h_{\pi}(\mathcal{X}, \sigma)$, the entropy $h_{\pi}(\mathcal{X}, \sigma)$ takes its maximum value at some measures $\pi \in \mathcal{P}(\mathcal{X}, \sigma)$. This maximum value coincides with the *topological entropy* of the shift (\mathcal{X}, σ) , defined by

$$h(\mathcal{X}, \sigma) \triangleq \lim_{n \rightarrow \infty} \frac{\log |L_{I_n}(\mathcal{X})|}{|I_n|} = \inf_{n \geq 0} \frac{\log |L_{I_n}(\mathcal{X})|}{|I_n|}, \tag{19}$$

which is the average combinatorial entropy per site of \mathcal{X} .

The following propositions are easy to prove, and are indeed valid for arbitrary dynamical systems.

Proposition 4 (Factoring) *Let $\Phi : \mathcal{X} \rightarrow \mathcal{Y}$ be a factor map between two shifts (\mathcal{X}, σ) and (\mathcal{Y}, σ) and $\pi \in \mathcal{P}(\mathcal{X}, \sigma)$ a probability measure on \mathcal{X} . Then, $h_{\Phi\pi}(\mathcal{Y}, \sigma) \leq h_{\pi}(\mathcal{X}, \sigma)$.*

Proposition 5 (Embedding) *Let $\Phi : \mathcal{Y} \rightarrow \mathcal{X}$ be an embedding of a shift (\mathcal{Y}, σ) in a shift (\mathcal{X}, σ) and $\pi \in \mathcal{P}(\mathcal{Y}, \sigma)$ a probability measure on \mathcal{Y} . Then, $h_{\pi}(\mathcal{Y}, \sigma) = h_{\Phi\pi}(\mathcal{X}, \sigma)$.*

Given a continuous observable $f \in C(\mathcal{X})$, the mapping $\pi \in \mathcal{P}(\mathcal{X}, \sigma) \mapsto \pi(f)$ is continuous and affine. Its range is closed, bounded, and convex, that is, a finite closed interval $[e_{\min}, e_{\max}] \subseteq \mathbb{R}$. For each $e \in [e_{\min}, e_{\max}]$, let us define

$$s_f(e) \triangleq \sup \{h_{\pi}(\mathcal{X}, \sigma) : \pi \in \mathcal{P}(\mathcal{X}, \sigma) \text{ and } \pi(f) = e\}. \tag{20}$$

Let $\mathcal{E}_{(f)=e}(\mathcal{X}, \sigma)$ denote the set of measures $\pi \in \mathcal{P}(\mathcal{X}, \sigma)$ with $\pi(f) = e$ and $h_\pi(\mathcal{X}, \sigma) = s_f(e)$, that is, the measures π that maximize entropy under the constraint $\pi(f) = e$. By the compactness of $\mathcal{P}(\mathcal{X}, \sigma)$ and the upper semi-continuity of $\pi \mapsto h_\pi(\mathcal{X}, \sigma)$, the set $\mathcal{E}_{(f)=e}(\mathcal{X}, \sigma)$ is non-empty (as long as $e \in [e_{\min}, e_{\max}]$). The mapping $s_f(\cdot)$ is concave and continuous. The measures in $\mathcal{E}_{(f)=e}(\mathcal{X}, \sigma)$ (and more generally, the solutions of similar entropy maximization problems with multiple constraints $\pi(f_1) = e_1, \pi(f_2) = e_2, \dots, \pi(f_n) = e_n$) could be implicitly identified after a Legendre transform.

The pressure associated to $f \in C(\mathcal{X})$ could be defined as

$$P_f(\mathcal{X}, \sigma) = \sup_{\nu \in \mathcal{P}(\mathcal{X}, \sigma)} [h_\nu(\mathcal{X}, \sigma) - \nu(f)]. \tag{21}$$

The functional $f \mapsto P_f(\mathcal{X}, \sigma)$ is convex and Lipschitz continuous. It is the convex conjugate of the entropy functional $\nu \mapsto h_\nu(\mathcal{X}, \sigma)$ (up to a negative sign), and we also have

$$h_\pi(\mathcal{X}, \sigma) = \inf_{g \in C(\mathcal{X})} [P_g(\mathcal{X}, \sigma) + \pi(g)] \tag{22}$$

(see [75], Theorem 3.12). Note that the pressure $P_0(\mathcal{X}, \sigma)$ associated to 0 is the same as the topological entropy of (\mathcal{X}, σ) . Again, the compactness of $\mathcal{P}(\mathcal{X}, \sigma)$ and the upper semi-continuity of $\nu \mapsto h_\nu(\mathcal{X}, \sigma)$ ensure that the supremum in (21) can be achieved. The set of shift-invariant probability measures $\pi \in \mathcal{P}(\mathcal{X}, \sigma)$ for which the equality in

$$h_\pi(\mathcal{X}, \sigma) - P_f(\mathcal{X}, \sigma) \leq \pi(f) \tag{23}$$

is satisfied will be denoted by $\mathcal{E}_f(\mathcal{X}, \sigma)$. Following the common terminology of statistical mechanics and ergodic theory, we call the elements of $\mathcal{E}_f(\mathcal{X}, \sigma)$ the *equilibrium measures* for f . Let us emphasize that this terminology lacks a dynamical justification that we are striving for. The Bayesian justification is further clarified below.

A celebrated theorem of Dobrushin, Lanford and Ruelle characterizes the equilibrium measures (for “short-ranged” observables over strongly irreducible shift spaces of finite type) as the associated shift-invariant Gibbs measures.

Theorem 1 (Characterization of Equilibrium Measures; see [75], Theorem 4.2, and [44], Sects. 5.2 and 5.3, and [57]) *Let $\mathcal{X} \subseteq S^{\mathbb{L}}$ be a strongly irreducible shift space of finite type. Let $f \in SV(\mathcal{X})$ be an observable with summable variations and Δ_f the Hamiltonian it generates. The set of equilibrium measures for f coincides with the set of shift-invariant Gibbs measures for Δ_f .*

Consider now an observable $f \in C(\mathcal{X})$, and as before, let $[e_{\min}, e_{\max}]$ be the set of possible values $\nu(f)$ for $\nu \in \mathcal{P}(\mathcal{X}, \sigma)$. For every $\beta \in \mathbb{R}$, we have

$$P_{\beta f}(\mathcal{X}, \sigma) = \sup\{s_f(e) - \beta e : e \in [e_{\min}, e_{\max}]\}. \tag{24}$$

That is, $\beta \in \mathbb{R} \mapsto P_{\beta f}$ is the Legendre transform of $e \mapsto s_f(e)$. If f has summable variations and the Hamiltonian Δ_f is not trivial, it can be shown that $\beta \mapsto P_{\beta f}$ is strictly convex (see [75], Sect. 4.6, or [35], Sect. III.4). It follows that $e \mapsto s_f(e)$ is continuously differentiable everywhere except at e_{\min} and e_{\max} , and

$$s_f(e) = \inf\{P_{\beta f}(\mathcal{X}, \sigma) + \beta e : \beta \in \mathbb{R}\} \tag{25}$$

for every $e \in (e_{\min}, e_{\max})$. For $e \in (e_{\min}, e_{\max})$, the above theorem identifies the elements of $\mathcal{E}_{(f)=e}(\mathcal{X}, \sigma)$ as the shift-invariant Gibbs measures for $\beta_e f$, where $\beta_e \in \mathbb{R}$ is the unique value at which $\beta \mapsto -P_{\beta f}(\mathcal{X}, \sigma)$ has a tangent with slope e . The mapping $e \mapsto \beta_e$ is

continuous and non-increasing. The set of slopes of tangents to $\beta \mapsto -P_{\beta f}(\mathcal{X}, \sigma)$ at a point $\beta \in \mathbb{R}$ is a closed interval $[e_{\beta}^-, e_{\beta}^+] \subseteq (e_{\min}, e_{\max})$. We have

$$\mathcal{E}_{\beta f}(\mathcal{X}, \sigma) = \bigcup_{e \in [e_{\beta}^-, e_{\beta}^+]} \mathcal{E}_{(f)=e}(\mathcal{X}, \sigma). \tag{26}$$

When f is interpreted as the energy contribution of a single site, $1/\beta$ is interpreted as the temperature and e as the mean energy per site. By a Bayesian reasoning, if $\mathcal{E}_{(f)=e}(\mathcal{X}, \sigma)$ is singleton, its unique element is an appropriate choice of the probability distribution of the system in thermal equilibrium when the mean energy per site is e . If $\mathcal{E}_{\beta f}(\mathcal{X}, \sigma)$ is singleton, the unique element is interpreted as a description of the system in thermal equilibrium at temperature $1/\beta$. The existence of more than one element in $\mathcal{E}_{\beta f}(\mathcal{X}, \sigma)$ (or in $\mathcal{E}_{(f)=e}(\mathcal{X}, \sigma)$) is interpreted as the existence of more than one phase (e.g., liquid or gas) at temperature $1/\beta$ (resp., with energy density e). The presence of distinct tangents to $\beta \mapsto -P_{\beta f}(\mathcal{X}, \sigma)$ at a given inverse temperature β implies the existence of distinct phases at temperature $1/\beta$ having different mean energy per site.

Note that since the elements of $\mathcal{E}_{\beta f}(\mathcal{X}, \sigma) = \mathcal{G}_{\beta \Delta_f}(\mathcal{X}, \sigma)$ are shift-invariant, they only offer a description of the equilibrium states that respect the translation symmetry of the model. By extrapolating the interpretation, one could consider the Gibbs measures $\pi \in \mathcal{G}_{\beta \Delta_f}(\mathcal{X})$ that are not shift-invariant as states of equilibrium in which the translation symmetry is broken.

2.5 Physical Equivalence of Observables

Let $\mathcal{X} \subseteq S^{\mathbb{L}}$ be a strongly irreducible shift space of finite type. Every local observable generates a finite-range Hamiltonian via Eq. (7). However, different local observables may generate the same Hamiltonians. Two local observables $f, g \in K(\mathcal{X})$ are *physically equivalent* (see [75], Sects. 4.6–4.7, [35], Sects. I.4 and III.4, or [27], Sect. 2.4), $f \sim g$ in symbols, if they identify the same Hamiltonian, that is, if $\Delta_f = \Delta_g$. The following proposition gives an alternate characterization of physical equivalence, which will allow us to extend the notion of physical equivalence to $C(\mathcal{X})$.

Proposition 6 *Let (\mathcal{X}, σ) be a strongly irreducible shift of finite type. Two observables $f, g \in K(\mathcal{X})$ are physically equivalent, if and only if there is a constant $c \in \mathbb{R}$ such that $\pi(f) = \pi(g) + c$ for every probability measure $\pi \in \mathcal{P}(\mathcal{X}, \sigma)$.*

Proof \Rightarrow) Let $h \triangleq f - g$. Let us pick an arbitrary configuration $\diamond \in \mathcal{X}$ with the property that the spatial average

$$c \triangleq \lim_{n \rightarrow \infty} \frac{\sum_{i \in I_n} h(\sigma^i \diamond)}{|I_n|} \tag{27}$$

(where $I_n \triangleq [-n, n]^d \subseteq \mathbb{L}$) exists. That such a configuration exists follows, for example, from the ergodic theorem.³ We claim that indeed

$$\lim_{n \rightarrow \infty} \frac{\sum_{i \in I_n} h(\sigma^i x)}{|I_n|} = c \tag{28}$$

³ We could simply choose \diamond to be a periodic configuration if we knew such a configuration existed. Unfortunately, it is not known whether every strongly irreducible shift of finite type (in more than two dimensions) has a periodic configuration.

for every configuration $x \in \mathcal{X}$. This follows from the fact that $\Delta_h = \Delta_f - \Delta_g = 0$. More specifically, let $0 \in M \subseteq \mathbb{L}$ be a neighborhood that witnesses the strong irreducibility of \mathcal{X} , and let $D \subseteq \mathbb{L}$ be a finite base for h (i.e., h is \mathfrak{F}_D -measurable). For each configuration $x \in \mathcal{X}$ and each $n \geq 0$, let x_n be a configuration that agrees with x on $I_n + D$ and with \diamond off $I_n + D + M - M$. Then

$$\sum_{i \in I_n} h(\sigma^i x) = \sum_{i \in I_n} h(\sigma^i x_n) \tag{29}$$

$$= \sum_{i \in I_n} h(\sigma^i \diamond) + \Delta_h(\diamond, x_n) + o(|I_n|) \tag{30}$$

$$= \sum_{i \in I_n} h(\sigma^i \diamond) + o(|I_n|), \tag{31}$$

and the claim follows. Now, the dominated convergence theorem concludes that $\pi(f) - \pi(g) = \pi(h) = c$, for every $\pi \in \mathcal{P}(\mathcal{X}, \sigma)$.

\Leftrightarrow) Following the definition, $P_f(\mathcal{X}, \sigma) = P_g(\mathcal{X}, \sigma) - c$, and f and g have the same equilibrium measures. Theorem 1 then implies that the shift-invariant Gibbs measures of Δ_f and Δ_g coincide, which in turn concludes that $\Delta_f = \Delta_g$. □

As a corollary, the physical equivalence relation is closed in $K(\mathcal{X}) \times K(\mathcal{X})$:

Corollary 1 *Let (\mathcal{X}, σ) be a strongly irreducible shift of finite type. Let h_1, h_2, \dots be local observables on \mathcal{X} such that $\Delta_{h_i} = 0$ for each i . If h_i converge to a local observable h , then $\Delta_h = 0$.*

The continuous extension of this relation (i.e., the closure of \sim in $C(\mathcal{X}) \times C(\mathcal{X})$) gives a notion of physical equivalence of arbitrary continuous observables.

Proposition 7 *Let (\mathcal{X}, σ) be a strongly irreducible shift of finite type. Two observables $f, g \in C(\mathcal{X})$ are physically equivalent if and only if there is a constant $c \in \mathbb{R}$ such that $\pi(f) = \pi(g) + c$ for every probability measure $\pi \in \mathcal{P}(\mathcal{X}, \sigma)$.*

Proof First, suppose that f and g are physically equivalent. Then, there exist sequences f_1, f_2, \dots and g_1, g_2, \dots of local observables such that $f_i \rightarrow f, g_i \rightarrow g$ and $f_i \sim g_i$. By Proposition 6, there are real numbers c_i such that for every $\pi \in \mathcal{P}(\mathcal{X}, \sigma), \pi(f_i) - \pi(g_i) = c_i$. Taking the limits as $i \rightarrow \infty$, we obtain $\pi(f) - \pi(g) = c$, where $c \triangleq \lim_i c_i$ is independent of π .

Conversely, suppose there is a constant $c \in \mathbb{R}$ such that $\pi(f) = \pi(g) + c$ for every probability measure $\pi \in \mathcal{P}(\mathcal{X}, \sigma)$. Let $h \triangleq f - g - c$. Then, according to Lemma 2, $h \in C(\mathcal{X}, \sigma)$. Therefore, by the denseness of $K(\mathcal{X})$ in $C(\mathcal{X})$, there exists a sequence of local observables $h_i \in C(\mathcal{X}, \sigma)$ such that $h_i \rightarrow h$. Choose another sequence of local observables g_i that converges to g , and set $f_i \triangleq h_i + g_i + c$. By Lemma 2, $\pi(f_i) = \pi(g_i) + c$ for every $\pi \in \mathcal{P}(\mathcal{X}, \sigma)$, which along with Proposition 6, implies that $\Delta_{f_i} = \Delta_{g_i}$. Taking the limit, we obtain that f and g are physically equivalent. □

Using Lemma 2, we also get the following characterization.

Corollary 2 *Let (\mathcal{X}, σ) be a strongly irreducible shift of finite type. Two observables $f, g \in C(\mathcal{X})$ are physically equivalent if and only if $f - g - c \in C(\mathcal{X}, \sigma)$ for some $c \in \mathbb{R}$.*

Physically equivalent observables define the same set of equilibrium measures. Moreover, the equilibrium measures of two observables with summable variations that are not physically equivalent are disjoint. (However, continuous observables that are not physically equivalent might in general share equilibrium measures; see [75], Corollary 3.17.)

Proposition 8 *Let (\mathcal{X}, σ) be a strongly irreducible shift of finite type. If two observables $f, g \in C(\mathcal{X})$ are physically equivalent, they have the same set of equilibrium measures. Conversely, if two observables $f, g \in SV(\mathcal{X})$ with summable variations share an equilibrium measure, they are physically equivalent.*

Proof The first claim is an easy consequence of the characterization of physical equivalence given in Proposition 7. The converse follows from the characterization of equilibrium measures as Gibbs measures (Theorem 1). □

3 Entropy-Preserving Maps

3.1 Entropy and Pre-injective Maps

The Garden-of-Eden theorem states that a cellular automaton over a strongly irreducible shift of finite type is surjective if and only if it is pre-injective [10,23,31,60,63]. This is one of the earliest results in the theory of cellular automata, and gives a characterization of when a cellular automaton has a so-called *Garden-of-Eden*, that is, a configuration with no pre-image. The Garden-of-Eden theorem can be proved by a counting argument. Alternatively, the argument can be phrased in terms of entropy (see [49], Theorem 8.1.16 and [9], Chapter 5).

Theorem 2 (see [49], Theorem 8.1.16 and [56], Theorem 3.6) *Let $\Phi: \mathcal{X} \rightarrow \mathcal{Y}$ be a factor map from a strongly irreducible shift of finite type (\mathcal{X}, σ) onto a shift (\mathcal{Y}, σ) . Then, $h(\mathcal{Y}, \sigma) \leq h(\mathcal{X}, \sigma)$ with equality if and only if Φ is pre-injective.*

Theorem 3 (see [14], Theorem 3.3, and [56], Lemma 4.1, and [23], Lemma 4.4) *Let (\mathcal{X}, σ) be a strongly irreducible shift of finite type and $\mathcal{Y} \subseteq \mathcal{X}$ a proper subsystem. Then, $h(\mathcal{Y}, \sigma) < h(\mathcal{X}, \sigma)$.*

Corollary 3 (Garden-of-Eden Theorem [10,23,60,63]) *Let $\Phi: \mathcal{X} \rightarrow \mathcal{X}$ be a cellular automaton on a strongly irreducible shift of finite type (\mathcal{X}, σ) . Then, Φ is surjective if and only if it is pre-injective.*

Proof

$$\begin{aligned} \mathcal{X} &\xrightarrow{\Phi} \Phi\mathcal{X} \xrightarrow{\subseteq} \mathcal{X}, \\ h(\mathcal{X}, \sigma) &\geq h(\Phi\mathcal{X}, \sigma) \leq h(\mathcal{X}, \sigma) \end{aligned} \tag{32}$$

□

Another corollary of Theorem 2 (along with Lemma 1 and Proposition 4) is the so-called *balance* property of pre-injective cellular automata.

Corollary 4 (see [14], Theorem 2.1, and [56], Theorems 3.3 and 3.6) *Let $\Phi: \mathcal{X} \rightarrow \mathcal{Y}$ be a pre-injective factor map from a strongly irreducible shift of finite type (\mathcal{X}, σ) onto a shift (\mathcal{Y}, σ) . Every maximum entropy measure $\nu \in \mathcal{P}(\mathcal{Y}, \sigma)$ has a maximum entropy pre-image $\pi \in \mathcal{P}(\mathcal{X}, \sigma)$.*

In particular, a cellular automaton on a full shift is surjective if and only if it preserves the uniform Bernoulli measure [31,55]. In Sect. 4.2, we shall find a generalization of this property.

The probabilistic version of Theorem 2 states that the pre-injective factor maps preserve the entropy of shift-invariant probability measures, and seems to be part of the folklore (see e.g. [32]).

Theorem 4 *Let $\Phi: \mathcal{X} \rightarrow \mathcal{Y}$ be a factor map from a shift of finite type (\mathcal{X}, σ) onto a shift (\mathcal{Y}, σ) . Let $\pi \in \mathcal{P}(\mathcal{X}, \sigma)$ be a probability measure. Then, $h_{\Phi\pi}(\mathcal{Y}, \sigma) \leq h_\pi(\mathcal{X}, \sigma)$ with equality if Φ is pre-injective.*

Proof For any factor map Φ , the inequality $h_{\Phi\pi}(\mathcal{Y}, \sigma) \leq h_\pi(\mathcal{X}, \sigma)$ holds by Proposition 4. Suppose that Φ is pre-injective. It is enough to show that $h_{\Phi\pi}(\mathcal{Y}, \sigma) \geq h_\pi(\mathcal{X}, \sigma)$.

Let $0 \subseteq M \subseteq \mathbb{L}$ be a neighborhood for Φ and a witness for the finite-type gluing property of \mathcal{X} (see Sect. 2.2). Let $A \subseteq \mathbb{L}$ be a finite set. By the pre-injectivity of Φ , for every $x \in \mathcal{X}$, the pattern $x|_{A \setminus M(A^c)}$ is uniquely determined by $x|_{\partial M(A)}$ and $(\Phi x)|_A$. Indeed, suppose that $x' \in \mathcal{X}$ is another configuration with $x'|_{\partial M(A)} = x|_{\partial M(A)}$ and $(\Phi x')|_A = (\Phi x)|_A$. Then, the configuration x'' that agrees with x on $M(A^c)$ and with x' on $M(A)$ is in \mathcal{X} and asymptotic to x . Since $(\Phi x'')|_A = (\Phi x')|_A = (\Phi x)|_A$, it follows that $\Phi x'' = \Phi x$. Therefore, $x'' = x$, and in particular, $x'|_{A \setminus M(A^c)} = x''|_{A \setminus M(A^c)} = x|_{A \setminus M(A^c)}$.

From the basic properties of the Shannon entropy, it follows that

$$H_\pi(\partial M(A)) + H_{\Phi\pi}(A) \geq H_\pi(A \setminus M(A^c)). \tag{33}$$

Now, choose the neighborhood M to be $I_r \triangleq [-r, r]^d \subseteq \mathbb{L}$ for a sufficiently large r . For $A \triangleq I_n = [-n, n]^d$, we obtain

$$H_{\Phi\pi}(I_n) \geq H_\pi(I_{n-r}) - H_\pi(I_{n+r} \setminus I_{n-r}). \tag{34}$$

Dividing by $|I_n|$ we get

$$\frac{H_{\Phi\pi}(I_n)}{|I_n|} \geq \frac{|I_{n-r}|}{|I_n|} \cdot \frac{H_\pi(I_{n-r})}{|I_{n-r}|} - \frac{o(|I_n|)}{|I_n|}, \tag{35}$$

which proves the theorem by letting $n \rightarrow \infty$. □

From Theorem 4 and Lemma 1, it immediately follows that the functionals $f \mapsto P_f$ and $f \mapsto s_f(\cdot)$ are preserved under the dual of a pre-injective factor map.

Corollary 5 *Let $\Phi: \mathcal{X} \rightarrow \mathcal{Y}$ be a factor map from a shift of finite type (\mathcal{X}, σ) onto a shift (\mathcal{Y}, σ) . Let $f \in C(\mathcal{Y})$ be an observable. Then, $P_{f \circ \Phi}(\mathcal{X}, \sigma) \geq P_f(\mathcal{Y}, \sigma)$ with equality if Φ is pre-injective.*

Corollary 6 *Let $\Phi: \mathcal{X} \rightarrow \mathcal{Y}$ be a factor map from a shift of finite type (\mathcal{X}, σ) onto a shift (\mathcal{Y}, σ) . Let $f \in C(\mathcal{Y})$ be an observable. Then, $s_{f \circ \Phi}(\cdot) \geq s_f(\cdot)$ with equality if Φ is pre-injective.*

Central to this article is the the following correspondence between the equilibrium (Gibbs) measures of a model and its pre-injective factors.

Corollary 7 *Let $\Phi: \mathcal{X} \rightarrow \mathcal{Y}$ be a pre-injective factor map from a shift of finite type (\mathcal{X}, σ) onto a shift (\mathcal{Y}, σ) . Let $f \in C(\mathcal{Y})$ be an observable and $\pi \in \mathcal{P}(\mathcal{X}, \sigma)$ a probability measure. Then $\pi \in \mathcal{E}_{f \circ \Phi}(\mathcal{X}, \sigma)$ if and only if $\Phi\pi \in \mathcal{E}_f(\mathcal{Y}, \sigma)$.*

Corollary 8 *Let $\Phi: \mathcal{X} \rightarrow \mathcal{Y}$ be a pre-injective factor map from a shift of finite type (\mathcal{X}, σ) onto a shift (\mathcal{Y}, σ) . Let $f \in C(\mathcal{Y})$ be an observable, $\pi \in \mathcal{P}(\mathcal{X}, \sigma)$ a probability measure, and $e \in \mathbb{R}$. Then, $\pi \in \mathcal{E}_{(f \circ \Phi)=e}(\mathcal{X}, \sigma)$ if and only if $\Phi\pi \in \mathcal{E}_{(f)=e}(\mathcal{Y}, \sigma)$.*

Example 4 Let $\mathcal{X} \subseteq \{0, 1, 2\}^{\mathbb{Z}}$ be the shift obtained by forbidding 11 and 22, and $\mathcal{Y} \subseteq \{0, 1, 2\}^{\mathbb{Z}}$ the shift obtained by forbidding 22 and 21. Then, both (\mathcal{X}, σ) and (\mathcal{Y}, σ) are mixing shifts of finite type. For every configuration $x \in \mathcal{X}$, let $\Phi x \in \{0, 1, 2\}^{\mathbb{Z}}$ be the configuration in which

$$(\Phi x)(i) = \begin{cases} 1 & \text{if } x(i) = 2 \text{ and } x(i + 1) = 1, \\ x(i) & \text{otherwise.} \end{cases} \tag{36}$$

Then, Φ is a pre-injective factor map from \mathcal{X} onto \mathcal{Y} .

Consider the observables $g_0, g_1, g_2: \mathcal{Y} \rightarrow \mathbb{R}$ defined by

$$g_0(y) \triangleq 1_{[0]_0}(y), \quad g_1(y) \triangleq 1_{[1]_0}(y), \quad g_2(y) \triangleq 1_{[2]_0}(y) \tag{37}$$

for $y \in \mathcal{Y}$. The Hamiltonians $\Delta_{g_0}, \Delta_{g_1}$ and Δ_{g_2} count the number of 0, 1 and 2 s, respectively. The unique Gibbs measures for $\Delta_{g_0}, \Delta_{g_1}$ and Δ_{g_2} are, respectively, the distribution of the bi-infinite Markov chains with transition matrices

$$A_0 \approx_1 \begin{matrix} & \begin{matrix} 0 & 1 & 2 \end{matrix} \\ \begin{matrix} 0 \\ 1 \\ 2 \end{matrix} & \begin{bmatrix} 0.230 & 0.626 & 0.144 \\ 0.230 & 0.626 & 0.144 \\ 1 & 0 & 0 \end{bmatrix} \end{matrix}, \quad A_1 \approx_1 \begin{matrix} & \begin{matrix} 0 & 1 & 2 \end{matrix} \\ \begin{matrix} 0 \\ 1 \\ 2 \end{matrix} & \begin{bmatrix} 0.528 & 0.194 & 0.278 \\ 0.528 & 0.194 & 0.278 \\ 1 & 0 & 0 \end{bmatrix} \end{matrix}, \quad A_2 \approx_1 \begin{matrix} & \begin{matrix} 0 & 1 & 2 \end{matrix} \\ \begin{matrix} 0 \\ 1 \\ 2 \end{matrix} & \begin{bmatrix} 0.461 & 0.461 & 0.078 \\ 0.461 & 0.461 & 0.078 \\ 1 & 1 & 0 \end{bmatrix} \end{matrix} \tag{38}$$

In general, every finite-range Gibbs measure on a one-dimensional mixing shift of finite type is the distribution of a bi-infinite Markov chain and vice versa (see [27], Theorem 3.5 and [11]). The observables induced by g_0, g_1 and g_2 on \mathcal{X} via Φ satisfy

$$(g_0 \circ \Phi)(x) = 1_{[0]_0}(x), \quad (g_1 \circ \Phi)(x) \triangleq (1_{[1]_0} + 1_{[21]_0})(x), \quad (g_2 \circ \Phi)(x) \triangleq 1_{[20]_0}(x). \tag{39}$$

for every $x \in \mathcal{X}$. The unique Gibbs measures for $\Delta_{g_0 \circ \Phi}, \Delta_{g_1 \circ \Phi}$ and $\Delta_{g_2 \circ \Phi}$ are, respectively, the distribution of the bi-infinite Markov chains with transition matrices

$$A_0 \approx_1 \begin{matrix} & \begin{matrix} 0 & 1 & 2 \end{matrix} \\ \begin{matrix} 0 \\ 1 \\ 2 \end{matrix} & \begin{bmatrix} 0.230 & 0.385 & 0.385 \\ 0.374 & 0 & 0.626 \\ 0.374 & 0.626 & 0 \end{bmatrix} \end{matrix}, \quad A_1 \approx_1 \begin{matrix} & \begin{matrix} 0 & 1 & 2 \end{matrix} \\ \begin{matrix} 0 \\ 1 \\ 2 \end{matrix} & \begin{bmatrix} 0.528 & 0.163 & 0.310 \\ 0.630 & 0 & 0.370 \\ 0.898 & 0.102 & 0 \end{bmatrix} \end{matrix}, \quad A_2 \approx_1 \begin{matrix} & \begin{matrix} 0 & 1 & 2 \end{matrix} \\ \begin{matrix} 0 \\ 1 \\ 2 \end{matrix} & \begin{bmatrix} 0.461 & 0.316 & 0.224 \\ 0.673 & 0 & 0.327 \\ 0.350 & 0.650 & 0 \end{bmatrix} \end{matrix} \tag{40}$$

By Corollary 7, we have $\Phi\pi_0 = \nu_0, \Phi\pi_1 = \nu_1$, and $\Phi\pi_2 = \nu_2$. ○

3.2 Complete Pre-injective Maps

In this section, we discuss the extension of Corollary 7 to the case of non-shift-invariant Gibbs measures (Conjecture 1, Theorem 5, and Corollary 9). We start with an example that deviates from the main line of this article (i.e., understanding macroscopic equilibrium in surjective cellular automata) but rather demonstrates an application of factor maps as a tool in the study of phase transitions in equilibrium statistical mechanics models. The (trivial) argument used in this example however serves as a model for the proof of Theorem 5.

Example 5 (Ising and contour models) There is a natural correspondence between the two-dimensional Ising model (Example 1) and the contour model (Example 2).

As before, let $\mathcal{X} = \{+, -\}^{\mathbb{Z}^2}$ and $\mathcal{Y} \triangleq T^{\mathbb{Z}^2}$ denote the configuration spaces of the Ising model and the contour model. Define a sliding block map $\Theta: \mathcal{X} \rightarrow T^{\mathbb{Z}^2}$ with neighborhood $N \triangleq \{(0, 0), (0, 1), (1, 0), (1, 1)\}$ and local rule $\theta: \{+, -\}^N \rightarrow T$, specified by

$$\begin{array}{cccccccc}
 \begin{array}{c} ++ \\ ++ \end{array} \mapsto \square & \begin{array}{c} ++ \\ +- \end{array} \mapsto \square \begin{array}{c} \square \\ \square \end{array} & \begin{array}{c} ++ \\ -+ \end{array} \mapsto \square \begin{array}{c} \square \\ \square \end{array} & \begin{array}{c} ++ \\ -- \end{array} \mapsto \square \begin{array}{c} \square \\ \square \end{array} & \begin{array}{c} +- \\ ++ \end{array} \mapsto \square \begin{array}{c} \square \\ \square \end{array} & \begin{array}{c} +- \\ +- \end{array} \mapsto \square \begin{array}{c} \square \\ \square \end{array} & \begin{array}{c} +- \\ -+ \end{array} \mapsto \square \begin{array}{c} \square \\ \square \end{array} & \begin{array}{c} +- \\ -- \end{array} \mapsto \square \begin{array}{c} \square \\ \square \end{array} \\
 \hline
 \begin{array}{c} -- \\ -- \end{array} \mapsto \square & \begin{array}{c} -- \\ +- \end{array} \mapsto \square \begin{array}{c} \square \\ \square \end{array} & \begin{array}{c} -- \\ +- \end{array} \mapsto \square \begin{array}{c} \square \\ \square \end{array} & \begin{array}{c} -- \\ ++ \end{array} \mapsto \square \begin{array}{c} \square \\ \square \end{array} & \begin{array}{c} -+ \\ -- \end{array} \mapsto \square \begin{array}{c} \square \\ \square \end{array} & \begin{array}{c} -+ \\ +- \end{array} \mapsto \square \begin{array}{c} \square \\ \square \end{array} & \begin{array}{c} -+ \\ -+ \end{array} \mapsto \square \begin{array}{c} \square \\ \square \end{array} & \begin{array}{c} -+ \\ ++ \end{array} \mapsto \square \begin{array}{c} \square \\ \square \end{array}
 \end{array} \tag{41}$$

(see Fig. 2). Then, Θ is a factor map onto \mathcal{Y} and is pre-injective. In fact, Θ is 2-to-1: every configuration $y \in \mathcal{Y}$ has exactly two pre-images $x, x' \in \mathcal{X}$, where $x' = -x$ (i.e., x' is obtained from x by flipping the direction of the spin at every site). Moreover, if f denotes the energy observable for the Ising model and g the contour length observable for the contour model, we have $\Delta_f = 2\Delta_g \circ \Theta$.

This relationship, which was first discovered by Peierls [67], is used to reduce the study of the Ising model to the study of the contour model (see e.g. [28,90]). The Gibbs measures for $\beta\Delta_f$ represent the states of thermal equilibrium for the Ising model at temperature $1/\beta$. According to Corollary 7 (and Theorem 1), the shift-invariant Gibbs measures $\pi \in \mathcal{G}_{\beta\Delta_f}(\mathcal{X}, \sigma)$ are precisely the Θ -pre-images of the shift-invariant Gibbs measures $\nu \in \mathcal{G}_{2\beta\Delta_g}(\mathcal{Y}, \sigma)$ for the contour model.

In fact, in this case it is also easy to show that the Θ -image of every Gibbs measure for $\beta\Delta_f$ (not necessarily shift-invariant) is a Gibbs measure for $2\beta\Delta_g$. Indeed, suppose that $\pi \in \mathcal{G}_{\beta\Delta_f}(\mathcal{X})$ is a Gibbs measure for $\beta\Delta_f$ and $\nu \triangleq \Theta\pi$ its image. Let $y, y' \in \mathcal{Y}$ be asymptotic configurations, and $E \supseteq \text{diff}(y, y')$ a sufficiently large finite set of sites. Let $x_1, x_2 \in \mathcal{X}$ be the pre-images of y , and $x'_1, x'_2 \in \mathcal{X}$ the pre-images of y' . Without loss of generality, we can assume that x_1 is asymptotic to x'_1 , and x_2 is asymptotic to x'_2 . It is easy to see that $\Theta^{-1}[y]_E = [x_1]_{N(E)} \cup [x_2]_{N(E)}$ and $\Theta^{-1}[y']_E = [x'_1]_{N(E)} \cup [x'_2]_{N(E)}$. Note that the cylinders $[x_1]_{N(E)}$ and $[x_2]_{N(E)}$ are disjoint, and so are the cylinders $[x'_1]_{N(E)}$ and $[x'_2]_{N(E)}$. Therefore,

$$\frac{\nu([y']_E)}{\nu([y]_E)} = \frac{\pi(\Theta^{-1}[y']_E)}{\pi(\Theta^{-1}[y]_E)} = \frac{\pi([x'_1]_{N(E)}) + \pi([x'_2]_{N(E)})}{\pi([x_1]_{N(E)}) + \pi([x_2]_{N(E)})}. \tag{42}$$

Since $N(E)$ is large and π is a Gibbs measure for $\beta\Delta_f$, we have $\pi([x'_1]_{N(E)}) = e^{-\beta\Delta_f(x_1, x'_1)}\pi([x_1]_{N(E)})$ and $\pi([x'_2]_{N(E)}) = e^{-\beta\Delta_f(x_2, x'_2)}\pi([x_2]_{N(E)})$. Since, $\Delta_f(x_1, x'_1) = \Delta_f(x_2, x'_2) = 2\Delta_g(y, y')$, it follows that $\nu([y']_E) = e^{-2\beta\Delta_g(y, y')} \nu([y]_E)$.

It has been proved that for any $0 < \beta < \infty$, the contour model with Hamiltonian $2\beta\Delta_g$ has a unique Gibbs measure [1,33]; the main difficulty is to show that the infinite contours are “unstable”, in the sense that, under every Gibbs measure, the probability of appearance of an infinite contour is zero.⁴ Let us denote the unique Gibbs measure for $2\beta\Delta_g$ by ν_β . It follows that the simplex of Gibbs measures for the Ising model at temperature $1/\beta$ is precisely $\Theta^{-1}\nu_\beta$. For, the set $\Theta^{-1}\nu_\beta$ includes $\mathcal{G}_{\beta\Delta_f}(\mathcal{X})$ (by the above observation) and is included in

⁴ In fact, the theorem of Aizenman and Higuchi states that the simplex of Gibbs measures for the two-dimensional Ising model at any temperature has at most two extremal elements. However, the uniqueness of the Gibbs measure for the contour model is implicit in their result, and constitutes the main ingredient of the proof.

$\mathcal{G}_{\beta\Delta_f}(\mathcal{X}, \sigma)$ (because ν_β must be shift-invariant). Therefore, the Gibbs measures for the Ising model at any temperature $1/\beta$ are shift-invariant and $\mathcal{G}_{\beta\Delta_f}(\mathcal{X}) = \mathcal{G}_{\beta\Delta_f}(\mathcal{X}, \sigma) = \Theta^{-1}\nu_\beta$.

It is not difficult to show that if $\Phi: \mathcal{X} \rightarrow \mathcal{Y}$ is a continuous k -to-1 map between two compact metric spaces, then every probability measure on \mathcal{Y} has at most k mutually singular pre-images under Φ . In particular, the simplex $\mathcal{G}_{\beta\Delta_f}(\mathcal{X}) = \mathcal{G}_{\beta\Delta_f}(\mathcal{X}, \sigma) = \Theta^{-1}\nu_\beta$ of Gibbs measures for the Ising model at temperature $1/\beta$ has at most 2 ergodic elements.

Whether the Ising model at temperature $1/\beta$ has two ergodic Gibbs measures or one depends on a specific geometric feature of the typical contour configurations under the measure ν_β . Roughly speaking, the contours of a contour configuration divide the two-dimensional plane into disjoint clusters. A configuration with no infinite contour generates either one or no infinite cluster, depending on whether each site is surrounded by a finite or infinite number of contours. Note that since ν_β is ergodic, the number of infinite clusters in a random configuration chosen according to ν_β is almost surely constant. If ν_β -almost every configuration has an infinite cluster, then it follows by symmetry that $\Theta^{-1}\nu_\beta$ contains two distinct ergodic measures, one in which the infinite cluster is colored with $+$ and one with $-$. The converse is also known to be true [76]: if ν_β -almost every configuration has no infinite cluster, then $\Theta^{-1}\nu_\beta$ has only one element.

Contour representations are used to study a wide range of statistical mechanics models, and are particularly fruitful to prove the “stability” of ground configurations at low temperature (see e.g. [20, 79]). ○

Let $\Phi: \mathcal{X} \rightarrow \mathcal{Y}$ be a pre-injective factor map between two strongly irreducible shifts of finite type (\mathcal{X}, σ) and (\mathcal{Y}, σ) . Let $f \in SV(\mathcal{Y})$ be an observable having summable variations and Δ_f the Hamiltonian defined by f . Then, according to Theorem 1, the equilibrium measures of f and $f \circ \Phi$ are precisely the shift-invariant Gibbs measures for the Hamiltonians Δ_f and $\Delta_{f \circ \Phi}$. A natural question is whether Corollary 7 remains valid for arbitrary Gibbs measures (not necessarily shift-invariant). If $\Phi: \mathcal{X} \rightarrow \mathcal{Y}$ is a morphism between two shifts and Δ is a Hamiltonian on \mathcal{Y} , let us denote by $\Phi^*\Delta$, the Hamiltonian on \mathcal{X} defined by $(\Phi^*\Delta)(x, y) \triangleq \Delta(\Phi x, \Phi y)$.

Conjecture 1 Let $\Phi: \mathcal{X} \rightarrow \mathcal{Y}$ be a pre-injective factor map between two strongly irreducible shifts of finite type (\mathcal{X}, σ) and (\mathcal{Y}, σ) . Let Δ be a Hamiltonian on \mathcal{Y} , and π a probability measure on \mathcal{X} . Then, π is a Gibbs measure for $\Phi^*\Delta$ if and only if $\Phi\pi$ is a Gibbs measure for Δ .

One direction of the latter conjecture is known to be true for a subclass of pre-injective factor maps. Let us say that a pre-injective factor map $\Phi: \mathcal{X} \rightarrow \mathcal{Y}$ between two shifts is *complete* if for every configuration $x \in \mathcal{X}$ and every configuration $y' \in \mathcal{Y}$ that is asymptotic to $y \triangleq \Phi x$, there is a (unique) configuration $x' \in \mathcal{X}$ asymptotic to x such that $\Phi x' = y'$.

Lemma 3 *Let $\Phi: \mathcal{X} \rightarrow \mathcal{Y}$ be a complete pre-injective factor map between two shifts of finite type (\mathcal{X}, σ) and (\mathcal{Y}, σ) . For every finite set $D \subseteq \mathbb{L}$, there is a finite set $E \subseteq \mathbb{L}$ such that every two asymptotic configurations $x, x' \in \mathcal{X}$ with $\text{diff}(\Phi x, \Phi x') \subseteq D$ satisfy $\text{diff}(x, x') \subseteq E$.*

Proof See Fig. 3 for an illustration.

For a configuration $x \in \mathcal{X}$, let \mathcal{A}_x be the set of all configurations x' asymptotic to x such that $\text{diff}(\Phi x, \Phi x') \subseteq D$. The set \mathcal{A}_x is finite. Therefore, there is a finite set E_x such that all the elements of \mathcal{A}_x agree outside E_x . We claim that if $C_x \supseteq E_x$ is a large enough finite set of sites, then for every configuration $x_1 \in [x]_{C_x}$, all the elements of \mathcal{A}_{x_1} agree outside E_x .

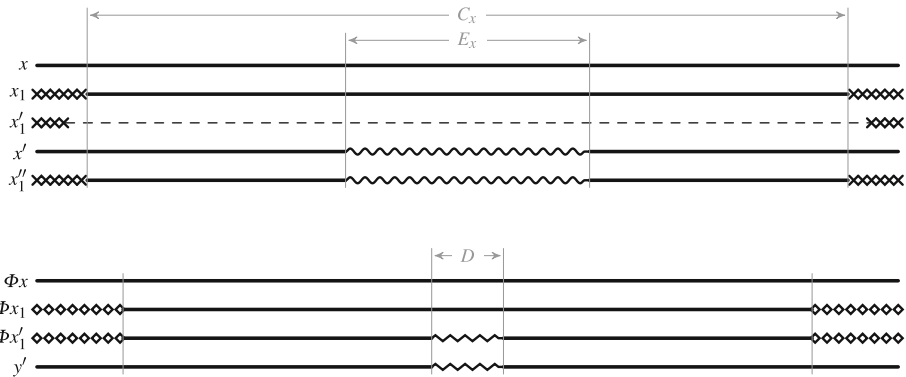


Fig. 3 Illustration of the proof of Lemma 3

To see this, suppose that C_x is large, and consider a configuration $x_1 \in [x]_{C_x}$. Let x'_1 be a configuration asymptotic to x_1 such that $\text{diff}(\Phi x_1, \Phi x'_1) \subseteq D$. By the gluing property of \mathcal{Y} , there is a configuration $y' \in \mathcal{Y}$ that agrees with $\Phi x'_1$ in a large neighborhood of D and with Φx outside D . Since Φ is a complete pre-injective factor map, there is a unique configuration x' asymptotic to x such that $\Phi x' = y'$. Now, by the gluing property of \mathcal{X} , there is a configuration x''_1 that agrees with x' in C_x and with x_1 outside E_x . Since C_x was chosen large, it follows that $\Phi x''_1 = \Phi x'_1$. Since x'_1 and x''_1 are asymptotic, the pre-injectivity of Φ ensures that $x''_1 = x'_1$. Therefore, x_1 and x'_1 agree outside E_x .

The cylinders $[x]_{C_x}$ form an open cover of \mathcal{X} . Therefore, by the compactness of \mathcal{X} , there is a finite set $\mathcal{S} \subseteq \mathcal{X}$ such that $\bigcup_{x \in \mathcal{S}} [x]_{C_x} \supseteq \mathcal{X}$. The set $E \triangleq \bigcup_{x \in \mathcal{S}} E_x$ has the desired property. \square

Theorem 5 (see [75], Proposition 2.5) *Let $\Phi : \mathcal{X} \rightarrow \mathcal{Y}$ be a complete pre-injective factor map between two strongly irreducible shifts of finite type (\mathcal{X}, σ) and (\mathcal{Y}, σ) . Let Δ be a Hamiltonian on \mathcal{Y} , and π a probability measure on \mathcal{X} . If π is a Gibbs measure for $\Phi^* \Delta$, then $\Phi \pi$ is a Gibbs measure for Δ .*

Proof Let $0 \in N \subseteq \mathbb{L}$ be a neighborhood for Φ . Let $0 \in M \subseteq \mathbb{L}$ be a neighborhood that witnesses the finite type gluing property of both \mathcal{X} and \mathcal{Y} . We write $\tilde{N} \triangleq N^{-1}(N)$ and $\tilde{M} \triangleq M^{-1}(M)$.

Let y and y' be two asymptotic configurations in \mathcal{Y} , and set $D \triangleq \text{diff}(y, y')$. For every configuration $x \in \Phi^{-1}[y]_{\tilde{M}(D)}$, there is a unique configuration $x' \in \Phi^{-1}[y']_{\tilde{M}(D)}$ that is asymptotic to x and such that $\text{diff}(\Phi x, \Phi x') \subseteq D$. (Namely, by the gluing property of \mathcal{Y} , the configuration y'_x that agrees with y' in $\tilde{M}(D)$ and with Φx outside D is in \mathcal{Y} . Since Φ is a complete pre-injective factor map, there is a unique configuration x' that is asymptotic to x and $\Phi x' = y'_x$.) The relation $x \mapsto x'$ is a one-to-one correspondence. By Lemma 3, there is a large enough finite set $E \subseteq \mathbb{L}$ such that for every $x \in \Phi^{-1}[y]_{\tilde{M}(D)}$, it holds $\text{diff}(x, x') \subseteq E$.

Consider a large finite set $\hat{D} \subseteq \mathbb{L}$ and another finite set $\hat{E} \subseteq \mathbb{L}$ that is much larger than \hat{D} . (More precisely, we need $\hat{D} \supseteq \tilde{M}(D)$ and $\hat{E} \supseteq N(\hat{D}) \cup \tilde{N}(E)$.) Let P_y denote the set of patterns $p \in L_{\hat{E}}(\mathcal{X})$ such that $\Phi[p]_{\hat{E}} \subseteq [y]_{\hat{D}}$. Then, $\Phi^{-1}[y]_{\hat{D}} = \bigcup_{p \in P_y} [p]_{\hat{E}}$ (provided $\hat{E} \supseteq N(\hat{D})$). Let $\mathcal{S} \subseteq \mathcal{X}$ be a finite set consisting of one representative from each cylinder $[p]_{\hat{E}}$, for $p \in A$. Then, $\Phi^{-1}[y]_{\hat{D}} = \bigcup_{x \in \mathcal{S}} [x]_{\hat{E}}$. Moreover, $\Phi^{-1}[y']_{\hat{D}} = \bigcup_{x \in \mathcal{S}} [x']_{\hat{E}}$

(provided $\hat{E} \supseteq \tilde{N}(E)$). Since the terms in each of the two latter unions are disjoint, we have

$$(\Phi\pi)[y]_{\hat{D}} = \sum_{x \in \mathcal{I}} \pi([x]_{\hat{E}}) \quad \text{and} \quad (\Phi\pi)[y']_{\hat{D}} = \sum_{x \in \mathcal{I}} \pi([x']_{\hat{E}}). \tag{43}$$

For each $x \in \Phi^{-1}[y]_{\hat{D}}$, we have

$$\frac{\pi([x']_{\hat{E}})}{\pi([x]_{\hat{E}})} - e^{-\Delta(y,y')} = \left(\frac{\pi([x']_{\hat{E}})}{\pi([x]_{\hat{E}})} - e^{-(\Phi^*\Delta)(x,x')} \right) + \left(e^{-\Delta(\Phi x, \Phi x')} - e^{-\Delta(y,y')} \right). \tag{44}$$

Let us denote the first term on the righthand side by $\delta_{\hat{E}}(x)$ and the second term by $\gamma_{\hat{D}}(x)$. Note that, since π is a Gibbs measure for $\Phi^*\Delta$ and $\text{diff}(x, x') \subseteq E$, $\delta_{\hat{E}}(x) \rightarrow 0$ uniformly over $\Phi^{-1}[y]_{\hat{D}}$ as $\hat{E} \nearrow \mathbb{L}$. Note also that, by the continuity property of Δ , $\gamma_{\hat{D}}(x) \rightarrow 0$ uniformly over $\Phi^{-1}[y]_{\hat{D}}$ as $\hat{D} \nearrow \mathbb{L}$. We can now write

$$\frac{(\Phi\pi)[y']_{\hat{D}}}{(\Phi\pi)[y]_{\hat{D}}} = \frac{\sum_{x \in \mathcal{I}} \pi([x']_{\hat{E}})}{\sum_{x \in \mathcal{I}} \pi([x]_{\hat{E}})} = \frac{\sum_{x \in \mathcal{I}} \left(e^{-\Delta(y,y')} + \delta_{\hat{E}}(x) + \gamma_{\hat{D}}(x) \right) \pi([x]_{\hat{E}})}{\sum_{x \in \mathcal{I}} \pi([x]_{\hat{E}})} \tag{45}$$

$$\frac{(\Phi\pi)[y']_{\hat{D}}}{(\Phi\pi)[y]_{\hat{D}}} = \frac{\sum_{x \in \mathcal{I}} \pi([x']_{\hat{E}})}{\sum_{x \in \mathcal{I}} \pi([x]_{\hat{E}})} = e^{-\Delta(y,y')} + \frac{\sum_{x \in \mathcal{I}} (\delta_{\hat{E}}(x) + \gamma_{\hat{D}}(x)) \pi([x]_{\hat{E}})}{\sum_{x \in \mathcal{I}} \pi([x]_{\hat{E}})}. \tag{46}$$

Consider a small number $\varepsilon > 0$. If \hat{D} is sufficiently large, we have $|\gamma_{\hat{D}}| < \varepsilon/2$. Moreover, after choosing \hat{D} , we can choose \hat{E} large enough so that $|\delta_{\hat{E}}| < \varepsilon/2$. Therefore, for \hat{D} sufficiently large we get

$$\left| \frac{(\Phi\pi)[y']_{\hat{D}}}{(\Phi\pi)[y]_{\hat{D}}} - e^{-\Delta(y,y)} \right| \leq \varepsilon. \tag{47}$$

It follows that

$$\left| \frac{(\Phi\pi)[y']_{\hat{D}}}{(\Phi\pi)[y]_{\hat{D}}} - e^{-\Delta(y,y)} \right| \rightarrow 0 \tag{48}$$

as $\hat{D} \nearrow \mathbb{L}$. Since this is valid for every two asymptotic configurations $y, y' \in \mathcal{Y}$, we conclude that $\Phi\pi$ is a Gibbs measure for Δ . □

Corollary 9 *Let $\Phi : \mathcal{X} \rightarrow \mathcal{Y}$ be a conjugacy between two strongly irreducible shifts of finite type (\mathcal{X}, σ) and (\mathcal{Y}, σ) . Let Δ be a Hamiltonian on \mathcal{Y} , and π a probability measure on \mathcal{X} . Then, π is a Gibbs measure for $\Phi^*\Delta$ if and only if $\Phi\pi$ is a Gibbs measure for Δ .*

3.3 The Image of a Gibbs Measure

Let $\Phi : \mathcal{X} \rightarrow \mathcal{Y}$ be a pre-injective factor map between two strongly irreducible shifts of finite type. According to Corollary 7, a pre-image of a shift-invariant Gibbs measure under the induced map $\mathcal{P}(\mathcal{X}, \sigma) \rightarrow \mathcal{P}(\mathcal{Y}, \sigma)$ is again a Gibbs measure. The image of a Gibbs measure, however, does not need to be a Gibbs measure as the following example demonstrates.

Example 6 (XOR map) Let $\mathcal{X} = \mathcal{Y} \triangleq \{0, 1\}^{\mathbb{Z}}$ be the binary full shift and Φ the so-called XOR map, defined by $(\Phi x)(i) \triangleq x(i) + x(i+1) \pmod{2}$. Let π be the shift-invariant Bernoulli measure on \mathcal{X} with marginals $1 \mapsto p$ and $0 \mapsto 1 - p$, where $0 < p < 1$. This is a Gibbs measure for the Hamiltonian Δ_f , where $f : \mathcal{X} \rightarrow \mathbb{R}$ is the single-site observable defined by $f(x) \triangleq -\log p$ if $x(0) = 1$ and $f(x) \triangleq -\log(1 - p)$ if $x(0) = 0$. We claim that unless $p = \frac{1}{2}$, $\Phi\pi$ is not a regular Gibbs measure (i.e., a Gibbs measure for a Hamiltonian generated by an observable with summable variations).

Suppose, on the contrary, that $p \neq \frac{1}{2}$ and $\Phi\pi$ is a Gibbs measure for Δ_g for some $g \in SV(\mathcal{X})$. Then π is also an equilibrium measure for $g \circ \Phi$ (Corollary 7), implying that f and $g \circ \Phi$ are physically equivalent (Proposition 8). Consider the two uniform configurations $\underline{0}$ and $\underline{1}$, where $\underline{0}(i) \triangleq 0$ and $\underline{1}(i) \triangleq 1$ for every $i \in \mathbb{Z}$. We have $f(\underline{0}) = -\log p \neq -\log(1 - p) = f(\underline{1})$, whereas $g \circ \Phi(\underline{0}) = g \circ \Phi(\underline{1})$. If $\delta_{\underline{0}}$ and $\delta_{\underline{1}}$ are, respectively, the probability measures concentrated on $\underline{0}$ and $\underline{1}$, we get that $\delta_{\underline{0}}(f) - \delta_{\underline{0}}(g \circ \Phi) \neq \delta_{\underline{1}}(f) - \delta_{\underline{1}}(g \circ \Phi)$. This is a contradiction with the physical equivalence of f and $g \circ \Phi$, because $\delta_{\underline{0}}, \delta_{\underline{1}} \in \mathcal{P}(\mathcal{X}, \sigma)$ (Proposition 7).

In fact, the same argument shows that none of the n -fold iterations $\Phi^n\pi$ are regular Gibbs measures, because $\Phi^n(\underline{0}) = \Phi^n(\underline{1})$ for every $n \geq 1$. On the other hand, it has been shown [50,58], that $\Phi^n\pi$ converges in density to the uniform Bernoulli measure, which is a Gibbs measure and is invariant under Φ . The question of approach to equilibrium will be discussed in Sect. 4.4. ○

The latter example was first suggested by van den Berg (see [51], Sect. 3.2) as an example of a measure that is *strongly non-Gibbsian*, in the sense that attempting to define a Hamiltonian for it via (15) would lead to a function Δ for which the continuity property fails *everywhere*. The question of when a measure is Gibbsian and the study of the symptoms of being non-Gibbsian is an active area of research as non-Gibbsianness sets boundaries on the applicability of the so-called renormalization group technique in statistical mechanics (see e.g. [19,21]).

The observation in Example 6 can be generalized as follows.

Proposition 9 *Let (\mathcal{X}, σ) be a strongly irreducible shift of finite type and $\pi \in \mathcal{P}(\mathcal{X}, \sigma)$ a Gibbs measure for a Hamiltonian Δ_f , where $f \in SV(\mathcal{X})$. Suppose that $\Phi : \mathcal{X} \rightarrow \mathcal{Y}$ is a pre-injective factor map from (\mathcal{X}, σ) onto another shift of finite type (\mathcal{Y}, σ) . A necessary condition for $\Phi\pi$ to be a regular Gibbs measure is that for every two measures $\mu_1, \mu_2 \in \mathcal{P}(\mathcal{X}, \sigma)$ with $\mu_1(f) \neq \mu_2(f)$ it holds $\Phi\mu_1 \neq \Phi\mu_2$.*

Example 7 (XOR map; Example 6 continued) The argument of Example 6 can be stretched to show that the iterations of the XOR map turn every Gibbs measure other than the uniform Bernoulli measure eventually to a non-Gibbs measure. More specifically, for every observable $f \in SV(\mathcal{X})$ that is not physically equivalent to 0 and every shift-invariant Gibbs measure π for Δ_f , there is an integer $n_0 \geq 1$ such that for any $n \geq n_0$, the measure $\Phi^n\pi$ is not a regular Gibbs measure.

This is a consequence of the self-similar behaviour of the XOR map. Namely, the map Φ satisfies $(\Phi^{2^k} x)(i) = x(i) + x(i + 2^k) \pmod{2}$ for every $i \in \mathbb{Z}$ and every $k \geq 1$. If f is not physically equivalent to 0, two periodic configurations $x, y \in \mathcal{X}$ with common period 2^k can be found such that $2^{-k} \sum_{i=0}^{2^k-1} f(\sigma^i x) \neq 2^{-k} \sum_{i=0}^{2^k-1} f(\sigma^i y)$. If μ_x and μ_y denote, respectively, the shift-invariant measures concentrated at the shift orbits of x and y , we obtain that $\mu_x(f) \neq \mu_y(f)$. Nevertheless, $\Phi^n x = \Phi^n y = \underline{0}$ for all $n \geq 2^k$, implying that $\Phi^n \mu_x = \Phi^n \mu_y = \delta_{\underline{0}}$. Therefore, according to Proposition 9, the measure $\Phi^n\pi$ cannot be a regular Gibbs measure. ○

With the interpretation of the shift-ergodic measures as the macroscopic states (see the Introduction), the above proposition reads as follows: a sufficient condition for the non-Gibbsianness of $\Phi\pi$ is that there are two macroscopic states that are distinguishable by the density of f and are mapped to the same state by Φ .

If the induced map $\Phi : \mathcal{P}(\mathcal{X}, \sigma) \rightarrow \mathcal{P}(\mathcal{Y}, \sigma)$ is not one-to-one, then there are Gibbs measures (even Markov measures) whose images are not Gibbs. For, suppose $\mu_1, \mu_2 \in \mathcal{P}(\mathcal{X}, \sigma)$ are distinct measures with $\Phi\mu_1 = \Phi\mu_2$. Then, there is a local observable $f \in K(\mathcal{X})$ such that $\mu_1(f) \neq \mu_2(f)$. Every shift-invariant Gibbs measure for Δ_f is mapped by Φ to a measure that is not regular Gibbs.

Question 2 Let $\Phi : \mathcal{X} \rightarrow \mathcal{Y}$ be a pre-injective factor map between two strongly irreducible shifts of finite type (\mathcal{X}, σ) and (\mathcal{Y}, σ) , and suppose that the induced map $\Phi : \mathcal{P}(\mathcal{X}, \sigma) \rightarrow \mathcal{P}(\mathcal{Y}, \sigma)$ is injective. Does Φ map every (regular, shift-invariant) Gibbs measure to a Gibbs measure?

4 Cellular Automata

4.1 Conservation Laws

Let $\Phi: \mathcal{X} \rightarrow \mathcal{X}$ be a cellular automaton on a strongly irreducible shift of finite type (\mathcal{X}, σ) . We say that Φ *conserves* (the energy-like quantity formalized by) a Hamiltonian Δ if $\Delta(\Phi x, \Phi y) = \Delta(x, y)$ for every two asymptotic configurations $x, y \in \mathcal{X}$. If $\Delta = \Delta_f$ is the Hamiltonian generated by a local observable $f \in K(\mathcal{X})$, then we may also say that Φ *conserves* f (in the aggregate). More generally, we say that a continuous observable $f \in C(\mathcal{X})$ is conserved by Φ if f and $f \circ \Phi$ are physically equivalent. According to Proposition 7, this is equivalent to the existence of a constant $c \in \mathbb{R}$ such that $(\Phi\pi)(f) = \pi(f) + c$ for every shift-invariant probability measure π . However, in this case c is always 0.

Proposition 10 *Let $\Phi: \mathcal{X} \rightarrow \mathcal{X}$ be a cellular automaton over a strongly irreducible shift of finite type (\mathcal{X}, σ) . A continuous observable $f \in C(\mathcal{X})$ is conserved by Φ if and only if $(\Phi\pi)(f) = \pi(f)$ for every probability measure $\pi \in \mathcal{P}(\mathcal{X}, \sigma)$.*

Proof Let $c \in \mathbb{R}$ be such that $(\Phi\pi)(f) = \pi(f) + c$ for every $\pi \in \mathcal{P}(\mathcal{X}, \sigma)$. Then, for every $n > 0$, $(\Phi^n\pi)(f) = \pi(f) + nc$. However, every continuous function on a compact space is bounded. Therefore, $c = 0$. □

If an observable f is conserved by a cellular automaton Φ , we say that f is bound by a *conservation law* under Φ . There is also a concept of *local* conservation law. Let D_0 be a finite generating set for the group $\mathbb{L} = \mathbb{Z}^d$. Suppose that $f \in C(\mathcal{X})$ is an observable that is conserved by a cellular automaton $\Phi : \mathcal{X} \rightarrow \mathcal{X}$. By Proposition 10 and Lemma 2, this means that $f \circ \Phi - f \in C(\mathcal{X}, \sigma)$, that is

$$f \circ \Phi - f = \lim_{n \rightarrow \infty} \sum_{i \in D_0} \left(h_i^{(n)} \circ \sigma^i - h_i^{(n)} \right) \tag{49}$$

for some $h_i^{(n)} \in K(\mathcal{X})$ (for $i \in D_0$ and $n = 0, 1, 2, \dots$). In other words, for every configuration $x \in \mathcal{X}$ it holds

$$f(\Phi x) = f(x) + \lim_{n \rightarrow \infty} \left[\sum_{i \in D_0} h_i^{(n)}(\sigma^i x) - \sum_{i \in D_0} h_i^{(n)}(x) \right]. \tag{50}$$

If furthermore $f \circ \Phi - f \in K(\mathcal{X}, \sigma) \subseteq C(\mathcal{X}, \sigma)$ (where $K(\mathcal{X}, \sigma)$ is defined as in (2)), then we have the more intuitive equation

$$f(\Phi x) = f(x) + \sum_{i \in D_0} h_i(\sigma^i x) - \sum_{i \in D_0} h_i(x) \tag{51}$$

for some $h_i \in K(\mathcal{X})$. In this case, we say that f is *locally conserved* by Φ (or satisfies a *local conservation law* under Φ). The value $h_i(\sigma^k x)$ is then interpreted as the *flow* (of the energy-like quantity captured by f) from site k to site $k - i$. The latter equation is a *continuity equation*, stating that at each site k , the changes in the observed quantity after one step should balance with the incoming and the outgoing flows. If \mathcal{X} is a full shift, it is known that every conserved local observable is locally conserved. The proof is similar to that of Proposition 1.

Local conservation laws enjoy a somewhat symmetric relationship with time and space. Namely, an observable $f \in K(\mathcal{X})$ is locally conserved by Φ if and only if the observable $\alpha \triangleq f \circ \Phi - f$ is in $K(\mathcal{X}, \Phi) \cap K(\mathcal{X}, \sigma)$. Moreover, to every observable $\alpha \in K(\mathcal{X}, \Phi) \cap K(\mathcal{X}, \sigma)$, there corresponds at least one observable $f \in K(\mathcal{X})$ such that $\alpha = f \circ \Phi - f$ and f is locally conserved by Φ . In general, there might be several observables f with the latter property. If $\alpha = f \circ \Phi - f = f' \circ \Phi - f'$ for two observables $f, f' \in K(\mathcal{X})$, then $(f - f') = (f - f') \circ \Phi$; that is, $f - f'$ is *invariant* under Φ . Every constant observable is invariant under any cellular automaton. The following is an example of a cellular automaton with non-constant invariant local observables.

Example 8 (Invariant observables) Let $\Phi : \{0, 1, 2\}^{\mathbb{Z}} \rightarrow \{0, 1, 2\}^{\mathbb{Z}}$ be the cellular automaton with

$$(\Phi x)(i) \triangleq \begin{cases} 2 & \text{if } x(i) = 2, \\ x(i) + x(i + 1) \pmod{2} & \text{otherwise} \end{cases} \tag{52}$$

(see Fig. 4). The observable $f : \{0, 1, 2\}^{\mathbb{Z}} \rightarrow \mathbb{R}$ defined by $f(x) \triangleq 1$ if $x(i) = 2$ and $f(x) \triangleq 0$ otherwise is obviously invariant. The Hamiltonian Δ_f counts the number of occurrences of symbol 2 and is conserved by Φ . In fact, there are infinitely many linearly independent, physically non-equivalent observables that are invariant under Φ . Namely, the relative position of the occurrences of 2 remain unchanged, and hence, for any finite set $D \subseteq \mathbb{Z}$, the logical conjunction of $f \circ \sigma^i$ for $i \in D$ is invariant. It follows that Φ has infinitely many distinct (and linearly independent) conservation laws.

Such abundance of conservation laws is common among all cellular automata having non-constant invariant local observables (see Lemma 2 of [25]), and has been suggested as the reason behind the “non-physical” behavior in these cellular automata (see e.g. [83]). Every surjective equicontinuous cellular automaton is periodic [5, 7] and hence has non-constant invariant local observables. It follows that every surjective cellular automaton that has a non-trivial equicontinuous cellular automaton as factor has non-constant invariant local observables and an infinity of linearly independent conservation laws. ○

Question 3 Does every surjective cellular automaton with equicontinuous points have non-constant local observables?

Every cellular automaton $\Phi: \mathcal{X} \rightarrow \mathcal{X}$ conserves the trivial Hamiltonian $\Delta \equiv 0$ on \mathcal{X} . Furthermore, every observable $f \in C(\mathcal{X})$ that is physically equivalent to 0 (i.e., $f - c \in C(\mathcal{X}, \sigma)$ for some $c \in \mathbb{R}$) is *trivially* conserved by Φ . Likewise, a local observable $f \in K(\mathcal{X})$ is *trivially* locally conserved by Φ if $f - c \in K(\mathcal{X}, \sigma)$ for some $c \in \mathbb{R}$. We shall say that two local observables $f, g \in K(\mathcal{X})$ are *locally physically equivalent* if

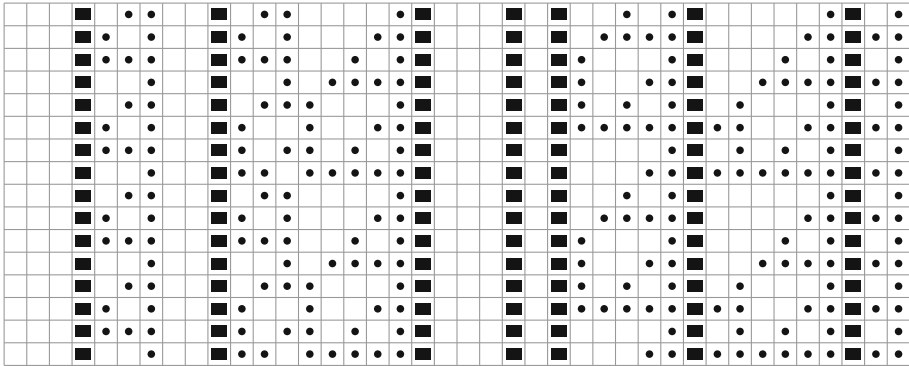


Fig. 4 A cellular automaton with infinitely many distinct conservation laws (see Example 8). *Black square* represents state 2 and *black dot* represents 1. Time goes downward

$f - g - c \in K(\mathcal{X}, \sigma)$ for some $c \in \mathbb{R}$. The following proposition is the analogue of Proposition 10.

Proposition 11 *Let $\Phi : \mathcal{X} \rightarrow \mathcal{X}$ be a cellular automaton over a strongly irreducible shift of finite type (\mathcal{X}, σ) . A local observable $f \in K(\mathcal{X})$ is locally conserved by Φ if and only if f and $f \circ \Phi$ are locally physically equivalent.*

4.2 Invariance of Gibbs Measures

As a corollary of the results of Sect. 3, we obtain a correspondence between the conservation laws of a surjective cellular automata and its invariant Gibbs measures. It is well-known that every surjective cellular automata over a full shift preserves the uniform Bernoulli measure (see [31], Theorem 5.4 and [55]). The invariance of the uniform Bernoulli measure is sometimes called the *balance property* of (the local update rule of) the surjective cellular automata. In case of surjective cellular automata over strongly irreducible shifts of finite type, a similar property is known to hold: every measure of maximum entropy is mapped to a measure of maximum entropy (see [14], Corollary 2.3 and [56], Theorems 3.3 and 3.6). The following two theorems can be seen as further generalizations of the balance property. Indeed, choosing $f \equiv 0$ in either of the two theorems implies that a surjective cellular automaton maps each measure of maximum entropy to a measure of maximum entropy. An elementary proof of Theorem 6 in the special case of surjective cellular automata on one-dimensional full shifts and single-site observables was earlier presented in [42].

Theorem 6 *Let $\Phi : \mathcal{X} \rightarrow \mathcal{X}$ be a surjective cellular automaton over a strongly irreducible shift of finite type (\mathcal{X}, σ) , and let $f \in SV(\mathcal{X})$ be an observable with summable variations. The following conditions are equivalent:*

- (a) Φ conserves f .
- (b) Φ maps the set $\mathcal{E}_f(\mathcal{X}, \sigma)$ of equilibrium measures for f onto itself.
- (c) There exist a measure in $\mathcal{E}_f(\mathcal{X}, \sigma)$ whose Φ -image is also in $\mathcal{E}_f(\mathcal{X}, \sigma)$.

If $f \in C(\mathcal{X})$ does not have summable variations, condition (a) still implies the other two conditions.

Proof

- a \Rightarrow b) Suppose that Φ conserves f . By Proposition 8 and Corollary 7 we have $\pi \in \mathcal{E}_f(\mathcal{X}, \sigma)$ if and only if $\Phi\pi \in \mathcal{E}_f(\mathcal{X}, \sigma)$. Using Lemma 1, we obtain $\Phi\mathcal{E}_f(\mathcal{X}, \sigma) = \mathcal{E}_f(\mathcal{X}, \sigma)$.
- b \Rightarrow c) Trivial.
- c \Rightarrow a) Let f have summable variations. Then, so does $f \circ \Phi$. Suppose that there exists a measure $\pi \in \mathcal{E}_f(\mathcal{X}, \sigma)$ such that $\Phi\pi \in \mathcal{E}_f(\mathcal{X}, \sigma)$. By Corollary 7, we also have $\pi \in \mathcal{E}_{f \circ \Phi}(\mathcal{X}, \sigma)$. Therefore, $\mathcal{E}_f(\mathcal{X}, \sigma) \cap \mathcal{E}_{f \circ \Phi}(\mathcal{X}, \sigma) \neq \emptyset$ and by Proposition 8, f and $f \circ \Phi$ are physically equivalent. That is, Φ conserves f .

□

Theorem 7 *Let $\Phi : \mathcal{X} \rightarrow \mathcal{X}$ be a surjective cellular automaton over a strongly irreducible shift of finite type (\mathcal{X}, σ) . Let $f \in C(\mathcal{X})$ be an observable and $e \in \mathbb{R}$. If Φ conserves f , then Φ maps $\mathcal{E}_{(f)=e}(\mathcal{X}, \sigma)$ onto itself.*

From Theorems 6 and 7 it follows that each of the (convex and compact) sets $\mathcal{E}_f(\mathcal{X}, \sigma)$ and $\mathcal{E}_{(f)=e}(\mathcal{X}, \sigma)$ contains an invariant measure for Φ , provided that Φ conserves f . However, following the common reasoning of statistical mechanics (see the Introduction), such an invariant measure should not be considered as a macroscopic equilibrium state unless it is shift-ergodic (see Example 9 below).

In the implication (c \Rightarrow a) of Theorem 6, the set $\mathcal{E}_f(\mathcal{X}, \sigma)$ of equilibrium measures for f can be replaced by the potentially larger set $\mathcal{G}_{\Delta_f}(\mathcal{X})$ of Gibbs measures for Δ_f .

Corollary 10 *Let $\Phi : \mathcal{X} \rightarrow \mathcal{X}$ be a surjective cellular automaton over a strongly irreducible shift of finite type (\mathcal{X}, σ) , and let $f \in SV(\mathcal{X})$ be an observable with summable variations. Suppose that there is a Gibbs measure for Δ_f whose Φ -image is also a Gibbs measure for Δ_f . Then, Φ conserves Δ_f .*

Proof Let π be a probability measure on \mathcal{X} such that $\pi, \Phi\pi \in \mathcal{G}_{\Delta_f}(\mathcal{X})$. Let \mathcal{H} denote the closed convex hull of the measures $\sigma^k\pi$ for $k \in \mathbb{L}$. Then, \mathcal{H} is a closed, convex, shift-invariant set, and therefore, contains a shift-invariant element ν . Moreover, both \mathcal{H} and $\Phi\mathcal{H}$ are subsets of $\mathcal{G}_{\Delta_f}(\mathcal{X})$. In particular, $\nu, \Phi\nu \in \mathcal{G}_{\Delta_f}(\mathcal{X})$. Hence, $\nu, \Phi\nu \in \mathcal{E}_f(\mathcal{X}, \sigma)$, and the claim follows from Theorem 6. □

For reversible cellular automata, Corollary 9 leads to a variant of Theorem 6 concerning all (not necessarily shift-invariant) Gibbs measures.

Theorem 8 *Let $\Phi : \mathcal{X} \rightarrow \mathcal{X}$ be a reversible cellular automaton over a strongly irreducible shift of finite type (\mathcal{X}, σ) , and let Δ be a Hamiltonian on \mathcal{X} . The following conditions are equivalent:*

- (a) Φ conserves Δ .
- (b) A probability measure is in $\mathcal{G}_{\Delta}(\mathcal{X})$ if and only if its Φ -image is in $\mathcal{G}_{\Delta}(\mathcal{X})$.
- (c) There exists a measure in $\mathcal{G}_{\Delta}(\mathcal{X})$ whose Φ -image is also in $\mathcal{G}_{\Delta}(\mathcal{X})$.

Proof If Φ conserves Δ , we have, by definition, $\Phi^*\Delta = \Delta$, and Corollary 9 (and Lemma 1) imply that $\Phi^{-1}\mathcal{G}_{\Delta}(\mathcal{X}) = \mathcal{G}_{\Delta}(\mathcal{X})$. Conversely, suppose that π is a probability measure such that $\pi, \Phi\pi \in \mathcal{G}_{\Delta}(\mathcal{X})$. Then, by Corollary 9, $\pi \in \mathcal{G}_{\Delta}(\mathcal{X}) \cap \mathcal{G}_{\Phi^*\Delta}(\mathcal{X})$, and it follows from the definition of a Gibbs measure that $\Phi^*\Delta = \Delta$. That is, Φ conserves Δ . □

Example 9 (Q2R cellular automaton) The Q2R model discussed in the Introduction is not, strictly speaking, a cellular automaton (with the standard definition), as it involves alternate application of two maps that do not commute with the shift. Simple tricks can however be used to turn it into a standard cellular automaton (see e.g. [88], Sect. 5.2).

Let $\mathcal{X} \triangleq \{+, -\}^{\mathbb{Z}^2}$ be the space of spin configurations, and denote by Φ_e the mapping $\mathcal{X} \rightarrow \mathcal{X}$ that updates the even sites. That is,

$$(\Phi_e x)(i) \triangleq \begin{cases} \overline{x_i} & \text{if } i \text{ an even site and } n_i^+(x) = n_i^-(x), \\ x_i & \text{otherwise,} \end{cases} \tag{53}$$

where the spin-flipping operation is denoted by overline, and $n_i^+(x)$ (resp., $n_i^-(x)$) represents the number of sites j among the four immediate neighbors of i such that $x(j) = +$ (resp., $x(j) = -$). Similarly, let Φ_o denotes the mapping that updates the odd sites. The composition $\Phi \triangleq \Phi_o \Phi_e$ commutes with the shifts σ^k , for k in the sub-lattice $(2\mathbb{Z})^2$, and (after a recoding) could be considered as a cellular automaton.

Let f denote the energy observable defined in Example 1. For every $\beta > 0$, the Hamiltonian $\Delta_{\beta f}$ is conserved by Φ . Therefore, according to Theorem 8, the set $\mathcal{G}_{\Delta_{\beta f}}(\mathcal{X})$ of Gibbs measures for $\Delta_{\beta f}$ is invariant under Φ . In fact, in this example, it is easy to show that Φ preserves every individual Gibbs measure in $\mathcal{G}_{\Delta_{\beta f}}(\mathcal{X})$.

It is natural to ask whether the preservation of individual elements of $\mathcal{G}_{\Delta_{\beta f}}(\mathcal{X})$ holds in general. This is however not the case. When β large enough, it is known that $\mathcal{G}_{\Delta_{\beta f}}(\mathcal{X})$ contains two distinct shift-ergodic measures, obtained from each other by a spin flip transformation (see Example 5). The cellular automaton $\Phi'x \triangleq \overline{\Phi x}$, which flips every spin after applying Φ , conserves $\Delta_{\beta f}$ but does not preserve either of the two distinct shift-ergodic Gibbs measures for $\Delta_{\beta f}$. ○

4.3 Absence of Conservation Laws

In light of the above connection, every statement about conservation laws in surjective cellular automata has an interpretation in terms of invariance of Gibbs measures, and vice versa. In this section, we see an example of such reinterpretation that leads to otherwise non-trivial results. Namely, proving the absence of conservation laws in two relatively rich families of surjective and reversible cellular automata, we obtain strong constraints on the invariant measures of the cellular automata within each family. Roughly speaking, strong chaotic behavior is incompatible with the presence of conservation laws. In contrast, any surjective cellular automaton with a non-trivial equicontinuous factor has an infinity of linearly independent conservation laws (see Example 8).

We say that a dynamical system (\mathcal{X}, Φ) is *strongly transitive* if for every point $z \in \mathcal{X}$, the set $\bigcup_{i=0}^{\infty} \Phi^{-i}z$ is dense in \mathcal{X} . Strong transitivity is stronger than transitivity (!) and weaker than minimality. A dynamical system $\Phi : \mathcal{X} \rightarrow \mathcal{X}$ is *minimal* if it has no non-trivial closed subsystems, and is *transitive* if for every pair of non-empty open sets $A, B \subseteq \mathcal{X}$, there is an integer $n \geq 0$ such that $A \cap \Phi^{-n}B \neq \emptyset$. In our setting (i.e., \mathcal{X} being compact), minimality is equivalent to the property that the only closed sets $E \subseteq \mathcal{X}$ with $E \subseteq \Phi E$ are \emptyset and \mathcal{X} , which is easily seen to imply strong transitivity. However, note that cellular automata over non-trivial strongly irreducible shifts of finite type cannot be minimal. This is because every strongly irreducible shift of finite type has configurations that are periodic in at least one direction. (More specifically, for each $k \in \mathbb{L} \setminus \{0\}$, there is a configuration x such that $\sigma^{pk}x = x$ for some $p > 0$.) Transitivity is often considered as one of the main indicators of

chaos (see e.g. [4,46]). Every transitive cellular automaton is known to be sensitive to initial conditions (i.e., uniformly unstable) [13,47].⁵

Example 10 (XOR cellular automata) The d -dimensional XOR cellular automaton with neighborhood $N \subseteq \mathbb{Z}^d$ is defined by the map $\Phi : \{0, 1\}^{\mathbb{Z}^d} \rightarrow \{0, 1\}^{\mathbb{Z}^d}$, where $(\Phi x)(i) \triangleq \sum_{i \in N} x(i) \pmod{2}$. To avoid the trivial case, we assume that the neighborhood has at least two elements. Examples 6 and 7 were about the one-dimensional XOR cellular automaton with neighborhood $\{0, 1\}$. Figure 5a depicts a sample run of the one-dimensional model with neighborhood $\{-1, 1\}$.

The XOR cellular automaton is strongly transitive. An argument similar to that in Example 7 shows that the uniform Bernoulli measure is the only regular Gibbs measure that is invariant under an XOR cellular automaton. Note, however, that there are many other (non-Gibbs) invariant measures. For example, the Dirac measure concentrated at the uniform configuration with 0 everywhere is invariant. So is the (atomic) measure uniformly distributed over any jointly periodic orbit (i.e., a finite orbit of (σ, Φ)).

In fact, much more is known about the invariant measures of the XOR cellular automata, with a strong indication that the uniform Bernoulli measure is the only “state of macroscopic equilibrium”. For instance, the uniform Bernoulli measure on $\{0, 1\}^{\mathbb{Z}}$ is known to be the only shift-ergodic probability measure that is invariant and of positive entropy for the XOR cellular automaton with neighborhood $\{0, 1\}$ [34]. Another such result states that the only measures that are strongly mixing for the shift and invariant under the XOR cellular automaton with neighborhood $\{-1, 1\}$ are the uniform Bernoulli measure and the Dirac measure concentrated at the uniform configuration with 0s everywhere [58]. (Note that the one-dimensional Gibbs measures are all strongly mixing.) Similar results have been obtained for broad classes of cellular automata with algebraic structure (e.g. [69,77,81]). See [70] for a survey. \circ

The following theorem is a slight generalization of Theorem 5 in [25].

Theorem 9 *Let $\Phi : \mathcal{X} \rightarrow \mathcal{X}$ be a strongly transitive cellular automaton over a shift of finite type (\mathcal{X}, σ) . Then, Φ does not conserve any non-trivial Hamiltonian.*

Proof Let $0 \in M \subseteq \mathbb{L}$ be a finite window that witnesses the finite type gluing property of \mathcal{X} .

Let Δ be a non-trivial Hamiltonian on \mathcal{X} , and suppose there exist two asymptotic configurations u and v such that $\varepsilon \triangleq \Delta(u, v) > 0$. By the continuity property of Δ , there is a finite set $D \supseteq M(M^{-1}(\text{diff}(u, v)))$ such that for every two asymptotic configurations $u' \in [u]_D$ and $v' \in [v]_D$ with $\text{diff}(u', v') = \text{diff}(u, v)$, $\Delta(u', v') \geq \varepsilon/2 > 0$.

Let z be a ground configuration for Δ (see Proposition 2). Since Φ is strongly transitive, there is a configuration $x \in [v]_D$ and a time $t \geq 0$ such that $\Phi^t x = z$. Construct a configuration $y \in \mathcal{X}$ that agrees with u on D and with x outside $\text{diff}(u, v)$. In particular, $y \in [u]_D$. Then, $\Delta(y, x) \geq \varepsilon/2$, whereas $\Delta(\Phi^t y, \Phi^t x) \leq 0$. Therefore, Δ is not conserved by Φ . \square

Corollary 11 *Let $\Phi : \mathcal{X} \rightarrow \mathcal{X}$ be a strongly transitive cellular automaton over a strongly irreducible shift of finite type (\mathcal{X}, σ) . Then, Φ does not preserve any regular Gibbs measure other than the Gibbs measures for the trivial Hamiltonian.*

A special case of the above corollary (for the permutive cellular automata and Bernoulli measures) is also proved in [2] (Corollary 3.6). Let us recall that the *shift-invariant* Gibbs measures for the trivial Hamiltonian on \mathcal{X} coincide with the measures of maximum entropy

⁵ In fact, transitive cellular automata are weakly mixing [61], which, in addition to sensitivity, also implies chaos in the sense of Li and Yorke (see [4,46]).

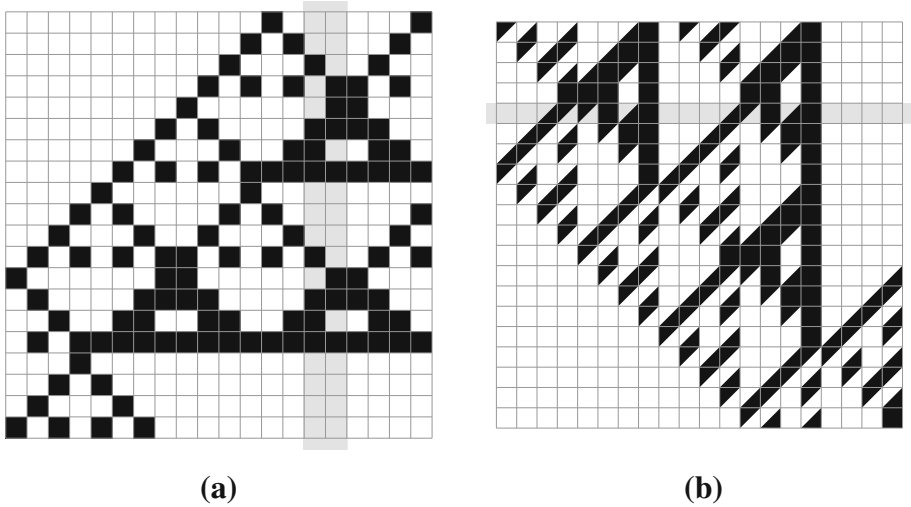


Fig. 5 Sample runs of **a** the one-dimensional XOR cellular automaton with neighborhood $\{-1, 1\}$ (see Example 10) and **b** its transpose (Example 11). Time goes downward

for (\mathcal{X}, σ) (Theorem 1). Therefore, according to Corollary 11, if Φ is strongly transitive, the measures of maximum entropy for (\mathcal{X}, σ) are the only candidates for Gibbs measures that are invariant under both σ and Φ . Since the set of measures with maximum entropy for (\mathcal{X}, σ) is closed and convex, and is preserved under Φ , it follows that at least one measure with maximum entropy is invariant under Φ . However, this measure does not need to be ergodic for the shift.

Next, we are going to introduce a class of one-dimensional *reversible* cellular automata with no local conservation law. The proof will be via reduction to Theorem 9. Note that reversible cellular automata over non-trivial strongly irreducible shifts of finite type cannot be strongly transitive: the inverse of a strongly transitive system is minimal, and as mentioned above, cellular automata over non-trivial strongly irreducible shifts of finite type cannot be minimal.

Example 11 (Transpose of XOR) Figure 5b depicts a sample space-time diagram of the reversible cellular automaton Φ on $(\{0, 1\} \times \{0, 1\})^{\mathbb{Z}}$ with neighbourhood $\{0, 1\}$ and local rule $((a, b), (c, d)) \mapsto (b, a + d)$, where the addition is modulo 2. Observe that rotating a space-time diagram of Φ by 90 degrees, we obtain what is essentially a space-time diagram of the XOR cellular automaton with neighbourhood $\{-1, 1\}$ (see Fig. 5a and Example 10).

As in Example 3 of [25], it is possible to show that Φ has no non-trivial finite-range conservation law. Below, we shall present an alternative proof (using its connection with the XOR cellular automaton) that covers a large class of similar reversible cellular automata. \circ

We shall say that two surjective one-dimensional cellular automata are *transpose* of each other if the bi-infinite space-time diagrams of each is obtained (up to a conjugacy) from the bi-infinite space-time diagrams of the other by swapping the role of space and time. To be more specific, let $\Phi: \mathcal{X} \rightarrow \mathcal{X}$ be a surjective cellular automaton on a one-dimensional mixing shift space of finite type $\mathcal{X} \subseteq S^{\mathbb{Z}}$. Define the continuous map $\Theta: S^{\mathbb{Z} \times \mathbb{Z}} \rightarrow S^{\mathbb{Z}}$ where $(\Theta z)(i) \triangleq z(i, 0)$, and let $\tilde{\mathcal{X}}$ be the two-dimensional shift space formed by all configurations $z \in S^{\mathbb{Z} \times \mathbb{Z}}$ such that

$$\dots \xrightarrow{\Phi} \Theta\sigma^{(0,-1)}_z \xrightarrow{\Phi} \Theta z \xrightarrow{\Phi} \Theta\sigma^{(0,1)}_z \xrightarrow{\Phi} \dots \tag{54}$$

is a bi-infinite orbit of Φ , that is $\Theta\sigma^{(0,k+1)}_z = \Phi\Theta\sigma^{(0,k)}_z$ for each $k \in \mathbb{Z}$. Set $V \triangleq (0, 1)$ and $H \triangleq (1, 0)$. The dynamical system $(\tilde{\mathcal{X}}, \sigma^V, \sigma^H)$ (together with the map Θ) is the *natural extension* of $(\mathcal{X}, \Phi, \sigma)$. Now, let $\Psi : \mathcal{Y} \rightarrow \mathcal{Y}$ be another surjective cellular automaton on a one-dimensional mixing shift space of finite type $\mathcal{Y} \subseteq T^{\mathbb{Z}}$. We say Ψ is a *transpose* of Φ if its natural extension is conjugate to $(\tilde{\mathcal{X}}, \sigma^H, \sigma^V)$. The transpose of Φ (if it exists) is unique only up to conjugacy. When there is no danger of confusion, we denote any representative of the transpose conjugacy class by Φ^\top .

Proposition 12 *A surjective cellular automaton on a one-dimensional mixing shift of finite type is mixing provided it has a transpose (acting on a mixing shift of finite type).*

Proof A dynamical system is mixing if and only if its natural extension is mixing. □

Obviously, not every cellular automaton has a transpose. A class of cellular automata that do have transposes is the class of those that are positively expansive. A dynamical system (\mathcal{X}, Φ) is *positively expansive* if there exists a real number $\varepsilon > 0$ such that for every two distinct points $x, y \in \mathcal{X}$, there is a time $t \geq 0$ such that $\Phi^t x$ and $\Phi^t y$ have distance at least ε . If (\mathcal{X}, σ) is a mixing shift of finite type and $\Phi : \mathcal{X} \rightarrow \mathcal{X}$ is a positively expansive cellular automaton, then Φ is surjective, and it is known that a transpose of Φ exists and is a reversible cellular automaton on a mixing shift of finite type (see [48], Sect. 5.5⁶). If, furthermore, (\mathcal{X}, σ) is a full shift, then the transpose of Φ also acts on a full shift (see [65], Theorem 3.12).

Proposition 13 *Every positively expansive cellular automaton on a one-dimensional mixing shift of finite type is strongly transitive.*

Proof Any continuous map $\Phi : \mathcal{X} \rightarrow \mathcal{X}$ on a compact metric space that is transitive, open, and positively expansive is strongly transitive [38]. Every positively expansive cellular automaton on a mixing shift of finite type is itself mixing (see the above paragraph) and open (see [48], Theorem 5.45).

Alternatively, every positively expansive cellular automaton on a mixing shift of finite type is conjugate to a mixing *one-sided* shift of finite type (see [48], Theorem 5.49), and hence strongly transitive. □

The local conservation laws of a cellular automaton and its transpose are in one-to-one correspondence.

Theorem 10 *Let $\Phi : \mathcal{X} \rightarrow \mathcal{X}$ and $\Phi^\top : \mathcal{X}^\top \rightarrow \mathcal{X}^\top$ be surjective cellular automata over one-dimensional mixing shifts of finite type \mathcal{X} and \mathcal{X}^\top , and suppose that Φ and Φ^\top are transpose of each other. There is a one-to-one correspondence (up to local physical equivalence) between the observables $f \in K(\mathcal{X})$ that are locally conserved by Φ and the observables $f^\top \in K(\mathcal{X}^\top)$ that are locally conserved by Φ^\top . Moreover, f is locally physically equivalent to 0 if and only if f^\top is so.*

⁶ The proof in [48] is presented for the case that (\mathcal{X}, σ) is a full shift, but the same proof, with slight adaptation, works for any arbitrary mixing shift of finite type. To prove the openness of Φ , see [64], Theorems 6.3 and 6.4, and note that Φ is both left- and right-closing.

Proof Recall that an observable $f \in K(\mathcal{X})$ is locally conserved by Φ if and only if it satisfies the continuity equation

$$f \circ \Phi = f + g \circ \sigma - g \tag{55}$$

for some observable $g \in K(\mathcal{X})$, where the terms $g \circ \sigma$ and g are interpreted, respectively, as the flow pouring into a site from its right neighbour and the flow leaving that site towards its left neighbour. This equation may alternatively be written as

$$g \circ \sigma = g + f \circ \Phi - f, \tag{56}$$

which can be interpreted as the local conservation of the observable g when the role of Φ and σ are exchanged.

To specify the correspondence between local conservation laws of Φ and Φ^\top more precisely, let $\tilde{\mathcal{X}}$ be the shift space of the space-time diagrams of Φ , so that $(\tilde{\mathcal{X}}, \sigma^V, \sigma^H)$ is the natural extension of $(\mathcal{X}, \Phi, \sigma)$, and $(\tilde{\mathcal{X}}, \sigma^H, \sigma^V)$ is the natural extension of $(\mathcal{X}^\top, \Phi^\top, \sigma)$, and let $\Theta : \tilde{\mathcal{X}} \rightarrow \mathcal{X}$ and $\Theta^\top : \tilde{\mathcal{X}} \rightarrow \mathcal{X}^\top$ be, respectively, the corresponding factor maps, extracting (up to a conjugacy) the 0th row and the 0th column of $\tilde{\mathcal{X}}$.

Let us use the following notation. Suppose that local observables $f, g \in K(\mathcal{X})$ and $f^\top, g^\top \in K(\mathcal{X}^\top)$ are such that $f \circ \Theta = g^\top \circ \Theta^\top$ and $f^\top \circ \Theta^\top = g \circ \Theta$, and setting $\tilde{f}_V \triangleq f \circ \Theta = g^\top \circ \Theta^\top$ and $\tilde{f}_H \triangleq f^\top \circ \Theta^\top = g \circ \Theta$, it holds

$$\tilde{f}_V \circ \sigma^V - \tilde{f}_V = \tilde{f}_H \circ \sigma^H - \tilde{f}_H. \tag{57}$$

Then, we write $f_1 \perp f_1^\top$ for any two local observables $f_1 \in K(\mathcal{X})$ and $f_1^\top \in K(\mathcal{X}^\top)$ that are locally physically equivalent to f and f^\top , respectively.

We verify that

- (i) a local observable $f \in K(\mathcal{X})$ is locally conserved by Φ if and only if $f \perp f^\top$ for some local observable $f^\top \in K(\mathcal{X}^\top)$,
- (ii) the relation \perp is linear, and
- (iii) $f \perp 0$ if and only if f is locally physically equivalent to 0.

Note that these three statements (along with the similar statements obtained by swapping f and f^\top) would imply that \perp is a one-to-one correspondence with the desired properties.

To prove the first statement, suppose that $f \perp f^\top$. Then,

$$\tilde{f}_V \circ \sigma^V - \tilde{f}_V = \tilde{f}_H \circ \sigma^H - \tilde{f}_H, \tag{58}$$

where $\tilde{f}_V = f \circ \Theta$ and $\tilde{f}_H = g \circ \Theta$ for some $g \in K(\mathcal{X})$. Rewriting this equation as

$$(f \circ \Phi - f) \circ \Theta = (g \circ \sigma - g) \circ \Theta, \tag{59}$$

we obtain, using Lemma 1 and the surjectivity of Θ , that f is locally conserved by Φ . Conversely, suppose that Φ locally conserves f , and let $g \in K(\mathcal{X})$ be such that $f \circ \Phi - f = g \circ \sigma - g$. Therefore,

$$f \circ \Theta \circ \sigma^V - f \circ \Theta = g \circ \Theta \circ \sigma^H - g \circ \Theta. \tag{60}$$

Since $f \circ \Theta$ and $g \circ \Theta$ are local observables, there exists a finite region $D \subseteq \mathbb{Z} \times \mathbb{Z}$ such that $f \circ \Theta, g \circ \Theta \in K_D(\tilde{\mathcal{X}})$. By the definition of natural extension, there is an integer $k > 0$ such that $z|_D$ is uniquely and continuously determined by $\Theta^\top \sigma^{-kH} z$ (i.e., column $-k$ of the space-time shift of Φ). Hence, there exist observables $f^\top, g^\top \in K(\mathcal{X}^\top)$ such that

$f \circ \Theta \circ \sigma^{kH} = g^T \circ \Theta^T$ and $g \circ \Theta \circ \sigma^{kV} = f^T \circ \Theta^T$. Now, setting $\tilde{f}_V \triangleq f \circ \sigma^k \circ \Theta = g^T \circ \Theta^T$ and $\tilde{f}_H \triangleq g \circ \sigma^k \circ \Theta = f^T \circ \Theta^T$, we can write

$$\tilde{f}_V \circ \sigma^V - \tilde{f}_V = \tilde{f}_H \circ \sigma^H - \tilde{f}_H, \tag{61}$$

which means $f \circ \sigma^k \perp f^T$. Finally, note that f and $f \circ \sigma^k$ are locally physically equivalent.

The linearity of \perp and the fact that $0 \perp 0$ are clear. It remains to show that if $f_1 \in K(\mathcal{X})$ is a local observable such that $f_1 \perp 0$, then f_1 is locally physically equivalent to 0. Suppose that $f_1 \perp 0$. Then, there is an observable $f \in K(\mathcal{X})$ locally physically equivalent to f_1 , and an observable $f^T \in K(\mathcal{X}^T)$ locally physically equivalent to 0 such that

$$f \circ \Theta \circ \sigma^V - f \circ \Theta = f^T \circ \Theta^T \circ \sigma^H - f^T \circ \Theta^T. \tag{62}$$

Since f^T is locally physically equivalent to 0, it has the form $f^T = h^T \circ \sigma - h^T + c$ for some observable $h^T \in K(\mathcal{X}^T)$ and some constant $c \in \mathbb{R}$. Therefore,

$$\begin{aligned} & f \circ \Theta \circ \sigma^V - f \circ \Theta \\ &= h^T \circ \Theta^T \circ \sigma^V \circ \sigma^H - h^T \circ \Theta^T \circ \sigma^V - h^T \circ \Theta^T \circ \sigma^H + h^T \circ \Theta^T. \end{aligned} \tag{63}$$

Since h^T is a local observable, we can find, as before, an integer $l > 0$ and a local observable $h \in K(\mathcal{X})$ such that $h^T \circ \sigma^l \circ \Theta^T = h \circ \Theta$. Therefore, composing both sides of (63) with σ^{lV} leads to

$$\begin{aligned} & f \circ \Phi^l \circ \Theta \circ \sigma^V - f \circ \Phi^l \circ \Theta \\ &= h \circ \Theta \circ \sigma^V \circ \sigma^H - h \circ \Theta \circ \sigma^V - h \circ \Theta \circ \sigma^H + h \circ \Theta, \end{aligned} \tag{64}$$

which, together with Lemma 1, gives

$$f \circ \Phi^l \circ \Phi - f \circ \Phi^l = h \circ \Phi \circ \sigma - h \circ \Phi - h \circ \sigma + h. \tag{65}$$

The latter equation can be rewritten as

$$(f \circ \Phi^l - h \circ \sigma + h) \circ \Phi = (f \circ \Phi^l - h \circ \sigma + h), \tag{66}$$

which says that $f \circ \Phi^l - h \circ \sigma + h$ is invariant under Φ . On the other hand, since (\mathcal{X}^T, σ) is a mixing shift, it follows from Proposition 12 that (\mathcal{X}, Φ) is also mixing. As a consequence, every continuous observable that is invariant under Φ is constant. In particular, $f \circ \Phi^l - h \circ \sigma + h = c'$ for some constant $c' \in \mathbb{R}$, which means $f \circ \Phi^l$ is locally physically equivalent to 0. Since f is locally conserved by Φ , the observable $f \circ \Phi^l$ is also locally physically equivalent to f , and this completes the proof. \square

Corollary 12 *Let $\Phi: \mathcal{X} \rightarrow \mathcal{X}$ be a reversible cellular automaton on a one-dimensional mixing shift of finite type (\mathcal{X}, σ) , and suppose that Φ has a positively expansive transpose. Then, Φ has no non-trivial local conservation law.*

As mentioned in Sect. 4.1, for cellular automata on full shifts, every conserved local observable is locally conserved.

Corollary 13 *Let $\Phi: \mathcal{X} \rightarrow \mathcal{X}$ be a reversible cellular automaton on a one-dimensional full shift (\mathcal{X}, σ) , and suppose that Φ has a positively expansive transpose. The uniform Bernoulli measure is the only finite-range Gibbs measure (\equiv full-support Markov measure) that is invariant under Φ .*

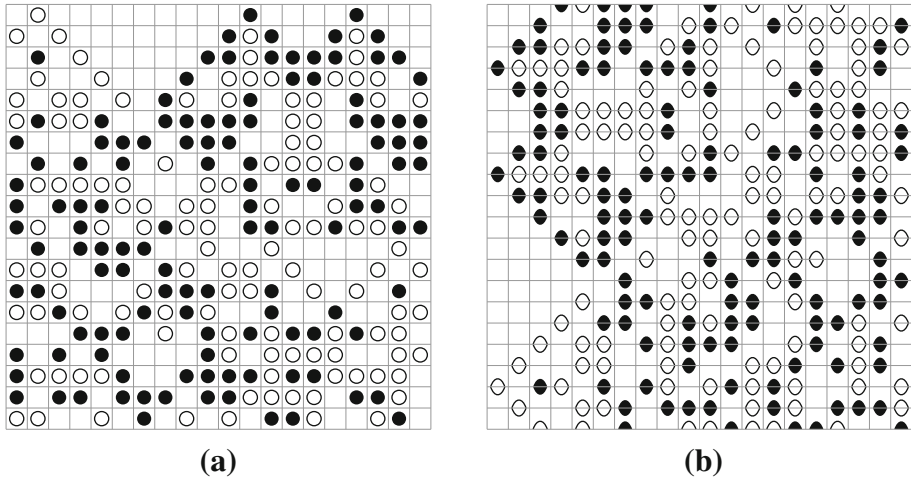


Fig. 6 Sample runs of **a** a one-dimensional bi-permutive cellular automaton and **b** its transpose. See Example 12. Time goes downward. *Black circle* represents 2 and *white circle* 1

Example 12 (Non-additive positively expansive) Let $\Phi : \{0, 1, 2\}^{\mathbb{Z}} \rightarrow \{0, 1, 2\}^{\mathbb{Z}}$ be the cellular automaton defined by neighborhood $N \triangleq \{-1, 0, 1\}$ and local update rule $\varphi : \{0, 1, 2\}^N \rightarrow \{0, 1, 2\}$ defined by

$$\varphi(a, b, c) \triangleq \begin{cases} a + c + 1 \pmod{3} & \text{if } b = 2, \\ a + c \pmod{3} & \text{otherwise.} \end{cases} \tag{67}$$

See Fig. 6a for a sample run. Note that the local rule is both left- and right-permutive (i.e., $a \mapsto \varphi(a, b, c)$ and $c \mapsto \varphi(a, b, c)$ are permutations). It follows that Φ is positively expansive, and hence also strongly transitive. Therefore, according to Theorem 9 and Corollary 11, Φ has no non-trivial conservation law and the uniform Bernoulli measure is the only regular Gibbs measure on $\{0, 1, 2\}^{\mathbb{Z}}$ that is invariant under Φ .

The cellular automaton Φ has a transpose $\Phi^T : (\{0, 1, 2\} \times \{0, 1, 2\})^{\mathbb{Z}} \rightarrow (\{0, 1, 2\} \times \{0, 1, 2\})^{\mathbb{Z}}$ defined with neighborhood $\{0, 1\}$ and local rule

$$((a, b), (a', b')) \mapsto \begin{cases} (b, b' - a - 1) & \text{if } b = 2, \\ (b, b' - a) & \text{otherwise,} \end{cases} \tag{68}$$

where the subtractions are modulo 3 (see Fig. 6b). This is a reversible cellular automaton. It follows from Corollaries 12 and 13 that Φ^T has no non-trivial local conservation law and no invariant full-support Markov measure other than the uniform Bernoulli measure. \circ

According to Corollary 11, if Φ is a strongly transitive cellular automaton on a full shift \mathcal{X} , the uniform Bernoulli measure on \mathcal{X} is the only regular Gibbs measure that is preserved by Φ . Likewise, Corollary 13 states that for a class of one-dimensional reversible cellular automata, the uniform Bernoulli measure is the only invariant full-support Markov measure. Note that even with these constraints, a cellular automaton in either of these two classes still has a large collection of other invariant measures. For example, for every d linearly independent vectors $k_1, k_2, \dots, k_d \in \mathbb{Z}^d$, the set of d -dimensional spatially periodic configurations having k_i as periods (i.e., $\{x : \sigma^{k_i} x = x \text{ for } i = 1, 2, \dots, d\}$) is finite and invariant under any cellular automaton, and therefore any cellular automaton has an (atomic) invariant measure supported

at such a set. Nevertheless, if we restrict our attention to sufficiently “smooth” measures, the uniform Bernoulli measure becomes the “unique” invariant measure for a cellular automaton in either of the above classes.⁷ In this sense, Corollaries 11 and 13 may be interpreted as weak indications of “absence of phase transition” for cellular automata in the two classes in question.

Question 4 Let (\mathcal{X}, σ) be a strongly irreducible shift of finite type. Which shift-ergodic measures can be invariant under a strongly transitive cellular automaton? Can a shift-ergodic measure with positive but sub-maximum entropy on (\mathcal{X}, σ) be invariant under a strongly transitive cellular automaton?

4.4 Randomization and Approach to Equilibrium

This section contains a few remarks and open questions regarding the problem of approach to equilibrium in surjective cellular automata.

Example 13 (Randomization in XOR cellular automata) The XOR cellular automata (Examples 10, 6 and 7) exhibit the same kind of “approach to equilibrium” as observed in the Q2R model (see the Introduction). Starting from a biased Bernoulli random configuration, the system quickly reaches a uniformly random state, where it remains (see Fig. 7). A mathematical explanation of this behavior was first found independently by Miyamoto [58] and Lind [50] (following Wolfram [93]) and has since been extended and strengthened by others.

Let $\mathcal{X} \triangleq \{0, 1\}^{\mathbb{Z}}$, and consider the XOR cellular automaton $\Phi : \mathcal{X} \rightarrow \mathcal{X}$ with neighborhood $\{0, 1\}$. If π is a shift-invariant probability measure on \mathcal{X} , the convergence of $\Phi^t \pi$ as $t \rightarrow \infty$ fails as long as π is strongly mixing and different from the uniform Bernoulli measure and the Dirac measures concentrated at one of the two uniform configurations [58, 59]. However, if π is a non-degenerate Bernoulli measure, the convergence holds if a negligible set of time steps are ignored. More precisely, there is a set $J \subseteq \mathbb{N}$ of density 1 such that for every non-degenerate Bernoulli measure π , the sequence $\{\Phi^t \pi\}_{t \in J}$ converges, as $t \rightarrow \infty$, to the uniform Bernoulli measure μ . In particular, we have the convergence of the Cesàro averages

$$\frac{1}{n} \sum_{t=0}^{n-1} \Phi^t \pi \rightarrow \mu \tag{69}$$

as $n \rightarrow \infty$ [50, 58].

The same type of convergence holds as long as π is harmonically mixing [71]. Similar results have been obtained for a wide range of algebraic cellular automata (see e.g. [8, 22, 34, 52, 71–73, 81]). In particular, the reversible cellular automaton of Example 11 has been shown to have the same randomizing effect [53]. See [70] for a survey.

It is also worth mentioning a similar result due to Johnson and Rudolph [37] regarding maps of the unit circle $\mathbb{T} \triangleq \mathbb{R}/\mathbb{Z}$. Namely, let π be a Borel measure on \mathbb{T} . They showed that if π is invariant, ergodic and of positive entropy for the map $3 \times : x \mapsto 3x \pmod{1}$, then it is randomized by the map $2 \times : x \mapsto 2x \pmod{1}$, in the sense that $(2 \times)^t \pi$ converges to the Lebesgue measure along a subsequence $J \subseteq \mathbb{N}$ of density 1. ○

⁷ The term “smoothness” here refers to the continuity of the conditional probabilities $\pi([p]_D | \mathfrak{F}_D)(z)$ for Gibbs measures (which is a defining property). Unfortunately, Corollary 11 restricts only the invariance of regular Gibbs measures (see Sect. 2.3). We do not know if every Hamiltonian is generated by an observable with summable variations. However, see [82] in this direction.

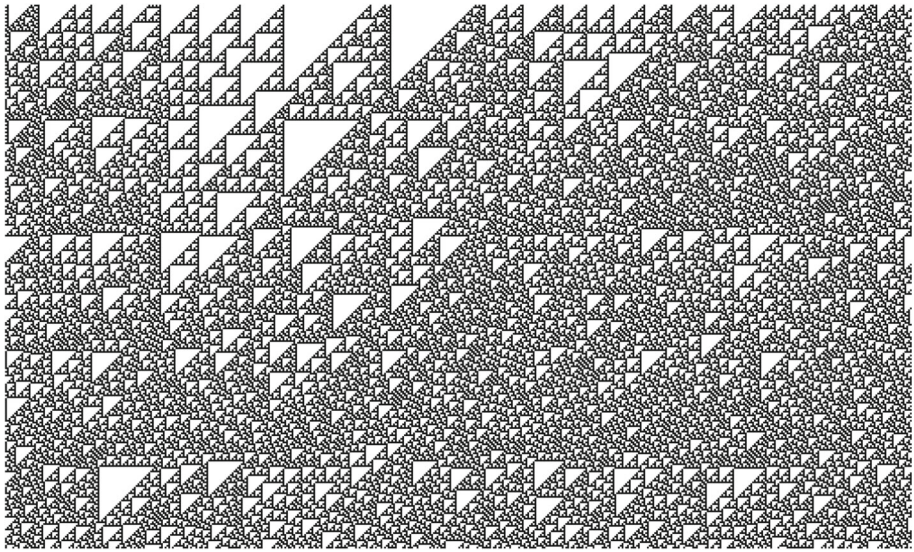


Fig. 7 Randomization effect of the XOR cellular automaton (see Example 13). Time goes downward. The initial configuration is chosen using coin flips with bias 1:9. The initial density of symbol 1 is 0.104. The density at time 300 is 0.504

Randomization behavior similar to that in the XOR cellular automaton has been observed in simulations of other (non-additive) cellular automata, but the mathematical results are so far limited to algebraic cellular automata. The uniform Bernoulli measure is the unique measure with maximum entropy on the full shift (\mathcal{X}, σ) (i.e., the “state of maximum randomness”). The convergence (in density) of $\Phi^t \pi$ to the uniform Bernoulli measure may thus be interpreted as a manifestation of the second law of thermodynamics [70].

We say that a cellular automaton $\Phi : \mathcal{X} \rightarrow \mathcal{X}$ (asymptotically) *randomizes* a probability measure $\pi \in \mathcal{P}(\mathcal{X})$, if there is a set $J \subseteq \mathbb{N}$ of density 1 such that the weak limit

$$\Phi^\infty \pi \triangleq \lim_{J \ni t \rightarrow \infty} \Phi^t \pi \tag{70}$$

exists and is a shift-invariant measure with maximum entropy, that is, $h_{\Phi^\infty \pi}(\mathcal{X}, \sigma) = h(\mathcal{X}, \sigma)$. The *density* of a set $J \subseteq \mathbb{N}$ is defined as

$$d(J) \triangleq \lim_{n \rightarrow \infty} \frac{|J \cap \{0, 1, \dots, n - 1\}|}{n}. \tag{71}$$

Note that the limit measure $\Phi^\infty \pi$ must be invariant under Φ , even if (\mathcal{X}, σ) has multiple measures with maximum entropy. If Φ randomizes a measure π , the Cesàro averages $(\sum_{t=0}^{n-1} \Phi^t \pi)/n$ will also converge to $\Phi^\infty \pi$. The converse is also true as long as π is shift-invariant and the limit measure is shift-ergodic:

Lemma 4 [see [37], Corollary 1.4] *Let \mathcal{X} be a compact metric space and $\mathcal{Q} \subseteq \mathcal{P}(\mathcal{X})$ a closed and convex set of probability measures on \mathcal{X} . Let π_1, π_2, \dots be a sequence of elements in \mathcal{Q} whose Cesàro averages $(\sum_{i=0}^{n-1} \pi_i)/n$ converge to a measure μ as $n \rightarrow \infty$. If μ is extremal in \mathcal{Q} , then there is a set $J \subseteq \mathbb{N}$ of density 1 such that $\pi_i \rightarrow \mu$ as $J \ni i \rightarrow \infty$.*

As mentioned in Example 13, the stronger notion of randomization fails for the XOR cellular automaton. We say that a cellular automaton Φ *strongly randomizes* a measure π if $\Phi^t \pi$ converges to a measure with maximum entropy.

Question 5 Are there examples of surjective or reversible cellular automata that strongly randomize all (say) Bernoulli measures? Is there a generic obstacle against strong randomization in surjective or reversible cellular automata?

If the cellular automaton Φ has non-trivial conservation laws, the orbit of a measure π will be entirely on the same “energy level”. Nevertheless, we could expect π to be randomized within its energy level. To evade an abundance of invariant measures, let us assume that Φ has only finitely many linearly independent conservation laws. More precisely, let $F = \{f_1, f_2, \dots, f_n\} \subseteq C(\mathcal{X})$ be a collection of observables conserved by Φ such that every observable $g \in C(\mathcal{X})$ conserved by Φ is physically equivalent to an element of the linear span of F . The measures $\Phi^t \pi$ as well as their accumulation points are confined in the closed convex set

$$\{v \in \mathcal{P}(\mathcal{X}) : v(f_i) = \pi(f_i) \text{ for } i = 1, 2, \dots, n\}. \tag{72}$$

Let us say that Φ *randomizes π modulo F* if there is a set $J \subseteq \mathbb{N}$ of density 1 such that

$$\Phi^\infty \pi \triangleq \lim_{J \ni t \rightarrow \infty} \Phi^t \pi \tag{73}$$

exists, is shift-invariant, and has entropy $s_{f_1, f_2, \dots, f_n}(\pi(f_1), \pi(f_2), \dots, \pi(f_n))$, where

$$s_{f_1, f_2, \dots, f_n}(e_1, e_2, \dots, e_n) = \sup\{h_v(\mathcal{X}, \sigma) : v \in \mathcal{P}(\mathcal{X}, \sigma) \text{ and } v(f_i) = e_i \text{ for } i = 1, 2, \dots, n\}. \tag{74}$$

Question 6 What are some examples of non-algebraic cellular automata (with or without non-trivial conservation laws) having a randomization property?

Suitable candidates to inspect for the occurrence of a randomization behavior are those that do not have any non-trivial conservation laws.

Question 7 Do strongly transitive cellular automata randomize every Gibbs measure?

Question 8 Does a one-dimensional reversible cellular automaton that has a positively expansive transpose randomize every Gibbs measure?

5 Conclusions

There is a wealth of open issues in connection with the statistical mechanics of reversible and surjective cellular automata. We have asked a few questions in this article. From the modeling point of view, there are at least three central problems that need to be addressed:

- What is a good description of macroscopic equilibrium states?
- What is a satisfactory description of approach to equilibrium?
- How do physical phenomena such as phase transition appear in the dynamical setting of cellular automata?

By virtue of their symbolic nature, various questions regarding cellular automata can be conveniently approached using computational and algorithmic methods. Nevertheless, many fundamental global properties of cellular automata have turned out to be algorithmically undecidable, at least in two and higher dimensions. For example, the question of whether a given two-dimensional cellular automaton is reversible (or surjective) is undecidable [39]. Similarly, *all* non-trivial properties of the limit sets of cellular automata are undecidable, even when restricted to the one-dimensional case [29,40] (see also [17]). Whether a given cellular automaton on a full shift conserves a given local observable can be verified using a simple algorithm [30], but whether a (one-dimensional) cellular automaton has any non-trivial local conservation law is undecidable [25]. It is an interesting open problem whether the latter undecidability statement remains true when restricted to the class of reversible (or surjective) cellular automata. We hope to address this and other algorithmic questions related to the statistical mechanics of cellular automata in a separate study.

Problems similar to those studied here have been addressed in different but related settings and with various motivations. Simple necessary and sufficient conditions have been obtained that characterize when a one-dimensional probabilistic cellular automaton has a Bernoulli or Markov invariant measure [54,89]. The equivalence of parts (b) and (c) in Theorem 6 is also true for positive-rate probabilistic cellular automata [16]. For positive-rate probabilistic cellular automata, however, the existence of an invariant Gibbs measure implies that all shift-invariant invariant Gibbs measures are Gibbs for the same Hamiltonian! The ergodicity problem of the probabilistic cellular automata (see e.g. [89]) has close similarity with the problem of randomization in surjective cellular automata.

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Appendix: Equivalence of the Definitions of a Gibbs Measure

Proposition 14 *Let Δ be a Hamiltonian on a shift space \mathcal{X} and $\pi \in \mathcal{P}(\mathcal{X})$ a probability measure. The following conditions are equivalent:*

(a) *For every finite set $D \subseteq \mathbb{L}$,*

$$\pi([q]_D \mid \mathfrak{F}_{D^c})(z) = e^{-\Delta(p \vee z|_{D^c}, q \vee z|_{D^c})} \pi([p]_D \mid \mathfrak{F}_{D^c})(z) \tag{75}$$

for π -almost every $z \in \mathcal{X}$ and every two patterns $p, q \in L_D(\mathcal{X} \mid z)$.

(b) *For every finite set $D \subseteq \mathbb{L}$,*

$$\frac{\pi([q \vee z|_{D^c}]_E)}{\pi([p \vee z|_{D^c}]_E)} \rightarrow e^{-\Delta(p \vee z|_{D^c}, q \vee z|_{D^c})} \tag{76}$$

uniformly in $z \in \text{supp}(\pi)$ and $p, q \in L_D(\mathcal{X} \mid z)$ as $E \nearrow \mathbb{L}$ along the directed family of finite subsets of \mathbb{L} .

c) For every configuration $x \in \mathcal{X}$ that is in the support of π and every configuration $y \in \mathcal{X}$ that is asymptotic to x ,

$$\frac{\pi([y]_E)}{\pi([x]_E)} \rightarrow e^{-\Delta(x,y)}, \tag{77}$$

as $E \nearrow \mathbb{L}$ along the directed family of finite subsets of \mathbb{L} .

Proof (a) \Rightarrow (b) Assume that condition (a) is satisfied. Let $D \subseteq \mathbb{L}$ be a finite set. Integrating (75), for any finite $E \supseteq D$ we get

$$\pi([q \vee z|_{D^c}]_E) = \int_{[z]_{E \setminus D}} e^{-\Delta(p \vee \zeta|_{D^c}, q \vee \zeta|_{D^c})} \pi([p]_D | \mathfrak{F}_{D^c})(\zeta) \pi(d\zeta). \tag{78}$$

Setting

$$\delta(z, \zeta \triangleq e^{-\Delta(p \vee \zeta|_{D^c}, q \vee \zeta|_{D^c})} - e^{-\Delta(p \vee z|_{D^c}, q \vee z|_{D^c})}, \tag{79}$$

we can write

$$\pi([q \vee z|_{D^c}]_E) = \int_{[z]_{E \setminus D}} \left(e^{-\Delta(p \vee z|_{D^c}, q \vee z|_{D^c})} + \delta(z, \zeta) \right) \pi([p]_D | \mathfrak{F}_{D^c})(\zeta) \pi(d\zeta) \tag{80}$$

$$\begin{aligned} \pi([q \vee z|_{D^c}]_E) &= e^{-\Delta(p \vee z|_{D^c}, q \vee z|_{D^c})} \pi([p \vee z|_{D^c}]_E) \\ &\quad + \int_{[z]_{E \setminus D}} \delta(z, \zeta) \pi([p]_D | \mathfrak{F}_{D^c})(\zeta) \pi(d\zeta). \end{aligned} \tag{81}$$

Now, let $p, q \in L_D(\mathcal{X})$ be fixed patterns with $\pi([p]_D), \pi([q]_D) > 0$, and let $\varepsilon > 0$. By the uniform continuity of $z \mapsto \Delta(p \vee z|_{D^c}, q \vee z|_{D^c})$, there is a sufficiently large finite set $E_\varepsilon \subseteq \mathbb{L}$ such that, for every $E \supseteq E_\varepsilon$ and every z, ζ with $z|_{E \setminus D} = \zeta|_{E \setminus D}$, we have $|\delta(z, \zeta)| < \varepsilon$. In particular, for every $E \supseteq E_\varepsilon$ and every $z \in \text{supp}(\pi)$ satisfying $p, q \in L_D(\mathcal{X} | z)$, we get

$$\left| \int_{[z]_{E \setminus D}} \delta(z, \zeta) \pi([p]_D | \mathfrak{F}_{D^c})(\zeta) \pi(d\zeta) \right| \leq \int_{[z]_{E \setminus D}} |\delta(z, \zeta)| \pi([p]_D | \mathfrak{F}_{D^c})(\zeta) \pi(d\zeta) \tag{82}$$

$$< \varepsilon \pi([p \vee z|_{D^c}]_E). \tag{83}$$

Substituting in (81), we obtain, for every $z \in \text{supp}(\pi)$ satisfying $p, q \in L_D(\mathcal{X} | z)$, that

$$\left| \pi([q \vee z|_{D^c}]_E) - e^{-\Delta(p \vee z|_{D^c}, q \vee z|_{D^c})} \pi([p \vee z|_{D^c}]_E) \right| < \varepsilon \pi([p \vee z|_{D^c}]_E) \tag{84}$$

provided $E \supseteq E_\varepsilon$. Dividing by $\pi([p \vee z|_{D^c}]_E)$ and letting $\varepsilon \rightarrow 0$ proves the claim.

(b) \Rightarrow (c) Trivial.

(c) \Rightarrow (a) Suppose that π satisfies condition (c). Let $I_1 \subseteq I_2 \subseteq \dots$ be an arbitrary chain of finite subsets of \mathbb{L} with $\bigcup_n I_n = \mathbb{L}$. Let $z \in \mathcal{X}$ be a configuration in the support of π and $D \subseteq \mathbb{L}$ a finite set. For every two patterns $p, q \in L_D(\mathcal{X} | z)$, we have

$$\frac{\pi([q]_D | [z]_{I_n \setminus D})}{\pi([p]_D | [z]_{I_n \setminus D})} = \frac{\pi([q \vee z|_{D^c}]_{I_n})}{\pi([p \vee z|_{D^c}]_{I_n})} \rightarrow e^{-\Delta(p \vee z|_{D^c}, q \vee z|_{D^c})} \tag{85}$$

as $n \rightarrow \infty$, implying that

$$\pi([q]_D | [z]_{I_n \setminus D}) - e^{-\Delta(p \vee z|_{D^c}, q \vee z|_{D^c})} \pi([p]_D | [z]_{I_n \setminus D}) \rightarrow 0 \tag{86}$$

as $n \rightarrow \infty$.

Note that the σ -algebra \mathfrak{F}_{D^c} is generated by the filtration $\mathfrak{F}_{I_1 \setminus D} \subseteq \mathfrak{F}_{I_2 \setminus D} \subseteq \dots$. Therefore, by the martingale convergence theorem, for π -almost every z , and every $p \in L_D(\mathcal{X}^z | z)$,

$$\pi([p]_D | [z]_{I_n \setminus D}) = \pi([p]_D | \mathfrak{F}_{I_n \setminus D})(z) \rightarrow \pi([p]_D | \mathfrak{F}_{D^c})(z) \quad (87)$$

as $n \rightarrow \infty$.

Combining (86) and (87), we obtain

$$\pi([q]_D | \mathfrak{F}_{D^c})(z) = e^{-\Delta(p \vee z|_{D^c} \cdot q \vee z|_{D^c})} \pi([p]_D | \mathfrak{F}_{D^c})(z) \quad (88)$$

for π -almost every $z \in \mathcal{X}$ and every $p, q \in L_D(\mathcal{X}^z | z)$. \square

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