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Conservation Laws in Cellular Automata

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To Farzaneh, Nasser, and Babak

Abstract

Conservation laws in physics are numerical invariants of the dynamics of a system. In cellular automata (CA), a similar concept has already been defined and studied. To each local pattern of cell states a real value is associated, interpreted as the "energy" (or "mass", or ...) of that pattern. The overall "energy" of a configuration is simply the sum of the energy of the local patterns appearing on different positions in the configuration. We have a conservation law for that energy, if the total energy of each configuration remains constant during the evolution of the CA.

For a given conservation law, it is desirable to find microscopic explanations for the dynamics of the conserved energy in terms of flows of energy from one region toward another. Often, it happens that the energy values are from non-negative integers, and are interpreted as the number of "particles" distributed on a configuration. In such cases, it is conjectured that one can always provide a microscopic explanation for the conservation laws by prescribing rules for the local movement of the particles. The one-dimensional case has already been solved by Fukś and Pivato. We extend this to two-dimensional cellular automata with radius-$\frac{1}{2}$ neighborhood on the square lattice.

We then consider conservation laws in which the energy values are chosen from a commutative group or semigroup. In this case, the class of all conservation laws for a CA form a partially ordered hierarchy. We study the structure of this hierarchy and prove some basic facts about it. Although the local properties of this hierarchy (at least in the group-valued case) are tractable, its global properties turn out to be algorithmically inaccessible. In particular, we prove that it is undecidable whether this hierarchy is trivial (i.e., if the CA has any non-trivial conservation law at all) or unbounded. We point out some interconnections between the structure of this hierarchy and the dynamical properties of the CA. We show that positively expansive CA do not have non-trivial conservation laws.

We also investigate a curious relationship between conservation laws and invariant Gibbs measures in reversible and surjective CA. Gibbs measures are known to coincide with the equilibrium states of a lattice system

defined in terms of a Hamiltonian. For reversible cellular automata, each conserved quantity may play the role of a Hamiltonian, and provides a Gibbs measure (or a set of Gibbs measures, in case of phase multiplicity) that is invariant. Conversely, every invariant Gibbs measure provides a conservation law for the CA. For surjective CA, the former statement also follows (in a slightly different form) from the variational characterization of the Gibbs measures. For one-dimensional surjective CA, we show that each invariant Gibbs measure provides a conservation law. We also prove that surjective CA almost surely preserve the average information content per cell with respect to any probability measure.

Acknowledgements

This thesis contains new contributions to the theory of conservation laws in cellular automata, as well as a survey of known results. The new results presented here are not mine alone. In particular, the results presented in Chapter 3 were obtained in collaboration with Jarkko Kari, and were partially communicated in The First Symposium on Cellular Automata (JAC 2008), held in Uzès, France [48]. The material of Chapter 4 is a product of collaboration with Enrico Formenti and Jarkko Kari, and was partially presented in The 3rd International Computer Science Symposium in Russia (CSR 2008), which was held in Moscow, Russia [27]. Chapter 5 is a report of an ongoing research together with Jarkko Kari.

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I am also grateful to Enrico Formenti for our fruitful and enjoyable collaboration, and for his hospitality during my two visits in Nice. My interest in the topic of this work was initiated by an earlier collaboration with Tim Boykett, which was reported in [15]. I thank him for posing an excellent problem.

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Nice, March 2009 Siamak Taati

Contents

CHAPTER 1

Introduction

The wonderful wheel of nature,
circling day and night,
resembles a lamp, to a fanciful sight.
The sun is the flame, the universe the lamp,
we, wandering shadows,
revolving around the light.

— Omar Khayyám (1048–1122)

MUCH of science arises from looking at nature through a highly selective glass that eliminates the irrelevant details and singles out a particular feature to be studied. This approach flourishes when the filtered feature has a nice description of its own, which is independent of the eliminated parts. A conservation law is the simplest of such descriptions. It asserts that a certain quantity associated with a system remains constant throughout the evolution of the system.

Perhaps the first example of a conservation law found in physics is the intriguing discovery by the German astronomer Johannes Kepler (1571–1630) of the laws governing the motion of the planets. Kepler knew from his large collection of data, gathered from astronomical observations, that each planet follows not a perfectly circular orbit, but an elliptic one, with the sun as one of the focal points. The speed of the planet is not uniform either. Whenever it is farther from the sun, the planet moves slowly, while once it comes closer to the sun, the planet circles around the sun faster. Kepler was able to put this quantitatively, by realizing that the axis connecting the planet to the sun sweeps out equal areas within equal time segments (Figure 1.1). In other words, all through its orbit, the area-sweeping rate dS/dt of each planet remains constant (cf. [1]).[1]

In this thesis, we study such laws in cellular automata. A *cellular automaton* (CA for short) is an abstract structure, consisting of a d-dimensional

[1] This was later coined as the law of conservation of angular momentum.

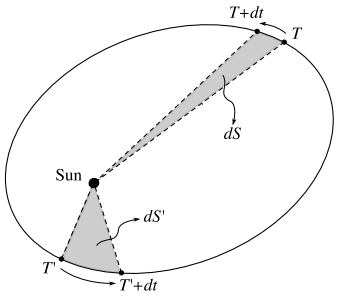


Figure 1.1: Kepler's selective observation: $dS' = dS$

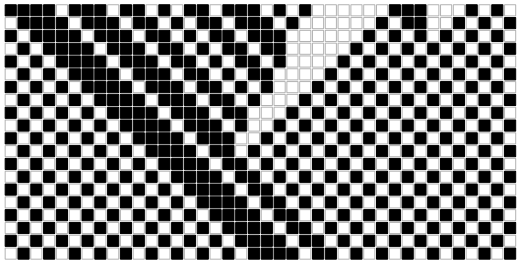
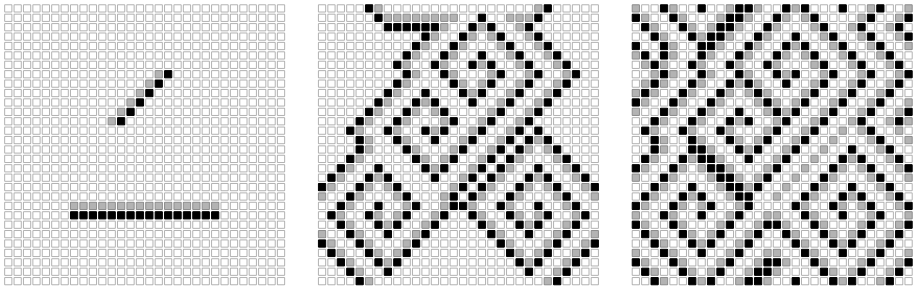


Figure 1.2: A typical space-time diagram of the Traffic CA. Time evolves downward. The highway is directed towards the left.

checkerboard ($d = 1, 2, 3, \ldots$). Each cell of the board has a state chosen from a finite set of states. The state of each cell changes with time, according to a uniform, deterministic rule, which takes into account the previous state of the cell itself and those in its neighborhood. The changes, however, happen synchronously, and in discrete time steps.

One of the simplest CA exhibiting a non-trivial conservation law is the *Traffic* CA, which resembles cars moving on a highway. This is a one-dimensional CA, consisting of an infinite number of cells arranged next to each other on a line. Each cell has two possible states: ■ (interpreted as a "car") or □ ("empty space"). At each step, a car moves one cell forward if and only if its front cell is empty. Figure 1.2 shows a typical space-time diagram of the evolution of the Traffic CA. Not surprisingly, the number of cars on the highway is preserved by the evolution of the CA.

As a two-dimensional example, consider the following discrete model of an excitable medium due to Greenberg and Hastings [35]. The CA runs on a two-dimensional board. Each cell is either "at rest" (state □), "excited" (state ■), or in a "refractory phase" (state ■). A cell which is at rest



(a) (b) (c)

Figure 1.3: Simulation of Greenberg-Hastings model on a spatially periodic configuration. (a) The initial configuration. (b) The configuration at time $t = 10$. (c) The configuration at time $t = 60$.

remains so unless it is "stimulated" by one or more of its four neighbors (i.e., if at least one of the neighbors is excited). An excited cell undergoes a 1-step refractory phase, before going back to rest. Typically, a configuration of the infinite board contains a number of "singularities" with waves continuously swirling around them. See Figure 1.3 for a few snapshots. The singularities are never created, nor are they destroyed. Therefore, the number of such singularities remains constant throughout time. To put it precisely, the singularities are the 2×2 blocks of cells with states  ,  , or  , or the rotations or mirror images of these blocks. It is a matter of mechanical verification to see that a singular 2×2 block remains singular after one step, and that a non-singular block remains non-singular. See [35, 34, 36] for the fascinating study of this CA and its generalizations.

1.1 Brief Historic Review

The early investigation of conservation laws in cellular automata was inspired by their immensely successful role in physics, and in connection with cellular automata models of physical phenomena (see e.g. [40, 35, 73, 82, 79, 80, 62]). Despite some modest efforts to develop a general theory (e.g. [73, 62]), the methods used were ad hoc, or simply imitated those used in physics.

The systematic study of additive conservation laws in CA was initiated by Hattori and Takesue [41], who formally defined such laws and showed how to algorithmically verify them. Similar results were obtained, inde-

pendently, by several others (e.g. [16]).

Meanwhile, and somewhat independently, a body of research was developed around the concept of number-conserving cellular automata (see e.g. [11, 29, 12, 65, 24, 26, 66, 13]). In these cellular automata, which are inspired by models of urban traffic, the state of a cell represents the number of particles in that cell, and the dynamics is such that the total number of particles is preserved.

Local representation of conservation laws using flows and particles were studied in [41, 29, 72, 52, 66]. Computational issues related to conservation laws were addressed, for example, in [41, 65, 24]. In [26], dynamical properties of number-conserving CA were studied. Characterization of conservation laws using average or expected energy per cell were given in [72, 52]. Generalizations of the original concept were discussed in [52, 66, 6, 13, 5, 10]. In [14], efforts were made to establish a correspondence between the conservation laws and algebraic structure of reversible CA.

1.2 Structure of the Thesis

The next section contains a quick review of the necessary background and terminology. In Chapter 2, we formalize the concept of conservation laws, and present various well-known characterizations of them. In Chapter 3, we discuss the problem of expressing conservation laws in terms of flows, or movements of the quanta of energy. Chapter 4 is devoted to the structural aspects of the class of all conservation laws for a given CA. In Chapter 5, we investigate the relationship between conservation laws and equilibrium states in surjective CA.

Appendix A contains a review of standard ergodic theory in the context of multi-dimensional shift spaces. Appendix B provides an example to illustrate the discussions in Chapter 5.

1.3 Preliminaries

In this section, we fix the terminology and notation, and review the basic combinatorial, topological and measure theoretic background needed in our discussions. For more thorough background material, we refer to [47, 53, 58, 83, 25, 23, 4, 56].

A cellular automaton (CA) is a collection of *cells* arranged regularly on a *lattice*, where a natural notion of *neighborhood* is present. Each cell is assigned a *state* from a finite number of possible states. The state of the cells is updated synchronously, in discrete time steps, according to a uniform *local*

update rule, which takes into account the current state of each cell and its neighbors.

The cells are often indexed by $\mathbb{Z}^d$ ($d \geq 1$), from which we obtain a *d-dimensional* CA. The index set $\mathbb{L} \triangleq \mathbb{Z}^d$ is called the d-dimensional *square* (or *integer*) lattice. The state set is a finite set S. An assignment $c : \mathbb{L} \to S$ of states to the cells of the lattice is referred to as a *configuration* (of the lattice). A *pattern* is a mapping $p : D \to S$ where $D \subseteq \mathbb{L}$. The pattern is *finite* if D is finite. If $A \subseteq D$, the restriction $p|_A$ is a *sub-pattern* of p. We write $q \preceq p$ when q is a sub-pattern of p. If two patterns $p : D \to S$ and $q : E \to S$ agree on the intersection $D \cap E$ of their domains, then $p \vee q : D \cup E \to S$ denotes the pattern which agrees with each of p and q on their domains. The *empty* pattern, denoted $\varnothing$, is the unique pattern with an empty domain. The *size* of a pattern p, denoted $|p|$, is the cardinality of its domain.

Let $p : D \to S$ be a pattern and $A \subseteq D$ a finite set. The *cylinder* with base p and support A is the set $\left\{x \in S^{\mathbb{L}} : x[i] = p[i] \text{ for all } i \in A\right\}$ and is denoted by $[p]_A$. For brevity, we sometimes write $[p]$ for $[p]_D$ whenever D is understood from the context. For every pattern $p : D \to S$, let us define an operator ζ_p that sets the state of D into p. That is, if $q : E \to S$ is any other pattern, then $\zeta_p q : D \cup E \to S$ is defined so that it agrees with p over D and with q elsewhere. For each finite $p : D \to S$, let δ_p be the characteristic function of the cylinder $[p]_D$. That is, for each configuration x, $\delta_p(x) = 1$ if $x|_D = p$, and $\delta_p(x) = 0$ otherwise.

For every pattern $p : D \to S$ and each vector $a \in \mathbb{L}$, $\sigma^a p$ is the *translation* of p by a; that is, $\sigma^a p[i] \triangleq p[a + i]$ when $a + i \in D$. When $d = 1$, we may write σ for σ^1. We write $p \equiv q \pmod{\sigma}$ if q is a translation of p. The equivalence class of p is denoted by $\langle p \rangle$. The collection of all finite patterns modulo translation is represented by $S^{\#}$. Whenever it causes no confusion, we may use p and $\langle p \rangle$ interchangeably.

The neighborhood is specified by a finite set $0 \in N \subseteq \mathbb{L}$. The neighborhood of a set $A \subseteq \mathbb{L}$ of cells is the set $N(A) \triangleq \{i + k : i \in A \text{ and } k \in N\}$. We denote by $N^{-1}(A) \triangleq \{i : N(i) \cap A \neq 0\} = \{i - k : i \in A \text{ and } k \in N\}$ the set of those cells which have a neighbor in A. We will also need to speak of the *boundary* of a group of cells (with respect to a neighborhood). The boundary of a set $A \subseteq \mathbb{L}$ is the set $\partial N(A) \triangleq N(A) \setminus A$. We identify a cell $i \in \mathbb{L}$ with the singleton $\{i\}$, and write $N(i)$ and $\partial N(i)$ for $N(\{i\})$ and $\partial N(\{i\})$.

The local update rule is a function $f : S^N \to S$. It naturally induces a mapping $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$, called the *global mapping*, which maps each configuration c to its follower configuration Fc, which appears on the lattice after one time step. Namely, $(Fc)[i] \triangleq f\left(c|_{N(i)}\right)$; that is, the state of the cell i in Fc is the result of the application of the local rule on the pattern of the neighborhood of i in c. We often identify a CA with its global mapping.

For each state $q \in S$, the *q-uniform* configuration is the configuration

with all cells in state q, and is denoted by $q^{\mathbb{L}}$. A *q-finite* configuration is one in which only finitely many cells are in states other than q. The set of all q-finite configurations is denoted by $\mathcal{C}_q[S]$. A *quiescent* state is a state $q \in S$ such that F maps the q-uniform configuration to itself; that is, $f(q^N) = q$. If q is a quiescent state, the image of every q-finite configuration is also q-finite. Two configurations x and y are *asymptotic* if they differ on no more than a finite number of cells. Cellular automata map asymptotic configurations into asymptotic configurations. A vector $a \in \mathbb{L}$ is a *period* of a configuration $x \in S^{\mathbb{L}}$ if $\sigma^a x = x$. A configuration x is said to be *(spatially) periodic* if the set $\{\sigma^a x : a \in \mathbb{L}\}$ is finite. The periods of every configuration form a subgroup of $\mathbb{L}$. A *fundamental domain* of a spatially periodic configuration x is a minimal subset $A \subseteq \mathbb{L}$, such that the value of x on A, together with the group $\mathbb{P}_x$ of periods of x, uniquely restricts the value of x on every cell in $\mathbb{L}$. In other words, it is a subset $A \subseteq \mathbb{L}$ that has exactly one element from each coset $a+\mathbb{P}_x$. By definition, every spatially periodic configuration has a finite fundamental domain. A configuration x is *temporally periodic* if $F^t x = x$, for some $t > 0$.

A *surjective* (resp., *injective*; *bijective*) cellular automaton has an onto (resp., one-to-one; onto and one-to-one) global mapping. The *Garden-of-Eden Theorem* [64, 67] states that a cellular automaton is surjective if and only if it is injective when restricted to q-finite configurations (q being an arbitrary state). Equivalently, surjective CA are exactly those that are *pre-injective*, that is, those that map distinct asymptotic configurations into distinct asymptotic configurations. As a result, every injective CA is also surjective.

Surjective CA have a characteristic *balance* property [42]: for all finite sets $A, B \subseteq \mathbb{L}$ with $B \supseteq N(A)$, and every pattern $p : A \to S$, the number of patterns $q : B \to S$ that are mapped by the local rule into p is independent of p. More specifically, the cardinality of the set $\left\{q \in S^B : F[q]_B \subseteq [p]_A\right\}$ equals $|S|^{|B|-|A|}$.

It is often useful to see a cellular automaton as a *dynamical system*. By a dynamical system we mean a topological (or measurable) space $\mathcal{X}$, together with a continuous (resp., measurable) mapping F on $\mathcal{X}$. More generally, we may have a group or semigroup of continuous (resp., measurable) transformations on $\mathcal{X}$. Hence, we now review the standard topological and measurable structures on the configuration space of a CA.

The most useful topology on the space $S^{\mathbb{L}}$ of all configurations is the *Cantor* topology $\mathscr{T}$. This is the product topology when S is discretely topologized. Equivalently, the Cantor topology is the topology in which convergence is defined as pointwise eventual agreement. It is compact, perfect, totally disconnected, and metrizable. Cylinders are clopen (both closed and open) and form a countable basis for $\mathscr{T}$. The celebrated *Curtis-*

Hedlund-Lyndon Theorem [42] states that the global mappings of cellular automata are exactly the mappings $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ that are continuous and translation-invariant. Bijective mappings between compact metric spaces are homeomorphisms. Thus, the inverse of a bijective cellular automaton is itself a cellular automaton. A bijective CA is often called *reversible*.

The action of σ on $S^{\mathbb{L}}$ defines a (topological) dynamical system which is called the *full shift*. The operator $\sigma : \mathbb{L} \times S^{\mathbb{L}} \to S^{\mathbb{L}}$ is called the *shift*. A compact subsystem of $(S^{\mathbb{L}}, \sigma)$ (i.e., a closed set $\mathcal{X} \subseteq S^{\mathbb{L}}$ with $\sigma^a \mathcal{X} \subseteq \mathcal{X}$ for every $a \in \mathbb{L}$) is called a *shift space* or a *subshift*. Shift spaces are exactly those subsets of $S^{\mathbb{L}}$ that can be defined by *forbidding* a collection of finite patterns: Given a collection $K \subseteq S^{\#}$ of finite patterns, we define the shift space

$$\mathcal{X}_K \triangleq \left\{ x \in S^{\mathbb{L}} : \langle x|_A \rangle \notin K \text{ for every finite } A \subseteq \mathbb{L} \right\} . \tag{1.1}$$

Every shift space has a representation of this form. For a shift space $\mathcal{X}$, let us denote by $L(\mathcal{X}) \subseteq S^{\#}$ the set of all finite patterns that occur in the configurations in $\mathcal{X}$. The compactness of $\mathcal{X}$ implies that $\mathcal{X}_{S^{\#} \setminus L(\mathcal{X})} = \mathcal{X}$. If K is finite, $\mathcal{X}_K$ is called a shift *of finite type* (SFT for short).

The *Borel* σ-algebra $\mathscr{B}$ on $S^{\mathbb{L}}$ is the σ-algebra generated by the open sets (equivalently, by the cylinders). It is the same as the product σ-algebra, where S is given the full σ-algebra. Every continuous mapping is Borel measurable. In particular, every cellular automaton is measurable.

The collection of Borel probability measures on $S^{\mathbb{L}}$ is denoted by $\mathscr{M}$. We see it as a topological space, with the topology of *weak* convergence (often called *weak** or *vague* topology). This is the weakest topology with respect to which, for every cylinder U, the mapping $\pi \overset{U}{\mapsto} \pi(U)$ is continuous. In particular, $\lim_{i\to\infty} \pi_i = \pi$ iff $\lim_{i\to\infty} \pi_i(U) = \pi(U)$ for every cylinder U. The space $\mathscr{M}$ is compact and metrizable. Every Borel probability measure on a metric space is regular, meaning that the measure of every Borel set B can be approximated arbitrarily closely by the measure of open sets $E \supseteq B$ or closed sets $C \subseteq B$. Therefore, every element $\pi \in \mathscr{M}$ is regular: for every Borel set $B \in \mathscr{B}$, we have

$$\pi(B) = \inf \{\pi(E) : \text{open } E \supseteq B\} \tag{1.2}$$

$$= \sup \{\pi(C) : \text{closed } C \subseteq B\} . \tag{1.3}$$

Every continuous mapping $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ naturally defines a mapping, also denoted by F, on the space $\mathscr{M}$ of Borel measures $\pi : \mathscr{B} \to [0, 1]$, by $(F\pi)(A) \triangleq \pi\left(F^{-1}A\right)$. The latter is continuous and affine. An *F-invariant* measure is a fixed point of F when acting on $\mathscr{M}$. The collection of F-invariant measures is a closed and convex subspace of $\mathscr{M}$ and is denoted by $\mathscr{M}_F$. A *translation-invariant* measure is a measure that is σ^a-invariant for every $a \in \mathbb{L}$.

Given a probability measure $\pi : \mathscr{B} \to [0,1]$, a pattern $p : D \to S$ is *probable* (more specifically, π-probable) if $\pi([p]_D) > 0$. An *improbable* pattern is one which is not probable. The *support* of a probability measure π is the smallest closed subset of $S^{\mathbb{L}}$ with measure 1; that is,

$$\operatorname{supp}(\pi) \triangleq \bigcap \{C : \pi(C) = 1 \text{ and } C \text{ closed}\} \ . \tag{1.4}$$

A *full-support* measure is a measure with support $S^{\mathbb{L}}$. The support of a translation-invariant measure π is the subshift in which improbable patterns are forbidden. On the other hand, given a subshift $\mathcal{X} \subseteq S^{\mathbb{L}}$, the set

$$\mathscr{M}_\sigma[\mathcal{X}] \triangleq \{\pi \in \mathscr{M}_\sigma : \operatorname{supp}(\pi) \subseteq \mathcal{X}\} \tag{1.5}$$

is a closed and convex subspace of $\mathscr{M}_\sigma$.

The collection of cylinders form a semi-algebra which generates $\mathscr{B}$. Therefore, a measure on $(S^{\mathbb{L}}, \mathscr{B})$ is completely determined by its values on the cylinders (see [83]). Furthermore, every family

$$\left\{\pi_D : S^D \to [0,1]\right\}_{D \subseteq \mathbb{L} \text{ finite}} \tag{1.6}$$

of probability distributions satisfying the consistency equations

$$\pi_D(p) = \sum_{\substack{q : E \to S \\ q|_D = p}} \pi_E(q) \tag{1.7}$$

for all finite $D \subseteq E \subseteq \mathbb{L}$ and $p : D \to S$, can be uniquely extended to a probability measure π on $\mathscr{B}$ with $\pi([p]_D) \triangleq \pi_D(p)$. For brevity, we sometimes write $\pi(p)$ for $\pi([p]_D)$, where $p : D \to S$ is a finite pattern, and there is no danger of confusion over the domain D.

A *Bernoulli* measure on $(S^{\mathbb{L}}, \mathscr{B})$ is a probability measure $\pi : \mathscr{B} \to [0,1]$ such that

$$\pi([p]_D \cap [q]_E) = \pi([p]_D) \cdot \pi([q]_E) \tag{1.8}$$

whenever $p : D \to S$ and $q : E \to S$ are finite patterns with $D \cap E = \varnothing$. A translation-invariant Bernoulli measure is identified by a probability distribution $\pi : S \to [0,1]$: for every finite pattern $p : D \to S$ we have $\pi([p]_D) = \prod_{i \in D} \pi(p[i])$. This is interpreted as the probability distribution where the state of each cell on the lattice is chosen randomly and independently, according to a given distribution over the state set. The average entropy per cell (entropy, for short) of a translation-invariant Bernoulli measure π equals $h_\pi(\sigma) = -\sum_{s \in S} \pi(s) \log \pi(s)$ (see Appendix A).

Let $K \subseteq \mathbb{L}$ be a finite set. The *K-block-presentation* of a configuration $x : \mathbb{L} \to S$ is a configuration $x^{(K)} : \mathbb{L} \to S^K$ where $x^{(K)}[i] = x|_{K(i)}$. That is, the state of the cell i in $x^{(K)}$ is the overall state of the K-neighborhood of cell i in x.

One-dimensional CA have a natural representation (up to composition with translations) using edge-labeled De Bruijn graphs. The *De Bruijn* graph of order k ($k > 0$) over an alphabet S is a graph $\mathcal{B}_k[S]$ with vertex set $V = S^k$ and edge set $E = S^{k+1}$, where for every $a, b \in S$ and $u \in S^{k-1}$, there is an edge aub from au to ub.

Let $F : S^{\mathbb{Z}} \to S^{\mathbb{Z}}$ be a one-dimensional CA with neighborhood $[-l, r] = \{-l, -l+1, \ldots, r\}$ and local rule $f : S^{[-l,r]} \to S$. For every $k \geq l + r$, the CA can be represented on the De Bruijn graph $\mathcal{B}_k[S]$ with labeling $\lambda : E \to S^{k-(l+r)}$ which is defined as follows: for every edge $u_0 u_1 \cdots u_k \in S^{k+1}$, let $\lambda(u_0 u_1 \cdots u_k) = v_l v_{l+1} \cdots v_{k-r}$, where $v_i = f\left(u_{i-l} u_{i-l+1} \cdots u_{i+r}\right)$.

The edge sequence $p = \{p[i]\}_{i \in \mathbb{Z}}$ of each bi-infinite path on $\mathcal{B}_k[S]$ is the $[0, k]$-block-presentation of a unique configuration $c : \mathbb{Z} \to S$, while its label sequence $\lambda(p) \triangleq \{\lambda(p[i])\}_{i \in \mathbb{Z}}$ is the $[l, k - r]$-block-presentation of Fc. Conversely, for every configuration $c : \mathbb{Z} \to S$, there is a unique infinite path on $\mathcal{B}_k[S]$ whose edge sequence is the $[0, k]$-block-presentation of c.

CHAPTER 2

Potentials and Conservation Laws

THIS chapter is dedicated to the precise formulation of conservation laws in cellular automata, and to reviewing the very many ways to characterize them. Though the results are more or less well-known, we take the opportunity to present them in a uniform and general setting.

By a conservation law we mean the invariance of an energy-like function under the dynamics of a CA. The essential features of the concept of energy that make it so useful in physics are its "additivity" and "locality". An energy function in a cellular automaton is, therefore, usually defined by sliding a local observable over the configuration and adding up the values it declares. There is, however, a technical difficulty in such a definition: the total energy of a configuration is an infinite sum, which is typically diverging and meaningless.

One way to circumvent this problem — the approach we choose in our main definition — is to consider only the *difference* between the energy of configurations that are only slightly perturbed from each other; instead of speaking of the energy level of a configuration x, we speak of the difference between the energy levels of two configurations x and x' that are different only on a finite region. This is also compatible with the physical picture, in that the difference between the energy levels of two systems is more fundamental (or more useful) a concept than the absolute energy of a system.

An alternate approach is to work with the average density of energy in a configuration. The drawback of this approach is that it is not algorithmic. Nevertheless, it gives us the opportunity to use the machinery of analysis and ergodic theory.

2.1 The Concept of Energy

We would like to formalize energy-like functions that are "local" and "additive". Intuitively, by additivity we mean that

> *"their values for a system composed of several parts whose interaction is negligible are equal to the sums of their values for the individual parts,"* [55]

and by locality we mean that there is no interaction between parts that are far enough apart.

More specifically, in our setting, additivity and locality translate into the following property: if changing a configuration x into configuration $\zeta_p x$ requires energy E_p, and changing x into $\zeta_q x$ requires energy E_q, and if p and q are distant enough, then changing x into $\zeta_q \zeta_p x$ would require energy $E_p + E_q$.

Let $\mathcal{X}$ be an arbitrary set. We say that a partial mapping $\Delta : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a *potential difference* on $\mathcal{X}$ if

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.

We say that a mapping $F : \mathcal{X} \to \mathcal{X}$ *conserves* Δ, if $\Delta(Fx, Fy) = \Delta(x, y)$ whenever $\Delta(x, y)$ exists.

A potential difference Δ on $S^{\mathbb{L}}$ is called *local* if

d) $\Delta(x, y)$ exists exactly 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) there exists a finite neighborhood $M \subseteq \mathbb{L}$, such that for every finite pattern $p : D \to S$ and every two configurations x, y that agree on $M(D)$, we have $\Delta(x, \zeta_p x) = \Delta(y, \zeta_p y)$.

Note that $\Delta(x, \sigma^a y)$ and $\Delta(x, y)$ do not necessarily have the same values.

A local potential difference captures the concept of a "local" and "additive" energy. Namely, for every configuration x, and every two finite patterns $p : D \to S$ and $q : E \to S$,

$$\Delta(x, \zeta_q \zeta_p x) = \Delta(x, \zeta_p x) + \Delta(\zeta_p x, \zeta_q \zeta_p x) \tag{2.1}$$

$$= \Delta(x, \zeta_p x) + \Delta(x, \zeta_q x)\ , \tag{2.2}$$

provided $D \cap M(E) = \varnothing$ (or similarly, if $M(D) \cap E = \varnothing$). The neighborhood M determines the "range of interaction" between the parts.

Let $\mathcal{X}$ be a compact topological space. An *observable* is a continuous mapping $\mu : \mathcal{X} \to \Gamma$ from $\mathcal{X}$ into another space Γ. If Γ is discretely topologized, we call μ a *discrete* observable. A discrete observable on $S^{\mathbb{L}}$ is also called a *local* observable. This name comes from the fact that for every discrete observable $\mu : S^{\mathbb{L}} \to \Gamma$, there is a finite neighborhood $M \subseteq \mathbb{L}$, and a function $g : S^M \to \Gamma$, where $\mu(x) = g\left(x|_M\right)$ for every configuration $x \in S^{\mathbb{L}}$. Every discrete observable $\mu : S^{\mathbb{L}} \to \mathbb{R}$ defines a local potential difference Δ on $S^{\mathbb{L}}$ via

$$\Delta(x, y) \triangleq \sum_{i \in \mathbb{L}} \left[\mu(\sigma^i y) - \mu(\sigma^i x)\right] \tag{2.3}$$

$$= \sum_{i \in \mathbb{L}} \left[g\left(y|_{M(i)}\right) - g\left(x|_{M(i)}\right)\right] \tag{2.4}$$

for every two asymptotic configurations x and y. In fact, every local potential difference on $S^{\mathbb{L}}$ is of this form.

Proposition 2.1. *Every local potential difference Δ on $S^{\mathbb{L}}$ is generated by a local observable.*

Proof. Let M be the neighborhood of Δ. We show that Δ is generated by a local observable μ with neighborhood M, via (2.3).

Let us distinguish an arbitrary state $\diamond \in S$ and call it blank. The $\diamond$-uniform configuration is denoted by $\diamondsuit$. Let $\preceq$ be the lexicographic order on $\mathbb{L}$ (or any total order which is preserved by σ). For every cell $i \in \mathbb{L}$, let $\gamma(i)$ be the successor of i according to $\preceq$. Recall that for every pattern $p : D \to S$, ζ_p is the operator that sets the state of the cells in D to their values in p. For every $k \in \mathbb{L}$, let us also define the operator ζ_k that sets the cells $i \succeq k$ to blank. Define a mapping $\mu : S^{\mathbb{L}} \to \mathbb{R}$ by $\mu(x) \triangleq \Delta(\zeta_0 x, \zeta_{\gamma(0)} x)$.

To see that μ is a local observable, define $g : S^M \to \mathbb{R}$ by $g(p) \triangleq \mu(\zeta_p \diamondsuit)$ for every $p \in S^M$. Let x be an arbitrary configuration, and let $p \triangleq x|_M$ be the pattern seen on M in x. We have

$$\mu(x) = \Delta(\zeta_0 x, \zeta_{\gamma(0)} x) \tag{2.5}$$

$$= \Delta(\zeta_0 \zeta_p \diamondsuit, \zeta_{\gamma(0)} \zeta_p \diamondsuit) \tag{2.6}$$

$$= \mu(\zeta_p \diamondsuit) \tag{2.7}$$

$$= g\left(x|_M\right) \ , \tag{2.8}$$

where (2.6) follows from the locality of Δ. So, μ is a local observable with neighborhood M.

Next, observe that if $\alpha_1, \alpha_2, \beta_1, \beta_2$ are any four asymptotic configurations, we have

$$\Delta(\beta_1, \beta_2) - \Delta(\alpha_1, \alpha_2) = \Delta(\alpha_2, \beta_2) - \Delta(\alpha_1, \beta_1) \ . \tag{2.9}$$

This follows from condition (c) in the definition of potential difference. Now, let x and y be two asymptotic configurations. Let $D \subseteq \mathbb{L}$ be the finite set on which x and y disagree, and suppose that $a_1 \prec a_2 \prec \cdots \prec a_n$ is the lexicographic ordering of the elements of $M^{-1}(D) \cup M(D)$. Notice that for $a \notin M^{-1}(D) \subseteq M^{-1}(D) \cup M(D)$, we have

$$\Delta(\zeta_a y, \zeta_{\gamma(a)} y) = \Delta(\zeta_a x, \zeta_{\gamma(a)} x) \ , \tag{2.10}$$

and for each $i = 1, 2, \ldots n-1$, we have

$$\Delta(\zeta_{\gamma(a_i)} x, \zeta_{\gamma(a_i)} y) = \Delta(\zeta_{a_{i+1}} x, \zeta_{a_{i+1}} y) \ . \tag{2.11}$$

Therefore, we can write

$$\sum_{a \in \mathbb{L}} [\mu(\sigma^a y) - \mu(\sigma^a x)] \tag{2.12}$$

$$= \sum_{a \in \mathbb{L}} \left[\Delta(\zeta_a y, \zeta_{\gamma(a)} y) - \Delta(\zeta_a x, \zeta_{\gamma(a)} x)\right] \tag{2.13}$$

$$= \sum_{i=1}^{n} \left[\Delta(\zeta_{a_i} y, \zeta_{\gamma(a_i)} y) - \Delta(\zeta_{a_i} x, \zeta_{\gamma(a_i)} x)\right] \tag{2.14}$$

$$= \sum_{i=1}^{n} \left[\Delta(\zeta_{\gamma(a_i)} x, \zeta_{\gamma(a_i)} y) - \Delta(\zeta_{a_i} x, \zeta_{a_i} y)\right] \tag{2.15}$$

$$= \Delta(\zeta_{\gamma(a_n)} x, \zeta_{\gamma(a_n)} y) - \Delta(\zeta_{a_1} x, \zeta_{a_1} y) \tag{2.16}$$

$$= \Delta(x, y) \ , \tag{2.17}$$

which completes the proof. □

In summary, potential differences generated by local observables formalize the concept of "energy", as desired.

As an example, recall that for each finite pattern $p : D \to S$, the characteristic function of the cylinder $[p]_D$ is denoted by δ_p. Clearly, δ_p is a local observable, with neighborhood D. The potential difference generated by δ_p represents the difference between the number of occurrences of p in two given configurations. In fact, every local observable on $S^{\mathbb{L}}$ is a linear combination of such *elementary* observables.

We remark that an observable $\mu : S^{\mathbb{L}} \to \mathbb{R}$ that is uniformly continuous with respect to the usual topology on $\mathbb{R}$ would also lead to a potential difference which is *quasilocal*, in the sense that the greater the distance between two parts of the system, the smaller their interaction (see e.g. [32]). In this thesis, we do not study such potential differences.

2.2 Conservation Laws

Suppose that a cellular automaton F conserves a local potential difference Δ. We call the statement

$$\Delta(Fx, Fy) = \Delta(x, y) \qquad \text{for all asymptotic } x \text{ and } y, \tag{2.18}$$

a *conservation law* for F. Is it possible to algorithmically verify the validness of a conservation law for a cellular automaton? Can we find all conservation laws governing the evolution of a CA? The former question has a positive answer, as was first realized by Hattori and Takesue (1991). A negative answer to the second question will be given later, in Chapter 4.

Theorem 2.2 ([41]). *Let $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ be a cellular automaton, and Δ a local potential difference on $S^{\mathbb{L}}$. The following statements are equivalent.*

i) $\Delta(Fx, Fy) = \Delta(x, y)$ *for every two asymptotic configurations x and y.*

ii) $\Delta(Fx, Fy) = \Delta(x, y)$ *for every two configurations x and y which differ on exactly one cell.*

Proof. The implication [i⇒ii] is trivial. To prove the converse implication, let x and y be asymptotic. Since x and y disagree on at most a finite number of cells, we can find a sequence $x = x_0, x_1, \ldots, x_n = y$ ($n \geq 0$) of configurations, such that, for each $i = 0, 1, \ldots, n-1$, x_i and x_{i+1} differ on exactly one cell. So, we can write

$$\Delta(Fx, Fy) = \sum_{i=0}^{n-1} \Delta(Fx_i, Fx_{i+1}) = \sum_{i=0}^{n-1} \Delta(x_i, x_{i+1}) = \Delta(x, y)\ . \tag{2.19}$$

□

The above theorem immediately gives rise to an algorithm for deciding whether a given CA conserves a given local potential difference. Let F be a CA with neighborhood N. Suppose that Δ is a potential difference on $S^{\mathbb{L}}$ which is generated by a local observable with neighborhood $M \subseteq \mathbb{L}$. Note that if two configurations x and y differ on only a single cell i, $\Delta(x, y)$ depends only on the values of x and y on $M(M^{-1}(i))$.[1] Likewise, $\Delta(Fx, Fy)$ depends only on the values of x and y on $M(M^{-1}(N^{-1}(i)))$. Therefore, in order to determine whether F conserves Δ, one need only verify

$$\Delta(F\zeta_p\diamondsuit, F\zeta_q\diamondsuit) = \Delta(\zeta_p\diamondsuit, \zeta_q\diamondsuit) \tag{2.20}$$

for each two patterns $p, q : M(M^{-1}(N^{-1})) \to S$ that agree everywhere but on the cell 0. Here $\diamondsuit$ can be any fixed arbitrarily chosen configuration.

[1] Recall that according to our definition, a *neighborhood* always contains the element 0.

In fact, in solving the system of equations (2.20) for μ, we can find at once the linear space of all potential differences that are conserved by F and generated by local observables with neighborhood M.

Let us next mention the following standard characterization of conservation laws in terms of finite configurations.

Theorem 2.3 ([41, 11, 16, 24])**.** *Let $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ be a cellular automaton, and Δ a local potential difference on $S^{\mathbb{L}}$. Let $\diamond \in S$ be an arbitrary state and $\diamondsuit$ the $\diamond$-uniform configuration. The following statements are equivalent.*

i) $\Delta(Fx, Fy) = \Delta(x, y)$ for every two asymptotic configurations x and y.

ii) $\Delta(F\diamondsuit, Fx) = \Delta(\diamondsuit, x)$ for every $\diamond$-finite configuration x.

Proof. That [i⇒ii] is trivial. Let us prove the other implication.

Let x and y be asymptotic, and $D \triangleq \{i : x[i] \neq y[i]\}$ be the set on which they disagree. Define $\diamond$-finite configurations $\hat{x}$ and $\hat{y}$ that agree, respectively, with x and y on a sufficiently large set $\overline{D} \supseteq D$ (namely, $\overline{D} \triangleq M(M^{-1}(N^{-1}(D)))$) and have state $\diamond$ on all the other cells. We have

$$\begin{aligned}
\Delta(Fx, Fy) &= \sum_{i \in M^{-1}(N^{-1}(D))} \big[\mu(\sigma^i Fy) - \mu(\sigma^i Fx)\big] && (2.21)\\
&= \sum_{i \in M^{-1}(N^{-1}(D))} \big[\mu(\sigma^i F\hat{y}) - \mu(\sigma^i F\hat{x})\big] && (2.22)\\
&= \Delta(F\hat{x}, F\hat{y}) && (2.23)\\
&= \Delta(F\diamondsuit, F\hat{y}) - \Delta(F\diamondsuit, F\hat{x}) && (2.24)\\
&= \Delta(\diamondsuit, \hat{y}) - \Delta(\diamondsuit, \hat{x}) && (2.25)\\
&= \Delta(\hat{x}, \hat{y}) && (2.26)\\
&= \sum_{i \in M^{-1}(D)} \big[\mu(\sigma^i \hat{y}) - \mu(\sigma^i \hat{x})\big] && (2.27)\\
&= \sum_{i \in M^{-1}(D)} \big[\mu(\sigma^i y) - \mu(\sigma^i x)\big] && (2.28)\\
&= \Delta(x, y)\ . && (2.29)
\end{aligned}$$

□

When the CA has a quiescent state $\diamond \in S$, we can choose $\diamondsuit$, the $\diamond$-uniform configuration, as a point of reference, and measure the energy of each $\diamond$-finite configuration x *relative to* $\diamondsuit$. In this case, the above characterization of conservation laws takes the following concise form.

Corollary 2.4. *Let $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ be a cellular automaton, and Δ a local potential difference on $S^{\mathbb{L}}$. Let $\diamond \in S$ be a quiescent state for F, and $\diamondsuit$ the $\diamond$-uniform*

configuration. For every $\diamond$-finite configuration x, define $\Delta(x) \triangleq \Delta(\diamondsuit, x)$. The following statements are equivalent.

i) $\Delta(Fx, Fy) = \Delta(x, y)$ *for every two asymptotic configurations x and y.*

ii) $\Delta(Fx) = \Delta(x)$ *for every $\diamond$-finite configuration x.*

2.3 Average Energy per Cell

Let $\mu : S^{\mathbb{L}} \to \mathbb{R}$ be a local observable with neighborhood $M \subseteq \mathbb{L}$. For every finite set $D \subseteq \mathbb{L}$, let us define a mapping $\mu_D : S^{\mathbb{L}} \to \mathbb{R}$ by

$$\mu_D(x) \triangleq \sum_{i \in D} \mu\left(\sigma^i x\right) \ , \tag{2.30}$$

which measures the *μ-content* of D on a given configuration x. Let us denote by $I_n \triangleq [-n, n]^d \subseteq \mathbb{L}$ the centered hyper-cube of side $2n+1$ in $\mathbb{L}$. The *upper average μ per cell* (or simply, the upper average energy per cell) of a configuration x is defined by

$$\overline{\mu}(x) \triangleq \limsup_{n \to \infty} \frac{\mu_{I_n}(x)}{|I_n|} \ . \tag{2.31}$$

The *lower average μ per cell* (or, the lower average energy per cell) of a configuration x is defined similarly, via

$$\underline{\mu}(x) \triangleq \liminf_{n \to \infty} \frac{\mu_{I_n}(x)}{|I_n|} \ . \tag{2.32}$$

For a probability measure $\pi \in \mathscr{M}$ on $S^{\mathbb{L}}$, the integral

$$\pi(\mu) \triangleq \int \mu \mathrm{d}\pi \triangleq \sum_{p : M \to S} g(p) \pi([p]) \tag{2.33}$$

is the *expected μ per cell* (or simply, the expected energy per cell) with respect to π.

The observable μ defines a potential difference Δ. In general, different observables may generate the same potential difference.[2] However, for a fixed Δ, the mappings $\overline{\mu}$ and $\underline{\mu}$ are (up to an additive constant) independent of the choice of μ.

Proposition 2.5. *Let Δ be a potential difference on $S^{\mathbb{L}}$. Let $\mu : S^{\mathbb{L}} \to \mathbb{R}$ be a local observable which generates Δ. Let $\diamond \in S$ be an arbitrary state, and $\diamondsuit$ the*

[2] We shall discuss this further in the next section.

$\diamond$-uniform configuration. For every $D \subseteq \mathbb{L}$, let ζ_D be the operator that sets the state of the cells in D to $\diamond$. For every configuration x,

$$\overline{\mu}(x) = \limsup_{n\to\infty} \frac{\Delta(\zeta_{I_n} x, x)}{|I_n|} + \mu(\diamondsuit) \ . \tag{2.34}$$

Proof. Let $x_n \triangleq \zeta_{I_n} x$. We have

$$\frac{\Delta(x_n, x)}{|I_n|} = \frac{\sum_{i\in M^{-1}(I_n)} \left[\mu(\sigma^i x) - \mu(\sigma^i x_n)\right]}{|I_n|} \tag{2.35}$$

$$= \frac{\sum_{i\in I_n} \mu(\sigma^i x)}{|I_n|} - \frac{\sum_{i\in I_n} \mu(\sigma^i \diamondsuit)}{|I_n|} + \frac{o(|I_n|)}{|I_n|} \ . \tag{2.36}$$

Letting $n \to \infty$ proves the claim. □

By definition, an observable μ is continuous with respect to the Cantor topology on $S^{\mathbb{L}}$. The average mapping $\overline{\mu}$ is not continuous in this sense. However, it is continuous if we consider the *Besicovitch* topology on $S^{\mathbb{L}}$ (see e.g. [18, 28]). The latter is defined using the pseudo-metric

$$d(x, y) \triangleq \limsup_{n\to\infty} \frac{|\{i \in I_n : x[i] \neq y[i]\}|}{|I_n|} \ . \tag{2.37}$$

Proposition 2.6. *For every local observable $\mu : S^{\mathbb{L}} \to \mathbb{R}$, the mapping $\overline{\mu} : S^{\mathbb{L}} \to \mathbb{R}$ is Lipschitz continuous with respect to the Besicovitch pseudo-metric.*

Proof. Suppose that μ has neighborhood M and local assignment $g : S^M \to \mathbb{R}$. Let

$$K \triangleq \sup\{|\mu(y) - \mu(x)| : x, y : \mathbb{L} \to S\} \tag{2.38}$$

$$= \max\{|g(q) - g(p)| : p, q : M \to S\} \ . \tag{2.39}$$

For every two configurations x and y, and every finite set $D \subseteq \mathbb{L}$, we have

$$|\mu_D(y) - \mu_D(x)| \leq \sum_{i\in D} |\mu(\sigma^i y) - \mu(\sigma^i x)| \tag{2.40}$$

$$\leq K \cdot |\{i \in D : x|_{M(i)} \neq y|_{M(i)}\}| \tag{2.41}$$

$$\leq K \cdot |M| \cdot |\{i \in D : x[i] \neq y[i]\}| \ . \tag{2.42}$$

Therefore,

$$|\overline{\mu}(y) - \overline{\mu}(x)| = \Big| \limsup_{n\to\infty} \frac{\mu_{I_n}(y)}{|I_n|} - \limsup_{n\to\infty} \frac{\mu_{I_n}(x)}{|I_n|} \Big| \tag{2.43}$$

$$\leq \limsup_{n\to\infty} \frac{|\mu_{I_n}(y) - \mu_{I_n}(x)|}{|I_n|} \tag{2.44}$$

$$\leq \limsup_{n\to\infty} \frac{K \cdot |M| \cdot |\{i \in D : x[i] \neq y[i]\}|}{|I_n|} \tag{2.45}$$

$$= K \cdot |M| \cdot \limsup_{n\to\infty} \frac{\{i \in D : x[i] \neq y[i]\}|}{|I_n|} \tag{2.46}$$

$$= K \cdot |M| \cdot d(x, y) \; . \tag{2.47}$$

□

Note that cellular automata are also Lipschitz continuous with respect to the Besicovitch pseudo-metric [18].

The mapping $\pi \mapsto \pi(\mu)$ is continuous with respect to weak convergence.

Proposition 2.7. *For every local observable $\mu : S^{\mathbb{L}} \to \mathbb{R}$, the mapping $\pi \mapsto \pi(\mu)$ (for $\pi \in \mathscr{M}$) is continuous with respect to the weak* topology.*

Proof. Suppose that μ has neighborhood $M \subseteq \mathbb{L}$ and local assignment $g : S^M \to \mathbb{R}$. For every converging sequence $\pi_1, \pi_2, \ldots$ in $\mathscr{M}$, we have

$$\lim_{n\to\infty} \pi_n(\mu) = \lim_{n\to\infty} \sum_{p:M\to S} g(p)\pi_n([p]) \tag{2.48}$$

$$= \sum_{p:M\to S} g(p) \lim_{n\to\infty} \pi_n([p]) \tag{2.49}$$

$$= \Big(\lim_{n\to\infty} \pi_n\Big)(\mu) \; . \tag{2.50}$$

□

We say that a configuration x is *generic* if for each finite pattern p we have $\overline{\delta_p}(x) = \underline{\delta_p}(x)$ (see e.g. [54, 28]). That is, a generic configuration is one for which the *frequency of occurrence* of each finite pattern is well-defined. It follows from the Ergodic Theorem (see Appendix A, Theorems A.4 and A.5) that the set of all generic configurations has probability 1 with respect to any translation-invariant probability measure $\pi \in \mathscr{M}_\sigma$ on $S^{\mathbb{L}}$. Every generic configuration x defines a translation-invariant Borel probability measure via $\pi_x([p]_D) \triangleq \overline{\delta}_p(x)$ for each finite pattern $p : D \to S$. In fact, by a theorem of Kakutani (see [71]), every translation-invariant probability measure is obtained from a generic configuration in this way.

Proposition 2.8 (e.g. [54, 28]). *Let $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ be a cellular automaton. If x is a generic configuration, so is Fx. If π_x is the probability measure associated to a generic configuration x, $F\pi_x$ is the probability measure associated to Fx.*

Proof. Let F have neighborhood N. For every finite pattern $p : D \to S$, let us denote by $F^{-1}p$ the set of patterns $q : N(D) \to S$ such that $F[q] \subseteq [p]$. We have

$$\delta_p(Fx) = \sum_{q \in F^{-1}p} \delta_q(x) \ . \tag{2.51}$$

Therefore,

$$\overline{\delta}_p(Fx) = \sum_{q \in F^{-1}p} \overline{\delta}_q(x) = \sum_{q \in F^{-1}p} \underline{\delta}_q(x) = \underline{\delta}_p(Fx) \ , \tag{2.52}$$

and

$$(F\pi_x)([p]) = \sum_{q \in F^{-1}p} \pi_x([q]) = \sum_{q \in F^{-1}p} \overline{\delta}_q(x) = \overline{\delta}_p(Fx) \ . \tag{2.53}$$

□

Proposition 2.9 (e.g. [54]). *Let $x : \mathbb{L} \to S$ be a generic configuration and $\pi_x \in \mathscr{M}_\sigma$ the corresponding probability measure. For every local observable $\mu : S^{\mathbb{L}} \to \mathbb{R}$, we have $\pi_x(\mu) = \overline{\mu}(x) = \underline{\mu}(x)$.*

Proof. Let μ have neighborhood $M \subseteq \mathbb{L}$ and local assignment $g : S^M \to \mathbb{R}$. For every finite $D \subseteq \mathbb{L}$, we have

$$\mu_D(x) = \sum_{i \in D} \mu(\sigma^i x) = \sum_{p : M \to S} \sum_{i \in D} \delta_p(x) g(p) = \sum_{p : M \to S} g(p) \sum_{i \in D} \delta_p(x) \ . \tag{2.54}$$

Therefore,

$$\overline{\mu}(x) = \sum_{p : M \to S} g(p) \overline{\delta}_p(x) = \sum_{p : M \to S} g(p) \cdot \pi_x([p]) = \pi_x(\mu) \ . \tag{2.55}$$

That $\underline{\mu}(x) = \pi_x(\mu)$ is similar. □

Clearly, each periodic configuration is generic. Let $\mathcal{P}$ denote the set of all spatially periodic configurations.

Proposition 2.10. *For each configuration x, there is a sequence $\{x_i\}_i$ in $\mathcal{P}$ converging to x (with Cantor topology), such that $\lim_{i \to \infty} \overline{\mu}(x_i) = \overline{\mu}(x)$.*

Proof. For every $n \geq 0$, let x_n be the periodic configuration with fundamental domain I_n that agrees with x on I_n. Clearly $\lim_{n\to\infty} x_n = x$ with Cantor topology. We have,

$$\frac{\sum_{i\in I_n} \mu(\sigma^i x)}{|I_n|} = \frac{\sum_{i\in I_n} \mu(\sigma^i x_n)}{|I_n|} + \frac{o(|I_n|)}{|I_n|} \tag{2.56}$$

$$= \overline{\mu}(x_n) + \frac{o(|I_n|)}{|I_n|} \,. \tag{2.57}$$

Letting $n \to \infty$ proves the claim. □

Corollary 2.11. *For every local observable $\mu : S^{\mathbb{L}} \to \mathbb{R}$, the set $\overline{\mu}(\mathcal{P})$ is dense in $\overline{\mu}(S^{\mathbb{L}})$.*

Conservation laws can be expressed in terms of average or expected energy per cell.

Theorem 2.12 ([72, 52, 16, 12])**.** *Let $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ be a cellular automaton. Let Δ be a local potential difference generated by a local observable $\mu : S^{\mathbb{L}} \to \mathbb{R}$. The following statements are equivalent:*

i) $\Delta(Fx, Fy) = \Delta(x, y)$ *for every two asymptotic configurations x and y.*

ii) $\overline{\mu}(Fx) = \overline{\mu}(x)$ *for every configuration x.*

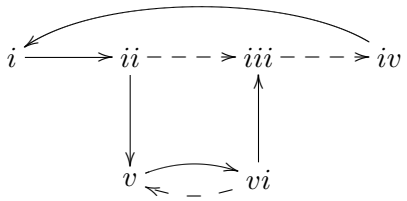
iii) $\overline{\mu}(Fx) = \overline{\mu}(x)$ *for every generic configuration x.*

iv) $\overline{\mu}(Fx) = \overline{\mu}(x)$ *for every periodic configuration x.*

v) $(F\pi)(\mu) = \pi(\mu)$ *for every translation-invariant σ-ergodic probability measure $\pi \in \mathscr{M}_\sigma$.*

vi) $(F\pi)(\mu) = \pi(\mu)$ *for every translation-invariant probability measure $\pi \in \mathscr{M}_\sigma$.*

Proof. The implications [ii⇒iii⇒iv], and [vi⇒v] are trivial. We prove the rest of the following implications:



Let F have neighborhood N and let μ have neighborhood M. For the sake of demonstration, we can assume $N = [-r, r]^d$ and $M = [-l, l]^d$, where $r, l \geq 0$. Let $\diamond \in S$ be an arbitrary state, and $\diamondsuit$ the $\diamond$-uniform configuration.

[i⇒ii] For each $D \subseteq \mathbb{L}$ and each configuration x, let $\zeta_D x$ be the configuration that has state $\diamond$ on every cell in D and agrees with x everywhere else. Note that, for each $t \geq 0$, $F^t\diamondsuit$ is a uniform configuration. Let x be an arbitrary configuration, and $t \geq 0$. If $n \geq 0$ is large, $F^t\zeta_{I_n}x$ agrees with $F^t\diamondsuit$ on a large finite set (namely, I_{n-tr}), while it is asymptotic to $F^t x$ (namely, it agrees with $F^t x$ on $\mathbb{L} \setminus I_{n+tr}$). We can write

$$\frac{\Delta\left(F^t\zeta_{I_n}x, F^t x\right)}{|I_n|} = \frac{\sum_{i\in M^{-1}(N^{-t}(I_n))}\left[\mu(\sigma^i F^t x) - \mu(\sigma^i F^t \zeta_{I_n} x)\right]}{|I_n|} \tag{2.58}$$

$$= \frac{\sum_{i\in I_n}\mu(\sigma^i F^t x)}{|I_n|} - \mu(F^t\diamondsuit) + \frac{o(|I_n|)}{|I_n|} \ . \tag{2.59}$$

Therefore, for a fixed $t \geq 0$ we have

$$\limsup_{n\to\infty} \frac{\Delta\left(F^t\zeta_{I_n}x, F^t x\right)}{|I_n|} = \overline{\mu}(F^t x) - \mu(F^t\diamondsuit) \ . \tag{2.60}$$

Since $\Delta(F^t\zeta_{I_n}x, F^t x) = \Delta(\zeta_{I_n}x, x)$, for each $t \geq 0$ we get

$$\overline{\mu}(F^t x) - \mu(F^t\diamondsuit) = \overline{\mu}(x) - \mu(\diamondsuit) \ . \tag{2.61}$$

It remains to show that for each $t \geq 0$, $\mu(F^t\diamondsuit) = \mu(\diamondsuit)$.

To prove the latter claim, substitute $F\diamondsuit$ for x in (2.61), and note that μ and $\overline{\mu}$ agree on uniform configurations. We obtain that

$$\mu(F^{t+1}\diamondsuit) - \mu(F^t\diamondsuit) = \mu(Fx) - \mu(\diamondsuit) \tag{2.62}$$

for each $t \geq 0$. However, the sequence $\diamondsuit, F\diamondsuit, \ldots$ is eventually periodic. That is, for some $k \geq 0$ and $p > 0$ we have $F^{k+p}\diamondsuit = F^k\diamondsuit$. Therefore,

$$0 = \mu(F^{k+p}\diamondsuit) - \mu(F^k\diamondsuit) = p \cdot (\mu(F\diamondsuit) - \mu(\diamondsuit)) \ . \tag{2.63}$$

That is, $\mu(F^t\diamondsuit) = \mu(\diamondsuit)$ for every $t \geq 0$.

[iv⇒i] Let x and y be two asymptotic configurations. Let $D \triangleq \{i : x[i] \neq y[i]\}$ be the set of cells on which x and y differ. Choose a hyper-cube

$$J \triangleq [a_1, b_1) \times [a_2, b_2) \times \cdots [a_d, b_d) \subseteq \mathbb{L} \ , \tag{2.64}$$

which contains $M(M^{-1}(D)) \cup M(M^{-1}(N^{-1}(D)))$. Define periodic configurations $\hat{x}$ and $\hat{y}$, with fundamental domain J, that agree with x and y on J. Namely, let

$$\hat{x}[i] \triangleq x[(i \bmod p) + a] \ , \tag{2.65}$$

$$\hat{y}[i] \triangleq y[(i \bmod p) + a] \tag{2.66}$$

for every $i = (i_1, i_2, \ldots, i_d) \in \mathbb{L}$, where

$$p \triangleq b - a \tag{2.67}$$
$$= (b_1, b_2, \ldots, b_d) - (a_1, a_2, \ldots, a_d) \; . \tag{2.68}$$

We have

$$\Delta(Fx, Fy) = \sum_{i \in M^{-1}(N^{-1}(D))} [\mu(\sigma^i Fy) - \mu(\sigma^i Fx)] \tag{2.69}$$
$$= \sum_{i \in M^{-1}(N^{-1}(D))} [\mu(\sigma^i F\hat{y}) - \mu(\sigma^i F\hat{x})] \tag{2.70}$$
$$= \sum_{i \in J} [\mu(\sigma^i F\hat{y}) - \mu(\sigma^i F\hat{x})] \tag{2.71}$$
$$= |J| \cdot [\overline{\mu}(F\hat{y}) - \overline{\mu}(F\hat{x})] \tag{2.72}$$
$$= |J| \cdot [\overline{\mu}(\hat{y}) - \overline{\mu}(\hat{x})] \tag{2.73}$$
$$= \sum_{i \in J} [\mu(\sigma^i \hat{y}) - \mu(\sigma^i \hat{x})] \tag{2.74}$$
$$= \sum_{i \in M^{-1}(D)} [\mu(\sigma^i \hat{y}) - \mu(\sigma^i \hat{x})] \tag{2.75}$$
$$= \sum_{i \in M^{-1}(D)} [\mu(\sigma^i y) - \mu(\sigma^i x)] \tag{2.76}$$
$$= \Delta(x, y) \; . \tag{2.77}$$

[ii⇒v] Let $\pi \in \mathscr{M}_\sigma$ be σ-ergodic. By Proposition A.2, $F\pi$ is also σ-ergodic. Let

$$\mathcal{A} \triangleq \{x : \overline{\mu}(x) = \pi(\mu)\} \; , \tag{2.78}$$
$$\mathcal{B} \triangleq \{y : \overline{\mu}(y) = (F\pi)(\mu)\} \; . \tag{2.79}$$

By the ergodic theorem (Theorem A.4), we have $\pi(\mathcal{A}) = 1$ and $(F\pi)(\mathcal{B}) = 1$. Therefore, $\pi(\mathcal{A} \cap F^{-1}\mathcal{B}) = 1$, which implies $\mathcal{A} \cap F^{-1}\mathcal{B} \neq \varnothing$. For each $x \in \mathcal{A} \cap F^{-1}\mathcal{B}$, we have $(F\pi)(\mu) = \overline{\mu}(Fx) = \overline{\mu}(x) = \pi(\mu)$.

[v⇒vi] Every probability measure $\pi \in \mathscr{M}_\sigma$ is a limit of convex combinations of σ-ergodic elements of $\mathscr{M}_\sigma$ (Theorem A.5). The claim follows from the fact that the mappings $\pi \mapsto \pi(\mu)$ and $\pi \mapsto F\pi$ are continuous and affine.

[vi⇒iii] For a generic configuration x, let π_x be the associated probability measure. By Propositions 2.8 and 2.9, we have

$$\overline{\mu}(Fx) = (F\pi_x)(\mu) = \pi_x(\mu) = \overline{\mu}(x) \; . \tag{2.80}$$

□

It is sometimes convenient to assume that a local observable is strictly positive. This often does not affect the generality of the discussion. For, if $\mu : S^{\mathbb{L}} \to \mathbb{R}$ is an arbitrary local observable, we can choose a constant $c \in \mathbb{R}$ such that $\mu^+ \triangleq \mu + c > 0$. Clearly, μ and μ^+ generate the same potential difference. Yet another way to characterize conservation laws is in terms of *expansion rate* of μ^+.

Theorem 2.13 ([24, 5]). *Let $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ be a cellular automaton, and Δ a local potential difference on $S^{\mathbb{L}}$. Let $\mu^+ : S^{\mathbb{L}} \to \mathbb{R}$ be a strictly positive local observable generating Δ. The following statements are equivalent:*

i) $\Delta(Fx, Fy) = \Delta(x, y)$ *for every two asymptotic configurations x and y.*

ii) $\lim_{n\to\infty} \dfrac{\mu^+_{I_n}(Fx)}{\mu^+_{I_n}(x)} = 1$ *for every configuration x.*

Proof. Let $\diamond \in S$ be an arbitrary state, and $\diamondsuit$ the $\diamond$-uniform configuration. As usual, for each $D \subseteq \mathbb{L}$ and each configuration x, let $\zeta_D x$ be the configuration which has state $\diamond$ on every cell in D and agrees with x everywhere else.

[i⇒ii] For $n \geq 0$ we have

$$\mu^+_{I_n}(x) = \Delta(\zeta_{I_n} x, x) + |I_n| \cdot \mu^+(\diamondsuit) + o(|I_n|) \;, \tag{2.81}$$

$$\mu^+_{I_n}(Fx) = \Delta(F\zeta_{I_n} x, Fx) + |I_n| \cdot \mu^+(F\diamondsuit) + o(|I_n|) \;. \tag{2.82}$$

By assumption, $\Delta(F\zeta_{I_n} x, Fx) = \Delta(\zeta_{I_n} x, x)$, and by Theorem 2.12 we know $\mu^+(F\diamondsuit) = \mu^+(\diamondsuit)$. Note also that $\mu^+_{I_n} \geq K \cdot |I_n|$ where $K = \inf_z \mu^+(z) > 0$. Therefore,

$$\lim_{n\to\infty} \frac{\mu^+_{I_n}(Fx)}{\mu^+_{I_n}(x)} = \lim_{n\to\infty} \frac{\Delta(F\zeta_{I_n} x, Fx) + |I_n| \cdot \mu^+(F\diamondsuit) + o(|I_n|)}{\Delta(\zeta_{I_n} x, x) + |I_n| \cdot \mu^+(\diamondsuit) + o(|I_n|)} \tag{2.83}$$

$$= 1 \;. \tag{2.84}$$

[ii⇒i] By Theorem 2.12, it is enough to show that, for each spatially periodic configuration x, we have $\overline{\mu}^+(Fx) = \overline{\mu}^+(x)$. Let x be a spatially periodic configuration. For $n \geq 0$ we have

$$\mu^+_{I_n}(x) = |I_n| \cdot \overline{\mu}^+(x) + o(|I_n|) \;, \tag{2.85}$$

$$\mu^+_{I_n}(Fx) = |I_n| \cdot \overline{\mu}^+(Fx) + o(|I_n|) \;. \tag{2.86}$$

Therefore,

$$1 = \lim_{n\to\infty} \frac{\mu^+_{I_n}(Fx)}{\mu^+_{I_n}(x)} = \lim_{n\to\infty} \frac{|I_n| \cdot \overline{\mu}^+(Fx) + o(|I_n|)}{|I_n| \cdot \overline{\mu}^+(x) + o(|I_n|)} = \frac{\overline{\mu}^+(Fx)}{\overline{\mu}^+(x)} \;. \tag{2.87}$$

□

2.4 Observables vs. Interaction Potentials

Let $\mathscr{D}$ be the set of all local potential differences on $S^{\mathbb{L}}$. This is a linear space. If Δ_1 and Δ_2 are generated by local observables μ_1 and μ_2, respectively, $a\Delta_1 + b\Delta_2$ $(a, b \in \mathbb{R})$ is generated by the local observable $a\mu_1 + b\mu_2$. Every cellular automaton $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ induces a linear operator F^* on $\mathscr{D}$, where for every $\Delta \in \mathscr{D}$, $F^*\Delta$ is defined via $(F^*\Delta)(x, y) \triangleq \Delta(Fx, Fy)$. If Δ is generated by a local observable $\mu : S^{\mathbb{L}} \to \mathbb{R}$, $F^*\Delta$ is generated by the local observable $\mu \circ F$. It is easy to see that $\overline{\mu \circ F} = \overline{\mu} \circ F$.

For every neighborhood $M \subseteq \mathbb{L}$, we have a linear subspace $\mathscr{D}[M] \subseteq \mathscr{D}$ of potential differences with neighborhood M. For a cellular automaton F with neighborhood N, F^* maps $\mathscr{D}[M]$ into $\mathscr{D}[N(M)]$. The potential differences conserved by a cellular automaton F form a subspace of $\mathscr{D}$, denoted by $\mathscr{D}_F$. As pointed out in Section 2.2, for every neighborhood M, one can identify algorithmically the finite dimensional space $\mathscr{D}_F[M]$.

In general, different local observables may generate the same potential difference. If observables μ_1 and μ_2 generate the same potential difference Δ, $\mu_2 - \mu_1$ generates the zero element of $\mathscr{D}$. We call an observable *void* if it generates the zero potential difference. Void local observables are exactly those with constant average.

Proposition 2.14. *A local observable $\mu : S^{\mathbb{L}} \to \mathbb{R}$ is void if and only if the average $\overline{\mu}$ is constant.*

Proof. Let μ be void; that is, $\Delta \equiv 0$. It follows from Proposition 2.5 that $\overline{\mu}$ is constant.

Conversely, suppose that $\Delta(x, y) \neq 0$ for asymptotic configurations x and y. Let $D \triangleq \{i : x[i] \neq y[i]\}$ be the set of cells over which x and y disagree. Let μ have neighborhood M. Choose a hyper-cube

$$J \triangleq [a_1, b_1) \times [a_2, b_2) \times \cdots [a_d, b_d) \subseteq \mathbb{L} \,, \tag{2.88}$$

which contains $M(M^{-1}(D))$. Define periodic configurations $\hat{x}$ and $\hat{y}$, with fundamental domain J, that agree with x and y on J. Namely, let

$$\hat{x}[i] \triangleq x[(i \bmod p) + a] \,, \tag{2.89}$$

$$\hat{y}[i] \triangleq y[(i \bmod p) + a] \tag{2.90}$$

for every $i = (i_1, i_2, \ldots, i_d) \in \mathbb{L}$, where

$$p \triangleq b - a \tag{2.91}$$

$$= (b_1, b_2, \ldots, b_d) - (a_1, a_2, \ldots, a_d) \,. \tag{2.92}$$

We have

$$\overline{\mu}(\hat{y}) - \overline{\mu}(\hat{x}) = \frac{\Delta(x,y)}{|J|} \neq 0 \ . \tag{2.93}$$

Hence, $\overline{\mu}$ is not constant. □

Void local observables form a linear subspace of the space of all local observables. Adding a void observable to an observable μ does not affect the potential difference μ generates. If Δ is a potential difference generated by μ, we can express the fact that a cellular automaton F conserves Δ by saying $\mu \circ F - \mu$ is void.

An alternative way to generate local potential differences is via *interaction potentials*, that is, by assigning energy to the interaction of the elements, rather than to the individual elements and their context. Although a bit cumbersome to work with, defining potential differences via interaction potentials has the advantage that it is often more compatible with the physical intuition. Furthermore, as we shall see, every local potential difference has a *canonical* interaction potential, which is in some sense the most natural.

Recall that $S^{\#}$ denotes the collection of finite patterns modulo translations. A (local) *interaction potential* is an assignment $\theta : S^{\#} \to \mathbb{R}$ such that

i) The set $\mathrm{supp}(\theta) \triangleq \{p \in S^{\#} : \theta(p) \neq 0\}$ is finite, and

ii) $\theta(\varnothing) = 0$.

(Recall that $\varnothing$ is the empty pattern.) Every interaction potential θ generates a local potential difference Δ via

$$\Delta(x,y) \triangleq \sum_{K \text{ finite}} [\theta(y|_K) - \theta(x|_K)] \tag{2.94}$$

for asymptotic configurations x and y.

Proposition 2.15. *The mapping defined via (2.94) is a local potential difference.*

Proof. That Δ is a potential difference is trivial. To see that Δ is local, first note that it is defined for each asymptotic x and y, and that $\Delta(\sigma^a x, \sigma^a y) = \Delta(x,y)$ for each $a \in \mathbb{L}$.

Choose a finite set $M \subseteq \mathbb{L}$ such that for each finite pattern $p : A \to S$ where $\langle p \rangle \in P_\theta$, either $0 \notin A$ or $A \subseteq M$. For example, if

$$\mathrm{supp}(\theta) = \{\langle p_1 \rangle, \langle p_2 \rangle, \ldots, \langle p_n \rangle\} \tag{2.95}$$

where p_k has domain A_k, we can choose

$$M \triangleq \bigcup_{k=1}^{n} A_k(A_k^{-1}) \ . \tag{2.96}$$

Let $q : D \to S$ be a finite pattern, and x and y two configurations that agree on $M(D)$. We have

$$\begin{aligned}
\Delta(y, \zeta_q y) &= \sum_{K \text{ finite}} [\theta(y|_K) - \theta(\zeta_q y|_K] && (2.97)\\
&= \sum_{K \subseteq M(D)} [\theta(y|_K) - \theta(\zeta_q y|_K] && (2.98)\\
&= \sum_{K \subseteq M(D)} [\theta(x|_K) - \theta(\zeta_q x|_K] && (2.99)\\
&= \sum_{K \text{ finite}} [\theta(x|_K) - \theta(\zeta_q x|_K] && (2.100)\\
&= \Delta(x, \zeta_q x) \ . && (2.101)
\end{aligned}$$

□

We are now going to show that each local potential difference has a canonical presentation in terms of an interaction potential. For this, we must single out one state $\diamond \in S$ which we will call *blank*. A non-blank state is called *active*. A pattern is active if all its cells are active. By convention, the empty pattern is non-active.

Proposition 2.16 ([39, 20])**.** *Every local potential difference is generated by a unique (up to the choice of the blank state) interaction potential that assigns zero to all non-active patterns.*

Proof. Let Δ be a local potential difference with neighborhood M. Let $\diamond \in S$ be the blank state, and $\diamondsuit$ the $\diamond$-uniform configuration. For every finite pattern $p : D \to S$, define $\Delta(p) \triangleq \Delta(\diamondsuit, \zeta_p \diamondsuit)$. Consider the equations

$$\sum_{q \preceq p} \theta(q) = \Delta(p) \tag{2.102}$$

for every finite pattern $p : D \to S$. The set of all sub-patterns of p is a finite partially ordered set isomorphic to $(2^D, \subseteq)$. Therefore, by the Möbius Inversion Theorem (see e.g. [81]), the system of equations (2.102) has a unique solution for θ, given by

$$\theta(p) \triangleq \sum_{q \preceq p} (-1)^{|p|-|q|} \Delta(q) \ . \tag{2.103}$$

Let $Q \triangleq \{p : \theta(p) \neq 0\}$. We show that, for every $p : D \to S$, θ vanishes whenever

a) there exist $i, j \in D$ with $M^{-1}(i) \cap M^{-1}(j) = \varnothing$, or

b) $p[i] = \diamond$ for some $i \in D$.

Since θ is translation-invariant, it follows that the quotient Q/σ is finite. We see that $\theta(\langle p \rangle) \triangleq \theta(p)$ (for every $\langle p \rangle \in S^{\#}$) is well-defined and is an interaction potential. We further show that

c) $\Delta(x, y) = \sum_{K \text{ finite}} [\theta(y|_K) - \theta(x|_K)]$ for each asymptotic x and y.

First, suppose there exist two cells $i, j \in D$, such that $M^{-1}(i) \cap M^{-1}(j) = \varnothing$; that is, for every $k \in \mathbb{L}$, either $i \notin M(k)$ or $j \notin M(k)$. We have

$$\theta(p) = \sum_{\substack{A \subseteq D \\ A \ni i, A \ni j}} (-1)^{|D|-|A|} \Delta(p|_A) + \sum_{\substack{A \subseteq D \\ A \ni i, A \not\ni j}} (-1)^{|D|-|A|} \Delta(p|_A) \tag{2.104}$$

$$+ \sum_{\substack{A \subseteq D \\ A \not\ni i, A \ni j}} (-1)^{|D|-|A|} \Delta(p|_A) + \sum_{\substack{A \subseteq D \\ A \not\ni i, A \not\ni j}} (-1)^{|D|-|A|} \Delta(p|_A) \tag{2.105}$$

$$= \sum_{\substack{A \subseteq D \\ A \ni i, A \ni j}} (-1)^{|D|-|A|} \left[\Delta_A - \Delta_{A \smallsetminus j} - \Delta_{A \smallsetminus i} + \Delta_{A \smallsetminus i \smallsetminus j}\right] , \tag{2.106}$$

where we have used the shorthand Δ_X for $\Delta(p|_X)$. But the additivity of Δ implies

$$\Delta_A - \Delta_{A \smallsetminus j} - \Delta_{A \smallsetminus i} + \Delta_{A \smallsetminus i \smallsetminus j} = 0 \tag{2.107}$$

(cf. Equations 2.1 and 2.2). Specifically,

$$\Delta_A - \Delta_{A \smallsetminus j} = \Delta(\zeta_{p|_{A \smallsetminus j}} \diamondsuit, \zeta_{p|_A} \diamondsuit) \tag{2.108}$$

$$= \Delta(\zeta_{p|_{A \smallsetminus i \smallsetminus j}} \diamondsuit, \zeta_{p|_{A \smallsetminus i}} \diamondsuit) \tag{2.109}$$

$$= \Delta_{A \smallsetminus i} - \Delta_{A \smallsetminus i \smallsetminus j} . \tag{2.110}$$

Hence, $\theta(p) = 0$.

Next, assume that $p[i] = \diamond$ for some $i \in D$. We have

$$\theta(p) = \sum_{A \subseteq D} (-1)^{|D|-|A|} \Delta(p|_A) \tag{2.111}$$

$$= \sum_{\substack{A \subseteq D \\ A \ni i}} (-1)^{|D|-|A|} \left[\Delta(p|_A) - \Delta(p|_{A \smallsetminus i})\right] . \tag{2.112}$$

But $\Delta(p|_A) = \Delta(p|_{A \smallsetminus i})$, because $\zeta_{p|_A} \diamondsuit = \zeta_{p|_{A \setminus i}} \diamondsuit$. Therefore, $\theta(p) = 0$.

Finally, let x and y be asymptotic. Let D be the set of cells on which x and y differ. Let $p \triangleq x|_{M(M^{-1}(D))}$ and $q \triangleq y|_{M(M^{-1}(D))}$. We have

$$\begin{aligned}
\Delta(x,y) &= \Delta(\zeta_p\diamondsuit, \zeta_q\diamondsuit) && (2.113)\\
&= \Delta(\diamondsuit, \zeta_q\diamondsuit) - \Delta(\diamondsuit, \zeta_p\diamondsuit) && (2.114)\\
&= \sum_{K\subseteq M(M^{-1}(D))} \theta(q|_K) - \sum_{K\subseteq M(M^{-1}(D))} \theta(p|_K) && (2.115)\\
&= \sum_{K\subseteq M(M^{-1}(D))} \theta(y|_K) - \sum_{K\subseteq M(M^{-1}(D))} \theta(x|_K) && (2.116)\\
&= \sum_{K \text{ finite}} \left[\theta(y|_K) - \theta(x|_K)\right] \ , && (2.117)
\end{aligned}$$

which concludes the proof. □

We will call the interaction potential provided by Proposition 2.16 the *canonical* interaction potential generating Δ.

Let θ be an interaction potential. For a configuration x and a finite set $A \subseteq \mathbb{L}$, we can define

$$\Theta_A(x) \triangleq \sum_{K\subseteq A} \theta(x|_A) \tag{2.118}$$

as the amount of energy on x which is concentrated in A. Likewise, for two disjoint finite sets $A, B \subseteq \mathbb{L}$, we can define

$$\Theta_{A,B}(x) \triangleq \sum_{\substack{K\subseteq A\cup B\\ K\cap A\neq\varnothing\\ K\cap B\neq\varnothing}} \theta(x|_K) \tag{2.119}$$

as the amount of energy in x resulting from the interaction of A and B. Clearly, whenever $A, B \in \mathbb{L}$ are finite and disjoint, we have

$$\Theta_{A\cup B} = \Theta_A + \Theta_B + \Theta_{A,B} \ . \tag{2.120}$$

If $\diamond \in S$ is the blank state, $\diamondsuit$ the $\diamond$-uniform configuration, and θ canonical, for every finite pattern $p : D \to S$ we can define $\Theta(\zeta_p\diamondsuit) \triangleq \Theta_D(\zeta_p\diamondsuit)$. If θ generates a potential difference Δ, for every $\diamond$-finite configuration x we have $\Theta(x) = \Delta(\diamondsuit, x)$.

The average energy per cell can equivalently be defined in terms of interaction potentials. Namely, if $\theta : S^{\#} \to \mathbb{R}$ is an interaction potential, for every configuration x, let

$$\overline{\theta}(x) \triangleq \limsup_{n\to\infty} \frac{\Theta_{I_n}(x)}{|I_n|} \ . \tag{2.121}$$

Proposition 2.17. *Let $\mu : S^{\mathbb{L}} \to \mathbb{R}$ be a local observable, and $\theta : S^{\#} \to \mathbb{R}$ an interaction potential, both generating a potential difference Δ. Then $\overline{\mu} - \overline{\theta}$ is constant.*

Proof. Let M be the neighborhood of Δ. Let x_n be the configuration which agrees with x outside I_n and has $\diamond$ on each cell inside I_n. By Proposition 2.5, it is enough to show that

$$\overline{\theta}(x) = \limsup_{n\to\infty} \frac{\Delta(x_n, x)}{|I_n|} + c \tag{2.122}$$

for a constant $c \in \mathbb{R}$. We have

$$\frac{\Delta(x_n, x)}{|I_n|} = \frac{\sum_{\substack{K \text{ finite} \\ K \cap I_n \neq \varnothing}} [\theta(x|_K) - \theta(x_n|_K)]}{|I_n|} \tag{2.123}$$

$$= \frac{\Theta_{I_n}(x) + \Theta_{I_n, \partial M(I_n)}(x)}{|I_n|} - \frac{\Theta_{I_n}(x_n) + \Theta_{I_n, \partial M(I_n)}(x_n)}{|I_n|} \tag{2.124}$$

$$= \frac{\Theta_{I_n}(x)}{|I_n|} - \frac{\Theta_{I_n}(\diamondsuit)}{|I_n|} + \frac{o(|I_n|)}{|I_n|} \,. \tag{2.125}$$

Letting $n \to \infty$ proves the claim. □

CHAPTER 3

Flows and Particles

A conservation law, as discussed in the previous chapter, is a global property of a CA. It asserts that certain local additive quantity, which we call energy, is globally preserved. It does not, however, provide any microscopic mechanism behind this. Namely, it does not elaborate how the energy is manipulated locally so that its global quantity remains intact. As we shall see, microscopic explanations can be given for any conservation law in CA in terms of "flows" of energy from one cell to another. Needless to say, such explanations are utterly conceptual (as are all mathematical models). They provide only a contrivance to make the phenomenon more intuitive and perhaps easier to treat with some of our mathematical or computational tools.

Since each conservation law may have many different "flow" explanations, we may look for restricted types of flow that have some desired properties. In the case that the energy concept of a conservation law has a certain physical interpretation, we would like our flow explanation to be compatible with that interpretation. An interesting case is when the energy of a configuration is interpreted as the number of objects or "particles" distributed over the cells. We then expect our flow to explain the movement of the particles. This gives rise to the concept of particle flows.

Finally, we might hope that following the approach in Section 2.4, we can find a "canonical" flow explanation for each conservation law. We will make an effort in this direction. The result, though not satisfactory, is perhaps worth mentioning.

3.1 Flows and Local Conservation Laws

We would like to find an explanation for the microscopic dynamics of a conserved energy, in terms of "flows" of energy from one cell to another.

Let $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ be an arbitrary CA. Let Δ be the potential difference generated by a local observable $\mu : S^{\mathbb{L}} \to \mathbb{R}$. If $x \in S^{\mathbb{L}}$ is a configuration,

and $a \in \mathbb{L}$ a cell on the lattice, we may think of $\mu(\sigma^a x)$ as the amount of energy in x which is associated with (or is coming from) cell a.[1] A "flow" would describe how this value is redistributed among the neighboring cells of a in one iteration of F.

Specifically, by a *flow* we mean a mapping $x, i, j \mapsto \Phi_{i\to j}(x) \in \mathbb{R}$ for $x \in S^{\mathbb{L}}$ and $i, j \in \mathbb{L}$ that satisfies the following conditions:

i) For every $i, j \in \mathbb{L}$, the mapping $x \mapsto \Phi_{i\to j}(x)$ is a local observable.

ii) For every configuration x, all cells $i, j \in \mathbb{L}$, and every $a \in \mathbb{L}$,

$$\Phi_{a+i\to a+j}(x) = \Phi_{i\to j}(\sigma^a x) \; . \tag{3.1}$$

iii) There is a finite set $I \subseteq \mathbb{L}$ such that, $\Phi_{i\to j} = 0$ unless $i - j \in I$.

Equivalently, a mapping $x, i, j \mapsto \Phi_{i\to j}(x)$ is called a flow if there exist finite sets $K, I \subseteq \mathbb{L}$, and a rule $\varphi : S^K \times I \to \mathbb{R}$ such that

$$\Phi_{i\to j}(x) = \begin{cases} \varphi(x|_{K(j)}, i - j) & \text{if } i - j \in I, \\ 0 & \text{otherwise} \end{cases} \tag{3.2}$$

for every $x \in S^{\mathbb{L}}$ and $i, j \in \mathbb{L}$. The value $\Phi_{i\to j}(x)$ is referred to as the flow *from* cell i *to* cell j in configuration x. The amount of flow to each cell is decided locally, by looking at a finite *neighborhood* K of that cell. The set I is the set of *directions* from which energy flows to a cell.

We say that a flow Φ is *compatible* with energy μ and cellular automaton F (or, Φ is a flow for μ, under the dynamics of F), if the following *continuity equations* hold (see Figure 3.1(a)):

a) For every configuration x and every cell a,

$$\mu(\sigma^a x) = \sum_{j\in\mathbb{L}} \Phi_{a\to j}(x) \; . \tag{3.3}$$

b) For every configuration x and every cell a,

$$\sum_{i\in\mathbb{L}} \Phi_{i\to a}(x) = \mu(\sigma^a F x) \; . \tag{3.4}$$

An energy μ is *locally conserved* by F if it has a flow under F. In fact, conservation laws and local conservation laws are equivalent concepts in cellular automata (see [41]):

[1] This is not, strictly speaking, a universal meaning induced by Δ, but rather, subjective to the specific observable μ. A different observable generating Δ would claim a different energy for cell a. We would like to see if the version of the story told by μ can be extended to cover the movements of the energy.

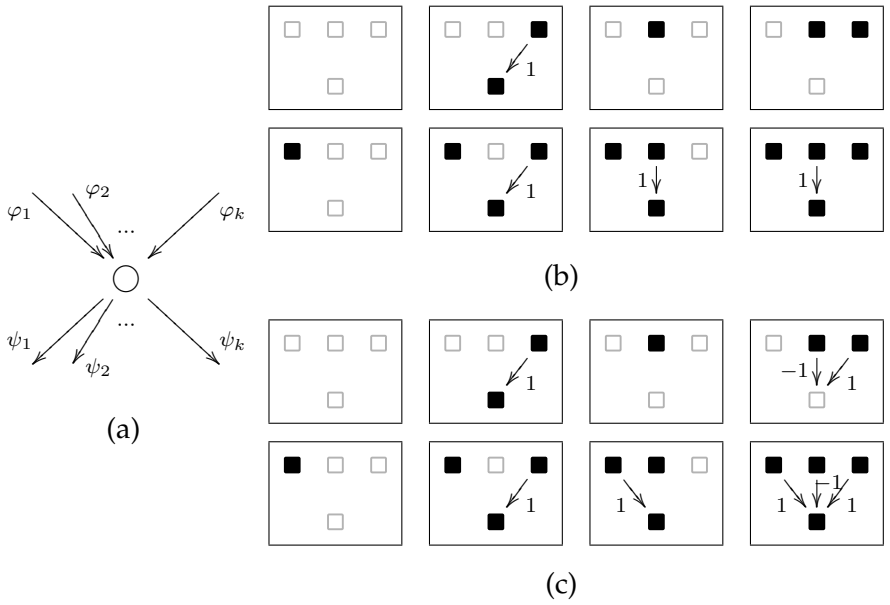


Figure 3.1: (a) Continuity of the flow: $\sum_i \varphi_i = \mu = \sum_j \psi_j$.
(b, c) Two different flows for the car conservation law in the Traffic CA.

Proposition 3.1. *Let Δ be a potential difference generated by a local observable μ. A cellular automaton F conserves Δ if and only if it locally conserves μ.*

Proof. [$\Leftarrow$] First, suppose that F locally conserves μ. Let Φ be a flow compatible with μ and F. For any two asymptotic configurations x and y, we have

$$\Delta(x,y) = \sum_{i\in\mathbb{L}} \big[\mu(\sigma^i y) - \mu(\sigma^i x)\big] \tag{3.5}$$

$$= \sum_{i\in\mathbb{L}} \left[\sum_{j\in\mathbb{L}} \Phi_{i\to j}(y) - \sum_{j\in\mathbb{L}} \Phi_{i\to j}(x)\right] \tag{3.6}$$

$$= \sum_{j\in\mathbb{L}} \left[\sum_{i\in\mathbb{L}} \Phi_{i\to j}(y) - \sum_{i\in\mathbb{L}} \Phi_{i\to j}(x)\right] \tag{3.7}$$

$$= \sum_{j\in\mathbb{L}} \big[\mu(\sigma^j F y) - \mu(\sigma^j F x)\big] \tag{3.8}$$

$$= \Delta(Fx, Fy)\ . \tag{3.9}$$

Therefore, F conserves Δ.

[⇒] Next, suppose that F conserves Δ. We construct a flow compatible with μ and F. The construction is similar to that in Proposition 2.1 where we proved that every local potential difference is generated by a local observable.

Let us distinguish an arbitrary state $\diamond \in S$, and denote the $\diamond$-uniform configuration by $\diamondsuit$. Let $\preceq$ be the lexicographic order on $\mathbb{L}$, and for every cell $i \in \mathbb{L}$, denote by $\gamma(i)$ the successor of i according to $\preceq$. Recall that for every pattern $p : D \to S$, the operator ζ_p turns every pattern $q : E \to S$ into $q|_{E\setminus D} \vee p$. For every cell $k \in \mathbb{L}$, let us use the shorthand ζ_k for the operator ζ_{r_k}, where r_k is the restriction of $\diamondsuit$ to $\{i \in \mathbb{L} : k \preceq i\}$. In other words, the operator ζ_k sets all the cells $i \succeq k$ to blank. Let $N \subseteq \mathbb{L}$ be the neighborhood of F and $M \subseteq \mathbb{L}$ the neighborhood of μ.

Let x be an arbitrary configuration. Roughly speaking, starting from the configuration $\diamondsuit$, we follow the order $\preceq$ and switch the state of the cells, one by one, to their values in x. At each step, we look at the change in the energy values of the cells before and after applying F, and try to match them with each other.

For every $a, i, j \in \mathbb{L}$, let us define

$$\varepsilon[a,i](x) \triangleq \mu\left(\sigma^i \zeta_{\gamma(a)} x\right) - \mu\left(\sigma^i \zeta_a x\right) \ , \tag{3.10}$$

$$\vartheta[a,j](x) \triangleq \mu\left(\sigma^j F \zeta_{\gamma(a)} x\right) - \mu\left(\sigma^j F \zeta_a x\right) \ . \tag{3.11}$$

Note that

a) $\sum_{i\in\mathbb{L}} \varepsilon[a,i](x) = \Delta(\zeta_a x, \zeta_{\gamma(a)} x) = \Delta(F\zeta_a x, F\zeta_{\gamma(a)} x) = \sum_{j\in\mathbb{L}} \vartheta[a,j](x)$,

b) $\varepsilon[a,i](x) = 0$, unless $i \in M^{-1}(a)$,

c) $\vartheta[a,j](x) = 0$, unless $j \in M^{-1}(N^{-1}(a))$,

d) $\varepsilon[a,i](x) = \varepsilon[a,i](x')$ if $x|_{M(M^{-1}(a))} = x'|_{M(M^{-1}(a))}$,

e) $\vartheta[a,j](x) = \vartheta[a,j](x')$ if $x|_{N(M(M^{-1}(N^{-1}(a))))} = x'|_{N(M(M^{-1}(N^{-1}(a))))}$.

For every configuration x, and all $a, i, j \in \mathbb{L}$ with $i \in M^{-1}(a)$ and $j \in M^{-1}(N^{-1}(a))$, let us choose $\delta\Phi[a, i \to j](x) \in \mathbb{R}$ in such a way that

$$\sum_{i\in M^{-1}(a)} \delta\Phi[a, i \to j](x) = \vartheta[a,j](x) \ , \tag{3.12}$$

$$\sum_{j\in M^{-1}(N^{-1}(a))} \delta\Phi[a, i \to j](x) = \varepsilon[a,i](x) \ . \tag{3.13}$$

Namely, for $i \neq a$, let us choose

$$\delta\Phi[a, i \to j](x) \triangleq \begin{cases} \varepsilon[a,i](x) & \text{if } j = i, \\ 0 & \text{otherwise,} \end{cases} \tag{3.14}$$

while we choose

$$\delta\Phi[a, a \to j](x) \triangleq \begin{cases} \vartheta[a, j](x) & \text{if } j = a, \\ \vartheta[a, j](x) - \varepsilon[a, j](x) & \text{otherwise.} \end{cases} \tag{3.15}$$

When $i \notin M^{-1}(a)$ or $j \notin M^{-1}(N^{-1}(a))$, define $\delta\Phi[a, i \to j](x) \triangleq 0$.

Now we can construct a flow as follows. For every configuration x, and every $i, j \in \mathbb{L}$, define

$$\Phi_{i\to j}(x) \triangleq \delta_{ij} \cdot \mu(\diamondsuit) + \sum_{a\in\mathbb{L}} \delta\Phi[a, i \to j](x) \ , \tag{3.16}$$

where $\delta_{ij} \triangleq 1$ if $i = j$ and $\delta_{ij} \triangleq 0$ otherwise. The translation-invariance of Φ (condition (ii)) follows from the translation-invariance of ε, ϑ and $\delta\Phi$. For fixed $a, i, j \in \mathbb{L}$, clearly $\varepsilon[a, i]$ and $\vartheta[a, j]$, and hence $\delta\Phi[a, i \to j]$, are local observables. Furthermore, $\delta\Phi[a, i \to j] = 0$, unless $a \in M(i) \cap N(M(j))$. Therefore, Φ is also a local observable (condition (i)). Finally, $\Phi_{i\to j} = 0$ whenever $M(i) \cap N(M(j)) = \varnothing$; that is, unless $i - j \in M^{-1}(N(M))$ (condition (iii)). Therefore, Φ is a flow.

Let us verify that Φ also satisfies the continuity equations. For every $x \in S^{\mathbb{L}}$ and $c \in \mathbb{L}$, we have

$$\begin{aligned} \mu(\sigma^c x) &= \mu(\diamondsuit) + \sum_{a\in\mathbb{L}} \left[\mu\left(\sigma^c \zeta_{\gamma(a)} x\right) - \mu\left(\sigma^c \zeta_a x\right)\right] && (3.17)\\ &= \mu(\diamondsuit) + \sum_{a\in\mathbb{L}} \varepsilon[a, c](x) && (3.18)\\ &= \mu(\diamondsuit) + \sum_{a\in\mathbb{L}} \sum_{j\in\mathbb{L}} \delta\Phi[a, c \to j](x) && (3.19)\\ &= \sum_{j\in\mathbb{L}} \left[\delta_{cj} \cdot \mu(\diamondsuit) + \sum_{a\in\mathbb{L}} \delta\Phi[a, c \to j](x)\right] && (3.20)\\ &= \sum_{j\in\mathbb{L}} \Phi_{c\to j}(x) \ . && (3.21) \end{aligned}$$

and

$$\begin{aligned} \sum_{i\in\mathbb{L}} \Phi_{i\to c}(x) &= \sum_{i\in\mathbb{L}} \left[\delta_{ic} \cdot \mu(\diamondsuit) + \sum_{a\in\mathbb{L}} \delta\Phi[a, i \to c](x)\right] && (3.22)\\ &= \mu(\diamondsuit) + \sum_{a\in\mathbb{L}} \sum_{i\in\mathbb{L}} \delta\Phi[a, i \to c](x) && (3.23)\\ &= \mu(\diamondsuit) + \sum_{a\in\mathbb{L}} \vartheta[a, c](x) && (3.24) \end{aligned}$$

$$= \mu(\diamondsuit) + \sum_{a \in \mathbb{L}} \left[\mu\left(\sigma^c F \zeta_{\gamma(a)} x\right) - \mu\left(\sigma^c F \zeta_a x\right) \right] \tag{3.25}$$

$$= \mu(\diamondsuit) + \mu(\sigma^c F x) - \mu(\sigma^c F \diamondsuit) \tag{3.26}$$

$$= \mu(\sigma^c F x) \; . \tag{3.27}$$

(That $\mu(F\diamondsuit) = \mu(\diamondsuit)$ follows, for example, from Theorem 2.12.) Therefore, Φ is compatible with μ and F, which means μ is locally conserved by F. □

It is clear that the choice of the flow Φ in the above construction was quite arbitrary. In fact, there are infinitely many different flows compatible with each conservation law. For example, Figure 3.1(b,c) shows two different flows for the car conservation law in the Traffic CA, which was referred to in the introduction. We next discuss the existence of a restricted type of flow for interaction-free energies; that is, energies which can be defined via local observables with singleton neighborhoods.

3.2 Particle Flows

In this section, we focus on *interaction-free* potentials; that is, those generated by observables with singleton neighborhood $\{0\}$. Moreover, we restrict ourselves to observables that take values in the set of non-negative integers.

Let $\mu : S^{\mathbb{L}} \to \mathbb{N}$ ($\mathbb{N} \triangleq \{0, 1, 2, \ldots\}$) be a local observable with neighborhood $\{0\}$. That is, μ is specified using an assignment $g : S \to \mathbb{N}$ via $\mu(x) \triangleq g(x[0])$. We interpret $g(s)$ as the number of "particles" attached to state s. Or we may say that a cell with state $s \in S$ carries $g(s)$ particles. If a CA F conserves the energy defined by μ, the total number of particles in a configuration x after one iteration of F remains the same. Can we explain this by providing an explicit recipe for the movement of each individual particle? In other words, can we find a flow for μ whose values are all non-negative integers? A flow Φ such that $\Phi_{i \to j}(x) \in \mathbb{N}$ for all i, j and x is called a *particle flow*. The value $\Phi_{i \to j}(x)$ suggests the number of particles in configuration x traveling from cell i to cell j in one iteration step of F.

Remark 3.1. Let Φ be a flow for an interaction-free observable μ, and suppose that Φ takes its values in $\mathbb{Z}$. If I is the set of directions from which Φ flows, for a sufficiently large $k \in \mathbb{Z}$, the flow

$$\Phi'_{i \to j} \triangleq \begin{cases} \Phi_{i \to j} + k & \text{if } i - j \in I, \\ 0 & \text{otherwise,} \end{cases} \tag{3.28}$$

takes its values in $\mathbb{N}$, and hence is a particle flow for the observable $\mu + k|I|$. ○

Remark 3.2. Recall that every finitely generated subgroup of $\mathbb{R}$ is isomorphic to $\mathbb{Z}^m$ for some $m \geq 0$. If an interaction-free energy $\mu : S^{\mathbb{L}} \to \mathbb{Z}^m$ is conserved by a cellular automaton F, each of its m components must be conserved independently. If we are able to find particle flows for each component, we can extend our interpretation for μ by assuming m different types of particles, which flow independently. ○

Let us call the assignment $g : S \to \mathbb{N}$, defining an interaction-free observable μ, a *particle assignment*. We say a CA F conserves g if it conserves the potential difference generated by μ. By a flow for g, we mean a flow for μ. Whether every conserved particle assignment has a particle flow is not known. However, the following theorem, due to Pivato, strongly suggests that such flows always exist. In the following two subsections, we will present constructions of particle flows for two special cases: for the one-dimensional CA (Fukś and Pivato) and for the two-dimensional CA with radius-$\frac{1}{2}$ neighborhood.

Theorem 3.2 ([72]). *A CA $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ with neighborhood N conserves a particle assignment $g : S \to \mathbb{N}$ if and only if*

$$\sum_{i \in A} g\left(x[i]\right) \leq \sum_{i \in N^{-1}(A)} g\left((Fx)[i]\right) \tag{3.29}$$

and

$$\sum_{i \in A} g\left((Fx)[i]\right) \leq \sum_{i \in N(A)} g\left(x[i]\right) \tag{3.30}$$

for every configuration x and every finite set $A \subseteq \mathbb{L}$.

Proof.
[⇒] Let Δ be the potential difference generated by g. Let $\diamond \in S$ be a state which minimizes g, and let $\diamondsuit$ be the $\diamond$-uniform configuration. Then $F\diamondsuit$ is $\diamond'$-uniform for some $\diamond' \in S$. It follows from Theorem 2.12 that $g(\diamond') = g(\diamond)$.

Let x be an arbitrary configuration and $A \subseteq \mathbb{L}$ a finite set of cells. Let $p \triangleq x|_{N(A)}$. We have

$$\begin{aligned}
\sum_{i \in N(A)} g\left(x[i]\right) &= \Delta(\diamondsuit, \zeta_p \diamondsuit) + |N(A)| \cdot g(\diamond) && (3.31)\\
&\geq \Delta(F\diamondsuit, F\zeta_p\diamondsuit) + |A| \cdot g(\diamond') && (3.32)\\
&= \sum_{i \in A} g\left((Fx)[i]\right) + \sum_{i \in N^{-1}(N(A)) \setminus A} \left[g((F\zeta_p\diamondsuit)[i]) - g(\diamond')\right] && (3.33)\\
&\geq \sum_{i \in A} g\left((Fx)[i]\right) \ . && (3.34)
\end{aligned}$$

Next, let $r \triangleq \diamondsuit|_A$ and $r' \triangleq (F\diamondsuit)|_{N^{-1}(A)}$. We have

$$\sum_{i\in A} g\left(x[i]\right) = \Delta(\zeta_r x, x) + |A| \cdot g(\diamond) \tag{3.35}$$

$$\leq \Delta(F\zeta_r x, Fx) + |N^{-1}(A)| \cdot g(\diamond') \tag{3.36}$$

$$= \Delta(\zeta_{r'} Fx, Fx) - \Delta(\zeta_{r'} Fx, F\zeta_r x) + |N^{-1}(A)| \cdot g(\diamond') \tag{3.37}$$

$$= \sum_{i\in N^{-1}(A)} g\left((Fx)[i]\right) - \sum_{i\in N^{-1}(A)} g\left((F\zeta_r x)[i]\right) \tag{3.38}$$

$$\leq \sum_{i\in N^{-1}(A)} g\left((Fx)[i]\right) \ . \tag{3.39}$$

[$\Leftarrow$] Let $\mu : S^{\mathbb{L}} \to \mathbb{N}$ be the observable defined by g. By Theorem 2.12, it is enough to show that $\overline{\mu}(Fx) = \overline{\mu}(x)$ for every configuration x.

Let x be a configuration, and $n \geq 0$. Recall that $I_n \triangleq [-n, n]^d$ is the central hyper-cube of size $(2n+1)^d$ in $\mathbb{L}$. Let $r \geq 0$ be such that $N \subseteq I_r$. Then for $n \geq r$ we have

$$N^{-1}(I_{n-r}) \subseteq I_n \ , \qquad \text{and} \qquad N(I_n) \subseteq I_{n+r} \ . \tag{3.40}$$

Substituting I_{n-r} and I_n for A in (3.29) and (3.30), we get

$$\frac{\sum_{i\in I_{n-r}} g\left(x[i]\right)}{|I_{n-r}|} \cdot \frac{|I_{n-r}|}{|I_n|} \leq \frac{\sum_{i\in I_n} g\left((Fx)[i]\right)}{|I_n|} \leq \frac{\sum_{i\in I_{n+r}} g\left(x[i]\right)}{|I_{n+r}|} \cdot \frac{|I_{n+r}|}{|I_n|} \ . \tag{3.41}$$

Letting $n \to \infty$ we obtain

$$\overline{\mu}(x) \leq \overline{\mu}(Fx) \leq \overline{\mu}(x) \ , \tag{3.42}$$

which implies $\overline{\mu}(Fx) = \overline{\mu}(x)$. □

Let $g : S \to \mathbb{N}$ be a particle assignment and N a finite neighborhood. Given two configurations x and y, let us construct a bipartite graph $G_N[g; x, y] = (U, V, E)$ as follows. For every particle in x, the graph has a vertex in U. Similarly, for every particle in y, there is a vertex in V. A particle $u \in U$ coming from cell i is connected by an edge to a particle $v \in V$ coming from cell j if and only if i is a neighbor of j; that is, if and only if $i - j \in N$.

A perfect matching in graph $G_N[g; x, y]$ is a way of identifying particles in x with particles in y in such a way that the position of each particle in x is a neighbor of its position in y. A necessary and sufficient condition for a (possibly infinite, but locally finite[2]) bipartite graph to have a perfect matching is given by Hall's Marriage Theorem (see e.g. [81]): a bipartite

[2] A graph is *locally finite* if every vertex has a finite degree.

graph $G = (U, V, E)$ has a matching that covers U if and only if for every finite set $A \subseteq U$, the number of vertices in V that are adjacent to A is at least $|A|$. If G has a matching that covers U and a matching that covers V, G has a perfect matching.

It follows from Theorem 3.2 that if a CA with neighborhood N conserves g, then for every configuration x, the graph $G_N[g; x, Fx]$ must have a perfect matching.

Corollary 3.3. *A CA $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ with neighborhood N conserves a particle assignment $g : S \to \mathbb{N}$ if and only if for every configuration x, the graph $G_N[g; x, Fx]$ has a perfect matching.*

3.2.1 One Dimension

For one-dimensional CA, it is known that every conserved particle assignment has a compatible particle flow. Such a particle flow is not unique. However, there are simple and natural criteria to single out one such particle flow.

Let $F : S^{\mathbb{Z}} \to S^{\mathbb{Z}}$ be a one-dimensional CA and $g : S \to \mathbb{N}$ a particle assignment that is conserved by F. Without loss of generality, we assume that F has neighborhood $N \triangleq [-r, r]$ for $r \geq 0$. Let $\diamond \in S$ be a state which minimizes g. Without loss of generality, we can assume $g(\diamond) = 0$. Let $\diamondsuit$ be the $\diamond$-uniform configuration and $\diamond' \in S$ the state of the cells in $F\diamondsuit$. By Theorem 2.12, we know that $g(\diamond') = g(\diamond) = 0$.

Let x be a $\diamond$-finite configuration. There are a finite number of particles on x, and the same number on Fx. If we assume that F preserves the order of the particles, we can uniquely[3] identify the particles on x with those on Fx. As we shall see, this identification can, in fact, be done locally, via a particle flow.

Using the above assumption, we can calculate the number of particles $\Phi_{i\to j}(x)$ which are moving from each cell i to any other cell j. Namely, for every $\diamond$-finite configuration x, and every $k \in \mathbb{Z}$, let us define

$$\ell_k(x) \triangleq \sum_{i \leq k} g\left(x[i]\right) \ . \tag{3.43}$$

It is easy to verify that

$$\Phi_{i\to j}(x) = \begin{cases} \ell_i(x) - \ell_{j-1}(Fx) & \text{if } \ell_{i-1}(x) \leq \ell_{j-1}(Fx) < \ell_i(x) \leq \ell_j(Fx), \\ g\left(x[i]\right) & \text{if } \ell_{j-1}(Fx) < \ell_{i-1}(x) \leq \ell_i(x) \leq \ell_j(Fx), \\ \ell_j(Fx) - \ell_{i-1}(x) & \text{if } \ell_{j-1}(Fx) \leq \ell_{i-1}(x) < \ell_j(Fx) \leq \ell_i(x), \\ g\left((Fx)[j]\right) & \text{if } \ell_{i-1}(x) < \ell_{j-1}(Fx) \leq \ell_j(Fx) \leq \ell_i(x), \\ 0 & \text{otherwise.} \end{cases} \tag{3.44}$$

[3] provided that we do not distinguish between two particles that are on the same cell.

Let $a, b \in \mathbb{Z}$. If $a \leq b$, let $x' \triangleq x|_{>a-r} \vee \diamondsuit|_{\leq a-r}$. Since F conserves g, we have

$$\ell_a(x) - \ell_b(Fx) = \sum_{i \leq a} g\left(x[i]\right) - \sum_{i \leq b} g\left((Fx)[i]\right) \tag{3.45}$$

$$= \sum_{i > b} g\left((Fx)[i]\right) - \sum_{i > a} g\left(x[i]\right) \tag{3.46}$$

$$= \sum_{i > b} g\left((Fx')[i]\right) - \sum_{i > a} g\left(x'[i]\right) \tag{3.47}$$

$$= \sum_{i \leq a} g\left(x'[i]\right) - \sum_{i \leq b} g\left((Fx')[i]\right) \ , \tag{3.48}$$

which depends only on the value of x on $(a - r, b + r]$. Similarly, if $b < a$, let $x'' \triangleq x|_{<a+r} \vee \diamondsuit|_{\geq a+r}$. Again, since F conserves g, we can write

$$\ell_a(x) - \ell_b(Fx) = \sum_{i \leq a} g\left(x[i]\right) - \sum_{i \leq b} g\left((Fx)[i]\right) \tag{3.49}$$

$$= \sum_{i \leq a} g\left(x''[i]\right) - \sum_{i \leq b} g\left((Fx'')[i]\right) \tag{3.50}$$

$$= \sum_{i > b} g\left((Fx'')[i]\right) - \sum_{i > a} g\left(x''[i]\right) \ , \tag{3.51}$$

which depends only on the value of x on $[b - r, a + r)$. So in either case, we obtain that $\ell_a(x) - \ell_b(Fx)$ is a local observable. Therefore, for every $i, j \in \mathbb{Z}$, the mapping $\Phi_{i \to j}$ is a local observable.

Next, it follows from Theorem 3.2 that whenever $i < j - r$, we have $\ell_i(x) \leq \ell_{j-1}(Fx)$, and hence $\Phi_{i \to j}(x) = 0$. Similarly, whenever $i > j + r$, we have $\ell_j(Fx) \leq \ell_{i-1}(x)$, and again $\Phi_{i \to j}(x) = 0$. Therefore, $\Phi_{i \to j}(x) = 0$, unless $i - j \in I \triangleq [-r, r]$.

Finally, Φ clearly takes its values in $\mathbb{N}$. Furthermore, for every $a \in \mathbb{L}$ we have $\Phi_{a+i \to a+j}(x) = \Phi_{i \to j}(\sigma^a x)$.

Note that $\Phi_{i \to j}$ is defined only on $\diamond$-finite configurations. However, since $\diamond$-finite configurations are dense in $S^{\mathbb{Z}}$, $\Phi_{i \to j}$ can be uniquely extended to a local observable on $S^{\mathbb{Z}}$. By the continuity of Φ, the above properties automatically extend to all configurations in $S^{\mathbb{Z}}$.

We conclude that Φ is a particle flow. Moreover, by construction, the continuity equations

$$g\left(x[a]\right) = \sum_{j \in I^{-1}(a)} \Phi_{a \to j}(x) \tag{3.52}$$

and

$$\sum_{i \in I(a)} \Phi_{i \to a}(x) = g\left((Fx)[a]\right) \tag{3.53}$$

hold for every $\diamond$-finite configuration x and every cell $a \in \mathbb{Z}$. On the other hand, the set of configurations for which the above continuity equations hold is obviously closed. Therefore, the equations hold for every configuration in $S^{\mathbb{Z}}$. That is, Φ is compatible with g and F.

Theorem 3.4 ([29, 72, 66]). *Let $F : S^{\mathbb{Z}} \to S^{\mathbb{Z}}$ be a one-dimensional cellular automaton and $g : S \to \mathbb{N}$ a particle assignment conserved by F. There is a particle flow compatible with g and F. Furthermore, provided $g(\diamond) = 0$ for some state $\diamond \in S$, there is exactly one such flow which preserves the order of the particles.*

Remark 3.3. There are very many particle flows compatible with a one-dimensional CA and a conserved particle assignment. The above construction yields the flow which preserves the order of the particles. Alternatively, we could pick this particular particle flow via a *variational principle* (as is customary in physics). Namely, the above-constructed flow is that which minimizes the total distance traveled by particles on each $\diamond$-finite configuration. ○

3.2.2 Two Dimensions

Let $F : S^{\mathbb{Z}^2} \to S^{\mathbb{Z}^2}$ be a two-dimensional CA with neighborhood

$$N = \{(0,0), (0,1), (1,1), (1,0)\} \tag{3.54}$$

and local rule $f : S^N \to S$. The neighbors $(0,0)$, $(0,1)$, $(1,1)$ and $(1,0)$ are interpreted, respectively, as the down-left (`dl`), up-left (`ul`), up-right (`ur`) and down-right (`dr`) neighbors. Such a neighborhood is often called a *radius-*$\frac{1}{2}$ neighborhood.

To simplify our exposition, let us distinguish between the *neighbors* of a cell i and the cells that are *adjacent* to it. The former are the cells $i + \texttt{dl}$, $i + \texttt{ul}$, $i + \texttt{ur}$ and $i + \texttt{dr}$ at the previous step, while the latter are the cells $i+\texttt{r}$, $i+\texttt{u}$, $i+\texttt{l}$ and $i+\texttt{d}$ at the current time step, where $\texttt{r} \triangleq (1,0)$, $\texttt{u} \triangleq (0,1)$, $\texttt{l} \triangleq (-1,0)$ and $\texttt{d} \triangleq (0,-1)$.

Let $g : S \to \mathbb{N}$ be a particle assignment which is conserved by F. As before, without loss of generality we can assume that $\mu(\diamond) = 0$ for a state $\diamond \in S$ which we call *blank*. For every state $x \in S$, we define the *free* flows going out of x by looking at the following configurations:

$$\begin{array}{ccc} \diamond & \diamond & \diamond \\ \diamond & x & \diamond \\ \diamond & \diamond & \diamond \end{array} \quad \xrightarrow{F} \quad \begin{array}{cc} x_2 & x_3 \\ x_1 & x_4 \end{array} . \tag{3.55}$$

That is,

$$\varphi_{\searrow}(x) \triangleq g(f(\begin{smallmatrix} x & \diamond \\ \diamond & \diamond \end{smallmatrix})) \,, \qquad \varphi_{\swarrow}(x) \triangleq g(f(\begin{smallmatrix} \diamond & x \\ \diamond & \diamond \end{smallmatrix})) \,, \tag{3.56}$$

$$\varphi_{\nearrow}(x) \triangleq g(f(\begin{smallmatrix} \diamond & \diamond \\ x & \diamond \end{smallmatrix})) \,, \qquad \varphi_{\nwarrow}(x) \triangleq g(f(\begin{smallmatrix} \diamond & \diamond \\ \diamond & x \end{smallmatrix})) \,. \tag{3.57}$$

Since F conserves g, we have

$$\varphi_{\swarrow}(x) + \varphi_{\nwarrow}(x) + \varphi_{\nearrow}(x) + \varphi_{\searrow}(x) = g(x) \,. \tag{3.58}$$

When two states are adjacent, their out-going flows *interfere* and as a result we have a flow *deflection* from one cell toward another.

$$\begin{matrix} \diamond & \diamond & \diamond & \diamond \\ \diamond & x & y & \diamond \\ \diamond & \diamond & \diamond & \diamond \end{matrix} \xrightarrow{F} \begin{matrix} x_2 & a & y_3 \\ x_1 & b & y_4 \end{matrix} . \tag{3.59}$$

Specifically, for every $x, y \in S$, define

$$\psi_{\uparrow}(x \;\; y) \triangleq \max\left\{0,\, g(f(\begin{smallmatrix} \diamond & \diamond \\ x & y \end{smallmatrix})) - \varphi_{\nearrow}(x) - \varphi_{\nwarrow}(y)\right\} \,, \tag{3.60}$$

$$\psi_{\downarrow}(x \;\; y) \triangleq \max\left\{0,\, g(f(\begin{smallmatrix} x & y \\ \diamond & \diamond \end{smallmatrix})) - \varphi_{\searrow}(x) - \varphi_{\swarrow}(y)\right\} \,. \tag{3.61}$$

Since F conserves g, we have

$$g(f(\begin{smallmatrix} \diamond & \diamond \\ x & y \end{smallmatrix})) = \varphi_{\nearrow}(x) + \varphi_{\nwarrow}(y) + \psi_{\uparrow}(x \;\; y) - \psi_{\downarrow}(x \;\; y) \,, \tag{3.62}$$

$$g(f(\begin{smallmatrix} x & y \\ \diamond & \diamond \end{smallmatrix})) = \varphi_{\searrow}(x) + \varphi_{\swarrow}(y) + \psi_{\downarrow}(x \;\; y) - \psi_{\uparrow}(x \;\; y) \,, \tag{3.63}$$

and either $\psi_{\downarrow}(x \;\; y)$ or $\psi_{\uparrow}(x \;\; y)$ is zero. The deflections $\psi_{\rightarrow}(\begin{smallmatrix} x \\ y \end{smallmatrix})$ and $\psi_{\leftarrow}(\begin{smallmatrix} x \\ y \end{smallmatrix})$ are defined similarly, and in the same way we have

$$g(f(\begin{smallmatrix} x & \diamond \\ y & \diamond \end{smallmatrix})) = \varphi_{\searrow}(x) + \varphi_{\nearrow}(y) + \psi_{\rightarrow}(\begin{smallmatrix} x \\ y \end{smallmatrix}) - \psi_{\leftarrow}(\begin{smallmatrix} x \\ y \end{smallmatrix}) \,, \tag{3.64}$$

$$g(f(\begin{smallmatrix} \diamond & x \\ \diamond & y \end{smallmatrix})) = \varphi_{\swarrow}(x) + \varphi_{\nwarrow}(y) + \psi_{\leftarrow}(\begin{smallmatrix} x \\ y \end{smallmatrix}) - \psi_{\rightarrow}(\begin{smallmatrix} x \\ y \end{smallmatrix}) \,, \tag{3.65}$$

and either $\psi_{\leftarrow}(\begin{smallmatrix} x \\ y \end{smallmatrix})$ or $\psi_{\rightarrow}(\begin{smallmatrix} x \\ y \end{smallmatrix})$ is zero. The deflections summarize all the interactions between the free flows:

Lemma 3.5. *For every $x, y, z, t \in S$ we have*

$$\begin{aligned} g(f(\begin{smallmatrix} y & z \\ x & t \end{smallmatrix})) = {} & \varphi_{\nearrow}(x) + \varphi_{\searrow}(y) + \varphi_{\swarrow}(z) + \varphi_{\nwarrow}(t) \\ & + \psi_{\rightarrow}(\begin{smallmatrix} y \\ x \end{smallmatrix}) + \psi_{\downarrow}(y \;\; z) + \psi_{\leftarrow}(\begin{smallmatrix} z \\ t \end{smallmatrix}) + \psi_{\uparrow}(x \;\; t) \\ & - \psi_{\leftarrow}(\begin{smallmatrix} y \\ x \end{smallmatrix}) - \psi_{\uparrow}(y \;\; z) - \psi_{\rightarrow}(\begin{smallmatrix} z \\ t \end{smallmatrix}) - \psi_{\downarrow}(x \;\; t) \,. \end{aligned} \tag{3.66}$$

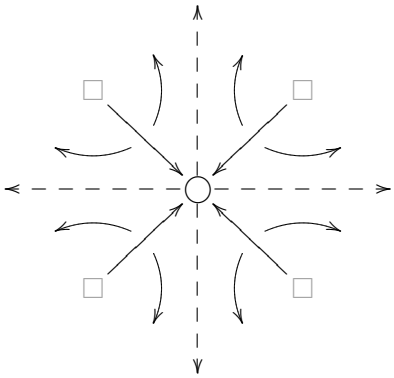
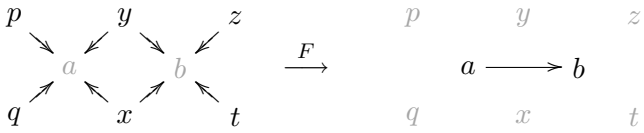


Figure 3.2: Correcting the flows.

We shall think of the free flows and the flow deflections as weighted arrows from one cell (in the space-time) to another. For example, in the consecutive configurations



, (3.67)

the free flow $\varphi_{\searrow}(p)$ is depicted by an arrow toward the cell with state a from its up-left neighbor in the previous time step, and so forth. Similarly, there is a deflection arrow from a to b with weight $\psi_{\rightarrow}\binom{y}{x} \geq 0$ and one in the opposite direction with weight $\psi_{\leftarrow}\binom{y}{x} \geq 0$, though at least one of their values is zero. For two consecutive configurations x and $y = Fx$, let us write $\Phi_{\nearrow}[i]$ for the free flow arrow with value $\varphi_{\nearrow}\,(x[i + \mathtt{dl}])$ from the cell $i + \mathtt{dl}$ (in x), to the cell i (in y), and so forth. Similarly, let $\Psi_{\uparrow}[i]$, $\Psi_{\rightarrow}[i]$, $\Psi_{\downarrow}[i]$ and $\Psi_{\leftarrow}[i]$ be the deflection arrows from i (in y) to the cells $i + \mathtt{u}$, $i + \mathtt{r}$, $i + \mathtt{d}$ and $i + \mathtt{l}$ (in y), respectively.

Deflections represent the deviation of g values from what is prescribed by the free flows. If we split each deflection $\psi_{\uparrow}$ (resp. $\psi_{\rightarrow}$, $\psi_{\downarrow}$, $\psi_{\leftarrow}$) into two parts $\psi_{\uparrow}$ and $\psi_{\uparrow}$ (resp. $\psi_{\rightharpoonup}$ and $\psi_{\rightharpoondown}$, $\psi_{\downharpoonright}$ and $\psi_{\downharpoonleft}$, $\psi_{\leftharpoondown}$ and $\psi_{\leftharpoonup}$) and use these parts to correct the free flows, we obtain a flow compatible with g and F. To be precise, at each cell i, the arrow $\Phi_{\nearrow}[i]$ is corrected to

$$\Phi'_{\nearrow}[i] \triangleq \Phi_{\nearrow}[i] - \Psi_{\downarrow}[i] + \Psi_{\uparrow}[i + \mathtt{d}] - \Psi_{\leftarrow}[i] + \Psi_{\rightarrow}[i + \mathtt{l}]\ , \tag{3.68}$$

and so forth (Figure 3.2). We require the splits $\psi_{\uparrow}, \psi_{\uparrow}, \ldots$ to be non-negative integers. In other respects the splitting can be arbitrary and may depend on

the local neighborhood pattern. The main challenge here is to do the splitting in such a way that the corrected flow has only non-negative integer values.

Let us say that a cell i on y is *balanced* if

a) $\Phi_{\searrow}[i] + \Phi_{\swarrow}[i] \geq \Psi_{\uparrow}[i]$ (and its rotations),

b) $\Phi_{\searrow}[i] + \Phi_{\swarrow}[i] + \Phi_{\nwarrow}[i] \geq \Psi_{\uparrow}[i] + \Psi_{\rightarrow}[i]$ (and its rotations), and

c) $\Phi_{\searrow}[i] + \Phi_{\swarrow}[i] + \Phi_{\nwarrow}[i] + \Phi_{\nearrow}[i] \geq \Psi_{\uparrow}[i] + \Psi_{\rightarrow}[i] + \Psi_{\downarrow}[i] + \Psi_{\leftarrow}[i]$.

Observation 3.6. For every $a, b, c \in S$ we have

a) $\varphi_{\searrow}(a) + \varphi_{\swarrow}(b) \geq \psi_{\uparrow}(\begin{smallmatrix} a & b \end{smallmatrix})$,

b) $\varphi_{\searrow}(a) + \varphi_{\swarrow}(b) + \varphi_{\nwarrow}(c) \geq \psi_{\uparrow}(\begin{smallmatrix} a & b \end{smallmatrix}) + \psi_{\rightarrow}(\begin{smallmatrix} b \\ c \end{smallmatrix})$.

Lemma 3.7. *If a cell is balanced, its out-going deflections can be split so that its corrected in-coming flows remain non-negative and integer.*

Proof. Let i be a balanced cell. Let us construct a bipartite graph $H = (X, Y, E)$ as follows. For each in-coming particle, put a vertex in X, and for each out-going particle, put a vertex in Y. Connect with an edge each particle associated with the in-coming free flow $\Phi_{\nearrow}[i]$ to each particle associated with the out-going deflections $\Psi_{\leftarrow}[i]$ and $\Psi_{\downarrow}[i]$, and so forth. The balancedness of i ensures that, for every subset $A \subseteq X$, the number of vertices in Y that are connected to A is at least $|A|$. Therefore, by Hall's Marriage Theorem (see e.g. [81]), H has a perfect matching $P \subseteq E$. Let $\Psi_{\leftarrow}[i]$ be the number of particles associated with $\Psi_{\leftarrow}[i]$ which are matched with particles associated with $\Phi_{\nearrow}[i]$, and similarly choose the other splits. □

Figure 3.3 shows the various deflection patterns that may occur around a cell. The other possibilities are all symmetrically identical to these five cases. According to Lemma 3.7, Observation 3.6 guarantees that, unless there is exactly one deflection directing toward a cell (i.e., the cases (1-4)), one can correct the in-coming free flows of that cell to satisfy its out-going deflections in such a way that the corrected flows remain non-negative. Let us call a cell *problematic* (represented by P) if the situation around it is as in case (5) (or its symmetrically identical variants). We call a cell *doubly problematic* (represented by $\tilde{\text{P}}$) if it is problematic, and if furthermore the endpoints of its out-going deflection arrows are also problematic (Figure 3.4). For two adjacent cells i and j, let us say j *follows* i if there is a deflection arrow from i to j.

Observation 3.8. If j follows i, i and j cannot both be doubly problematic at the same time.

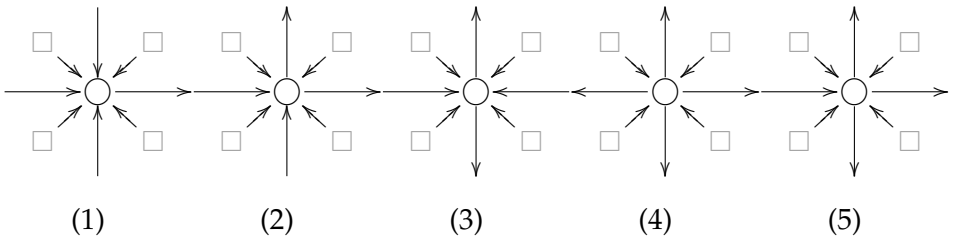


Figure 3.3: The deflection patterns that may occur around a cell.

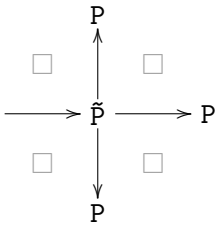


Figure 3.4: Doubly problematic cell.

Theorem 3.9 ([48]). *Let $F : S^{\mathbb{Z}^2} \to S^{\mathbb{Z}^2}$ be a two-dimensional radius-$\frac{1}{2}$ cellular automaton and $g : S \to \mathbb{N}$ a particle assignment conserved by F. There is a particle flow compatible with g and F.*

Proof. Let x and y be two consecutive configurations in $S^{\mathbb{Z}^2}$. Let us set the free flows as an initial approximation of the desired flow. That is, let $\Phi_d^{(0)} \triangleq \Phi_d$ ($d \in \{\nearrow, \searrow, \swarrow, \nwarrow\}$). We construct a particle flow for g by correcting this approximation in three steps. At each step a number of deflections are split and redistributed into the affected flows.

Step 1
SPLITTING. For every cell i around which the pattern of deflection arrows is in either of the cases (1-4) of Figure 3.3, we split the out-going deflections as suggested in Lemma 3.7. If the cell is doubly problematic, we leave the splitting of its out-going deflections for the next step. If the cell is problematic but not doubly problematic, we leave for the next step one of its out-going deflections leading to a non-problematic cell and split the other two, as described in Lemma 3.7.
CORRECTING. We use the already split deflections to correct the flows. Let $\Phi_d^{(1)}$ ($d \in \{\nearrow, \searrow, \swarrow, \nwarrow\}$) be the corrected flow arrows of this step.

Step 2
SPLITTING. Let i be a problematic cell. Notice that unless i follows a doubly problematic cell, its in-coming deflection has already been resolved in the previous step. In this case, i is no longer problematic, and we can split its out-going deflections as explained in Lemma 3.7. In particular, all out-going deflections of (formerly) doubly problematic cells are split in this step (Observation 3.8).
CORRECTING. We correct the flows using the newly split deflections. Let $\Phi_d^{(2)}$ ($d \in \{\nearrow, \searrow, \swarrow, \nwarrow\}$) be the corrected flow arrows of this step.

Step 3
SPLITTING. The only unresolved deflections are those originating from a problematic cell (such as i) that follows an initially doubly problematic cell. But the out-going deflections of the doubly problematic cells are already resolved. So i is no longer problematic. We split its unresolved out-going deflection using Lemma 3.7.
CORRECTING. We correct the flows using the newly split deflections. Let $\Phi_d^{(3)}$ ($d \in \{\nearrow, \searrow, \swarrow, \nwarrow\}$) be the corrected flow arrows of this step.

At this point, all the deflections are resolved. The corrected arrows $\Phi_d^{(3)}$ define a flow Φ by

$$\Phi_{i\to j} \triangleq \begin{cases} \Phi^{(3)}_{\nearrow}[j] & \text{if } i = j + \mathtt{dl}, \\ \Phi^{(3)}_{\searrow}[j] & \text{if } i = j + \mathtt{ul}, \\ \Phi^{(3)}_{\swarrow}[j] & \text{if } i = j + \mathtt{ur}, \\ \Phi^{(3)}_{\nwarrow}[j] & \text{if } i = j + \mathtt{dr}, \\ 0 & \text{otherwise}, \end{cases} \tag{3.69}$$

which satisfies the continuity equations. Also, by construction, the values of Φ are all non-negative integers. Therefore, Φ is a particle flow compatible with g and F. □

3.3 Interaction-type Flows

In this section, we take a different point of view to obtain a microscopic explanation of a conservation law when presented in terms of interaction potentials. Namely, we try to identify the contribution of a finite group of cells to the energy of another finite group of cells one step later, by tinkering around with the inclusion-exclusion principle as in Section 2.4.

Let $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ be a CA. For simplicity, in this section we assume that F has a quiescent state $\diamond \in S$. Denote the $\diamond$-uniform configuration by $\diamondsuit$.

Let Δ be a local potential difference which is conserved by F. By Corollary 2.4, this means that $\Delta(Fx) = \Delta(x)$ for every $\diamond$-finite configuration x. Let $\theta : S^{\#} \to \mathbb{R}$ be the canonical interaction potential (with respect to $\diamond$) generating Δ.

Let $\mathscr{K} \subseteq 2^{\mathbb{L}}$ denote the collection of finite subsets of $\mathbb{L}$. We are going to work with elements of $\mathbb{R}^{\mathscr{K}}$; that is, the mappings which assign real values to each finite set of cells. For every finite pattern $p : D \to S$, let us define $G(p) \in \mathbb{R}^{\mathscr{K}}$ as follows. For every finite $K \subseteq \mathbb{L}$, let $G(p)[K] \triangleq \theta\left((F\zeta_p\diamondsuit)|_K\right)$, that is the energy resulting from the interaction of the cells in K on the configuration $F\zeta_p\diamondsuit$. For every finite $p : D \to S$, define

$$H(p) \triangleq \sum_{q \preceq p} (-1)^{|p|-|q|} G(q) \in \mathbb{R}^{\mathscr{K}} \ . \tag{3.70}$$

By the Möbius Inversion Theorem (see e.g. [81]), or equivalently by the inclusion-exclusion principle, for every finite $p : D \to S$ we have

$$G(p) = \sum_{q \preceq p} H(q) \ . \tag{3.71}$$

For every configuration x and each two finite sets $A, B \subseteq \mathbb{L}$, let us define

$$\Phi_{A \to B}(x) \triangleq H(x|_A)[B] \ . \tag{3.72}$$

The following proposition shows that this can indeed be seen as the "flow" of energy from A to B in one iteration of F on x.

Proposition 3.10. *Let F, Δ, θ and Φ be as above. Let N be the neighborhood of F and M the neighborhood of Δ. We have*

i) $\Phi_{A \to B}(x) = 0$, *unless for all $i, j \in B$, we have $M^{-1}(i) \cap M^{-1}(j) \neq \varnothing$.*

ii) $\Phi_{A \to B}(x) = 0$, *unless $A \subseteq N(B)$.*

iii) $\Phi_{A \to B}(x) = 0$ *if $x[a] = \diamond$ for some $a \in A$.*

iv) For every $B \in \mathscr{K}$, we have

$$\sum_{A \in \mathscr{K}} \Phi_{A \to B}(x) = \theta\left((Fx)|_B\right) \ . \tag{3.73}$$

v) For every $A \in \mathscr{K}$, we have

$$\sum_{B \in \mathscr{K}} \Phi_{A \to B}(x) = \theta\left(x|_B\right) \ . \tag{3.74}$$

Proof.

i) Recall from the proof of Proposition 2.16, that for every finite pattern $p : D \to S$, $\theta(p) = 0$, unless $M^{-1}(i) \cap M^{-1}(j) \neq \varnothing$ for all $i, j \in D$.

Suppose that for $B \in \mathscr{K}$, there exist $i, j \in B$ with $M^{-1}(i) \cap M^{-1}(j) = \varnothing$. Then for each finite pattern p, we have $G(p)[B] = 0$. Hence for each finite pattern p, we also have $H(p)[B] = 0$.

ii) Suppose that $A \not\subseteq N(B)$. Let $a \in A \setminus N(B)$. We have

$$H(x|_A) = \sum_{\substack{C \subseteq A \\ C \ni a}} (-1)^{|A|-|C|} \left[G(x|_C) - G(x|_{C \smallsetminus a}) \right] \ . \tag{3.75}$$

But the state of the cell a does not affect the state of the cells in B one step later. Therefore, $G(x|_C)[B] = G(x|_{C \smallsetminus a})[B]$ for each $C \in \mathscr{K}$. Therefore, $H(x|_A)[B] = 0$.

iii) Suppose that $x[a] = \diamond$ for some $a \in A$. Then for every $C \ni a$ we have $\zeta_{x|_C} \diamondsuit = \zeta_{x|_{C \smallsetminus a}} \diamondsuit$. Therefore,

$$H(x|_A) = \sum_{\substack{C \subseteq A \\ C \ni a}} (-1)^{|A|-|C|} \left[G(x|_C) - G(x|_{C \smallsetminus a}) \right] = 0 \ . \tag{3.76}$$

iv) We have

$$\begin{aligned} \sum_{A \in \mathscr{K}} \Phi_{A \to B}(x) &= \sum_{A \subseteq N(B)} H(x|_A)[B] && (3.77) \\ &= G(x|_{N(B)})[B] && (3.78) \\ &= \theta \left((F \zeta_{x|_{N(B)}} \diamondsuit)|_B \right) && (3.79) \\ &= \theta \left((Fx)|_B \right) \ . && (3.80) \end{aligned}$$

v) We have

$$\begin{aligned} \sum_{B \in \mathscr{K}} \Phi_{A \to B}(x) &= \sum_{B \in \mathscr{K}} H(x|_A)[B] && (3.81) \\ &= \sum_{B \in \mathscr{K}} \sum_{C \subseteq A} (-1)^{|A|-|C|} G(x|_C)[B] && (3.82) \\ &= \sum_{C \subseteq A} (-1)^{|A|-|C|} \sum_{B \subseteq \mathscr{K}} G(C)[B] && (3.83) \\ &= \sum_{C \subseteq A} (-1)^{|A|-|C|} \sum_{B \subseteq \mathscr{K}} \theta \left((F \zeta_{x|_C} \diamondsuit)|_B \right) && (3.84) \end{aligned}$$

$$= \sum_{C \subseteq A} (-1)^{|A|-|C|} \Delta \left(F\zeta_{x|_C} \diamondsuit \right) \tag{3.85}$$

$$= \sum_{C \subseteq A} (-1)^{|A|-|C|} \Delta \left(\zeta_{x|_C} \diamondsuit \right) \tag{3.86}$$

$$= \theta(x|_A) \ , \tag{3.87}$$

where the last equality follows from the construction of θ in the proof of Proposition 2.16 (i.e., by the Möbius Inversion Theorem). □

CHAPTER 4

The Hierarchy of Conservation Laws

RECALL from Chapter 2, that for every cellular automaton F, the collection $\mathscr{D}_F[M]$ of local potential differences with neighborhood M that are conserved by F form a finite dimensional linear space, which can effectively be found. If $M' \supseteq M$ is a larger neighborhood, the space $\mathscr{D}_F[M']$ contains $\mathscr{D}_F[M]$ as a subspace. Therefore, we have a hierarchy of linear spaces whose structure we may want to understand. In particular, we may wonder if for a large enough neighborhood M, all the conservation laws of F are covered in $\mathscr{D}_F[M]$ (i.e., if $\mathscr{D}_F = \mathscr{D}_F[M]$). Or we may ask whether F has any non-trivial conservation law at all (i.e., whether $\mathscr{D}_F$ is a non-trivial space). In this chapter, we address such questions.

More generally, we study the structure of the hierarchy of conservation laws for a CA. For this, it seems appropriate to consider a more general class of conservation laws in which the energy values are from an arbitrary commutative group (or semigroup). A remarkable (though easily recognized) fact is that for each CA, among all conservation laws with a given range of interaction, there is one which is the most general: it extracts whatever information about the CA that can be expressed in terms of conservation laws with that range. Any other conservation law with that range can be derived from the most general one by applying an algebraic homomorphism. Therefore, our hierarchy can be seen as a hierarchy of more and more general conservation laws.

We provide an example that the group-valued conservation laws give strictly more information than the real-valued ones, and an example in which the semigroup-valued conservation laws are strictly more general than the group-valued ones. Needless to say, the semigroup-valued conservation laws can be quite expressive. Nevertheless, we prove that for one-dimensional CA, the most general conservation law of each range, as well as a finite presentation of the corresponding semigroup, can effectively

be constructed. This is a good news, because the Word Problem for commutative semigroups is also decidable (see e.g. [8]). Therefore the whole theory, in the one-dimensional case, is algorithmically effective. For example, we can effectively determine whether two (finite) configurations have the same total energy, or if a given CA conserves a given energy. In higher dimensions, however, no such construction for the most general semigroup-valued conservation laws is possible.

We also consider the interconnection between the hierarchy of conservation laws and the dynamical behavior of the CA. We identify some restrictions that the existence of conservation laws imposes on the dynamics of the CA.

4.1 Group-valued Conservation Laws

In this section, we consider the broader class of conservation laws, in which the energy values are chosen from a commutative group. Let $\mathbb{G}$ be a commutative group. A $\mathbb{G}$-valued potential difference is defined in the same way as a real-valued potential difference, except that it takes its values from $\mathbb{G}$. Also, similar to the real-valued case, a $\mathbb{G}$-valued local potential difference can be generated either by a local observable (Proposition 2.1) or by a $\mathbb{G}$-valued interaction potential (Proposition 2.16). Likewise, conservation laws are defined in the same way. However, in this setup, the notion of average energy per cell is no longer meaningful.

Example 4.1 (XOR)**.** Consider the one-dimensional XOR CA F, which has state set $S \triangleq \{0, 1\}$, neighborhood $N \triangleq \{-1, 0, 1\}$, and local rule $f(a, b, c) = a + b + c \pmod 2$. Figure 4.1 shows a typical snapshot. The time axis in the figure goes downward. A well-known property of the XOR CA (and in general, of every linear CA) is its replicating behavior. Specifically, every finite pattern, after a finite number of steps, is replicated into three copies with large 0 blocks in between. (Figure 4.1 depicts an example. This fact is easy to verify using generating functions; see e.g. [75].) This implies that F cannot have any non-trivial real-valued conservation law. On the other hand, F preserves the parity of the configurations. Let $\mathbb{G} \triangleq \mathbb{Z}_2$ be the binary cyclic group, and consider the $\mathbb{G}$-valued observable $\mu : S^{\mathbb{Z}} \to \mathbb{Z}_2$ defined by $\mu(x) \triangleq x[0]$. The potential difference Δ generated by μ compares the parity of the number of 1's in two asymptotic configurations, and is conserved by F. ○

Let $\mathbb{G}$ be a commutative group and Δ a $\mathbb{G}$-valued local potential difference on $S^{\mathbb{L}}$. By the *realizable* subgroup of $\mathbb{G}$ we mean the subgroup

$$\breve{\mathbb{G}} \triangleq \mathbb{G}\langle \Delta(x, y) : x \text{ and } y \text{ asymptotic} \rangle \tag{4.1}$$

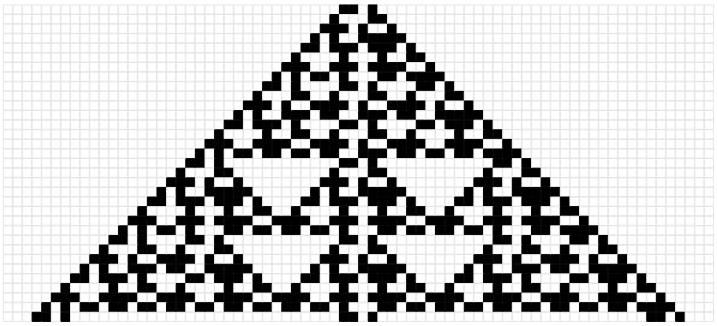


Figure 4.1: A space-time snapshot from the CA in Example 4.1.

generated by the range of Δ. Two local potential differences $\Delta_1 : S^{\mathbb{L}} \times S^{\mathbb{L}} \to \mathbb{G}_1$ and $\Delta_2 : S^{\mathbb{L}} \times S^{\mathbb{L}} \to \mathbb{G}_2$ are considered to be *equivalent*, written $\Delta_1 \equiv \Delta_2$, if there is a group isomorphism $\iota : \breve{\mathbb{G}}_1 \to \breve{\mathbb{G}}_2$ such that $\Delta_2 = \iota \circ \Delta_1$. We say that Δ_1 is *at least as general* as Δ_2, written $\Delta_2 \sqsubseteq \Delta_1$, if there is a group homomorphism $h : \breve{\mathbb{G}}_1 \to \breve{\mathbb{G}}_2$ such that $\Delta_2 = h \circ \Delta_1$. This defines a partial ordering (up to equivalence) on the collection of group-valued local potential differences on $S^{\mathbb{L}}$. The *join* of Δ_1 and Δ_2 is the local potential difference $\Delta_1 \vee \Delta_2 : S^{\mathbb{L}} \times S^{\mathbb{L}} \to \mathbb{G}_1 \times \mathbb{G}_2$, where $(\Delta_1 \vee \Delta_2)(x, y) \triangleq (\Delta_1(x, y), \Delta_2(x, y))$ whenever x and y are asymptotic. It is the least general potential difference which is at least as general as Δ_1 and Δ_2. A local potential difference $\Delta : S^{\mathbb{L}} \times S^{\mathbb{L}} \to \mathbb{G}$ is *trivial* if the realizable subgroup $\breve{\mathbb{G}}$ is trivial. If a cellular automaton $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ conserves a local potential difference Δ, it also conserves every local potential difference $\Delta' \sqsubseteq \Delta$ that is less general than Δ. If F conserves two local potential differences Δ_1 and Δ_2, it also conserves $\Delta_1 \vee \Delta_2$. The trivial local potential difference on $S^{\mathbb{L}}$ is conserved by every cellular automaton.

Let Δ be a $\mathbb{G}$-valued local potential difference on $S^{\mathbb{L}}$. Notice that either of Propositions 2.1 or 2.16 implies that the realizable subgroup $\breve{\mathbb{G}}$ is finitely generated. In fact, if $\theta : S^{\#} \to \mathbb{G}$ is the canonical interaction potential (with any choice of the blank state) generating Δ, Equation (2.103) implies that $\breve{\mathbb{G}}$ is exactly the subgroup generated by the values of θ.

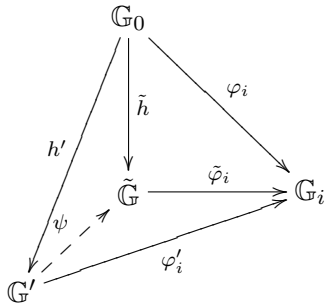
An interesting observation is that any collection of group-valued local potential differences with bounded "range of interaction" has a least upper-bound with respect to $\sqsubseteq$ that is itself a local potential difference. In particular, we can merge any collection of conservation laws with bounded range of interaction to obtain a single conservation law that embodies all of them. Let $\diamond \in S$ be a fixed state which we will call blank.

Proposition 4.1. *Let $\{\Delta_i\}_{i \in I}$ be a collection of local potential differences on $S^{\mathbb{L}}$. For every $i \in I$, let θ_i be the canonical interaction potential generating Δ_i.*

If $\mathcal{A} \triangleq \bigcup_{i\in I} \mathrm{supp}(\theta_i)$ is finite, there is a unique (up to equivalence) least general local potential difference $\bigvee_{i\in I} \Delta_i$ that is at least as general as each Δ_i. It is generated by a canonical interaction potential $\tilde{\theta}$ with $\mathrm{supp}(\tilde{\theta}) = \mathcal{A}$. A cellular automaton F conserves $\bigvee_{i\in I} \Delta_i$ if and only if it conserves every Δ_i.

Proof. For each $i \in I$, let Δ_i take its values from a group $\mathbb{G}_i$. Let $\breve{\mathbb{G}}_i$ be the realizable subgroup of $\mathbb{G}_i$.

Let $\mathbb{G}_0$ be the free commutative group generated by $S^\#$. For every $i \in I$, let us extend $\theta_i : S^\# \to \breve{\mathbb{G}}_i$ to a group homomorphism $\varphi_i : \mathbb{G}_0 \to \breve{\mathbb{G}}_i$. Denote by $\sim_i$ the congruence on $\mathbb{G}_0$ that is induced by φ_i. Then $\sim \triangleq \bigcap_{i\in I} \sim_i$ is the least discriminating congruence on $\mathbb{G}_0$ that is more discriminating than each $\sim_i$. Let $\tilde{\mathbb{G}} \triangleq \mathbb{G}_0/\!\sim$, and denote by $\tilde{h} : \mathbb{G}_0 \to \tilde{\mathbb{G}}$ the corresponding natural homomorphism. For each $i \in I$, there is a unique homomorphism $\tilde{\varphi}_i : \tilde{\mathbb{G}} \to \breve{\mathbb{G}}_i$ such that $\varphi_i = \tilde{\varphi}_i \circ \tilde{h}$. Furthermore, if $\mathbb{G}'$ is any other factor of $\mathbb{G}_0$ and $h' : \mathbb{G}_0 \to \mathbb{G}'$ and $\varphi'_i : \mathbb{G}' \to \breve{\mathbb{G}}_i$ are homomorphisms with $\varphi_i = \varphi'_i \circ h'$, there is another homomorphism $\psi : \mathbb{G}' \to \tilde{\mathbb{G}}$ such that $\tilde{h} = \psi \circ h'$ and $\varphi'_i = \tilde{\varphi}_i \circ \psi$. These are summarized in the following commuting diagram:



(4.2)

Let us define $\tilde{\theta} : S^\# \to \tilde{\mathbb{G}}$ by $\tilde{\theta}(p) \triangleq \tilde{h}(p)$. By assumption, whenever $p \in S^\# \setminus \mathcal{A}$, we have $\theta_i(p) = 0$ for each $i \in I$. Therefore, for each $i \in I$ we have $\varphi_i(p) = 0$ and $p \sim_i 0$. This implies that $p \sim 0$ and $\tilde{\theta}(p) = \tilde{h}(p) = 0$. Hence, $\tilde{\theta}$ is an interaction potential. Let $\tilde{\Delta}$ be the potential difference generated by $\tilde{\theta}$. Since the elements of $\mathcal{A}$ are all active patterns, $\tilde{\theta}$ is the canonical interaction potential generating $\tilde{\Delta}$.

For each $i \in I$ and $p \in \mathcal{A}$ we have

$$\theta_i(p) = \varphi_i(p) = \tilde{\varphi}_i \circ \tilde{h}(p) = \tilde{\varphi}_i \circ \tilde{\theta}(p) \ . \tag{4.3}$$

Therefore, $\Delta_i = \tilde{\varphi}_i \circ \tilde{\Delta}$, which means that $\Delta_i \sqsubseteq \tilde{\Delta}$.

On the other hand, let Δ' be any other local potential difference such that $\Delta_i \sqsubseteq \Delta'$ for each $i \in I$. Let $\theta' : S^\# \to \mathbb{G}'$ be the canonical interaction potential generating Δ', and let $\breve{\mathbb{G}}'$ be the realizable subgroup of $\mathbb{G}'$. Let $h' : \mathbb{G}_0 \to \breve{\mathbb{G}}'$ be the extension of θ' to a group homomorphism. For each $i \in I$, there is a group homomorphism $\varphi'_i : \breve{\mathbb{G}}' \to \mathbb{G}_i$ so that $\varphi'_i \circ \Delta' = \Delta_i$, or

equivalently $\varphi_i' \circ \theta' = \theta_i$. Therefore, $\varphi_i' \circ h' = \varphi_i$. Now, the above universal property of $\tilde{\mathbb{G}}$ ensures that there exists a homomorphism $\psi : \breve{\mathbb{G}}' \to \tilde{\mathbb{G}}$ such that $\tilde{h} = \psi \circ h'$. Therefore, $\tilde{\theta} = \psi \circ \theta'$, or equivalently, $\tilde{\Delta} = \psi \circ \Delta'$. Hence, $\tilde{\Delta} \sqsubseteq \Delta'$.

We conclude that $\bigvee_{i \in I} \Delta_i \triangleq \tilde{\Delta}$ is the least general local potential difference that is at least as general as each Δ_i. Any other potential difference with the same property is as general as $\tilde{\Delta}$, and hence equivalent with it.

Next, let $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ be a cellular automaton. If F conserves $\tilde{\Delta}$, it also conserves each Δ_i, because $\Delta_i \sqsubseteq \tilde{\Delta}$. Conversely, suppose that F conserves each Δ_i.

Let $\theta_0^{\mathcal{A}} : S^{\#} \to \mathbb{G}_0$ be the *formal* interaction potential defined by

$$\theta_0^{\mathcal{A}}(p) \triangleq \begin{cases} p & \text{if } p \in \mathcal{A}, \\ 0 & \text{otherwise.} \end{cases} \tag{4.4}$$

Let $\Delta_0^{\mathcal{A}}$ be the potential difference generated by $\theta_0^{\mathcal{A}}$. Clearly, $\theta_i = \varphi_i \circ \theta_0^{\mathcal{A}}$ (for each $i \in I$) and $\tilde{\theta} = \tilde{h} \circ \theta_0^{\mathcal{A}}$. Therefore, $\Delta_i = \varphi_i \circ \Delta_0^{\mathcal{A}}$ (for each $i \in I$), and $\tilde{\Delta} = \tilde{h} \circ \Delta_0^{\mathcal{A}}$.

Let x and y be two asymptotic configurations. For each $i \in I$, we have $\Delta_i(Fx, Fy) = \Delta_i(x, y)$, which means that $\Delta_0^{\mathcal{A}}(Fx, Fy) \sim_i \Delta_0^{\mathcal{A}}(x, y)$. So, $\Delta_0^{\mathcal{A}}(Fx, Fy) \sim \Delta_0^{\mathcal{A}}(x, y)$, which implies $\tilde{\Delta}(Fx, Fy) = \tilde{\Delta}(x, y)$. Therefore, F also conserves $\tilde{\Delta}$. □

The previous proposition implies that for every CA, there is no more than a finite amount of information in conservation laws with a certain range of interaction. In fact, using Theorem 2.2, we can algorithmically construct the most general of such conservation laws.

Let $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ be a CA and $\mathcal{A} \subseteq S^{\#}$ a finite set of active patterns. As before, let $\mathbb{G}_0$ be the free commutative group generated by $S^{\#}$, and define the formal interaction potential $\theta_0^{\mathcal{A}} : S^{\#} \to \mathbb{G}_0$ by

$$\theta_0^{\mathcal{A}}(p) \triangleq \begin{cases} p & \text{if } p \in \mathcal{A}, \\ 0 & \text{otherwise.} \end{cases} \tag{4.5}$$

Let $\Delta_0^{\mathcal{A}}$ be the potential difference generated by $\theta_0^{\mathcal{A}}$. The realizable subgroup of $\mathbb{G}_0$ is the free commutative group $\mathbb{G}_0^{\mathcal{A}}$ generated by $\mathcal{A}$. Let $\mathbb{G}_F^{\mathcal{A}}$ be the commutative group generated by $\mathcal{A}$ with relations

$$\Delta_0^{\mathcal{A}}(Fx, Fy) \sim \Delta_0^{\mathcal{A}}(x, y) \tag{4.6}$$

for all asymptotic x and y. This is the freest factor of $\mathbb{G}_0^{\mathcal{A}}$ that equalizes $\Delta_0^{\mathcal{A}}(x, y)$ and $\Delta_0^{\mathcal{A}}(Fx, Fy)$ for each asymptotic x and y. Let $h_F^{\mathcal{A}} : \mathbb{G}_0^{\mathcal{A}} \to \mathbb{G}_F^{\mathcal{A}}$

be the corresponding natural homomorphism, and define

$$\Delta_F^{\mathcal{A}} \triangleq h_F^{\mathcal{A}} \circ \Delta_0^{\mathcal{A}} , \tag{4.7}$$

$$\theta_F^{\mathcal{A}} \triangleq h_F^{\mathcal{A}} \circ \theta_0^{\mathcal{A}} . \tag{4.8}$$

It is easy to verify that $\Delta_F^{\mathcal{A}}$ is the most general potential difference conserved by F that is generated by a canonical interaction potential θ with $\mathrm{supp}(\theta) \subseteq \mathcal{A}$.

However, following the argument of Theorem 2.2, we see that $\mathbb{G}_F^{\mathcal{A}}$ is equivalently generated with relations

$$\Delta_0^{\mathcal{A}}(Fx, Fy) \sim \Delta_0^{\mathcal{A}}(x, y) \tag{4.9}$$

whenever x and y differ on exactly one cell. There are finitely many such relations, which we can effectively find (see the comments after the proof of Theorem 2.2). In conclusion, we can algorithmically construct a finite presentation of the group $\mathbb{G}_F^{\mathcal{A}}$.

Proposition 4.2 ([27])**.** *Let $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ be a CA and $\mathcal{A} \subseteq S^{\#}$ a finite set of patterns. There is an algorithm to identify the most general conservation law for F whose canonical interaction potential associates non-zero values only to the elements of $\mathcal{A}$. In particular, we can construct the canonical interaction potential of this conservation law, as well as a finite presentation of the corresponding group.*

4.2 Semigroup-valued Conservation Laws

Let us extend our framework even further and allow energy values to be chosen from a commutative monoid. There is no well-defined concept of semigroup-valued potential difference. We should therefore use a different approach to define conservation laws. For simplicity, in this section we restrict ourselves to those CA which have a quiescent state. We specify energies using observables or interaction potentials, and define conservation laws using the characterization given in Corollary 2.4.

Example 4.2 (Spreading 1's)**.** Let F be the one-dimensional CA with state set $S \triangleq \{0, 1\}$, neighborhood $N \triangleq \{-1, 0, 1\}$, and local rule $f(a, b, c) = a \vee b \vee c$. See Figure 4.2 for a typical snapshot. It is easy to see that every group-valued conservation law for F is trivial. Notice that every non-quiescent 0-finite configuration eventually turns into a single ever-growing block of ones. In contrast, F has a non-trivial semigroup-valued conservation law. Let $\Phi = \{0, 1\}$ be the commutative semigroup with binary operation $a + b \triangleq a \vee b$. Consider the observable $\mu : S^{\mathbb{L}} \to \Phi$ defined by $\mu(x) \triangleq x[0]$, and the energy it specifies. The 0-uniform configuration has total energy 0, while every other 0-finite configuration has total energy 1. ○

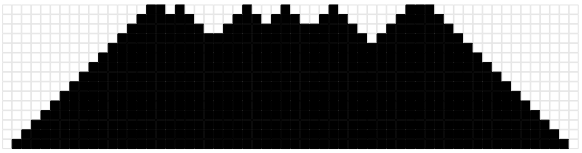


Figure 4.2: A space-time snapshot from the CA in Example 4.2.

Let Φ be an arbitrary commutative monoid. We denote its binary operation by $+$ and its identity element by 0. Let us fix a state $\diamond \in S$ and denote the $\diamond$-finite configuration with $\diamondsuit$. We restrict ourselves to local observables $\mu : S^{\mathbb{L}} \to \Phi$ with $\mu(\diamondsuit) = 0$. The *potential* generated by μ is the mapping $\Delta : \mathcal{C}_\diamond[S] \to \Phi$ defined by

$$\Delta(x) \triangleq \sum_{i \in \mathbb{L}} \mu\left(\sigma^i x\right) \ , \tag{4.10}$$

which measures the *total energy* of $\diamond$-finite configurations. This is well-defined, because when x is a $\diamond$-finite configuration, $\mu\left(\sigma^i x\right) \neq 0$ for no more than a finite number of choices of i. Let $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ be a CA in which $\diamond$ is quiescent. We say that F *conserves* Δ if for every $\diamond$-finite configuration x we have $\Delta(Fx) = \Delta(x)$.

Let Φ be a commutative monoid and Δ a Φ-valued potential (generated by some local observable). Similarly to the previous section, by the *realizable* sub-monoid of Φ we mean the sub-monoid

$$\breve{\Phi} \triangleq \Phi\langle \Delta(x) : x \diamond\text{-finite} \rangle \tag{4.11}$$

generated by the total energy of the $\diamond$-finite configurations. Two potentials $\Delta_1 : \mathcal{C}_\diamond[S] \to \Phi_1$ and $\Delta_2 : \mathcal{C}_\diamond[S] \to \Phi_2$ are considered to be *equivalent*, written $\Delta_1 \equiv \Delta_2$, if there is a monoid isomorphism $\iota : \breve{\Phi}_1 \to \breve{\Phi}_2$ such that $\Delta_2 = \iota \circ \Delta_1$. We say that Δ_1 is *at least as general* as Δ_2, written $\Delta_2 \sqsubseteq \Delta_1$, if there is a monoid homomorphism $h : \breve{\Phi}_1 \to \breve{\Phi}_2$ such that $\Delta_2 = h \circ \Delta_1$. As before, this defines a partial ordering (up to equivalence) on the collection of monoid-valued potentials on $S^{\mathbb{L}}$. The *join* of Δ_1 and Δ_2 is the potential $\Delta_1 \vee \Delta_2 : \mathcal{C}_\diamond[S] \to \Phi_1 \times \Phi_2$, where $(\Delta_1 \vee \Delta_2)(x) \triangleq (\Delta_1(x), \Delta_2(x))$ whenever x is $\diamond$-finite. It is the least general potential which is at least as general as Δ_1 and Δ_2. If Δ_1 is generated by the observable $\mu_1 : S^{\mathbb{L}} \to \Phi_1$ and Δ_2 is generated by the observable $\mu_2 : S^{\mathbb{L}} \to \Phi_2$, then $\Delta_1 \vee \Delta_2$ is generated by the observable $\mu_1 \vee \mu_2 : S^{\mathbb{L}} \to \Phi_1 \times \Phi_2$, where $(\mu_1 \vee \mu_2)(x) \triangleq (\mu_1(x), \mu_2(x))$. A potential $\Delta : \mathcal{C}_\diamond[S] \to \Phi$ is *trivial* if the realizable sub-monoid $\breve{\Phi}$ is trivial. If a cellular automaton $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ conserves a potential Δ, it also conserves every potential $\Delta' \sqsubseteq \Delta$ which is less general than Δ. If F conserves two

potentials Δ_1 and Δ_2, it also conserves $\Delta_1 \vee \Delta_2$. The trivial potential on $S^{\mathbb{L}}$ is conserved by every cellular automaton.

Monoid-valued potentials can equivalently be generated using interaction potentials. However, unlike in the group-valued case, here we cannot identify a unique canonical interaction potential generating a given potential. In particular, there is no immediate way to identify the realizable sub-monoid. More importantly, the algorithm for deciding whether a CA conserves a given real-valued (or group-valued) energy does not work for monoid-valued energies.

On the other hand, as in the group-valued case, among all monoid-valued conservation laws with a fixed "range of interaction", there is one which is the most general.

Proposition 4.3 ([27]). *Let $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ be a cellular automaton for which $\diamond$ is a quiescent state, and let $M \subseteq \mathbb{L}$ be a finite neighborhood. Among all monoid-valued conservation laws which are defined using observables with neighborhood M, there is one which is the most general.*

Proof. Let Φ_0^M be the free commutative monoid generated by $S^M \setminus \{\diamond^M\}$. Let $\mu_0^M : S^{\mathbb{L}} \to \Phi_0^M$ be the formal observable defined by

$$\mu_0^M(x) \triangleq \begin{cases} x|_M & \text{if } x|_M \neq \diamondsuit|_M, \\ 0 & \text{otherwise,} \end{cases} \tag{4.12}$$

and let $\Delta_0^M : \mathcal{C}_\diamond[S] \to \Phi_0^M$ be the potential it generates. Let $\sim$ be the smallest congruence on Φ_0^M such that $\Delta_0^M(Fx) \sim \Delta_0^M(x)$ for every $\diamond$-finite configuration x. Define $\Phi_F^M \triangleq \Phi_0^M/\!\sim$, and let $h_F^M : \Phi_0^M \to \Phi_F^M$ be the corresponding natural homomorphism. Define the potential $\Delta_F^M \triangleq h_F^M \circ \Delta_0^M$, which is generated by the local observable $\mu_F^M \triangleq h_F^M \circ \mu_0^M$.

For every $\diamond$-finite configuration x we have

$$\Delta_F^M(Fx) = h_F^M \circ \Delta_0^M(Fx) = h_F^M \circ \Delta_0^M(x) = \Delta_F^M(x)\ . \tag{4.13}$$

Hence, F conserves Δ.

On the other hand, let Δ' be any other monoid-valued potential which is conserved by F and is generated by an observable $\mu' : S^{\mathbb{L}} \to \Phi'$ with neighborhood M and $\mu'(\diamondsuit) = 0$. Let $g' : S^M \to \Phi'$ be the local assignment which defines μ'. For each $p \in S^M \setminus \{\diamond^M\}$, let $h'(p) \triangleq g'(p)$ and extend h' to a monoid homomorphism $h' : \Phi_0^M \to \Phi'$. We have $\mu' = h' \circ \mu_0^M$ and $\Delta' = h' \circ \Delta_0^M$. Let $\sim'$ be the congruence on Φ_0^M that is induced by h'. Since $\Delta'(Fx) = \Delta'(x)$ for every $\diamond$-finite configuration x, we have $\sim' \supseteq \sim$. Therefore, there is a homomorphism $\psi : \Phi_F^M \to \Phi'$ such that $h' = \psi \circ h_F^M$. For every $\diamond$-finite x, we have

$$\Delta'(x) = h'\left(\Delta_0^M(x)\right) = \psi \circ h_F^M\left(\Delta_0^M(x)\right) = \psi\left(\Delta_F^M(x)\right)\ . \tag{4.14}$$

Therefore, Δ_F^M is at least as general as Δ'. □

Naturally, we would like to be able to find the most general monoid-valued conservation law corresponding to a given neighborhood. In particular, we would like to have an algorithm that, given a cellular automaton F and a neighborhood M, constructs the monoid Φ_F^M and the observable $\mu_F^M : S^{\mathbb{L}} \to \Phi_F^M$ defined in the proof of Proposition 4.3. Note that since Φ_F^M is finitely generated, it has a finite presentation (see e.g. [38]). However, it is not clear how to find such a finite presentation. A finite presentation is needed if, for example, we want to algorithmically verify whether two configurations have the same total energy (see e.g. [8]).

It turns out that for 2- or higher-dimensional CA, no algorithm can construct such a finite presentation for the monoid Φ_F^M. For one-dimensional CA, we will show how to construct Φ_F^M and μ_F^M.

Let $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ be a CA with a quiescent state $\diamond$. Clearly, $(\diamond, \diamond)$ is a quiescent state for the product $F \times F : (S \times S)^{\mathbb{L}} \to (S \times S)^{\mathbb{L}}$. Let $\Phi \triangleq \{0, 1\}$ be the Boolean monoid with $a + b \triangleq a \vee b$ for every $a, b \in \Phi$. Define the local observable $\mu : (S \times S)^{\mathbb{L}} \to \Phi$ by

$$\mu(x) \triangleq \begin{cases} 0 & \text{if } x[0] = (a, a) \text{ for some } a \in S, \\ 1 & \text{otherwise,} \end{cases} \tag{4.15}$$

and let Δ be the potential generated by μ. The CA $F \times F$ conserves Δ if and only if F is injective when restricted to $\diamond$-finite configurations. According to the Garden-of-Eden Theorem, F is injective on $\diamond$-finite configurations if and only if it is surjective. However, the question of whether a given 2- or higher-dimensional CA is surjective is undecidable [45]. Therefore, no algorithm can verify, for a given F, whether $F \times F$ conserves Δ.

Proposition 4.4 ([27])**.** *There is no algorithm that, given a 2- or higher-dimensional CA F and a local observable μ with values from a finitely presented commutative monoid, determines whether F conserves the potential generated by μ.*

Corollary 4.5 ([27])**.** *There is no algorithm that, given a 2- or higher-dimensional CA $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ and a finite neighborhood M, computes a finite presentation of the semigroup Φ_F^M and the observable $\mu_F^M : S^{\mathbb{L}} \to \Phi_F^M$ that, among the observables with neighborhood M, generates the most general potential conserved by F.*

Let us now focus on one-dimensional CA. Let $F : S^{\mathbb{Z}} \to S^{\mathbb{Z}}$ be a one-dimensional CA with a quiescent state $\diamond \in S$. Let Φ be a commutative monoid and $\mu : S^{\mathbb{Z}} \to \Phi$ a local observable with $\mu(\diamondsuit) = 0$. Without loss of generality we assume that F has a neighborhood $[-l, r]$ with $l + r \geq 0$, and that μ has a neighborhood $[0, m)$. Let $g : S^m \to \Phi$ be the local assignment defining μ. Let Δ be the potential generated by μ.

For $k \triangleq l + r + m$, consider the kth order De Bruijn representation $(\mathcal{B}_k[S], \lambda)$ of F. This has a vertex $\diamond^k$, with a loop edge $\diamond^{k+1}$ that is labeled by $\diamond^m$. Any path corresponding to a $\diamond$-finite configuration starts by circulating in the loop, and after possibly passing through a finite number of other edges, eventually returns to this loop.

To each edge $u_0u_1 \cdots u_k \in S^{k+1}$ let us assign two elements

$$\alpha(u_0u_1 \cdots u_k) \triangleq g(u_0u_1 \cdots u_{m-1}) \tag{4.16}$$

and

$$\beta(u_0u_1 \cdots u_k) \triangleq g(v_lv_{l+1} \cdots v_{l+m-1}) \tag{4.17}$$

from Φ, where $v_lv_{l+1} \cdots v_{k-r} \triangleq \lambda(u_0u_1 \cdots u_k)$ is the label of $u_0u_1 \cdots u_k$. The total energy of a $\diamond$-finite configuration x can be calculated by adding up the values of α over the edges of the corresponding bi-infinite path on $\mathcal{B}_k[S]$. Likewise, the sum of the β values on this path gives the total energy of Fx. Note that the initial and final parts of such a path, where it is circulating in the loop $\diamond^{k+1}$, do not contribute to the total energy, because $g(\diamond^m) = 0$. For any path $p = p_1p_2 \cdots p_n$ (p_i being the ith edge of the path), let us use the notation $\alpha(p)$ for the sum of the values of α over the edges of p; that is,

$$\alpha(p) \triangleq \sum_{i=1}^{n} \alpha(p_i) \ . \tag{4.18}$$

Similarly, let $\beta(p)$ be the sum of the values of β over the edges of p.

The requirements imposed by the conservation of Δ can now be translated in terms of the values of α and β over finite paths on the graph $\mathcal{B}_k[S]$: the CA F conserves Δ if and only if for each finite path p starting and ending at vertex $\diamond^k$, we have $\alpha(p) = \beta(p)$.

Luckily, we can algorithmically verify this condition. Moreover, by running the algorithm on a formally generated potential, we can construct the most general monoid-valued conservation law for F that is defined using an observable with a given neighborhood.

Proposition 4.6 ([27]). *Let G be a (finite, directed) graph with vertex set V and edge set E, and let Σ be a finite symbol set. Let $\alpha, \beta : E \to \Sigma^*$ be arbitrary and $A, B \subseteq V$. Let Φ be the largest commutative monoid generated by Σ satisfying the equation*

$$\alpha(p) = \beta(p) \tag{4.19}$$

for every finite path p starting from A and ending at B. There is an algorithmically constructible finite subset of the above equations, such that any commutative monoid generated by Σ satisfying those equations is a factor of Φ.

Proof. We start by introducing the finite subset in question. For any vertex $v \in V$, define the following three sets:

P_v: The set of all simple paths starting from A and ending at v,

Q_v: The set of all simple paths starting from v and ending at B, and

C_v: The set of all simple cycles (including the empty one) passing through v.

For any v, the set $P_vC_vQ_v$ is finite, because each of P_v, C_v and Q_v is finite. The elements of $P_vC_vQ_v$ are paths starting from A, passing through v (and possibly a cycle around v), and ending at B. Define

$$R \triangleq \bigcup_{v \in V} P_v C_v Q_v \ . \tag{4.20}$$

We claim that, if for some monoid Φ' generated by Σ, Equation (4.19) holds for all paths $r \in R$, it also holds for any other path p from A to B.

The proof is by induction on the length of the path p. Note that any sufficiently short path p from A to B is simple and passes through a vertex like v. Therefore p is of the form xy where $x \in P_v$ and $y \in Q_v$. That is, $p \in R$ and Equation (4.19) holds by the assumption.

Suppose that Equation (4.19) holds for all paths of length at most n, and let p be a path of length $n+1$ from A to B. If p is not simple, it contains at least one non-empty simple cycle, and hence can be written in the form xcy where x is a (not necessarily simple) path from A to a vertex v, c is a non-empty simple cycle starting and ending at v, and y is a (not necessarily simple) path from v to B. On the other hand, x contains a subsequence $\tilde{x}$ that is a simple path from A to v, and we can write

$$\alpha(x) = \sum_i \alpha(x_i) = \gamma_x + \sum_i \alpha(\tilde{x}_i) = \gamma_x + \alpha(\tilde{x}) \ , \tag{4.21}$$

where $\gamma_x \in \Phi$ is the sum of α over those edges from x that are not in $\tilde{x}$. Similarly y contains a subsequence $\tilde{y}$ that is a simple path from v to B, and we can write

$$\alpha(y) = \gamma_y + \alpha(\tilde{y}) \tag{4.22}$$

for some $\gamma_y \in \Phi$. Writing Equation (4.19) for the paths $\tilde{x}\tilde{y}$ and $\tilde{x}c\tilde{y}$ (note that $\tilde{x}\tilde{y}, \tilde{x}c\tilde{y} \in R$) and for the path xy (by induction hypothesis), we have

$$\alpha(\tilde{x}) + \alpha(\tilde{y}) = \beta(\tilde{x}) + \beta(\tilde{y}) \ , \tag{4.23}$$

$$\alpha(\tilde{x}) + \alpha(c) + \alpha(\tilde{y}) = \beta(\tilde{x}) + \beta(c) + \beta(\tilde{y}) \ , \tag{4.24}$$

$$\alpha(x) + \alpha(y) = \beta(x) + \beta(y) \ , \tag{4.25}$$

from which we obtain that

$$\begin{aligned}
\alpha(p) &= \alpha(x) + \alpha(c) + \alpha(y) && (4.26)\\
&= \gamma_x + \gamma_y + \alpha(\tilde{x}) + \alpha(c) + \alpha(\tilde{y}) && (4.27)\\
&= \gamma_x + \gamma_y + \beta(\tilde{x}) + \beta(c) + \beta(\tilde{y}) && (4.28)\\
&= \gamma_x + \gamma_y + \alpha(\tilde{x}) + \alpha(\tilde{y}) + \beta(c) && (4.29)\\
&= \alpha(x) + \alpha(y) + \beta(c) && (4.30)\\
&= \beta(x) + \beta(y) + \beta(c) && (4.31)\\
&= \beta(p)\ , && (4.32)
\end{aligned}$$

which is what we wanted to prove. Therefore, any equation satisfied by the monoid Φ is also satisfied by Φ', and Φ' is a factor of Φ. □

Corollary 4.7 ([27]). *Let $F : S^{\mathbb{Z}} \to S^{\mathbb{Z}}$ be a one-dimensional CA and $M \subseteq \mathbb{Z}$ an arbitrary neighborhood. There is an algorithm to identify the most general monoid-valued conservation law for F among those which are defined using observables with neighborhood M. In particular, we can construct both a finite presentation of the monoid Φ_F^M, and the observable μ_F^M defining this conservation law.*

Remark 4.1. In terms of formal language theory, Proposition 4.6 can be translated into the following: let Σ and Γ be finite symbol sets, $\alpha, \beta : \Sigma^* \to \Gamma^*$ arbitrary morphisms, and $L \subseteq \Sigma^*$ a regular language. Then the largest commutative monoid generated by Γ satisfying the equations

$$\alpha(w) = \beta(w) \qquad \text{(for all } w \in L\text{)} \tag{4.33}$$

is effectively finitely presentable. ○

Remark 4.2. Another problematic issue is identifying the realizable submonoid $\breve{\Phi} \subseteq \Phi$ associated with a potential $\Delta : \mathcal{C}_\diamond[S] \to \Phi$. For example, it is not even clear whether $\breve{\Phi}$ is finitely generated or not. However, in the one-dimensional case we can use Proposition 4.6, to decide whether a given monoid-valued potential Δ is trivial. ○

4.3 The Existence Problem

Given a cellular automaton, we would like to understand the hierarchy of its conservation laws. We already know that the conservation laws of a given CA are partially ordered, and that for each fixed range of interaction, there is a maximal conservation law that incorporates all the others with that range. Furthermore, at least in the group-valued hierarchy, we can algorithmically find these maximal laws. For a given CA, two extreme possibilities regarding this hierarchy are imaginable:

I. The hierarchy is trivial. That is, the CA has no non-trivial conservation law.

II. The hierarchy is unbounded. In other words, looking at larger and larger ranges of interactions, we always find new conservation laws.

A CA which maps every configuration to a unique quiescent configuration belongs to the first case. An example of the second case is the identity CA, which keeps every configuration unchanged. The XOR CA from Example 4.1 rests in neither of these two categories (see Section 4.4). As we shall see, each of these two extreme cases is algorithmically undecidable. Even worse, the two categories are algorithmically inseparable; no terminating algorithm can distinguish between the two cases.

Let us introduce a rather large class of CA which belong to Category I. Recall that a CA with a quiescent state $\diamond$ is said to be nilpotent over $\diamond$-finite configurations if every $\diamond$-finite configuration eventually changes to the quiescent configuration $\diamondsuit$.

Lemma 4.8. *Let $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ be a cellular automaton with a quiescent state $\diamond$. Suppose that F is nilpotent over $\diamond$-finite configurations. Then F has no non-trivial (real-valued/group-valued/semigroup-valued) conservation law.*

Recall that a local observable $\mu : S^{\mathbb{L}} \to \Sigma$ partitions the space $S^{\mathbb{L}}$ into clopen sets. If μ is invariant under a cellular automaton $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$, each block $\mu^{-1}(a)$ of the partition is the basin of an attractor of F (see e.g. [53, 51]). Any CA which has a non-trivial invariant local observable belongs to Category II.

Lemma 4.9. *Let $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ be a cellular automaton and $\mu : S^{\mathbb{L}} \to \Sigma$ a non-trivial local observable that is invariant under F. Then F has an unbounded hierarchy of conservation laws.*

Proof. We present the proof in the group-valued setting. The same argument can be translated for the semigroup-valued or real-valued hierarchy.

Suppose that the hierarchy of conservation laws for F is bounded. Then there is a local potential difference $\bar{\Delta}$ that is more general than any local potential difference conserved by F. Such a potential difference is generated by a local observable $\bar{\mu} : S^{\mathbb{L}} \to \bar{\mathbb{G}}$ that has a neighborhood $\bar{M}$. We construct a local potential difference Δ' that is conserved by F, and yet $\Delta' \not\sqsubseteq \bar{\Delta}$; hence a contradiction.

First, note that F conserves any potential difference that is generated by a group-valued F-invariant local observable. Let $a \in \mathbb{L}$, and define the observable

$$\mu' \triangleq \mu \vee (\sigma^a \circ \mu) : S^{\mathbb{L}} \to \Sigma \times \Sigma \,. \tag{4.34}$$

If μ has neighborhood M, μ' has neighborhood $M' \triangleq M \cup M(a)$. Since μ is invariant under F, so is μ'. Let $\mathbb{G}'_0$ be the free commutative group generated by $\Sigma \times \Sigma$.[1] Then F conserves the $\mathbb{G}'_0$-valued potential difference Δ' generated by μ'. We show that $\Delta' \not\sqsubseteq \bar{\Delta}$, provided a is far enough from the origin, namely, if $a \notin M^{-1}(\bar{M}(\bar{M}^{-1}(M)))$ and $a \notin M^{-1}(M(M^{-1}(M)))$. To do this, it is sufficient to find two asymptotic configurations x and y such that $\bar{\Delta}(x, y) = 0$ but $\Delta'(x, y) \neq 0$.

Let $\diamond \in S$ be an arbitrary state, and denote the $\diamond$-uniform configuration by $\diamondsuit$. Let $p : M \to S$ be a pattern such that $\mu(\zeta_p \diamondsuit) \neq \mu(\diamondsuit)$. Such a pattern exists because μ is assumed to be non-trivial. Let $\alpha \triangleq \mu(\diamondsuit)$ and $\beta \triangleq \mu(\zeta_p \diamondsuit)$. We have $\alpha, \beta \in \Sigma$ and $\alpha \neq \beta$.

Choose $b \notin M^{-1}(M'(M'^{-1}(M)))$. Define two configurations

$$x \triangleq \zeta_{\sigma^{-a}p} \zeta_p \diamondsuit \,, \qquad \text{and} \qquad y \triangleq \zeta_{\sigma^{-b}p} \zeta_p \diamondsuit \,. \tag{4.35}$$

The idea is that on x and y, the two copies of p are too far away from each other for $\bar{\Delta}$ to sense the difference between x and y. On the other hand, Δ' can distinguish between x and y.

More precisely, since $\bar{\mu}$ has neighborhood $\bar{M}$, it is easy to see that $\bar{\Delta}$ has neighborhood $\bar{M}(\bar{M}^{-1})$. Therefore,

$$\begin{aligned} \bar{\Delta}(\diamondsuit, x) &= \bar{\Delta}(\diamondsuit, \zeta_{\sigma^{-a}p} \diamondsuit) + \bar{\Delta}(\zeta_{\sigma^{-a}p} \diamondsuit, x) && (4.36) \\ &= \bar{\Delta}(\diamondsuit, \zeta_{\sigma^{-b}p} \diamondsuit) + \bar{\Delta}(\zeta_{\sigma^{-b}p} \diamondsuit, y) && (4.37) \\ &= \bar{\Delta}(\diamondsuit, y) \,, && (4.38) \end{aligned}$$

which implies $\bar{\Delta}(x, y) = 0$. On the other hand, while every summand in $\Delta'(\diamondsuit, y)$ is a pair of the form (u, α) or (α, v) for $u, v \in \Sigma$, $\Delta'(\diamondsuit, x)$ contains a summand (β, β), and we know that $\beta \neq \alpha$. Since $\Sigma \times \Sigma$ is a free generating set for $\mathbb{G}'_0$, we conclude that $\Delta'(\diamondsuit, x) \neq \Delta'(\diamondsuit, y)$ and hence $\Delta'(x, y) \neq 0$. □

To prove the undecidability of Categories I and II, we use the following theorem, due to Blondel, Cassaigne and Nichitiu. By a 2-*counter machine* we mean a finite automaton equipped with two unbounded *counters*. The machine can increase or decrease the value of each counter, and can test if either has value zero. 2-counter machines are known to be equivalent in power to Turing machines — any algorithm can be implemented on a 2-counter machine (see e.g. [63]). Following Blondel et al. [9], we identify a 2-counter machine by a finite *state set* Q and a *transition rule* $\delta : Q \times \{0, 1\}^2 \to Q \times \{1, 2\} \times \{-, 0, +\}$.[2] A *configuration* of the machine consists of its current state $q \in Q$, and the current value of its two *registers*

[1] Note that this is *not* the same as the direct product $\mathbb{G}_0 \times \mathbb{G}_0$ where $\mathbb{G}_0$ is the free commutative group generated by Σ.

[2] For our purposes there are no designated initial and halting states.

$x_1, x_2 \in \mathbb{N}$. The transition rule reads the current state, checks whether either of the registers contains zero (1 means the value of the register is zero, and 0 means otherwise), decides the new state, chooses one of the registers (1 or 2 as the index of the chosen register), and instructs whether the chosen register should be decreased ($-$), left unchanged (0) or increased ($+$). Thus, it defines a dynamics on the configuration space $Q \times \mathbb{N} \times \mathbb{N}$.

Theorem 4.10 ([9])**.** *It is undecidable whether a given 2-counter machine (without initial and halting states) has a periodic orbit.*

Theorem 4.11 ([27])**.** *There is no algorithm to distinguish between Categories I and II. In particular, given a (one-dimensional) cellular automaton F, the following questions are undecidable:*

i) Does F have any non-trivial (real-valued/group-valued/semigroup-valued) conservation law?

ii) Does F have an unbounded hierarchy of (real-valued/group-valued/semigroup-valued) conservation laws?

Proof. We show how to reduce the problem of whether a given 2-counter machine has a periodic orbit to the problem of distinguishing between one-dimensional CA which have no non-trivial conservation law and those with an unbounded hierarchy of conservation laws. Since there is no algorithm for the former, none can either exist for the latter.

Let $\mathcal{A}$ be a 2-counter machine with state set Q, two registers x_1 and x_2, and transition rule $\delta : Q \times \{0,1\}^2 \to Q \times \{1,2\} \times \{-,0,+\}$. We construct a CA F with a designated quiescent state $\diamond$, such that

i) if $\mathcal{A}$ has no periodic orbit, F is nilpotent over $\diamond$-finite configurations (and hence, by Lemma 4.8, has no non-trivial conservation law), while

ii) if $\mathcal{A}$ has a periodic orbit, there is a non-trivial (real-valued) local observable which is invariant under F (therefore, by Lemma 4.9, F has an unbounded hierarchy of conservation laws).

The CA F has two states L and R which are *end-markers*. In the interval between a left end-marker L and a right end-marker R, the CA simulates the machine $\mathcal{A}$. The CA also constantly verifies the syntax of each block between two end-markers to ensure that it corresponds with an actual simulation. If a syntax error is found, or if the simulation overflows the end-markers, the CA erases the whole block by replacing the cell contents with $\diamond$. Blocks without end-markers are also erased.

If a machine $\mathcal{A}$ has no periodic orbit, every syntactically correct simulation of $\mathcal{A}$ on a finite block eventually overflows its boundaries. Therefore,

every $\diamond$-finite configuration eventually goes quiescent; that is, F is nilpotent over $\diamond$-finite configurations.

On the other hand, if $\mathcal{A}$ has a periodic configuration, one can choose a sufficiently large simulation block in F which evolves periodically and never overflows. Let us fix a snapshot of such a periodic simulation block (including its end-markers), and denote it by $B = Lb_1b_2\cdots b_{n-1}R$. Let us denote by $\mathcal{B}$ the set of all simulation blocks $B' \in S^{n+1}$ that eventually turn into B. Since no new end-marker is ever created by F, and since the information cannot pass through the end-markers, we can argue that the set $\mathcal{B}$ is "stable"; once we know that a block in $\mathcal{B}$ occurs in a certain position at a certain time during the evolution of the CA, we also know that in any other time a block in $\mathcal{B}$ occurs in that same position. In other words, the observable

$$\mu(x) \triangleq \begin{cases} 1 & \text{if } x|_{[0,n]} \in \mathcal{B}, \\ 0 & \text{otherwise} \end{cases} \tag{4.39}$$

is invariant under F.

Let us now describe the construction in detail. Let $E \triangleq \{L, R\}$, $X \triangleq \{0, 1\}$, $K \triangleq \{1, 2\}$ and $C \triangleq \{0, +, -, 1\}$. The state set of F is $S \triangleq \{q\} \cup E \cup Q \cup (X \times X \times K \times C)$, and its neighborhood is $N = \{-1, 0, 1\}$. Each simulation block starts with a left end-marker L, followed by an element from Q representing the state of the machine, and ends with a right end-marker R. The space between the Q state and the right end-marker stores the content of the two registers and manages the required signaling. The first and the second components of $X \times X \times K \times C$ keep the unary value of the registers x_1 and x_2 in the form of stacks extending to the right. The K component corresponds to the second component of the range of δ, indexing the register to be increased or decreased. The C component carries a signal indicating whether the indexed counter should be increased ($+$), decreased ($-$), or left unchanged (0), and an acknowledgment signal (1) which returns to the left to initiate the simulation of the next step. The local rule $f : S^3 \to S$ of the CA is presented in Table 4.1. A sample syntactically correct simulation block is depicted in Figure 4.3. □

4.4 Restrictions on the Dynamics

In the previous section, we saw two simple examples of what the dynamical properties of a CA may tell us about the structure of the hierarchy of its conservation laws: according to Lemma 4.8, nilpotent CA have no non-trivial conservation laws, while Lemma 4.9 implies that every non-nilpotent equicontinuous CA has an unbounded hierarchy of conservation laws. In this section, we will see two less trivial results about the inter-

a_{-1}	a_0	a_1	$f(a_{-1}a_0a_1)$	Condition
	q		q	
	L	x	L	$x \in Q$
	L	x	q	$x \notin Q$
$(0,0,k,c)$	R		R	$k \in K$ and $c \neq 0$
x	R		q	$x \notin \{0\} \times \{0\} \times K \times \{+,-,1\}$
L	x	$(b_1,b_2,k,1)$	x'	$x \in Q$ and $\delta(x,\neg b_1,\neg b_2)$ $= (x',k',c')$
L	x	(b_1,b_2,k,c)	x	$x \in Q$ and $c \neq 1$
y	x		q	$x \in Q$ but $y \neq L$
	x	R	q	$x \in Q$
x	$(b_1,b_2,k,1)$	y	(b_1,b_2,k',c')	$x \in Q$ and $y \notin \{q,L\}$ and $\delta(x,\neg b_1,\neg b_2)$ $= (x',k',c')$
(b_1',b_2',k',c')	$(b_1,b_2,k,1)$	y	(b_1,b_2,k',c')	$c' \neq 0$ and $y \notin \{q,L\}$
$(b_1',b_2',k',0)$	$(b_1,b_2,k,1)$	y	$(b_1,b_2,k,1)$	$y \notin \{q,L\}$
x	$(b_1,b_2,k,0)$	$(b_1',b_2',k',1)$	$(b_1,b_2,k,1)$	$x \notin \{q,L,R\}$
x	$(b_1,b_2,k,0)$	(b_1',b_2',k',c)	$(b_1,b_2,k,0)$	$c \neq 1$ and $x \notin \{q,L,R\}$
x	$(0,b_2,1,+)$	y	$(1,b_2,1,1)$	$x \in Q$ and $y \notin \{q,L\}$
(b_1',b_2',k',c')	$(0,b_2,1,+)$	y	$(b_1',b_2,1,1)$	$y \notin \{q,L\}$
x	$(1,b_2,1,+)$	y	$(1,b_2,1,0)$	$x \notin \{q,L,R\}$ and $y \notin \{q,L\}$
x	$(b_1,0,2,+)$	y	$(b_1,1,2,1)$	$x \in Q$ and $y \notin \{q,L\}$
(b_1',b_2',k',c')	$(b_1,0,2,+)$	y	$(b_1,b_2',2,1)$	$y \notin \{q,L\}$
x	$(b_1,1,2,+)$	y	$(b_1,1,2,0)$	$x \notin \{q,L,R\}$ and $y \notin \{q,L\}$
x	$(0,b_2,1,-)$	y	$(0,b_2,1,1)$	$x \notin \{q,L,R\}$ and $y \notin \{q,L\}$
x	$(1,b_2,1,-)$	$(0,b_2',k',c')$	$(0,b_2,1,1)$	$x \notin \{q,L,R\}$
x	$(1,b_2,1,-)$	$(1,b_2',k',c')$	$(1,b_2,1,0)$	$x \notin \{q,L,R\}$
x	$(b_1,0,1,-)$	y	$(b_1,0,1,1)$	$x \notin \{q,L,R\}$ and $y \notin \{q,L\}$
x	$(b_1,1,1,-)$	$(b_1',0,k',c')$	$(b_1,0,1,1)$	$x \notin \{q,L,R\}$
x	$(b_1,1,1,-)$	$(b_1',1,k',c')$	$(b_1,1,1,0)$	$x \notin \{q,L,R\}$
L	x		q	$x \neq Q$
	x	R	q	$x \notin \{0\} \times \{0\} \times K \times \{+,-,1\}$
y	x		q	$x \neq L$ and $y \in \{q,R\}$
	x	y	q	$x \neq R$ and $y \in \{q,L\}$

Table 4.1: The local rule of the CA described in the proof of Theorem 4.11.

$$\cdots\ q\ \ q\ \ q\ \ L\ \ x\ \begin{array}{|c|c|c|c|c|c|c|c|c|c|c|}\hline 0&0&0&+&1&1&1&1&-&1\\\hline 2&2&2&2&1&1&1&1&1&1\\\hline 1&1&0&0&0&0&0&0&0&0\\\hline 1&1&1&1&1&1&0&0&0&0\\\hline\end{array}\ R\ \ q\ \ q\ \ q\ \cdots$$

Figure 4.3: A syntactically correct simulation block in the CA described in the proof of Theorem 4.11. The simulated machine is in state $x \in Q$. The first register contains 2, while the second register contains 6. A signal is moving to the right, commanding the second register to increase.

connection between the dynamics of a CA and its hierarchy of conservation laws. First, we show that a positively expansive CA cannot have any non-trivial real-valued conservation law. Next, we mention a result, due to Formenti and Grange, that every surjective CA with a particular kind of conserved energy has a dense set of temporally periodic points.

Given a real-valued potential difference Δ on $S^{\mathbb{L}}$, let us call an element $x \in S^{\mathbb{L}}$ a *ground* configuration if for every configuration y asymptotic to x, we have $\Delta(x, y) \geq 0$. Let us first show that for every local potential difference, ground configurations exist.

Proposition 4.12. *Every real-valued local potential difference has at least one ground configuration.*

Proof. Let $\diamondsuit$ be an arbitrary configuration. Let $M \subseteq \mathbb{L}$ be the neighborhood of Δ. Recall that for every $n \in \mathbb{N}$, $I_n \triangleq [-n, n]^d$ denotes the central hypercubic region of size $(2n+1)^d$.

For every $n \in \mathbb{N}$, let us choose a pattern $p_n : I_n \to S$ such that $\Delta(\diamondsuit, \zeta_{p_n}\diamondsuit)$ takes its minimum value. Since S^{I_n} is finite, such a minimum exists. For every other pattern $q : I_n \to S$ we have

$$\Delta(\zeta_{p_n}\diamondsuit, \zeta_q\diamondsuit) = \Delta(\diamondsuit, \zeta_q\diamondsuit) - \Delta(\diamondsuit, \zeta_{p_n}\diamondsuit) \geq 0 \,. \tag{4.40}$$

Let $x_n \triangleq \zeta_{p_n}\diamondsuit$, and consider the sequence $x_0, x_1, \ldots$ of configurations. Since $S^{\mathbb{L}}$ is compact, there is a subsequence $x_{n_0}, x_{n_1}, \ldots$ that converges in $S^{\mathbb{L}}$. Let $x \triangleq \lim_{i\to\infty} x_{n_i}$. We claim that x is a ground configuration.

Let y be any configuration that is asymptotic to x. Let $D \triangleq \{i : x[i] \neq y[i]\}$ be the set of cells on which x and y differ. Let $k \in \mathbb{N}$ be large enough such that

i) $I_{n_k} \supseteq M(D)$, and

ii) x_{n_i} and x agree on $M(D)$, for every $i \geq k$.

Let y' be a configuration which agrees with y on $M(D)$, with x_{n_k} on $I_{n_k} \setminus M(D)$, and with $\diamondsuit$ everywhere else. We have

$$\Delta(x, y) = \Delta(x_{n_i}, y') \geq 0 \,. \tag{4.41}$$

Therefore, x is a ground configuration for Δ. □

Let us denote the set of ground configurations of Δ by $\mathcal{Z}_\Delta$. Let $\mu : S^{\mathbb{L}} \to \mathbb{R}$ be a local observable generating Δ. Ground configurations minimize the (upper) average energy per cell $\overline{\mu}$.

Proposition 4.13. *Let Δ be a real-valued local potential difference generated by an observable $\mu : S^{\mathbb{L}} \to \mathbb{R}$. For every ground configuration $z \in \mathcal{Z}_\Delta$ we have $\overline{\mu}(z) \triangleq \inf_{x\in S^{\mathbb{L}}} \overline{\mu}(x)$.*

Proof. Let x be an arbitrary configuration. For every $n \in \mathbb{L}$, let $p_n \triangleq x|_{I_n}$ and $x_n \triangleq \zeta_{p_n} z$. That is, x_n is the configuration which agrees with x on I_n and with z everywhere else. We have

$$\mu_{I_n}(x) = \mu_{I_n}(z) + \Delta(z, x_n) + o(|I_n|) \ . \tag{4.42}$$

Therefore,

$$\begin{aligned}
\overline{\mu}(x) &= \limsup_{n\to\infty} \frac{\mu_{I_n}(x)}{|I_n|} && (4.43)\\
&= \limsup_{n\to\infty} \frac{\mu_{I_n}(z) + \Delta(z, x_n) + o(|I_n|)}{|I_n|} && (4.44)\\
&\geq \limsup_{n\to\infty} \frac{\mu_{I_n}(z)}{|I_n|} && (4.45)\\
&= \overline{\mu}(z) \ . && (4.46)
\end{aligned}$$

□

Remark 4.3. Recalling Corollary 2.11, one might expect that every local potential difference has periodic ground configurations. In one dimension, this is indeed the case, as one may prove using the De Bruijn graph. However, in higher dimensions, using an aperiodic set of Wang tiles (see e.g. [46]), one can construct an energy for which no periodic configuration achieves the minimum average energy per cell. ○

We can measure the *total energy* of every configuration relative to the ground configurations. Namely, for every configuration x, let us define

$$\Delta_{\mathcal{Z}}(x) \triangleq \begin{cases} \Delta(z, x) & \text{if } x \text{ asymptotic to } z \in \mathcal{Z}_\Delta, \\ +\infty & \text{otherwise.} \end{cases} \tag{4.47}$$

Note that if x is asymptotic to two different ground configurations $z_1, z_2 \in \mathcal{Z}_\Delta$, z_1 and z_2 are also asymptotic to each other, and we have $\Delta(z_1, z_2) = 0$. Thus, $\Delta(z_1, x) = \Delta(z_2, x)$ and the total energy mapping $\Delta_{\mathcal{Z}} : S^{\mathbb{L}} \to [0, +\infty]$ is well-defined.

Lemma 4.14. *Let Δ be a real-valued local potential difference, and x an arbitrary configuration. Then*

i) $\Delta_{\mathcal{Z}}(x) = 0$ if and only if x is a ground configuration.

ii) $\Delta_{\mathcal{Z}}(x) = +\infty$ if and only if for every $a \in \mathbb{R}$, there is a configuration x' which is asymptotic to x and $\Delta(x', x) > a$.

Proof. The first part is trivial. Let us prove the second part.

First, note that for every real-valued local potential difference, there is a positive number $\varepsilon > 0$ such that whenever $\Delta(x, y) > 0$, we also have $\Delta(x, y) > \varepsilon$. This follows from the fact that Δ takes its values from a finitely generated subgroup of $\mathbb{R}$.

Assume that $\Delta_{\mathcal{Z}}(x) = +\infty$. This implies that x is not a ground configuration. So there is a configuration x_1 that is asymptotic to x, and we have $\Delta(x_1, x) > \varepsilon > 0$. Notice that x_1 itself is not a ground configuration, because it is asymptotic to x. Therefore, there is yet another configuration x_2 which is asymptotic to x_1 and we have $\Delta(x_2, x_1) > \varepsilon > 0$. Clearly, x and x_2 are also asymptotic, and we can write

$$\Delta(x_2, x) = \Delta(x_2, x_1) + \Delta(x_1, x) > 2\varepsilon \; . \tag{4.48}$$

Repeating this, we find a configuration x_n that is asymptotic to x, and $\Delta(x_n, x) > \lceil \frac{a}{\varepsilon} \rceil \varepsilon \geq a$.

Conversely, suppose that $\Delta_{\mathcal{Z}}(x) < +\infty$. Then there is a ground configuration z that is asymptotic to x and $\Delta(z, x) = \Delta_{\mathcal{Z}}(x) < +\infty$. For every other configuration x' that is asymptotic to x we can write

$$\Delta(x', x) = \Delta(z, x) - \Delta(z, x') \leq \Delta_{\mathcal{Z}}(x) \; . \tag{4.49}$$

□

The total energy mapping $\Delta_{\mathcal{Z}}$ has a weak continuity property.

Proposition 4.15. *Let Δ be a real-valued local potential difference. The total energy mapping $\Delta_{\mathcal{Z}} : S^{\mathbb{L}} \to [0, +\infty]$ is lower semi-continuous; for every $a \geq 0$, the set $\{x : \Delta_{\mathcal{Z}}(x) > a\}$ is open.*

Proof. Let M be the neighborhood of Δ. Let $A \triangleq \{x : \Delta_{\mathcal{Z}}(x) > a\}$. For each $x \in A$, we show that there is a cylinder around x which is included in A.

For every $x \in A$, there is a configuration x' asymptotic to x such that $\Delta(x', x) > a$. If $\Delta_{\mathcal{Z}}(x) = +\infty$, this is guaranteed by Lemma 4.14. If $\Delta_{\mathcal{Z}}(x) < +\infty$, there is a ground configuration $x' \in \mathcal{Z}_\Delta$ which is asymptotic to x and we have $\Delta(x', x) = \Delta_{\mathcal{Z}}(x) > a$.

Define $D \triangleq \{i : x[i] \neq x'[i]\}$. We claim that $[x]_{M(D)} \subseteq A$. Let $y \in [x]_{M(D)}$. If y is not asymptotic to any ground configuration, we have $\Delta_{\mathcal{Z}}(y) = +\infty > a$, and hence $y \in A$. Suppose that y is asymptotic to a ground configuration z. Let y' be a configuration which agrees with x' on $M(D)$ and with y outside $M(D)$. We have

$$\begin{aligned} \Delta_{\mathcal{Z}}(y) &= \Delta(z, y) && (4.50)\\ &= \Delta(z, y') + \Delta(y', y) && (4.51)\\ &= \Delta(z, y') + \Delta(x', x) && (4.52)\\ &> a \; . && (4.53) \end{aligned}$$

Therefore, $y \in A$. □

Lemma 4.16. *Let $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ be a cellular automaton and Δ a real-valued local potential difference conserved by F. For every $x \in S^{\mathbb{L}}$, we have $\Delta_{\mathcal{Z}}(x) \leq \Delta_{\mathcal{Z}}(Fx)$.*

Proof. For every real number $a < \Delta_{\mathcal{Z}}(x)$, there is a configuration y asymptotic to x such that $\Delta(y, x) > a$. Then $\Delta(Fy, Fx) > a$, which means that $\Delta_{\mathcal{Z}}(Fx) > a$. Therefore, $\Delta_{\mathcal{Z}}(Fx) \geq \Delta_{\mathcal{Z}}(x)$. □

A dynamical system $(\mathcal{X}, F)$ is *strongly transitive* if for every $x \in \mathcal{X}$, the set $\bigcup_{t>0} F^{-t}x$ is dense (see [61]). Equivalently, this means that for every open set $U \subseteq \mathcal{X}$ and every point $x \in \mathcal{X}$, there is a time $t > 0$ such that $x \in F^t U$.

Theorem 4.17. *A CA with a non-trivial real-valued conservation law cannot be strongly transitive.*

Proof. Let $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ be a strongly transitive CA, and let Δ be a real-valued local potential difference which is conserved by F. Let $z \in \mathcal{Z}_\Delta$ be an arbitrary ground configuration.

Since F is strongly transitive, the set $\bigcup_{t>0} F^{-t}z$ is dense. Then for every configuration x, there is a sequence $z_1, z_2, \ldots$ of configurations converging to x such that $F^{t_i} z_i = z$ for some $t_i > 0$. Since F conserves Δ, by Lemma 4.16 we have that for each i, $\Delta_{\mathcal{Z}}(z_i) \leq \Delta_{\mathcal{Z}}(z) = 0$. Now, the lower semi-continuity of $\Delta_{\mathcal{Z}}$ implies that

$$\Delta_{\mathcal{Z}}(x) = \Delta_{\mathcal{Z}}(\lim_{i\to\infty} z_i) \leq 0 \,, \tag{4.54}$$

which means that $\Delta_{\mathcal{Z}}(x) = 0$. Therefore, Δ is trivial. □

Every positively expansive CA is topologically conjugate to a mixing one-sided shift space of finite type [68, 50]. Every transitive one-sided shift space of finite type is, in fact, strongly transitive. Therefore, every positively expansive CA is strongly transitive.

Corollary 4.18. *Positively expansive CA have no non-trivial real-valued conservation laws.*

The XOR cellular automaton in Example 4.1 is positively expansive, and as we already knew, has no non-trivial real-valued conservation law. On the other hand, we saw that it has at least one non-trivial group-valued conservation law. The following proposition implies that the parity conservation law is, in fact, its only non-trivial conservation law.

A CA with neighborhood N and local rule $f : S^N \to S$ is *permutive* on a neighbor $k \in N$ if for every pattern $p : N \setminus \{k\} \to S$, the mapping

$x \mapsto f(p \vee x)$ (for $x \in S^{\{k\}}$) is bijective. A one-dimensional CA, with neighborhood $[l, r]$, where $l < r$, that is permutive on both l and r is said to be *bi-permutive*. Bi-permutive CA are positively expansive, so they cannot have non-trivial real-valued conservation laws. We show that they also have a bounded hierarchy of group-valued conservation laws.

Proposition 4.19 ([16])**.** *Every bi-permutive one-dimensional CA has a bounded hierarchy of group-valued conservation laws. Its most general conservation law is determined by an interaction-free potential difference.*

Proof. Let F be a bi-permutive one-dimensional CA and Δ a local potential difference with values from a commutative group $\mathbb{G}$ that is conserved by F. Suppose that Δ has neighborhood $M \triangleq [-m, m]$ and F has neighborhood $[-l, r]$, where $m > 0$ and $-l < r$. Note that, without loss of generality, we can assume $r + l \geq m$. Otherwise, instead of F we can take F^t for a large enough $t > 0$ such that $tr + tl \geq m$. Clearly, F^t is still bi-permutive with neighborhood $[-tl, tr]$, and conserves Δ.

Let $\diamond' \in S$ be a fixed state, and denote by $\diamondsuit'$ the $\diamond'$-uniform configuration. Then $\diamondsuit \triangleq F\diamondsuit'$ is also $\diamond$-uniform for some state $\diamond \in S$. Let $p : [a, b] \to S$ and $q : [c, d] \to S$ be any two finite patterns with $a \leq b < c \leq d$. We show that

$$\Delta(\diamondsuit, \zeta_p\zeta_q\diamondsuit) = \Delta(\diamondsuit, \zeta_p\diamondsuit) + \Delta(\diamondsuit, \zeta_q\diamondsuit) \; . \tag{4.55}$$

For the depiction of the following argument, see Figure 4.4. Let $x \triangleq \zeta_p\zeta_q\diamondsuit$. Since F is bi-permutive, there is a configuration x' with $x'[i] = \diamond'$ for every $b - l < i < c + r$, such that $Fx' = x$. Let $p' \triangleq x'|_{[a-m-l,b-l]}$ and $q' \triangleq x'|_{[c+r,d+m+r]}$. Let $y' \triangleq \zeta_{p'}\zeta_{q'}\diamondsuit'$ and $y \triangleq Fy'$. Let $u \triangleq y|_{[a-m-l-r,a-m]}$ and $v \triangleq y|_{[d+m,d+m+r+l]}$. Then clearly $y = \zeta_u\zeta_p\zeta_q\zeta_v\diamondsuit$. Moreover,

$$F\zeta_{p'}\diamondsuit' = \zeta_u\zeta_p\diamondsuit \qquad \text{and} \qquad F\zeta_{q'}\diamondsuit' = \zeta_q\zeta_v\diamondsuit \; . \tag{4.56}$$

By the additivity of Δ (since Δ has neighborhood $[-m, m]$), on the one hand we can write

$$\Delta(\diamondsuit, \zeta_u\zeta_p\zeta_q\zeta_v\diamondsuit) = \Delta(\diamondsuit, \zeta_p\zeta_q\diamondsuit) + \Delta(\diamondsuit, \zeta_u\diamondsuit) + \Delta(\diamondsuit, \zeta_v\diamondsuit) \; , \tag{4.57}$$

and on the other hand we have

$$\begin{aligned}
\Delta(\diamondsuit, \zeta_u\zeta_p\zeta_q\zeta_v\diamondsuit) &= \Delta(\diamondsuit', \zeta_{p'}\zeta_{q'}\diamondsuit') && (4.58)\\
&= \Delta(\diamondsuit', \zeta_{p'}\diamondsuit') + \Delta(\diamondsuit', \zeta_{q'}\diamondsuit') && (4.59)\\
&= \Delta(\diamondsuit, \zeta_u\zeta_p\diamondsuit) + \Delta(\diamondsuit, \zeta_q\zeta_v\diamondsuit) && (4.60)\\
&= \Delta(\diamondsuit, \zeta_p\diamondsuit) + \Delta(\diamondsuit, \zeta_q\diamondsuit) + \Delta(\diamondsuit, \zeta_u\diamondsuit) + \Delta(\diamondsuit, \zeta_v\diamondsuit) \; . && (4.61)
\end{aligned}$$

Putting these together, we obtain

$$\Delta(\diamondsuit, \zeta_p\zeta_q\diamondsuit) = \Delta(\diamondsuit, \zeta_p\diamondsuit) + \Delta(\diamondsuit, \zeta_q\diamondsuit) \; . \tag{4.62}$$

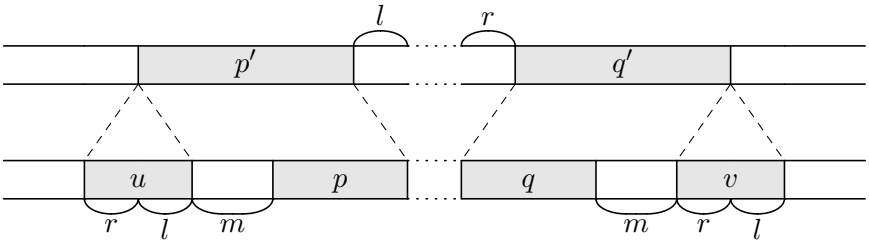


Figure 4.4: Illustration of the proof of Proposition 4.19.

For every state $s \in S$, let x_s be the configuration with $x[0] \triangleq s$ and $x[i] = \diamond$ for $i \neq 0$. Define $\theta(s) \triangleq \Delta(\diamondsuit, x_s)$ and $\theta(p) \triangleq 0$ for any pattern $p \in S^{\#}$ with more than one cell. It is easy to see that θ generates Δ.

We conclude that every local potential difference conserved by F is interaction-free. □

According to Devaney's formulation [22], a *chaotic* dynamical system is one which is sensitive and transitive, and has a dense set of periodic points. For infinite compact metric spaces (including all cellular automata), the sensitivity condition is implied by the other two conditions [3, 33] (see [52]). It is conjectured that every surjective cellular automaton (in particular, every transitive one) has a dense set of temporally periodic configurations (see e.g. [47, 17]).

We will now prove that a one-dimensional surjective CA has a dense set of temporally periodic configurations, provided it has a real-valued conservation law with a unique ground configuration. The result is due to Formenti and Grange, though in a slightly different setting.

Let Δ be a real-valued local potential difference on $S^{\mathbb{L}}$. If Δ has a unique ground configuration, that unique ground configuration is necessarily a uniform configuration like $\diamondsuit$, in which every cell is in a state $\diamond \in S$. If a CA $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ conserves Δ, then by Lemma 4.16, we must also have $F\diamondsuit = \diamondsuit$; that is, $\diamond$ is a quiescent state.

Theorem 4.20 ([26]). *Let $F : S^{\mathbb{Z}} \to S^{\mathbb{Z}}$ be a one-dimensional surjective CA. Suppose that there is a real-valued local potential difference Δ that has a unique ground configuration and that is conserved by F. Then, the set of temporally periodic points under F is dense in $S^{\mathbb{Z}}$.*

Proof. Let $\diamondsuit$ be the unique ground configuration for Δ. Then $\diamondsuit$ is $\diamond$-uniform for some quiescent state $\diamond \in S$, which we will call *blank*. Since F is surjective, by the Garden-of-Eden Theorem we have that each $\diamond$-finite configuration has at most one $\diamond$-finite pre-image. On the other hand, by Lemma 4.16,

every pre-image of a $\diamond$-finite configuration has a finite total energy, and hence is itself a $\diamond$-finite configuration. We conclude that every $\diamond$-finite configuration has a unique pre-image which is itself $\diamond$-finite.

Let F have neighborhood $N \triangleq [-r, r]$. Let x be an arbitrary $\diamond$-finite configuration. Then $x = \zeta_p \diamondsuit$, where $p : [a, b] \to S$ is a finite pattern with $a \leq b$. Let y be the unique pre-image of x. It is easy to verify that $y = \zeta_q \diamondsuit$ for some finite pattern $q : [a - (2^{2r} + r - 1), b + (2^{2r} + r - 1)] \to S$. Otherwise, one could make a periodic configuration $z \neq \diamondsuit$ with $Fz = \diamondsuit$, which is impossible. Set $R \triangleq [-(2^{2r} + r - 1), (2^{2r} + r - 1)]$.

On a configuration x, let us connect two non-blank cells i and j by an edge if $N^{-1}(R(i)) \cap N^{-1}(R(j)) \neq \varnothing$. Let us call a maximal connected collection of non-blank cells a *cluster*. The pre-images of disjoint finite clusters do not interact.

To state the latter claim precisely, suppose that a configuration x consists of finite clusters $D_1, D_2, \ldots$. Then $x \triangleq \zeta_{(p_1 \vee p_2 \vee \cdots)} \diamondsuit$, where $p_i \triangleq x|_{D_i}$. For each i, let $\zeta_{q_i} \diamondsuit$ be the unique pre-image of $\zeta_{p_i} \diamondsuit$, where $q_i : R(D_i) \to S$ is a finite pattern. Since the sets $N^{-1}(R(D_i))$ are mutually disjoint, it follows that $y \triangleq \zeta_{(q_1 \vee q_2 \vee \cdots)} \diamondsuit$ is a pre-image of x.

Let $\mu : S^{\mathbb{Z}} \to \mathbb{R}$ be a local observable generating Δ that has neighborhood $M \triangleq [0, m)$, and let $\mu(\diamondsuit) = 0$. We claim that for each real number E, there is a number T_E such that every spatially periodic configuration x, with period $k \geq T_E$ and energy per period $k\overline{\mu}(x) \leq E$, has only finite clusters.

For, suppose that for every $t > 0$, there is a periodic configuration x_t, with period $k_t \geq t$ and energy per period at most E, that has an infinite cluster. Without loss of generality, we can assume that on each x_t, the cell 0 belongs to this infinite cluster. By compactness, the sequence $\{x_n\}_{n=0}^{\infty}$ has a converging sub-sequence $\{x_{n_i}\}_{i=0}^{\infty}$. Let $x \triangleq \lim_{i \to \infty} x_{n_i}$. Clearly, x has an infinite cluster which contains cell 0. In particular, x cannot be $\diamond$-finite.

On the other hand, x can be written as the limit $x = \lim_{i \to \infty} \zeta_{p_i} \diamondsuit$ where $p_i \triangleq x_{n_i}|_{D_{n_i}}$ and

$$D_{n_i} \triangleq [-\lfloor \frac{k_{n_i}}{2} \rfloor, \lceil \frac{k_{n_i}}{2} \rceil - 1] \; . \tag{4.63}$$

Set $y_i \triangleq \zeta_{p_i} \diamondsuit$. It is easy to see that for each i we have

$$\Delta_{\mathcal{Z}}(y_i) \leq k\overline{\mu}(x_{n_i}) + \delta \leq E + \delta \; , \tag{4.64}$$

where $\delta \geq 0$ is a sufficiently large constant. But according to Proposition 4.15, this means that $\Delta_{\mathcal{Z}}(x) \leq E + \delta < +\infty$. Since $\diamondsuit$ is the only ground configuration, it follows that x is asymptotic to $\diamondsuit$, which is a contradiction.

Next, we show that every spatially periodic configuration with sufficiently small average energy per cell is temporally periodic. Namely, for

every $E > 0$ and $k \geq T_k$, define the set $P_{E,k}$ of all spatially periodic configurations with period k and energy per period at most E. We show that F acts periodically on $P_{E,k}$. Since $P_{E,k}$ is a finite set, it is enough to show that every element of $P_{E,k}$ has a pre-image in $P_{E,k}$.

Let x be an arbitrary element of $P_{E,k}$. Then x has no infinite clusters. Let $D_1, D_2, \ldots$ be the finite clusters of x. These are translations of a finite number of different clusters. We can write

$$x = \zeta_{(\bigvee_{i\in I}\bigvee_{j\in\mathbb{Z}}\sigma^{-jk}p_i)}\diamondsuit\,, \tag{4.65}$$

where $p_i \triangleq x|_{D_i}$ and I is a finite set. For every $i \in I$, let $q_i : R(D_i) \to S$ be such that $F\zeta_{q_i}\diamondsuit = \zeta_{p_i}\diamondsuit$. Then

$$y \triangleq \zeta_{(\bigvee_{i\in I}\bigvee_{j\in\mathbb{Z}}\sigma^{-jk}q_i)}\diamondsuit \tag{4.66}$$

is a pre-image of x. Clearly, y has period k and its energy per period is at most E. Therefore $y \in P_{E,k}$.

Let U be a non-empty open set. Choose a finite pattern $p : D \to S$ such that U contains the cylinder $[p]_D$. Let $E \triangleq \Delta_{\mathcal{Z}}(\zeta_p\diamondsuit)$, and choose a sufficiently large $k \geq T_E$ so that the sets $kj + M(N^{-1}(R(D)))$ ($j \in \mathbb{Z}$) are mutually disjoint. The configuration

$$x \triangleq \zeta_{(\bigvee_{j\in\mathbb{Z}}\sigma^{-jk}p)}\diamondsuit \tag{4.67}$$

is clearly in $[p]_D \subseteq U$. It is also in $P_{E,k}$, because it has spatial period k and energy per period E. Hence, it is temporally periodic. □

CHAPTER 5

Statistical Mechanics in Surjective CA

STATISTICAL physics is the attempt to deduce macroscopic physical phenomena by statistical analysis of microscopic models of the underlying processes. Classic examples are the study of thermodynamics via microscopic models of a gas or liquid consisting of a huge number of interacting particles, and the study of ferromagnetism by analyzing the magnetic field of the tiniest pieces of the material and their interactions. Often this underlying process can be approximated on a lattice. Each cell of the lattice is assigned a state (typically from a finite set) representing, for example, the number of particles in that approximate position or the magnetic field vector resulting from that piece of the material.

The similarity to our framework is already apparent. In both cellular automata and lattice statistical mechanics, the space $S^{\mathbb{L}}$ (or its subspaces) serves as the overall state space of the system. The concepts of observables, potential differences and interaction potentials in our formalism are borrowed from statistical mechanics. In fact, Takesue's early study of conservation laws in cellular automata was motivated by problems of statistical mechanics [79].

This chapter is dedicated to the connection between conservation laws and equilibrium states in reversible and surjective cellular automata. An *equilibrium state* of a statistical mechanics system refers to a probability measure that describes a typical state of the system in equilibrium. In equilibrium statistical mechanics, the model does not include any dynamics. Rather, the system is microscopically modeled via its Hamiltonian. The Hamiltonian, which corresponds to our concept of potential difference, is specified by assigning energy to the interaction of different parts of the system, corresponding to interaction potentials in our setting. The equilibrium states are then (macroscopically) identified via a variational principle, as is customary in the classical approach to physics. A fundamental theorem

of equilibrium statistical mechanics due to Dobrushin, Lanford and Ruelle characterizes the equilibrium states as the translation-invariant Gibbs measures associated with the Hamiltonian of the system.

In cellular automata, the equilibrium condition is naturally understood as time-invariance. It turns out, as one might expect, that in surjective CA, the equilibrium states as offered by the variational principle are indeed invariant (at least in some suitable sense). In reversible CA, even more can be said: a Gibbs measure is invariant (in the same suitable sense) if and only if it is associated with a conserved potential difference. Curiously, the latter has a simple proof independent of the above-mentioned fundamental theorem.

In Section 5.1 we will review the basic theory of Gibbs measures. Each Gibbs measure is defined by means of a local potential difference. Alternatively, these are the measures satisfying a certain Markovian property. In particular, the one-dimensional Gibbs measures coincide with the usual notion of Markov chains. Next, in Section 5.2, we prove the correspondence between conservation laws and Gibbs measures in reversible CA. One direction of this correspondence can be extended to one-dimensional surjective CA. For general surjective CA, an even more general correspondence can be proved in the almost sure sense. This is done in Section 5.3. Finally, in Section 5.4, we exploit the fundamental theorem of equilibrium statistical mechanics to prove one direction of the correspondence for general surjective CA.

5.1 Gibbs-Markov Measures

In this section, we review the definition of Gibbs-Markov measures and some basic facts about them. Gibbs measures were introduced by Dobrushin, Lanford and Ruelle in the late 1960's, as a natural extension of the Gibbs distribution to infinite lattices (see e.g., [31, 77, 78, 74, 37]). Soon after, it was shown by Averintsev and Spitzer that Gibbs measures are exactly those measures that satisfy certain a Markovian property (see e.g. [74, 37]). Here, we define these measures using this Markovian property and show their connection with potential differences.

Let $M \subseteq \mathbb{L}$ be a finite neighborhood. A *Markov* measure on $S^{\mathbb{L}}$ with neighborhood M is a Borel probability measure $\pi : \mathscr{B} \to [0,1]$ with the following property: for each finite set $D \subseteq \mathbb{L}$, and each finite pattern $p : E \to S$, where $E \supseteq M(D)$ and $\pi([p]_{E \setminus D}) > 0$, we have

$$\pi\left([p]_D \mid [p]_{E \setminus D}\right) = \pi\left([p]_D \mid [p]_{\partial M(D)}\right) \ . \tag{5.1}$$

(Recall that $\partial M(D) = M(D) \setminus D$ denotes the M-boundary of D.) We say that π is *locally Markovian* if (5.1) holds for all singletons $D = \{i\}$.

If π is a Markov measure with neighborhood M, the collection of conditional probabilities $\pi([p] \mid [\partial p])$, for finite $p : D \to S$ and $\partial p : \partial M(D) \to S$ with $\pi([\partial p]) > 0$, is called the (conditional) *specification*[1] of π. More generally, let M be an arbitrary neighborhood and suppose that for each finite set $D \subseteq \mathbb{L}$ and each pattern $\partial p : \partial M(D) \to S$, we are given a probability distribution $\gamma_D(\cdot \mid \partial p) : S^D \to [0,1]$. The family $\gamma = \{\gamma_D(\cdot \mid \partial p)\}_{D,\partial p}$ is called a *Markovian specification* if for all finite sets of cells D and $E \supseteq D$, and for each pattern $w : M(E) \to S$, it satisfies the consistency equation:

$$\gamma_E\left(q \mid \partial q\right) = \left[\sum_{p' : D \to S} \gamma_E\left(p' \vee r \mid \partial q\right)\right] \cdot \gamma_D\left(p \mid \partial p\right) \ , \tag{5.2}$$

where $q \triangleq w|_E$, $\partial q \triangleq w|_{\partial M(E)}$, $p \triangleq w|_D$, $\partial p \triangleq w|_{\partial M(D)}$, and $r \triangleq w|_{E \setminus D}$. A *positive* specification is one with non-zero values. A specification γ with neighborhood M is *translation-invariant* if

$$\gamma_{i+D}(\sigma^{-i}p \mid \sigma^{-i}\partial p) = \gamma_D(p \mid \partial p) \tag{5.3}$$

for every $i \in \mathbb{L}$, and for all finite $p : D \to S$ and $\partial p : \partial M(D) \to S$. We say that a probability measure π is *specified* by (or is *compatible* with) γ if for all finite sets D and $E \supseteq M(D)$, and for each finite pattern $p : E \to S$ with $\pi([p]_{E \setminus D}) > 0$, we have

$$\pi([p]_D \mid [p]_{E \setminus D}) = \gamma_D\left(p|_D \,\middle|\, p|_{\partial M(D)}\right) \ . \tag{5.4}$$

Clearly, every probability measure specified by a Markovian specification is a Markov measure.

Proposition 5.1 (see e.g. [31, 74])**.** *For every [translation-invariant] Markovian specification γ, there is at least one [translation-invariant] measure π compatible with γ.*

Proof. Let M be the neighborhood of γ. Let $\diamond \in S$ be an arbitrary state and $\diamondsuit$ the $\diamond$-uniform configuration. We prove the existence of a measure compatible with γ using the compactness of the space $\mathscr{M}$. We choose $\diamondsuit$ as the boundary condition, and construct measures in $\mathscr{M}$ which are compatible with γ on larger and larger finite sets.

For a finite set $A \subseteq \mathbb{L}$, let us define the measure π_A such that outside A, all its probability mass is concentrated on $\diamondsuit|_{\mathbb{L} \setminus A}$, while inside A it agrees with $\gamma_A(\cdot \mid \diamondsuit|_{\partial M(A)})$. Namely, for every $E \supseteq M(A)$ and every $p : E \to S$, let

$$\pi_A([p]_E) \triangleq \begin{cases} \gamma\left(p|_A \,\middle|\, \diamondsuit|_{\partial M(A)}\right) & \text{if } p|_{E \setminus A} = \diamondsuit|_{E \setminus A}, \\ 0 & \text{otherwise.} \end{cases} \tag{5.5}$$

[1] Such conditional specifications can also be defined for arbitrary measures, which however involves technical difficulties that are irrelevant to our discussion. See [31].

This clearly defines a probability measure, because $\gamma_A(\cdot \mid \Diamond|_{\partial M(A)})$ is a probability distribution. Note that it automatically follows from this definition that for every D and $E \supseteq M(D)$ with $E \subseteq A$, and for all $p : E \to S$ with $\pi_A([p]_{E\setminus D}) > 0$, π_A satisfies (5.4). This is guaranteed by the consistency condition (5.2) of Markovian specifications. Namely, let $q : M(A) \to S$ be any extension of p with $\pi_A([q]_{M(A)\setminus D}) > 0$. We have

$$\pi_A([q]_D \mid [q]_{M(A)\setminus D}) = \frac{\pi_A([q]_A \mid [q]_{\partial M(A)})}{\pi_A([q]_{A\setminus D} \mid [q]_{\partial M(A)})} \tag{5.6}$$

$$= \frac{\gamma_A\left(q|_A \,\middle|\, q|_{\partial M(A)}\right)}{\sum_{p':D\to S} \gamma_A\left(q|_{A\setminus D} \vee p' \,\middle|\, q|_{\partial M(A)}\right)} \tag{5.7}$$

$$= \gamma_D\left(p|_D \,\middle|\, p|_{\partial M(D)}\right) \ . \tag{5.8}$$

It follows that

$$\pi_A([p]_D \mid [p]_{E\setminus D}) = \sum_{r:M(A)\setminus E\to S} \pi_A([r]_{M(A)\setminus E}) \cdot \pi_A([p]_D \mid [p \vee r]_{M(A)\setminus D}) \tag{5.9}$$

$$= \sum_{r:M(A)\setminus E\to S} \pi_A([r]_{M(A)\setminus E}) \cdot \gamma_D\left(p|_D \,\middle|\, p|_{\partial M(D)}\right) \tag{5.10}$$

$$= \gamma_D\left(p|_D \,\middle|\, p|_{\partial M(D)}\right) \ . \tag{5.11}$$

Now, consider the sequence $\{\pi_{I_n}\}_n$, where, as usual, $I_n \triangleq [-n, n]^d$ denotes the central hyper-cube with sides of length $2n + 1$ on $\mathbb{L}$. Since $\mathscr{M}$ is compact, there is a sequence $0 < n_1 < n_2 < \cdots$ such that the subsequence $\{\pi_{I_{n_i}}\}_i$ converges to a measure $\pi \in \mathscr{M}$. We claim that π is compatible with γ.

Let us use the shorthand $\pi_i \triangleq \pi_{I_{n_i}}$. Let D and $E \supseteq M(D)$ be finite sets and $p : E \to S$ a pattern with $\pi([p]_{E\setminus D}) > 0$. Then $\pi_i([p]_{E\setminus D}) > 0$ for all sufficiently large i. On the other hand, for sufficiently large i, I_{n_i} contains E. Therefore,

$$\pi([p]_D \mid [p]_{E\setminus D}) = \lim_{i\to\infty} \pi_i([p]_D \mid [p]_{E\setminus D}) \tag{5.12}$$

$$= \lim_{i\to\infty} \gamma_D\left(p|_D \,\middle|\, p|_{E\setminus D}\right) \tag{5.13}$$

$$= \gamma_D\left(p|_D \,\middle|\, p|_{E\setminus D}\right) \ . \tag{5.14}$$

Therefore, π is compatible with γ.

Next, suppose that γ is translation-invariant. Let $\mathscr{G}$ be the set of measures compatible with γ. The set $\mathscr{G}$ is a non-empty, closed, convex, and translation-invariant subset of $\mathscr{M}$. Choose an arbitrary element π of $\mathscr{G}$. For every finite $D \subseteq \mathbb{L}$, the measure

$$\nu_D \triangleq \frac{\sum_{i\in D} \sigma^i \pi}{|D|} \tag{5.15}$$

is in $\mathscr{G}$. Consider the sequence $\{\nu_{I_m}\}_m$. Since $\mathscr{M}$ is compact, there is a sequence $0 < m_1 < m_2 < \cdots$ such that the sequence $\{\nu_{I_{m_i}}\}_i$ converges. Since $\mathscr{G}$ is closed, the limit measure ν is also in $\mathscr{G}$. We claim that ν is translation-invariant.

Let $p : D \to S$ be an arbitrary pattern and $k \in \mathbb{L}$. For $m > 0$, we have

$$\nu_{I_m}(\sigma^{-k}[p]) - \nu_{I_m}([p]) = \frac{\sum_{i\in I_m}\left[\pi(\sigma^{-k-i}[p]) - \pi(\sigma^{-i}[p])\right]}{|I_m|} \tag{5.16}$$

$$= \frac{\sum_{i\in (k+I_m)\setminus I_m}\pi(\sigma^{-i}[p])}{|I_m|} \tag{5.17}$$

$$- \frac{\sum_{i\in I_m\setminus (k+I_m)}\pi(\sigma^{-i}[p])}{|I_m|} \tag{5.18}$$

$$= \frac{o(|I_m|)}{|I_m|}\ . \tag{5.19}$$

Therefore,

$$(\sigma^k\nu)([p]) - \nu([p]) = \lim_{i\to\infty}\nu_{I_{m_i}}(\sigma^{-k}[p]) - \lim_{i\to\infty}\nu_{I_{m_i}}([p]) \tag{5.20}$$

$$= \lim_{i\to\infty}\left[\nu_{I_{m_i}}(\sigma^{-k}[p]) - \nu_{I_{m_i}}([p])\right] \tag{5.21}$$

$$= 0\ . \tag{5.22}$$

Hence ν is translation-invariant. □

Proposition 5.2 (e.g. [20]). *A positive Markovian specification γ is uniquely determined by those of its elements $\gamma_D(\cdot \,|\, \partial p)$ in which D is singleton.*

Proof. Let $\breve{\gamma}$ denote the family $\{\gamma_i(\cdot \,|\, \partial p)\}_{i,\partial p}$. The claim is that $\breve{\gamma}$ uniquely determines γ.

Let M be the neighborhood of γ and $D \subseteq \mathbb{L}$ any finite set. By the consistency condition of γ, for a pattern $p : M(D) \to S$ and a cell $i \in D$, we can write

$$\gamma_D\left(p|_D \,\middle|\, p|_{\partial M(D)}\right) = \gamma_D\left(p|_{D\setminus i} \,\middle|\, p|_{\partial M(D)}\right)\cdot\gamma_i\left(p|_i \,\middle|\, p|_{\partial M(i)}\right)\ , \tag{5.23}$$

where we have used the natural shorthand

$$\gamma_D\left(p|_{D\setminus i} \,\middle|\, p|_{\partial M(D)}\right) \triangleq \sum_{r:\{i\}\to S}\gamma_D\left(p|_{D\setminus i}\vee r \,\middle|\, p|_{\partial M(D)}\right)\ . \tag{5.24}$$

Therefore, if $p' : M(D) \to S$ is any other pattern which agrees with p everywhere except on i, the value

$$\frac{\gamma_D\left(p'|_D \,\middle|\, p'|_{\partial M(D)}\right)}{\gamma_D\left(p|_D \,\middle|\, p|_{\partial M(D)}\right)} = \frac{\gamma_i\left(p'|_i \,\middle|\, p'|_{\partial M(i)}\right)}{\gamma_i\left(p|_i \,\middle|\, p|_{\partial M(i)}\right)} \tag{5.25}$$

is uniquely determined by $\breve{\gamma}$.

Since D is finite, we have that for every two patterns $x, y \in S^D$, there is a finite sequence $x = x_0, x_1, \ldots, x_k = y$ of elements of S^D such that x_i and x_{i+1} agree everywhere but on a single cell. It follows that for every $x, y \in S^D$, the value

$$c(x,y) \triangleq \frac{\gamma_D\left(y \,\middle|\, p|_{\partial M(D)}\right)}{\gamma_D\left(x \,\middle|\, p|_{\partial M(D)}\right)} \tag{5.26}$$

is uniquely determined by $\breve{\gamma}$.

It is easy to see that the system of equations

$$h(y) = c(x,y) \cdot h(x) \quad (\forall x, y \in S^D) \,, \tag{5.27}$$

$$\sum_{x \in S^D} h(x) = 1 \,, \tag{5.28}$$

has exactly one solution $h : S^D \to [0,1]$. Hence the value

$$\gamma_D\left(x \,\middle|\, p|_{\partial M(D)}\right) = h(x) \tag{5.29}$$

is uniquely determined by $\breve{\gamma}$. □

Corollary 5.3. *Every full-support locally Markovian measure is a Markov measure.*

A full-support Markov measure has a positive specification. The converse, however, is not true in general; a measure compatible with a positive specification is not necessarily full-support. Similarly, the specification of a translation-invariant Markov measure is clearly translation-invariant, but a Markov measure with a translation-invariant specification does not need to be translation-invariant. There is a nice connection between positive translation-invariant Markovian specifications and local potential differences.

Proposition 5.4 (see e.g. [37])**.** *There is a one-to-one correspondence $\gamma \leftrightarrow \Delta$ between positive translation-invariant Markovian specifications and local potential differences on $S^{\mathbb{L}}$.*

Proof. Let $\Delta \in \mathscr{D}$ be a local potential difference with neighborhood $M \subseteq \mathbb{L}$ on $S^{\mathbb{L}}$. Let $\diamond \in S$ be an arbitrary state and $\diamondsuit$ the $\diamond$-uniform configuration. For all finite patterns $p : D \to S$ and $\partial p : \partial M(D) \to S$, define

$$\gamma_D(p \,|\, \partial p) \triangleq Z_{D,\partial p}^{-1} \cdot 2^{-\Delta(\zeta_{\partial p}\diamondsuit, \zeta_p \zeta_{\partial p}\diamondsuit)} \,, \tag{5.30}$$

where

$$Z_{D,\partial p} \triangleq \sum_{q : D \to S} 2^{-\Delta(\zeta_{\partial p}\diamondsuit, \zeta_q \zeta_{\partial p}\diamondsuit)} \,. \tag{5.31}$$

(The normalizing constant $Z_{D,\partial p}$ is often called the *partition function*.)

In order to show that $\gamma \triangleq \{\gamma_D(\cdot \,|\, \partial p)\}_{D,\partial p}$ is a Markovian specification, we need to prove that it satisfies the consistency equations (5.2). Let D and $E \supseteq D$ be finite, let $w : M(E) \to S$ be a pattern, and suppose that q, ∂q, p, ∂p and r are defined as in (5.2). Since Δ is a local potential difference, for every $p' : D \to S$ we have

$$\begin{aligned}\Delta(\zeta_{\partial q}\diamondsuit, \zeta_{p'}\zeta_r\zeta_{\partial q}\diamondsuit) &= \Delta(\zeta_{\partial q}\diamondsuit, \zeta_r\zeta_{\partial q}\diamondsuit) + \Delta(\zeta_r\zeta_{\partial q}\diamondsuit, \zeta_{p'}\zeta_r\zeta_{\partial q}\diamondsuit) &(5.32)\\ &= \Delta(\zeta_{\partial q}\diamondsuit, \zeta_r\zeta_{\partial q}\diamondsuit) + \Delta(\zeta_{\partial p}\diamondsuit, \zeta_{p'}\zeta_{\partial p}\diamondsuit)\ . &(5.33)\end{aligned}$$

Therefore,

$$\begin{aligned}&\sum_{p':D\to S} \gamma_E\left(p' \vee r \,|\, \partial q\right) &(5.34)\\ &= Z_{E,\partial q}^{-1} \cdot \sum_{p':D\to S} 2^{-\Delta(\zeta_{\partial q}\diamondsuit, \zeta_{p'}\zeta_r\zeta_{\partial q}\diamondsuit)} &(5.35)\\ &= Z_{E,\partial q}^{-1} \cdot 2^{-\Delta(\zeta_{\partial q}\diamondsuit, \zeta_r\zeta_{\partial q}\diamondsuit)} \cdot \sum_{p':D\to S} 2^{-\Delta(\zeta_{\partial p}\diamondsuit, \zeta_{p'}\zeta_{\partial p}\diamondsuit)} &(5.36)\\ &= Z_{E,\partial q}^{-1} \cdot 2^{-\Delta(\zeta_{\partial q}\diamondsuit, \zeta_r\zeta_{\partial q}\diamondsuit)} \cdot Z_{D,\partial p}\ , &(5.37)\end{aligned}$$

and so

$$\begin{aligned}&\left[\sum_{p':D\to S} \gamma_E\left(p' \vee r \,|\, \partial q\right)\right] \cdot \gamma_D\left(p \,|\, \partial p\right) &(5.38)\\ &= \left[Z_{E,\partial q}^{-1} \cdot 2^{-\Delta(\zeta_{\partial q}\diamondsuit, \zeta_r\zeta_{\partial q}\diamondsuit)} \cdot Z_{D,\partial p}\right] \cdot Z_{D,\partial p}^{-1} \cdot 2^{-\Delta(\zeta_{\partial p}\diamondsuit, \zeta_p\zeta_{\partial p}\diamondsuit)} &(5.39)\\ &= Z_{E,\partial q}^{-1} \cdot 2^{-\Delta(\zeta_{\partial q}\diamondsuit, \zeta_r\zeta_{\partial q}\diamondsuit) - \Delta(\zeta_{\partial p}\diamondsuit, \zeta_p\zeta_{\partial p}\diamondsuit)} &(5.40)\\ &= Z_{E,\partial q}^{-1} \cdot 2^{-\Delta(\zeta_{\partial q}\diamondsuit, \zeta_q\zeta_{\partial q}\diamondsuit)} &(5.41)\\ &= \gamma_E(q \,|\, \partial q)\ . &(5.42)\end{aligned}$$

Hence, γ is a Markovian specification. That γ is positive is trivial. That γ is translation-invariant follows from the fact that Δ is translation-invariant.

Next, let γ be a positive translation-invariant Markovian specification with neighborhood M. For every two asymptotic configurations x and y with $D \triangleq \{i : x[i] \neq y[i]\}$, define

$$\Delta(x, y) \triangleq -\log \frac{\gamma_D\left(y|_D \,\middle|\, y|_{\partial M(D)}\right)}{\gamma_D\left(x|_D \,\middle|\, x|_{\partial M(D)}\right)}\ . \tag{5.43}$$

It is easy to see that Δ is a potential difference. Since γ is positive, Δ is defined for all asymptotic pairs of configurations. Since γ is translation-invariant, so is Δ. Let $p : D \to S$ be a finite pattern, and let x and y be two

configurations that agree on $M(D)$. We have

$$\Delta(y, \zeta_p y) = -\log \frac{\gamma_D\left(p \,\middle|\, y|_{\partial M(D)}\right)}{\gamma_D\left(y|_D \,\middle|\, y|_{\partial M(D)}\right)} \tag{5.44}$$

$$= -\log \frac{\gamma_D\left(p \,\middle|\, x|_{\partial M(D)}\right)}{\gamma_D\left(x|_D \,\middle|\, x|_{\partial M(D)}\right)} \tag{5.45}$$

$$= \Delta(x, \zeta_p x)\,. \tag{5.46}$$

Therefore, Δ is local.

Finally, it is easy to see that γ is the specification associated to Δ if and only if Δ is the potential difference derived from γ. □

Let $\Delta \in \mathscr{D}$ be a local potential difference on $S^{\mathbb{L}}$ with neighborhood M. A *Gibbs* measure with potential Δ is a probability measure $\pi \in \mathscr{M}$ such that for every two asymptotic configurations x and y, with $D \triangleq \{i : x[i] \neq y[i]\}$, and for every finite set $E \supseteq M(D)$ with $\pi([x]_{E\setminus D}) > 0$, we have

$$\pi\left([y]_D \,|\, [y]_{E\setminus D}\right) = 2^{-\Delta(x,y)} \cdot \pi\left([x]_D \,|\, [x]_{E\setminus D}\right)\,. \tag{5.47}$$

From the proof of Proposition 5.4, we know that Gibbs measures (in our setting) are exactly those Markov measures which have positive translation-invariant specifications. For such measures we may interchangeably use the names Gibbs or Markov measures. From now on, we shall work only with positive, translation-invariant Markovian specifications, which we may call simply specifications.

Lemma 5.5. *Let $\pi \in \mathscr{M}$ be a Gibbs measure with local potential difference $\Delta \in \mathscr{D}$. Let x and y be asymptotic configurations in the support of π, where $D \triangleq \{i : x[i] \neq y[i]\}$ and $q \triangleq y|_D$.*

a) For every finite $A \supseteq D$ and $B \supseteq M(A)$, we have

$$\Delta(x, y) = -\log \frac{\pi\left([y]_A \,\middle|\, [y]_{B\setminus A}\right)}{\pi\left([x]_A \,\middle|\, [x]_{B\setminus A}\right)} = -\log \frac{\pi\left([y]_B\right)}{\pi\left([x]_B\right)}\,. \tag{5.48}$$

b) For every Borel set $U \subseteq [x]_{M(D)}$ with $\pi(U) > 0$, we have

$$\Delta(x, y) = -\log \frac{\pi(\zeta_q U)}{\pi(U)} = -\log \pi(\zeta_q U) + \log \pi(U)\,. \tag{5.49}$$

Proof.

a) We have

$$\frac{\pi\left([y]_B\right)}{\pi\left([x]_B\right)} = \frac{\pi\left([y]_{B\setminus A}\right)\cdot\pi\left([y]_A \,\middle|\, [y]_{B\setminus A}\right)}{\pi\left([x]_{B\setminus A}\right)\cdot\pi\left([x]_A \,\middle|\, [x]_{B\setminus A}\right)} = \frac{\pi\left([y]_A \,\middle|\, [y]_{B\setminus A}\right)}{\pi\left([x]_A \,\middle|\, [x]_{B\setminus A}\right)}\ , \tag{5.50}$$

because $y|_{B\setminus A} = x|_{B\setminus A}$. This is true in particular for $A = D$.

b) First suppose that U is open. Then U is a countable union of disjoint cylinders, and we can write

$$U = \bigcup_{(\alpha,A)\in J} [\alpha]_A\ , \tag{5.51}$$

where J is a countable set consisting of pairs (α, A), where $A \supseteq M(D)$ is a finite set and $\alpha : A \to S$ a pattern that agrees with x on $M(D)$. Similarly, $\zeta_q U$ can be written as the disjoint union

$$\zeta_q U = \bigcup_{(\alpha,A)\in J} [\zeta_q\alpha]_A\ . \tag{5.52}$$

Note that for every $(\alpha, A) \in J$, we have on the one hand $\alpha|_{M(D)} = x|_{M(D)}$ and $(\zeta_q\alpha)|_{M(D)} = y|_{M(D)}$, and on the other hand $(\zeta_q\alpha)|_{A\setminus D} = \alpha|_{A\setminus D}$. So we can write

$$\begin{aligned}
\frac{\pi(\zeta_q U)}{\pi(U)} &= \frac{\sum_{(\alpha,A)\in J}\pi\left([\zeta_q\alpha]_A\right)}{\sum_{(\alpha,A)\in J}\pi\left([\alpha]_A\right)} && (5.53)\\
&= \frac{\sum_{(\alpha,A)\in J}\pi\left([\zeta_q\alpha]_{A\setminus D}\right)\cdot\pi\left([\zeta_q\alpha]_D \,\middle|\, [\zeta_q\alpha]_{\partial M(D)}\right)}{\sum_{(\alpha,A)\in J}\pi\left([\alpha]_{A\setminus D}\right)\cdot\pi\left([\alpha]_D \,\middle|\, [\alpha]_{\partial M(D)}\right)} && (5.54)\\
&= \frac{\pi\left([y]_D \,\middle|\, [y]_{\partial M(D)}\right)\cdot\sum_{(\alpha,A)\in J}\pi\left([\zeta_q\alpha]_{A\setminus D}\right)}{\pi\left([x]_D \,\middle|\, [x]_{\partial M(D)}\right)\cdot\sum_{(\alpha,A)\in J}\pi\left([\alpha]_{A\setminus D}\right)} && (5.55)\\
&= \frac{\pi\left([y]_D \,\middle|\, [y]_{\partial M(D)}\right)}{\pi\left([x]_D \,\middle|\, [x]_{\partial M(D)}\right)}\ . && (5.56)
\end{aligned}$$

We obtain that

$$-\log\frac{\pi(\zeta_q U)}{\pi(U)} = \Delta(x,y)\ . \tag{5.57}$$

For an arbitrary Borel set $U \subseteq [x]_{M(D)}$, the result follows from the regularity of π. Let $[x]_{M(D)} \supseteq E_1 \supseteq E_2 \supseteq \cdots \supseteq U$ be a sequence of open sets such that

$$\pi(U) = \lim_{i\to\infty}\pi(E_i)\ , \qquad \text{and} \qquad \pi(\zeta_q U) = \lim_{i\to\infty}\pi(\zeta_q E_i)\ . \tag{5.58}$$

We have

$$-\log \frac{\pi(\zeta_q U)}{\pi(U)} = -\log \frac{\lim_{i\to\infty} \pi(\zeta_q E_i)}{\lim_{i\to\infty} \pi(E_i)} \tag{5.59}$$

$$= \lim_{i\to\infty} -\log \frac{\pi(\zeta_q E_i)}{\pi(E_i)} \tag{5.60}$$

$$= \Delta(x, y) \ . \tag{5.61}$$

□

Let γ be a positive, translation-invariant Markovian specification, and let Δ the corresponding potential difference. The collection of probability measures compatible with γ is denoted by $\mathscr{G}(\gamma)$ or $\mathscr{G}(\Delta)$. The set of translation-invariant elements of $\mathscr{G}(\gamma)$ is denoted by $\mathscr{G}_\sigma(\gamma)$ or $\mathscr{G}_\sigma(\Delta)$. In general, $\mathscr{G}(\Delta)$ (and $\mathscr{G}_\sigma(\Delta)$) may contain more than one element. This is interpreted in statistical mechanics, as the possibility of the existence of multiple phases into which a system in equilibrium can settle (see [78, 31, 32]). The sets $\mathscr{G}(\Delta)$ and $\mathscr{G}_\sigma(\Delta)$ are clearly convex and compact. The extreme elements of $\mathscr{G}(\Delta)$ are called the *phases* of γ (or of the system it is modeling).[2] See Appendix B for an example of a Markovian specification with multiple phases. On the other hand, the extreme elements of $\mathscr{G}_\sigma(\Delta)$ are exactly those which are σ-ergodic (see [31, 77]).

One-dimensional Markov measures agree with the usual notion of finite-state (time-invariant) Markov chains. A Markov chain with memory $m \geq 0$ is identified by its probability distribution — a probability measure π on $S^{\mathbb{Z}}$ which satisfies the *one-sided* Markov property: for every two patterns $w : [a, b] \to S$ and $u : [a - l, a) \to S$ with $a \leq b$ and $l \geq m$, we have

$$\pi\left([w]_{[a,b]} \,|\, [u]_{[a-l,a)}\right) = \pi\left([w]_{[a,b]} \,|\, [u]_{[a-m,a)}\right) \ , \tag{5.62}$$

provided $\pi([u]_{[a-l,a)}) > 0$. The transition probabilities of a time-invariant Markov chain are summarized in its transition matrix $P = [P(u, v)]_{u,v\in S^m}$. This is an *m-stochastic* matrix;[3] that is, $P(u, v) = 0$, unless $ub = av$ for some $a, b \in S$, while $\sum_{b\in S} P(aw, wb) = 1$ for all $a \in S$ and $w \in S^{m-1}$. If the matrix P is also *m-positive*, that is, if all the transition probabilities $P(aw, wb)$ (for $a, b \in S$ and $w \in S^{m-1}$) are positive, it uniquely determines the measure π. Specifically, in this case P is primitive, that is, $P^n > 0$ for some $n > 0$, and according to Perron-Frobenius Theorem (see e.g. [30]), there is a unique positive probability vector $\nu : S^m \to [0, 1]$ such that

[2] See [32] for the beautiful justification of the name.

[3] Non-standard term.

$\nu P = \nu$. The measure π is uniquely identified via

$$\begin{aligned}\pi([w]_{[i,j)}) = \nu(w|_{[i,i+m)}) &\cdot P(w|_{[i,i+m)}, w|_{[i+1,i+m+1)}) \\ &\cdot P(w|_{[i+1,i+m+1)}, w|_{[i+2,i+m+2)}) \\ &\cdot \dots \\ &\cdot P(w|_{[j-m-1,j-1)}, w|_{[j-m,j)})\end{aligned} \tag{5.63}$$

for all $w : [i, j) \to S$ with $i + m \leq j$. In particular, π is translation-invariant and full-support.

Proposition 5.6 (see e.g. [31, 37])**.** *The distribution of a Markov chain with memory m is a Markov measure with neighborhood $[-m, m]$.*

Proof. Let π be the distribution of a Markov chain with memory $m \geq 0$. Let $M \triangleq [-m, m]$. Let $D \subseteq \mathbb{Z}$ and $E \supseteq M(D)$ be finite, and let $p : E \to S$ an arbitrary pattern with $\pi\left([p]_{E\setminus D}\right) > 0$. Without loss of generality, we can assume that $D = [a, b]$ and $E = [a - l, b + r]$, where $a \leq b$ and $l, r \geq m$. Let $u \triangleq p|_{[a-l,a)}$, $w \triangleq p|_{[a,b]}$ and $v \triangleq p|_{(b,b+r]}$. Let $\hat{u} \triangleq u|_{[a-m,a)}$ and $\hat{v} \triangleq v|_{(b,b+m]}$. For brevity, let us write $\pi(w)$ for $\pi([w]_{[a,b]})$, and so forth. We have

$$\pi(w \,|\, u \vee v) = \frac{\pi(u \vee w \vee v)}{\pi(u \vee v)} \tag{5.64}$$

$$= \frac{\pi(u \vee w \vee v)}{\sum_{w':[a,b]\to S} \pi(u \vee w' \vee v)} \tag{5.65}$$

$$= \frac{\pi(u) \cdot \pi(w \vee \hat{v} \,|\, \hat{u}) \cdot \pi(v \,|\, \hat{v})}{\sum_{w':[a,b]\to S} \pi(u) \cdot \pi(w' \vee \hat{v} \,|\, \hat{u}) \cdot \pi(v \,|\, \hat{v})} \tag{5.66}$$

$$= \frac{\pi(\hat{u}) \cdot \pi(w \vee \hat{v} \,|\, \hat{u})}{\sum_{w':[a,b]\to S} \pi(\hat{u}) \cdot \pi(w' \vee \hat{v} \,|\, \hat{u})} \tag{5.67}$$

$$= \pi(w \,|\, \hat{u} \vee \hat{v}) \,. \tag{5.68}$$

Therefore, π is a Markov measure with neighborhood $[-m, m]$. □

The converse has more dramatic implications for us. We state it without the proof.

Theorem 5.7 (see e.g. [31])**.** *Every one-dimensional Markov measure π with neighborhood $[-m, m]$ and positive, translation-invariant specification is the distribution of a Markov chain with memory m. Moreover, the specification of π uniquely determines the transition matrix of the associated Markov chain.*

Corollary 5.8. *Every one-dimensional, positive, translation-invariant, Markovian specification has a unique phase which is translation-invariant.*

Remark 5.1. Let π be the unique measure specified by a one-dimensional, positive, translation-invariant Markovian specification γ with neighborhood $[-m, m]$, where $m > 0$. By Theorem 5.7, π is the distribution of a Markov chain with memory m. The potential difference Δ, corresponding to γ, has a simple form in terms of the transition matrix of the Markov chain. Namely, it is easy to verify that an observable with local assignment

$$g(awb) \triangleq -\log \pi(wb \,|\, aw) \qquad \text{(for all } a, b \in S \text{ and } w \in S^{m-1}) \tag{5.69}$$

generates Δ. When $m = 0$ (i.e., when π is a Bernoulli measure), Δ can be generated by an observable with local assignment

$$g(a) \triangleq -\log \pi(a) \qquad \text{(for all } a \in S) \ . \tag{5.70}$$

○

5.2 Conservation Laws and Invariant Gibbs Measures

In this section, we will show that the correspondence given by Proposition 5.4 is respected by reversible cellular automata. In particular, for every "locally" invariant Gibbs measure, there is a corresponding conservation law, and vice versa. By *locally* invariant, we mean here that π and $F\pi$ have the same Markovian specification. We do not know if the same correspondence holds for surjective CA in general; we will, however, prove some partial results.

The following theorem was proved by Ruelle [77] in a slightly different, more general setup. Let $\mathscr{G}^+(\Delta)$ denote the set of full-support elements of $\mathscr{G}(\Delta)$.

Theorem 5.9 ([77]). *Let F be a reversible cellular automaton and Δ a local potential difference. Then F conserves Δ if and only if it maps $\mathscr{G}^+(\Delta)$ into itself.*

Proof. Let γ be the Markovian specification corresponding to Δ. Let M be the neighborhood of Δ and N' the neighborhood of F^{-1}. Since π is full-support, so is $F\pi$.

[$\Leftarrow$] Let $F\pi$ be also a Gibbs measure with potential Δ, that is, a Markov measure with specification γ. Let x and y be asymptotic configurations, and let $x' \triangleq Fx$ and $y' \triangleq Fy$. Let $D \triangleq \{i : x[i] \neq y[i]\}$ and $D' \triangleq \{i : x'[i] \neq y'[i]\}$. Note that $D \subseteq N'^{-1}(D')$. Let $B \supseteq N'\left(N'^{-1}(D')\right)$ be a finite set. Clearly $F^{-1}[x']_{M(B)} \subseteq [x]_{M(D)}$ and $F^{-1}[y']_{M(B)} \subseteq [y]_{M(D)}$.

Let $q \triangleq y|_D$. Let us verify that $\zeta_q F^{-1}[x']_{M(B)} = F^{-1}[y']_{M(B)}$. Let $\bar{x} \in F^{-1}[x']_{M(B)}$. If $q' \triangleq y'|_{D'}$, we have $\zeta_{q'} F\bar{x} \in [y']_{M(B)}$. We claim that $\zeta_{q'} F\bar{x} = F\zeta_q \bar{x}$. We have $(\zeta_{q'} F\bar{x})|_{N'(N'^{-1}(D'))} = y'|_{N'(N'^{-1}(D'))}$. Therefore,

$$(F^{-1}\zeta_{q'} F\bar{x})|_{N'^{-1}(D')} = y|_{N'^{-1}(D')} = (\zeta_q \bar{x})|_{N'^{-1}(D')} \ . \tag{5.71}$$

On the other hand, we have $(\zeta_{q'} F\bar{x})|_{\mathbb{L}\setminus D'} = \bar{x}|_{\mathbb{L}\setminus D'}$, which implies

$$(F^{-1}\zeta_{q'} F\bar{x})|_{\mathbb{L}\setminus N'^{-1}(D')} = \bar{x}|_{\mathbb{L}\setminus N'^{-1}(D')} = (\zeta_q \bar{x})|_{\mathbb{L}\setminus N'^{-1}(D')} \ . \tag{5.72}$$

All in all, we have $\zeta_{q'} F\bar{x} = F\zeta_q \bar{x}$. Therefore, $\zeta_q F^{-1}[x']_{M(B)} \subseteq F^{-1}[y']_{M(B)}$. Similarly, if $p \triangleq x|_D$, we obtain that $\zeta_p F^{-1}[y']_{M(B)} \subseteq F^{-1}[x']_{M(B)}$. But for every $\bar{y} \in F^{-1}[y']_{M(B)}$ we have $\zeta_q \zeta_p \bar{y} = \bar{y}$. Therefore $F^{-1}[y']_{M(B)} \subseteq \zeta_q F^{-1}[x']_{M(B)}$. We conclude that $\zeta_q F^{-1}[x']_{M(B)} = F^{-1}[y']_{M(B)}$.

By Lemma 5.5 we can write

$$\begin{aligned}
\Delta(Fx, Fy) &= -\log \frac{\pi\left([y']_B \,\middle|\, [y']_{\partial M(B)}\right)}{\pi\left([x']_B \,\middle|\, [x']_{\partial M(B)}\right)} && (5.73)\\
&= -\log \frac{(F\pi)\left([y']_B \,\middle|\, [y']_{\partial M(B)}\right)}{(F\pi)\left([x']_B \,\middle|\, [x']_{\partial M(B)}\right)} && (5.74)\\
&= -\log \frac{(F\pi)\left([y']_{M(B)}\right)}{(F\pi)\left([x']_{M(B)}\right)} && (5.75)\\
&= -\log \frac{\pi\left(F^{-1}[y']_{M(B)}\right)}{\pi\left(F^{-1}[x']_{M(B)}\right)} && (5.76)\\
&= \Delta(x, y) \ . && (5.77)
\end{aligned}$$

[⇒] Suppose that $F\pi$ is not compatible with γ. Pick finite sets D and $E \supseteq M(D)$ and patterns $p, q : D \to S$ and $r : E \setminus D \to S$ such that

$$\begin{aligned}
(F\pi)\left([p]_D \,\middle|\, [r]_{E\setminus D}\right) &> \pi\left([p]_D \,\middle|\, [r]_{E\setminus D}\right) \ , && (5.78)\\
(F\pi)\left([q]_D \,\middle|\, [r]_{E\setminus D}\right) &< \pi\left([q]_D \,\middle|\, [r]_{E\setminus D}\right) \ . && (5.79)
\end{aligned}$$

Dividing (5.79) by (5.78) we get

$$(F\pi)\left([q]_D \,\middle|\, [r]_{E\setminus D}\right) < \frac{\pi\left([q]_D \,\middle|\, [r]_{E\setminus D}\right)}{\pi\left([p]_D \,\middle|\, [r]_{E\setminus D}\right)} \cdot (F\pi)\left([p]_D \,\middle|\, [r]_{E\setminus D}\right) \ , \tag{5.80}$$

which can rewritten

$$(F\pi)\left([q]_D \cap [r]_{E\setminus D}\right) < \frac{\pi\left([q]_D \,\middle|\, [r]_{E\setminus D}\right)}{\pi\left([p]_D \,\middle|\, [r]_{E\setminus D}\right)} \cdot (F\pi)\left([p]_D \cap [r]_{E\setminus D}\right) \ . \tag{5.81}$$

For $B \supseteq N'\left(N'^{-1}(E)\right)$ this is equivalent to

$$\begin{aligned}
&\sum_{w : M(B)\setminus E \to S} (F\pi)\left([q]_D \cap [r]_{E\setminus D} \cap [w]_{M(B)\setminus E}\right)\\
&< \sum_{w : M(B)\setminus E \to S} \frac{\pi\left([q]_D \,\middle|\, [r]_{E\setminus D}\right)}{\pi\left([p]_D \,\middle|\, [r]_{E\setminus D}\right)} \cdot (F\pi)\left([p]_D \cap [r]_{E\setminus D} \cap [w]_{M(B)\setminus E}\right) \ . \qquad (5.82)
\end{aligned}$$

Therefore, for some $w : M(B) \setminus E \to S$ we have

$$\begin{aligned}&(F\pi)\left([q]_D \cap [r]_{E\setminus D} \cap [w]_{M(B)\setminus E}\right)\\ &< \frac{\pi\left([q]_D \,\middle|\, [r]_{E\setminus D}\right)}{\pi\left([p]_D \,\middle|\, [r]_{E\setminus D}\right)} \cdot (F\pi)\left([p]_D \cap [r]_{E\setminus D} \cap [w]_{M(B)\setminus E}\right) \ . \end{aligned} \tag{5.83}$$

Choose two configurations x and y with

$$x|_D = p \ , \tag{5.84}$$
$$y|_D = q \ , \tag{5.85}$$
$$x|_{E\setminus D} = y|_{E\setminus D} = r \ , \tag{5.86}$$
$$x|_{M(B)\setminus E} = y|_{M(B)\setminus E} = w \ , \tag{5.87}$$

and $x|_{\mathbb{L}\setminus M(B)} = y|_{\mathbb{L}\setminus M(B)}$. We have

$$\frac{\pi\left(F^{-1}[y]_{M(B)}\right)}{\pi\left(F^{-1}[x]_{M(B)}\right)} = \frac{(F\pi)\left([y]_{M(B)}\right)}{(F\pi)\left([x]_{M(B)}\right)} < \frac{\pi\left([y]_D \,\middle|\, [y]_{E\setminus D}\right)}{\pi\left([x]_D \,\middle|\, [x]_{E\setminus D}\right)} \ . \tag{5.88}$$

If $q' \triangleq (Fy)|_{N'^{-1}(D)}$, similarly to the above, we can verify that $\zeta_{q'} F^{-1}[x]_{M(B)} = F^{-1}[y]_{M(B)}$. Therefore, by Lemma 5.5 we obtain that

$$\Delta(F^{-1}x, F^{-1}y) = -\log \frac{\pi\left(F^{-1}[y]_{M(B)}\right)}{\pi\left(F^{-1}[x]_{M(B)}\right)} \tag{5.89}$$
$$> -\log \frac{\pi\left([y]_D \,\middle|\, [y]_{E\setminus D}\right)}{\pi\left([x]_D \,\middle|\, [x]_{E\setminus D}\right)} \tag{5.90}$$
$$= \Delta(x, y) \ , \tag{5.91}$$

which completes the proof. □

In one dimension, we can prove one direction of the above correspondence even when the CA is assumed to be merely surjective.

Lemma 5.10. *Let $c_1, c_2, \ldots, c_k > 0$ and $z_1, z_2, \ldots, z_k \geq 0$. Suppose that for infinitely many integers $t > 0$, we have*

$$c_1 z_1^t + c_2 z_2^t + \cdots + c_k z_k^t = 1 \ . \tag{5.92}$$

Then for each $i \in \{1, 2, \ldots, k\}$, either $z_i = 0$ or $z_i = 1$.

Theorem 5.11. *Let F be a one-dimensional surjective CA, Δ a local potential difference, and π the (unique) Gibbs measure with potential Δ. If F preserves π, it also conserves Δ.*

Proof. Let $[-r, r]$ be the neighborhood of F. According to Theorem 5.7, π is the distribution of a Markov chain with memory $m \geq 0$. Let μ be the observable given in Remark 5.1 which generates Δ. It follows from the balance property of surjective CA that F is finite-to-one. In particular, this implies that each pre-image of a spatially periodic configuration is itself spatially periodic.

Suppose that π is F-invariant. Let y be a spatially periodic configuration and $F^{-1}y = \{x_1, x_2, \ldots, x_k\}$. Let $p > 2r, m$ be a common period of $x_1, x_2, \ldots, x_k$ and y. Let us consider the cylinders $[y]_{[-tp,tp)}$ for sufficiently large integers $t > 0$. We have

$$\pi\left([y]_{[-pt,pt)}\right) = \pi\left([y]_{[-p,0)}\right) \cdot \left[\pi\left([y]_{[0,p)} \,\middle|\, [y]_{[-m,0)}\right)\right]^{2t-1} . \tag{5.93}$$

Let $b > 0$ be an integer constant such that for every sufficiently large t, each pre-image of $[y]_{[-tp,tp)}$ agrees on $[-(t-b)p - m, (t-b)p + m)$ with some x_i ($i = 1, 2, \ldots, k$). That such a constant exists is easy to see. Define

$$U_i \triangleq \left\{u \in S^{[-bp-r,0)} : F([u] \cap [x_i]_{[0,p+r)}) \subseteq [y]_{[-bp,p)}\right\} , \tag{5.94}$$

$$V_i \triangleq \left\{v \in S^{[0,bp+r)} : F([v] \cap [x_i]_{[-p-r,0)}) \subseteq [y]_{[-p,bp)}\right\} . \tag{5.95}$$

We have (see Figure 5.1)

$$F^{-1}[y]_{[-pt,pt)} = \bigcup_{i=1}^{k} \bigcup_{u \in U_i} \bigcup_{v \in V_i} \left([\sigma^{(t-b)p}u] \cap [x_i]_{[-(t-b)p,(t-b)p)} \cap [\sigma^{-(t-b)p}v]\right) . \tag{5.96}$$

Note that, by construction, every $u \in U_i$ agrees with x_i on $[-m, 0)$, and similarly, every $v \in V_i$ agrees with x_i on $[0, m)$. Therefore,

$$\begin{aligned} &\pi\left([y]_{[-pt,pt)}\right) \\ &= \sum_{i=1}^{k} \sum_{\substack{u \in U_i \\ v \in V_i}} \pi([u]) \cdot \left[\pi\left([x_i]_{[0,p)} \,\middle|\, [x_i]_{[-m,0)}\right)\right]^{2t-2b} \cdot \pi\left([v] \,\middle|\, [x_i]_{[-m,0)}\right) \qquad (5.97) \\ &= \sum_{i=1}^{k} \left(\sum_{\substack{u \in U_i \\ v \in V_i}} \pi([u]) \cdot \pi\left([v] \,\middle|\, [x_i]_{[-m,0)}\right) \right) \cdot \left[\pi\left([x_i]_{[0,p)} \,\middle|\, [x_i]_{[-m,0)}\right)\right]^{2t-2b} . \qquad (5.98) \end{aligned}$$

Dividing (5.98) by (5.93) we obtain

$$1 = \sum_{i=1}^{k} \alpha_i \left(\frac{\pi\left([x_i]_{[0,p)} \,\middle|\, [x_i]_{[-m,0)}\right)}{\pi\left([y]_{[0,p)} \,\middle|\, [y]_{[-m,0)}\right)} \right)^{2t} , \tag{5.99}$$

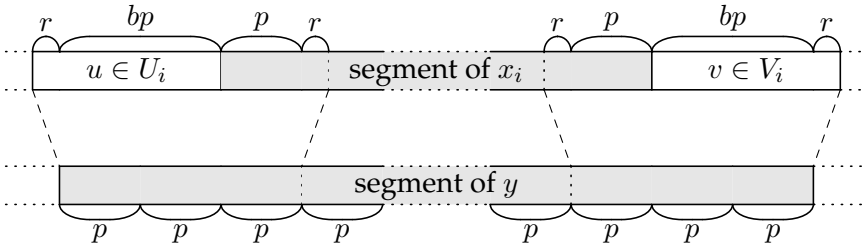


Figure 5.1: Illustration of the proof of Theorem 5.11.

where α_i ($i = 1, 2, \ldots, k$) are positive constants independent of t. Note that since π is full-support, both $\pi\left([x_i]_{[0,p)} \,\middle|\, [x_i]_{[-m,0)}\right)$ and $\pi\left([y]_{[0,p)} \,\middle|\, [y]_{[-m,0)}\right)$ are positive.

Since (5.99) holds for all sufficiently large $t > 0$, Lemma 5.10 implies that for each $i = 1, 2, \ldots, k$, we must have

$$\pi\left([x_i]_{[0,p)} \,\middle|\, [x_i]_{[-m,0)}\right) = \pi\left([y]_{[0,p)} \,\middle|\, [y]_{[-m,0)}\right) \ . \tag{5.100}$$

Therefore,

$$\overline{\mu}(x_i) = \frac{-\log \pi\left([x_i]_{[0,p)} \,\middle|\, [x_i]_{[-m,0)}\right)}{p} \tag{5.101}$$

$$= \frac{-\log \pi\left([y]_{[0,p)} \,\middle|\, [y]_{[-m,0)}\right)}{p} \tag{5.102}$$

$$= \overline{\mu}(y) \ , \tag{5.103}$$

which by Theorem 2.12 means that F conserves Δ. □

5.3 Almost-sure Correspondence

In this section, we prove a variant of the correspondence discussed in the previous section that is true for every probability measure and every surjective CA, but is true only in the probabilistic sense.

For every probability measure π and every $x \in \mathrm{supp}(\pi)$, define

$$\overline{\mu}_\pi(x) \triangleq \limsup_{n\to\infty} \frac{-\log \pi\left([x]_{I_n}\right)}{|I_n|} \ , \tag{5.104}$$

where $I_n \triangleq [-n, n]^d$ is the central hyper-cube of size $(2n+1)^d$. We show that, for every surjective CA F and for every probability measure π, we have $\overline{\mu}_{F\pi}(Fx) = \overline{\mu}_\pi(x)$ for π-almost all x.

If we were to interpret $\overline{\mu}_\pi$ as the average information content per cell on x with respect to π, the result would indicate that surjective CA conserve

information content, almost surely. That surjective CA in some sense conserve information is already suggested by the Garden-of-Eden Theorem, which is also used in the proof of the following theorem. A closely related result was obtained by Helvik, Lindgren and Nordahl [43].

Theorem 5.12. *For every probability measure π and every surjective CA F,*

$$\overline{\mu}_{F\pi}(Fx) = \overline{\mu}_{\pi}(x) \tag{5.105}$$

for π-almost all x.

Proof. Let $x \in \mathrm{supp}(\pi)$ be arbitrary and let $y = Fx$. Let $N = [r, r]^d$ be the neighborhood of F. Recall that for every $A \subseteq \mathbb{L}$, $\partial N(A)$ denotes the boundary of A, that is, the set $N(A) \backslash A$. Let us use an additional notation; let us define the *inside-outside* boundary of A by $\overline{\partial} N(A) \triangleq N(A) \setminus \{i : N^{-1}(i) \subseteq A\}$.

By the Garden-of-Eden Theorem, for every finite $D \subseteq \mathbb{L}$ we have

$$F^{-1}[y]_D \cap [x]_{\overline{\partial} N(D)} = [x]_{N(D)} \ , \tag{5.106}$$

and hence,

$$\begin{aligned} \frac{-\log \pi\left([x]_{N(D)}\right)}{|N(D)|} &= \frac{-\log \pi\left(F^{-1}[y]_D \cap [x]_{\overline{\partial} N(D)}\right)}{|N(D)|} && (5.107) \\ &= \left[\frac{-\log \pi\left(F^{-1}[y]_D\right)}{|D|} \cdot \frac{|D|}{|N(D)|}\right. \\ &\quad \left. + \frac{-\log \pi\left([x]_{\overline{\partial} N(D)} \,\middle|\, F^{-1}[y]_D\right)}{|N(D)|}\right] \ . && (5.108) \end{aligned}$$

Let $D \subseteq \mathbb{L}$ be finite. Let us define

$$A \triangleq \left\{(p, \partial q) : p : D \to S, \partial q : \overline{\partial} N(D) \to S, F^{-1}[p]_D \cap [\partial q]_{\overline{\partial} N(D)} \neq \varnothing\right\} \ , \tag{5.109}$$

and use pA and $A\partial q$ with their natural meanings. By the Gibbs inequality, for every $p : D \to S$ we have

$$\begin{aligned} &- \sum_{\partial q \in pA} \pi\left([\partial q] \,|\, F^{-1}[p]\right) \log \pi\left([\partial q] \,|\, F^{-1}[p]\right) \\ &\qquad \leq - \sum_{\partial q \in pA} \pi\left([\partial q] \,|\, F^{-1}[p]\right) \log \frac{1}{|pA|} = \log |pA| \ , \end{aligned} \tag{5.110}$$

in which $0 \log 0$ is interpreted as 0. By the balance property of the surjective CA, we have $|pA| = |S|^{|\partial N(D)|}$. Therefore,

$$- \sum_{(p,\partial q)\in A} \pi\left([\partial q] \cap F^{-1}[p]\right) \log \pi\left([\partial q] \,|\, F^{-1}[p]\right) \leq \sum_{p\in S^D} \pi(F^{-1}[p]) \log |pA| = |\partial N(D)| \log |S| \,. \tag{5.111}$$

By the Markov inequality, for every $K > 0$ this implies

$$\pi\left\{x : -\log \pi\left([x]_{\overline{\partial} N(D)} \,\middle|\, F^{-1}[Fx]_D\right) \geq K|\partial N(D)| \log |S|\right\} \leq \frac{1}{K} \,. \tag{5.112}$$

This means that for every $K > 0$, with a probability of at least $1 - \frac{1}{K}$ we have

$$\frac{-\log \pi\left([x]_{N(I_n)}\right)}{|N(I_n)|} = \frac{-\log \pi\left(F^{-1}[y]_{I_n}\right)}{|N(I_n)|} + \frac{-\log \pi\left([x]_{\overline{\partial} N(I_n)} \,\middle|\, F^{-1}[y]_{I_n}\right)}{|N(I_n)|} \tag{5.113}$$

$$= \frac{-\log \pi\left(F^{-1}[y]_{I_n}\right)}{|I_n|} \cdot \frac{|I_n|}{|N(I_n)|} + \frac{o(|I_n|)}{|N(I_n)|} \,. \tag{5.114}$$

Hence, for every $K > 0$, with a probability of at least $1 - \frac{1}{K}$ we have

$$\limsup_{n\to\infty} \frac{-\log \pi\left(F^{-1}[y]_{I_n}\right)}{|I_n|} = \limsup_{n\to\infty} \frac{-\log \pi\left([x]_{N(I_n)}\right)}{|N(I_n)|} \tag{5.115}$$

$$= \limsup_{n\to\infty} \frac{-\log \pi\left([x]_{I_{n+r}}\right)}{|I_{n+r}|} \,, \tag{5.116}$$

which means $\overline{\mu}_{F\pi}(Fx) = \overline{\mu}_\pi(x)$ for π-almost all x. □

Remark 5.2. Let M be a finite neighborhood. Using a similar argument, we can show that for every probability measure π,

$$\overline{\mu}_\pi(x) = \limsup_{n\to\infty} \frac{-\log \pi\left([x]_{I_n} \,|\, [x]_{\partial M(I_n)}\right)}{|I_n|} \tag{5.117}$$

for π-almost all x. This is true in particular when π is a Gibbs measure with potential difference Δ and neighborhood M, in which case $\overline{\mu}_\pi$ is the same as the average energy per cell with respect to Δ. ○

Remark 5.3. Suppose that π is translation-invariant and σ-ergodic. According to the Shannon-McMillan-Breiman Theorem (Theorem A.15), $\overline{\mu}_\pi(x)$ is

π-almost surely equal to $h_\pi(\sigma)$, the entropy of the shift space $(S^{\mathbb{L}}, \sigma)$ with respect to π. Recall that if π is σ-ergodic, so is $F\pi$ (Proposition A.2). It follows from Theorem 5.12 that whenever π is σ-ergodic and F is surjective, $h_{F\pi}(\sigma) = h_\pi(\sigma)$. This is, in fact, true even when π is not σ-ergodic: surjective CA preserve the average entropy per cell (Proposition A.13). ○

5.4 Equilibrium States and Surjective CA

As mentioned earlier, Gibbs measures characterize the macroscopic equilibrium of statistical mechanical systems. The macroscopic equilibrium is formulated via a variational principle: an *equilibrium state* is a state that maximizes the difference between entropy (per cell) and energy (per cell). More precisely, for every local observable μ on $S^{\mathbb{L}}$, let

$$P(\mu) \triangleq \sup_{\pi \in \mathscr{M}_\sigma} [h_\pi(\sigma) - \pi(\mu)] \ . \tag{5.118}$$

Depending on the physical context, the value $P(\mu)$ may be interpreted as *pressure* or as *free energy*. Observe that, since both $h_\pi(\sigma)$ and $\pi(\mu)$ are bounded, the value $P(\mu)$ always exists and is in $\mathbb{R}$. Furthermore, the compactness of $\mathscr{M}_\sigma$ ensures that the supremum is achieved for some elements in $\mathscr{M}_\sigma$. A measure $\pi \in \mathscr{M}_\sigma$ for which the supremum is achieved is called an *equilibrium state* for energy μ. Note that the equilibrium states are indeed a property of the energy defined by μ. Namely, if two observables μ and μ' generate the same potential difference, they have the same equilibrium states (Proposition 2.5). The set of all equilibrium states for μ is denoted by $\mathscr{E}(\mu)$; that is,

$$\mathscr{E}(\mu) \triangleq \{\pi \in \mathscr{M}_\sigma : h_\pi(\sigma) - \pi(\mu) = P(\mu)\} \ . \tag{5.119}$$

If μ generates a potential difference Δ, we may also write $\mathscr{E}(\Delta)$ for $\mathscr{E}(\mu)$. The following theorem, due to Dobrushin, Lanford and Ruelle, establishes the connection between equilibrium states and Gibbs measures.

Theorem 5.13 (see e.g. [77, 31])**.** *The equilibrium states for a local potential difference Δ on $S^{\mathbb{L}}$ are exactly the translation-invariant Gibbs measures with potential Δ. That is, $\mathscr{E}(\Delta) = \mathscr{G}_\sigma(\Delta)$ for every $\Delta \in \mathscr{D}$.*

In reversible cellular automata, the assertion of Theorem 5.9 is compatible with this picture: if Δ is a conserved potential difference, the Gibbs measures with potential Δ are exactly those that are "locally" invariant. Recall that by local invariance we mean that the CA maps $\mathscr{G}(\Delta)$ into $\mathscr{G}(\Delta)$. However, a few points are worth mentioning:

i) In reversible CA, the potential Δ is not unique; hence there is no unique concept of the pressure or free energy of a reversible CA. The equilibrium states, as specified by the variational principle, are meaningful for a reversible CA only in connection with a specific conserved energy.

ii) The variational principle, and therefore also Theorem 5.13, speak only of translation-invariant measures. In Theorem 5.9, the translation-invariance is not assumed, but the measures are required to be full-support.

iii) Theorem 5.9 does not say anything about the invariance of arbitrary measures. It only characterizes the Gibbs measures that are (locally) invariant.

Exploiting Theorem 5.13, we immediately obtain a one-sided connection between Gibbs measures and conservation laws in the more general class of surjective cellular automata. Surjective CA preserve the equilibrium associated with conserved energies.

Proposition 5.14. *Let F be a surjective cellular automaton and Δ a local potential difference. If F conserves Δ, it also maps $\mathscr{E}(\Delta)$ into itself.*

Proof. Let $\mu : S^{\mathbb{L}} \to \mathbb{R}$ be a local observable generating Δ. Since F conserves Δ, we have by Theorem 2.12 that for every measure $\pi \in \mathscr{M}_\sigma$, $(F\pi)(\mu) = \pi(\mu)$. Since F is surjective, we have by Proposition A.13 that it preserves entropy; that is, for every $\pi \in \mathscr{M}_\sigma$, we have $h_{F\pi}(\sigma) = h_\pi(\sigma)$. Therefore, for every $\pi \in \mathscr{E}(\Delta)$ we have

$$h_{F\pi}(\sigma) - (F\pi)(\mu) = h_\pi(\sigma) - \pi(\mu) \tag{5.120}$$

$$= P(\mu) \; . \tag{5.121}$$

Hence, $F\pi \in \mathscr{E}(\Delta)$. □

Corollary 5.15. *Let F be a surjective cellular automaton and Δ a local potential difference. If F conserves Δ, it also maps $\mathscr{G}_\sigma(\Delta)$ into itself.*

CHAPTER 6

Conclusion

We have studied conservation laws in cellular automata from different points of view. We now conclude the thesis with a number of comments and open problems.

The problem of finding a particle representation for arbitrary interaction-free conservation laws in higher-dimensional CA remains open. A drawback of our solution for the two-dimensional CA is the arbitrariness involved. There is an infinite number of ways in which one can assign a flow to a given conservation law. Can we (possibly by introducing additional constraints, or by formalizing the concept of the flows in a different way) obtain a *unique* "natural" flow for each conservation law? One criterion for naturalness is that for a reversible CA, the flows in the backward direction of time should be obtainable from the flows in the forward direction, merely by reversing the direction of the arrows.

Another open issue is the possible relationship between the conservation laws and the symmetries of (reversible) cellular automata. Several researchers (e.g., Margolus [62], Baez and Gilliam [2], Boykett [14, 15], and Bernardi [70]) have proposed variants of Noether's theorem (see e.g. [55, 1]) that are applicable to classes of cellular automata.

Group-valued conservation laws are more descriptive than those that are real-valued, and equally tractable. Semigroup-valued conservation laws are even more expressive, but unless for one-dimensional CA, they are not algorithmically verifiable. The hierarchy of conservation laws for a CA seems to provide useful information about the behavior of the CA. Further study of the relationship between this hierarchy and the dynamical properties of the CA may be rewarding.

Reversible CA, as a particularly important class of CA, are worth special attention. We do not know whether every reversible CA has at least one real-valued conservation law (though there are examples that suggest a negative answer). Finding specialized flow explanations for this class of CA would also be interesting.

The connection between the conservation laws and the equilibrium states of a reversible CA needs further exploration. Statistical mechanics and cellular automata are two fields of research which have been developed independently, though they concern the same kind of question: each tries to deduce information about the macroscopic behavior of a system consisting of a huge number of tiny interacting elements. Applying tools and insight from one field to another would be fruitful.

Finally, let us state two miscellaneous questions, which, to our knowledge, are open:

Question 6.1. Let F be a CA and Δ a potential difference conserved by F. Is the image of every ground configuration itself a ground configuration? If so, conservation laws can be expressed in terms of total energy relative to the ground configurations.

Question 6.2. Given a local potential difference Δ, is it decidable whether $|\mathscr{G}(\Delta)| > 1$?

APPENDIX A

Basic Ergodic Theory for Shift Spaces

Throughout the thesis, we occasionally need to apply a modest level of ergodic theory to multi-dimensional shift spaces. However, the standard texts in ergodic theory, such as [83], often base their treatment on one-dimensional dynamics. It therefore seems appropriate to go through the basic theory, retold in the multi-dimensional setting.

A.1 Ergodicity

Let $\mathcal{X} \subseteq S^{\mathbb{L}}$ be a shift space, and let $\mathscr{M}_\sigma[\mathcal{X}]$ be the set of translation-invariant Borel probability measures on $\mathcal{X}$. As usual, $I_n \triangleq [-n, n]^d \subseteq \mathbb{L}$ denotes the centered hyper-cube of side $2n+1$ in $\mathbb{L}$. A *σ-invariant* set is a set B such that $\sigma^{-a}B = B$ for all $a \in \mathbb{L}$. A mapping $g : \mathcal{X} \to \mathbb{R}$ is *σ-invariant* if $g \circ \sigma^a = g$ for all $a \in \mathbb{L}$. A measure $\pi \in \mathscr{M}_\sigma[\mathcal{X}]$ is *σ-ergodic* (or *shift-ergodic*) if for every σ-invariant Borel set $B \subseteq \mathcal{X}$, either $\pi(B) = 0$ or $\pi(B) = 1$.

Theorem A.1 (Theorems 1.5 and 1.6 in [83])**.** *Let $\pi \in \mathscr{M}_\sigma[\mathcal{X}]$ be a probability measure. The following statements are equivalent.*

i) *π is σ-ergodic.*

ii) *For every Borel set $B \subseteq \mathcal{X}$ with $\pi(B) > 0$, we have $\pi\left(\bigcup_{a\in\mathbb{L}} \sigma^{-a}B\right) = 1$.*

iii) *For every Borel sets $A, B \subseteq \mathcal{X}$ with $\pi(A), \pi(B) > 0$, there exists $a \in \mathbb{L}$ with $\pi\left(A \cap \sigma^{-a}B\right) > 0$.*

iv) *For every measurable function $g : \mathcal{X} \to \mathbb{R}$ such that $g\left(\sigma^a x\right) = g(x)$ for every $a \in \mathbb{L}$ and π-almost all x, there exists $\overline{g} \in \mathbb{R}$ such that $g(x) = \overline{g}$ for π-almost all x.*

Proof.
[i⇒ii] The set $\bigcup_{a\in\mathbb{L}} \sigma^{-a}B$ is σ-invariant and contains B.

[ii⇒iii] Let $A, B \subseteq \mathcal{X}$ be Borel sets with $\pi(A), \pi(B) > 0$. Choose $n > 0$ such that $\pi\left(\bigcup_{a\in I_n} \sigma^{-a}B\right) > 1 - \pi(A)$. Then

$$\sum_{a\in I_n} \pi\left(A \cap \sigma^{-a}B\right) \geq \pi\left(A \cap \bigcup_{a\in I_n} \sigma^{-a}B\right) > 0\,, \tag{A.1}$$

which implies $\pi\left(A \cap \sigma^{-a}B\right) > 0$ for some $a \in I_n$.

[iii⇒i] Suppose that B is σ-invariant, but $\pi(B), \pi\left(\mathcal{X} \setminus B\right) > 0$. There exists $a \in \mathbb{L}$ such that $\pi\left(\sigma^{-a}B \cap \left(\mathcal{X} \setminus B\right)\right) > 0$. Since B is σ-invariant, this gives $\pi\left(B \cap \left(\mathcal{X} \setminus B\right)\right) > 0$, which is a contradiction.

[i⇒iv] For every $n \in \mathbb{Z}^+$ let us partition $\mathbb{R}$ into intervals of length 2^{-n}, and denote the ith interval by $J_n(i)$. Namely, for every $i \in \mathbb{Z}$, let $J_n(i) \triangleq [i/2^n, (i+1)/2^n) \subseteq \mathbb{R}$. For every $n \in \mathbb{Z}^+$ and $i \in \mathbb{Z}$, consider the set

$$A_n(i) \triangleq \left\{x \in \mathcal{X} : g\left(\sigma^a x\right) \in J_n(i) \text{ for every } a \in \mathbb{L}\right\}\,. \tag{A.2}$$

Every $A_n(i)$ is σ-invariant, hence either $\pi\left(A_n(i)\right) = 0$ or $\pi\left(A_n(i)\right) = 1$. Furthermore, by assumption, for every n, the sets $A_n(i)$ cover π-almost all elements of $\mathcal{X}$; that is,

$$\sum_{i\in\mathbb{Z}} \pi\left(A_n(i)\right) = \pi\left(\bigcup_{i\in\mathbb{Z}} A_n(i)\right) = 1\,. \tag{A.3}$$

Therefore, there is a unique $i_n \in \mathbb{Z}$ such that $\pi\left(A_n(i_n)\right) = 1$. It follows that $J_1(i_1) \supseteq J_2(i_2) \supseteq \cdots$. Let $\overline{g}$ be the unique element of $\bigcap_{n>0} J_n(i_n)$. We have $\pi\left(\bigcap_{n>0} A_n(i_n)\right) = 1$ and $g(x) = \overline{g}$ for every $x \in \bigcap_{n>0} A_n(i_n)$.

[iv⇒i] Let B be σ-invariant. Consider its characteristic function χ_B. We have $\chi_B \circ \sigma^a = \chi_B$. Therefore, there exists $\overline{b} \in \mathbb{R}$ such that $\chi_B(x) = \overline{b}$ for π-almost every x. Either $\overline{b} = 0$, which means that $\pi(B) = 0$, or $\overline{b} = 1$, which implies $\pi(B) = 1$. □

Cellular automata preserve the ergodicity.

Proposition A.2. *Let F be a CA with $F\mathcal{X} \subseteq \mathcal{X}$. If $\pi \in \mathscr{M}_\sigma[\mathcal{X}]$ is σ-ergodic, so is $F\pi$.*

Proof. Clearly $F\pi$ is translation-invariant. If $B \subseteq \mathcal{X}$ is a σ-invariant Borel set, so is $F^{-1}B$. Therefore, either $(F\pi)(B) = \pi(F^{-1}B) = 0$ or $(F\pi)(B) = \pi(F^{-1}B) = 1$. □

A.2 Ergodic Theorem

For every bounded measurable mapping $g : \mathcal{X} \to \mathbb{R}$ and every finite set $D \subseteq \mathbb{L}$, let us define the *spatial average* $\mathcal{R}_D g : \mathcal{X} \to \mathbb{R}$ of g over D by

$$\mathcal{R}_D g(x) \triangleq \frac{\sum_{i \in D} g\left(\sigma^i x\right)}{|D|} \ . \tag{A.4}$$

Define the *upper* and the *lower* averages $\overline{\mathcal{R}} g, \underline{\mathcal{R}} g : \mathcal{X} \to \mathbb{R}$ by

$$\overline{\mathcal{R}} g(x) \triangleq \limsup_{n \to \infty} \mathcal{R}_{I_n} g(x) \ , \qquad \underline{\mathcal{R}} g(x) \triangleq \liminf_{n \to \infty} \mathcal{R}_{I_n} g(x) \ . \tag{A.5}$$

Proposition A.3. *For every bounded measurable mapping $g : \mathcal{X} \to \mathbb{R}$, the averages $\overline{\mathcal{R}} g$ and $\underline{\mathcal{R}} g$ are measurable and σ-invariant.*

Proof. The Borel σ-algebra on $\mathbb{R}$ is generated by the intervals $(a, +\infty)$ with $a \in \mathbb{R}$. For each $a \in \mathbb{R}$, the set

$$\left(\overline{\mathcal{R}} g\right)^{-1} (a, +\infty) = \bigcap_{n>0} \bigcup_{i>n} \left(\mathcal{R}_{I_i} g\right)^{-1} (a, +\infty) \tag{A.6}$$

is measurable. So $\overline{\mathcal{R}} g$ (and similarly, $\underline{\mathcal{R}} g$) is measurable.

For every finite $D \subseteq \mathbb{L}$ and all $a \in \mathbb{L}$, we have

$$\begin{aligned} \mathcal{R}_D g\left(\sigma^a x\right) - \mathcal{R}_D g(x) &= \frac{1}{|D|} \sum_{i \in D} g\left(\sigma^{a+i} x\right) - \frac{1}{|D|} \sum_{i \in D} g\left(\sigma^i x\right) && \text{(A.7)} \\ &= \frac{|(a+D) \setminus D|}{|D|} \mathcal{R}_{(a+D) \setminus D} g(x) \\ &- \frac{|D \setminus (a+D)|}{|D|} \mathcal{R}_{D \setminus (a+D)} g(x) \ . && \text{(A.8)} \end{aligned}$$

Since g is bounded, we get

$$\mathcal{R}_{I_n} g\left(\sigma^a x\right) - \mathcal{R}_{I_n} g(x) = \frac{o(|I_n|)}{|I_n|} O(1) \to 0 \tag{A.9}$$

as $n \to \infty$. Hence $\overline{\mathcal{R}} g$ and $\underline{\mathcal{R}} g$ must be σ-invariant. □

We will denote the integral $\int g \mathrm{d}\pi$ by $\pi(g)$. The following weak form of the (Pointwise) *Ergodic Theorem*, due to Birkhoff ($\mathbb{L} = \mathbb{Z}$) and Weiner ($\mathbb{L} = \mathbb{Z}^d$, $d \geq 1$), is sufficient for our purposes. Its proof can be found in [31]. See [69] for more general variants.

Theorem A.4 (Theorem 1.14 in [83] or Theorem 14.A8 in [31])**.** *Let $\pi \in \mathscr{M}_\sigma[\mathcal{X}]$ be σ-ergodic. For every bounded measurable mapping $g : \mathcal{X} \to \mathbb{R}$ we have $\overline{\mathcal{R}} g(x) = \underline{\mathcal{R}} g(x) = \pi(g)$ for π-almost every x.*

A.3 Geometry of $\mathscr{M}_\sigma[\mathcal{X}]$

By an *extreme* point of a convex set $\mathcal{U}$ we mean a point $x \in \mathcal{U}$ such that every convex combination $\sum_{i=1}^{n} \lambda_i x_i = x$ with $x_i \in \mathcal{U}$ is trivial; that is, for each $i = 1, 2, \ldots, n$, either $\lambda_i = 0$ or $x_i = x$. Two measures π, π' on $\mathcal{X}$ are *mutually singular* if there exists a Borel set $B \subseteq \mathcal{X}$ with $\pi(B) = \pi'(\mathcal{X} \setminus B) = 0$.

Theorem A.5 (Theorem 6.10 in [83])**.**

i) $\mathscr{M}_\sigma[\mathcal{X}]$ is compact.

ii) $\mathscr{M}_\sigma[\mathcal{X}]$ is convex.

iii) A measure $\pi \in \mathscr{M}_\sigma[\mathcal{X}]$ is σ-ergodic if and only if it is an extreme point of $\mathscr{M}_\sigma[\mathcal{X}]$.

iv) Every element of $\mathscr{M}_\sigma[\mathcal{X}]$ is a limit of convex combinations of σ-ergodic elements of $\mathscr{M}_\sigma[\mathcal{X}]$.

v) Distinct σ-ergodic measures in $\mathscr{M}_\sigma[\mathcal{X}]$ are mutually singular.

Proof.

i) $\mathscr{M}_\sigma[\mathcal{X}]$ is a closed subset of the compact space $\mathscr{M}$.

ii) Trivial.

iii) [$\Leftarrow$] Suppose that π is not σ-ergodic. There is a σ-invariant Borel set $B \subseteq \mathcal{X}$ with $0 < \pi(B) < 1$. Define the measures π_1, π_2 by

$$\pi_1(A) \triangleq \frac{\pi(A \cap B)}{\pi(B)} \quad \text{and} \quad \pi_2(A) \triangleq \frac{\pi(A \cap (\mathcal{X} \setminus B))}{\pi(\mathcal{X} \setminus B)} \tag{A.10}$$

for every $A \subseteq \mathscr{B}$. Clearly π_1 and π_2 are in $\mathscr{M}_\sigma[\mathcal{X}]$. Furthermore, $\pi = \pi(B) \cdot \pi_1 + \pi(\mathcal{X} \setminus B) \cdot \pi_2$.

[$\Rightarrow$] Suppose that π is σ-ergodic, and that $\pi = \lambda\pi_1 + (1 - \lambda)\pi_2$ for some $0 < \lambda < 1$ and $\pi_1, \pi_2 \in \mathscr{M}_\sigma[\mathcal{X}]$. For every σ-invariant B, if $\pi(B) = 0$, we have $\pi_1(B) = \pi_2(B) = 0$, and if $\pi(B) = 1$, we have $\pi_1(B) = \pi_2(B) = 1$. So, π_1 and π_2 are both σ-ergodic. Let $B \subseteq \mathscr{B}$ be arbitrary. Consider the characteristic function χ_B of B. By the Ergodic Theorem, we have $\overline{\mathcal{R}}\chi_B(x) = \pi(\chi_B) = \pi(B)$ on a set $Y \subseteq \mathcal{X}$ with $\pi(Y) = 1$. Similarly, for $i = 1, 2$, we have $\overline{\mathcal{R}}\chi_B(x) = \pi_i(\chi_B) = \pi_i(B)$ on a set $Y_i \subseteq \mathcal{X}$ with $\pi_i(Y) = 1$. But $\pi(Y) = 1$ implies $\pi_i(Y) = 1$. So $\pi_i(Y \cap Y_i) = 1$, which means that $Y \cap Y_i \neq \varnothing$. For each $x \in Y \cap Y_i$ we have $\pi(B) = \overline{\mathcal{R}}\chi_B(x) = \pi_i(B)$. Therefore, $\pi_1 = \pi_2 = \pi$.

iv) This follows from the Krein-Milman Theorem, which states that every compact and convex subset of a locally convex topological vector space (i.e., a topological vector space that has a basis consisting of convex sets) is the closure of the convex hull of its extreme points. See e.g. [76] for the proof of this.

v) Let π_1 and π_2 be two distinct σ-ergodic measures in $\mathscr{M}_\sigma[\mathcal{X}]$. There exists a Borel set $B \subseteq \mathcal{X}$ such that $\pi_1(B) \neq \pi_2(B)$. Consider the characteristic function χ_B of B. By the Ergodic Theorem, the average $\overline{\mathcal{R}}\chi_B(x)$ is equal to $\pi_1(B)$ on a set E_1 with $\pi_1(E_1) = 1$, and equal to $\pi_2(B)$ on a set E_2 with $\pi_2(E_2) = 1$. The fact that $\pi_1(B) \neq \pi_2(B)$ implies that E_1 and E_2 are disjoint, which means that π_1 and π_2 are mutually singular. □

A.4 Entropy

Let $\mathscr{A}$ be a finite sub-σ-algebra of $\mathscr{B}$, the Borel subsets of $\mathcal{X}$. We see $\mathscr{A}$ as a finite variety of distinguishable events on $\mathcal{X}$. The minimal non-empty elements of $\mathscr{A}$ form a finite partition of $\mathcal{X}$, which is denoted by $\xi(\mathscr{A})$. These are the primitive events in $\mathscr{A}$. Every other event is a conjunction of the primitive events. Every finite measurable partition of $\mathcal{X}$ generates a finite sub-σ-algebra of $\mathscr{B}$.

Given two finite sub-σ-algebras $\mathscr{A}, \mathscr{C}$, we denote by $\mathscr{A} \vee \mathscr{C}$ the coarsest (i.e., the smallest) σ-algebra containing $\mathscr{A}$ and $\mathscr{C}$. The elements of the partition $\xi(\mathscr{A} \vee \mathscr{C})$ are the non-empty intersections of the elements of $\xi(\mathscr{A})$ and $\xi(\mathscr{C})$. For every measurable mapping $F : \mathcal{X} \to \mathcal{X}$, $F^{-1}\mathscr{A}$ denotes the sub-σ-algebra $\{F^{-1}A : A \in \mathscr{A}\}$. For example, $\sigma^{-a}\mathscr{A}$ consists of the events similar to those in $\mathscr{A}$, but occurring around position a. Note that $F^{-1}\xi(\mathscr{A}) = \xi(F^{-1}\mathscr{A})$ and $F^{-1}(\mathscr{A} \vee \mathscr{C}) = F^{-1}\mathscr{A} \vee F^{-1}\mathscr{C}$.

Let π be a Borel probability measure on $\mathcal{X}$, and let $\mathscr{A}$ be a finite sub-σ-algebra of $\mathscr{B}$. Let $\xi(\mathscr{A}) = \{A_1, A_2, \ldots, A_n\}$ be the partition generating $\mathscr{A}$. The *entropy* of $\mathscr{A}$ with respect to π is defined by

$$H_\pi(\mathscr{A}) \triangleq -\sum_{i=1}^{n} \pi(A_i) \log \pi(A_i) \,, \tag{A.11}$$

in which $0 \log 0$ is interpreted as 0. When $\mathscr{A}$ and $\mathscr{C}$ are two finite sub-σ-algebras, the entropy of $\mathscr{A}$ *given* $\mathscr{C}$ is defined to be

$$H_\pi(\mathscr{A} \,|\, \mathscr{C}) \triangleq H_\pi(\mathscr{A} \vee \mathscr{C}) - H_\pi(\mathscr{C}) \,. \tag{A.12}$$

The following proposition summarizes some basic properties of entropy. See [83, 21, 44].

Proposition A.6. *Let $\mathscr{A}$, $\mathscr{C}$ and $\mathscr{D}$ be finite sub-σ-algebras of the Borel sets of $\mathcal{X}$, and let π be a probability measure on $\mathcal{X}$. We have*

i) $0 \leq H_\pi(\mathscr{A}) \leq \log|\xi(\mathscr{A})|$.

ii) $0 \leq H_\pi(\mathscr{A} \,|\, \mathscr{C}) \leq H_\pi(\mathscr{A})$.

iii) $H_\pi(\mathscr{C}) \leq H_\pi(\mathscr{C} \vee \mathscr{D}) \leq H_\pi(\mathscr{C}) + H_\pi(\mathscr{D})$.

iv) If $\mathscr{C} \subseteq \mathscr{D}$, then $H_\pi(\mathscr{C}) \leq H_\pi(\mathscr{D})$.

v) If $\mathscr{C} \subseteq \mathscr{D}$, then $H_\pi(\mathscr{A} \,|\, \mathscr{D}) \leq H_\pi(\mathscr{A} \,|\, \mathscr{C})$.

vi) $H_\pi(F^{-1}\mathscr{A}) = H_{F\pi}(\mathscr{A})$ *for every measurable* $F : \mathcal{X} \to \mathcal{X}$.

Proposition A.7 (Theorem 2.7.3 in [21])**.** *The mapping $\pi \mapsto H_\pi(\cdot)$ is concave. That is, for every π_1, π_2 and $0 \leq \lambda \leq 1$, we have*

$$\lambda H_{\pi_1} + (1-\lambda)H_{\pi_2} \leq H_{\lambda\pi_1+(1-\lambda)\pi_2} \leq \lambda H_{\pi_1} + (1-\lambda)H_{\pi_2} + \delta \;, \tag{A.13}$$

where $\delta \triangleq -\lambda\log\lambda - (1-\lambda)\log(1-\lambda)$.

Let $J \subseteq \mathbb{L}$ be a finite set of cells. Let $\mathscr{A}(J)$ be the sub-σ-algebra generated by the cylinders $[x]_J$ for all $x : J \to S$. This is the algebra of events occurring on J. We sometimes use the intuitive shorthand $H_\pi(J)$ for $H_\pi(\mathscr{A}(J))$, and call it the *entropy of the cells J* (with respect to π).

Recall that $I_n \triangleq [-n, n]^d$ is the centered hyper-cube of size $(2n+1)^d$ on the lattice. In order to define the entropy of a shift space, we need the following technical lemma.

Lemma A.8 (Theorem 4.9 in [83])**.** *Let $\{s_U\}_U$ be a family of real numbers where U ranges over the finite subsets of $\mathbb{L}$. Suppose that*

i) $s_{a+U} = s_U$ *for every finite set $U \subseteq \mathbb{L}$ and all $a \in \mathbb{L}$, and*

ii) $s_{U\cup V} \leq s_U + s_V$ *for every two disjoint finite sets $U, V \subseteq \mathbb{L}$.*

Then the sequence $\{s_{I_n}/|I_n|\}_{n=0}^\infty$ converges to its infimum.

Proof. Fix $p > 0$. Let $n \geq 0$ be arbitrary. We have $(2n+1) = k(2p+1) + i$ for some $k \geq 0$ and $0 \leq i < 2p+1$. We can pack k^d copies of I_p inside I_n, leaving $o(|I_n|)$ cells uncovered. Therefore,

$$\frac{s_{I_n}}{|I_n|} \leq \frac{k^d s_{I_p} + o(|I_n|)}{|I_n|} = \frac{k^d|I_p|}{|I_n|} \cdot \frac{s_{I_p}}{|I_p|} + \frac{o(|I_n|)}{|I_n|} \;, \tag{A.14}$$

which as $n \to \infty$, gives

$$\limsup_{n\to\infty} \frac{s_{I_n}}{|I_n|} \leq \frac{s_{I_p}}{|I_p|} \;. \tag{A.15}$$

Hence,

$$\limsup_{n\to\infty} \frac{s_{I_n}}{|I_n|} \leq \inf_p \frac{s_{I_p}}{|I_p|} \leq \liminf_{n\to\infty} \frac{s_{I_n}}{|I_n|} \ , \tag{A.16}$$

which proves the claim. □

Let $\pi \in \mathscr{M}_\sigma[\mathcal{X}]$ be a translation-invariant probability measure on $\mathcal{X}$. For every finite sub-σ-algebra $\mathscr{A}$, define

$$h_\pi(\sigma, \mathscr{A}) \triangleq \lim_{n\to\infty} \frac{H_\pi\left(\bigvee_{i\in I_n} \sigma^{-i}\mathscr{A}\right)}{|I_n|} \ . \tag{A.17}$$

Lemma A.8 and Proposition A.6.iii ensure that the above limit always exists.

Proposition A.9. *Let $\mathscr{C}$ and $\mathscr{D}$ be finite sub-σ-algebras of the Borel sets of $\mathcal{X}$, and let π be a translation-invariant probability measure on $\mathcal{X}$. We have*

i) $0 \leq h_\pi(\sigma, \mathscr{C}) \leq H_\pi(\mathscr{C})$.

ii) $h_\pi(\sigma, \mathscr{C}) \leq h_\pi(\sigma, \mathscr{C} \vee \mathscr{D}) \leq h_\pi(\sigma, \mathscr{C}) + h_\pi(\sigma, \mathscr{D})$.

iii) If $\mathscr{C} \subseteq \mathscr{D}$, *then* $h_\pi(\sigma, \mathscr{C}) \leq h_\pi(\sigma, \mathscr{D})$.

iv) $h_\pi(\sigma, \mathscr{C}) \leq h_\pi(\sigma, \mathscr{D}) + H_\pi(\mathscr{C} \mid \mathscr{D})$.

v) $h_\pi(\sigma, F^{-1}\mathscr{C}) = h_{F\pi}(\sigma, \mathscr{C})$ *for every cellular automaton* $F : \mathcal{X} \to \mathcal{X}$.

Proposition A.10. *The mapping $\pi \mapsto h_\pi(\sigma, \cdot)$ is affine. That is, for every π_1, π_2 and $0 \leq \lambda \leq 1$, we have*

$$h_{\lambda\pi_1+(1-\lambda)\pi_2}(\sigma, \cdot) = \lambda h_{\pi_1}(\sigma, \cdot) + (1-\lambda) h_{\pi_2}(\sigma, \cdot) \ . \tag{A.18}$$

Proof. Let $\mathscr{A}_n \triangleq \bigvee_{i\in I_n} \sigma^{-i}\mathscr{A}$. According to Proposition A.7, we have

$$\begin{aligned} &\lambda H_{\pi_1}(\mathscr{A}_n) + (1-\lambda) H_{\pi_2}(\mathscr{A}_n) \\ &\leq H_{\lambda\pi_1+(1-\lambda)\pi_2}(\mathscr{A}_n) \qquad (A.19) \\ &\leq \lambda H_{\pi_1}(\mathscr{A}_n) + (1-\lambda) H_{\pi_2}(\mathscr{A}_n) + \delta \ , \qquad (A.20) \end{aligned}$$

where δ is a constant. Dividing these expressions by $|I_n|$ and letting n go to infinity gives the result. □

The (Kolmogorov-Sinai) *entropy* of the dynamical system $(\mathcal{X}, \sigma)$ with respect to π is $h_\pi(\sigma) \triangleq \sup_{\mathscr{A}} h_\pi(\sigma, \mathscr{A})$, where the supremum is taken over all finite sub-σ-algebras $\mathscr{A}$ of $\mathscr{B}$.

Proposition A.11. *Let π be a translation-invariant probability measure on $\mathcal{X}$, and let $F : \mathcal{X} \to \mathcal{X}$ be a cellular automaton. Then $h_{F\pi}(\sigma) \leq h_\pi(\sigma)$.*

The following is a special case of the *Kolmogorov-Sinai Theorem* (Theorem 4.17 in [83]).

Theorem A.12. *For every translation-invariant probability measure $\pi \in \mathscr{M}_\sigma[\mathcal{X}]$ we have*

$$h_\pi(\sigma) = \lim_{n\to\infty} \frac{H_\pi(I_n)}{|I_n|} = \inf_{n\geq 0} \frac{H_\pi(I_n)}{|I_n|} \,. \tag{A.21}$$

Proof. The second equality follows from Lemma A.8. For every $n \geq 0$, let $\mathscr{A}_n \triangleq \mathscr{A}(I_n)$ be the σ-algebra of events occurring on I_n. Observe that $\mathscr{A}_{m+n} = \bigvee_{i\in I_n} \sigma^{-i}\mathscr{A}_m$ whenever $m, n \geq 0$. Therefore, for $m \geq 0$, we get

$$h_\pi(\sigma, \mathscr{A}_m) = \lim_{n\to\infty} \frac{H_\pi\left(\bigvee_{i\in I_n} \sigma^{-i}\mathscr{A}_m\right)}{|I_n|} \tag{A.22}$$

$$= \lim_{n\to\infty} \frac{|I_{m+n}|}{|I_n|} \cdot \frac{H_\pi(\mathscr{A}_{m+n})}{|I_{m+n}|} \tag{A.23}$$

$$= \lim_{n\to\infty} \frac{H_\pi(I_n)}{|I_n|} \,. \tag{A.24}$$

Let $\mathscr{C}$ be any finite sub-σ-algebra of $\mathscr{B}$. By Proposition A.9.iv, for every $n \geq 0$, we have

$$h_\pi(\sigma, \mathscr{C}) \leq h_\pi(\sigma, \mathscr{A}_n) + H_\pi(\mathscr{C} \,|\, \mathscr{A}_n) \,. \tag{A.25}$$

It remains to show that $\lim_{n\to\infty} H_\pi(\mathscr{C} \,|\, \mathscr{A}_n) = 0$.

Let $\xi(\mathscr{C}) = \{C_1, C_2, \ldots, C_k\}$ be the partition generating $\mathscr{C}$. Since π is regular, for each $l = 1, 2, \ldots, k$ and every $\varepsilon > 0$, there is an open set $U \supseteq C_l$ such that $\pi(U \setminus C_l) < \varepsilon$. Recall that the cylinders $[p]_{I_n}$ (where $p : I_n \to S$) form a basis for the topology of $\mathcal{X}$. So U is a countable union $\pi(U) = \bigcup_{i=0}^{\infty} A_i$, where $A_i \in \mathscr{A}_i$. Since $\mathscr{A}_0 \subseteq \mathscr{A}_1 \subseteq \cdots$, we have $B_i \triangleq \bigcup_{k=0}^{i} A_k \subseteq \mathscr{A}_i$. So $U = \bigcup_{i=0}^{\infty} B_i$, where $B_i \in \mathscr{A}_i$ and $B_0 \subseteq B_1 \subseteq \cdots$. For every $\varepsilon' > 0$, we can find $m \geq 0$ such that $\pi(U \setminus B_m) < \varepsilon'$. Altogether, we obtain that $\pi(C_l \triangle B_m) < \varepsilon + \varepsilon'$.

Let $\delta > 0$ be arbitrary. The above discussion implies that for $m \geq 0$ large enough, there is a sub-σ-algebra $\mathscr{D} \subseteq \mathscr{A}_m$ with generating partition $\xi(\mathscr{D}) = \{D_1, D_2, \ldots, D_k\}$ such that for each $l = 1, 2, \ldots, k$, we have $\pi(C_l \triangle D_l) < \delta$. In particular, we can choose $m \geq 0$ and $\mathscr{D} \subseteq \mathscr{A}_m$ so that $\pi(C_i \,|\, D_i) > 1 - \delta$ while $\pi(C_i \,|\, D_j) < \delta$ for each i and $j \neq i$.

This implies that by choosing $m \geq 0$ large enough, one can make $H_\pi(\mathscr{C} \,|\, \mathscr{D})$ arbitrarily small. But $H_\pi(\mathscr{C} \,|\, \mathscr{A}_m) \leq H_\pi(\mathscr{C} \,|\, \mathscr{D})$. Hence,

$$\lim_{m\to\infty} H_\pi(\mathscr{C} \,|\, \mathscr{A}_m) = 0 \,, \tag{A.26}$$

concluding the proof. □

Note that this, together with Proposition A.6.i, implies that $h_\pi(\sigma) \leq \log|S| < \infty$. Inspired by the above theorem, we call $h_\pi(\sigma)$ the *average entropy per cell* of measure π. Theorem A.12 also implies that surjective cellular automata preserve entropy.

Proposition A.13 ([60]). *Let π be a translation-invariant probability measure on $S^{\mathbb{L}}$, and let $F : S^{\mathbb{L}} \to S^{\mathbb{L}}$ be a surjective cellular automaton. Then $h_{F\pi}(\sigma) = h_\pi(\sigma)$.*

Proof. According to Proposition A.11, $h_{F\pi}(\sigma) \leq h_\pi(\sigma)$. We show that when F is surjective, $h_{F\pi}(\sigma) \geq h_\pi(\sigma)$. Let $[-r,r]^d$ ($r \geq 0$) be a neighborhood for F. For every $n \geq 0$, we have

$$\begin{aligned} H_{F\pi}\left(\mathscr{A}(I_n)\right) &= H_\pi\left(F^{-1}\mathscr{A}(I_n)\right) && \text{(A.27)}\\ &\leq H_\pi\left(\mathscr{A}(I_{n+r})\right) && \text{(A.28)}\\ &\leq H_\pi\left(F^{-1}\mathscr{A}(I_n)\right) + |I_{n+r} \setminus I_n| \cdot \log|S| && \text{(A.29)}\\ &= H_{F\pi}\left(\mathscr{A}(I_n)\right) + o(|I_n|)\,, && \text{(A.30)} \end{aligned}$$

where (A.27) and (A.30) follow from Proposition A.6.vi, (A.28) from Proposition A.6.iv, and (A.29) from the balance property of surjective CA and Proposition A.6.iii. Dividing by $|I_n|$, we get

$$\frac{|I_{n+r}|}{|I_n|} \cdot \frac{H_\pi\left(\mathscr{A}(I_{n+r})\right)}{|I_{n+r}|} \leq \frac{H_{F\pi}\left(\mathscr{A}(I_n)\right)}{|I_n|} + \frac{o(|I_n|)}{|I_n|}\,, \tag{A.31}$$

which as $n \to \infty$ proves the claim. □

Theorem A.14 (Theorem 8.1 in [83]). *The mapping $\pi \mapsto h_\pi(\sigma)$ is affine. That is, for every π_1, π_2 and $0 \leq \lambda \leq 1$, we have*

$$h_{\lambda\pi_1+(1-\lambda)\pi_2}(\sigma) = \lambda h_{\pi_1}(\sigma) + (1-\lambda)h_{\pi_2}(\sigma)\,. \tag{A.32}$$

Proof. From Proposition A.10 we immediately get

$$h_{\lambda\pi_1+(1-\lambda)\pi_2}(\sigma) \leq \lambda h_{\pi_1}(\sigma) + (1-\lambda)h_{\pi_2}(\sigma)\,. \tag{A.33}$$

Let $\varepsilon > 0$ be arbitrary. Choose sub-σ-algebras $\mathscr{A}_1, \mathscr{A}_2$ such that

$$h_{\pi_1}(\sigma, \mathscr{A}_1) > h_{\pi_1}(\sigma) - \varepsilon \qquad \text{and} \qquad h_{\pi_2}(\sigma, \mathscr{A}_2) > h_{\pi_2}(\sigma) - \varepsilon\,. \tag{A.34}$$

Let $\mathscr{A} \triangleq \mathscr{A}_1 \vee \mathscr{A}_2$. Then

$$\begin{aligned} h_{\lambda\pi_1+(1-\lambda)\pi_2}(\sigma, \mathscr{A}) &= \lambda h_{\pi_1}(\sigma, \mathscr{A}) + (1-\lambda)h_{\pi_2}(\sigma, \mathscr{A}) && \text{(A.35)}\\ &\geq \lambda h_{\pi_1}(\sigma, \mathscr{A}_1) + (1-\lambda)h_{\pi_2}(\sigma, \mathscr{A}_2) && \text{(A.36)}\\ &> \lambda h_{\pi_1}(\sigma) + (1-\lambda)h_{\pi_2}(\sigma) - \varepsilon\,. && \text{(A.37)} \end{aligned}$$

Since ε is arbitrary, we obtain that

$$h_{\lambda\pi_1+(1-\lambda)\pi_2}(\sigma) \geq \lambda h_{\pi_1}(\sigma) + (1-\lambda)h_{\pi_2}(\sigma) \;, \tag{A.38}$$

which together with (A.33) proves the claim. □

The following is the *Shannon-McMillan-Breiman Theorem*. See [59] for a more general variant.

Theorem A.15 (Theorem 13.1 in [7])**.** *For every σ-ergodic measure $\pi \in \mathscr{M}_\sigma[\mathcal{X}]$ we have*

$$\limsup_{n\to\infty} \frac{-\log \pi\left([x]_{I_n}\right)}{|I_n|} = \liminf_{n\to\infty} \frac{-\log \pi\left([x]_{I_n}\right)}{|I_n|} = h_\pi(\sigma) \;, \tag{A.39}$$

for π-almost every $x \in \mathcal{X}$.

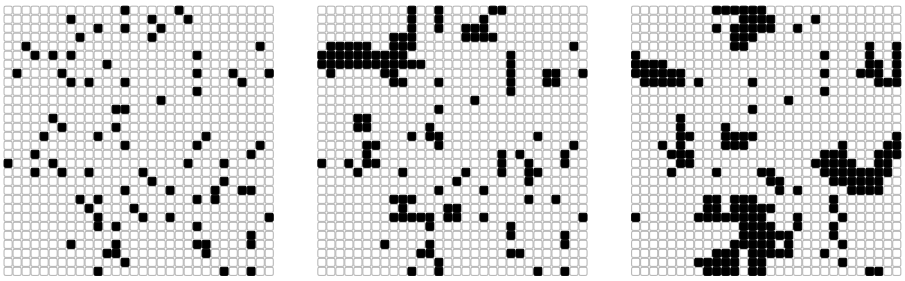
APPENDIX B

Example: The Ising Model

The Ising model, suggested by Lenz and Ising, is intended to describe the phase transition in ferromagnetic material (see e.g. [78, 31, 32]). A piece of iron can form a permanent magnet at room temperature. However, there is a certain critical temperature, above which the iron loses its magnetic property. The main reason for interest in the Ising model is that, despite its simplistic construction, it exhibits such phase transition. Understanding phase transition is one of the central goals of statistical physics (see e.g. [77, 31, 78, 57]).

In the Ising model, each cell on the lattice represents a tiny piece of a ferromagnetic material having a *spin* (i.e., a magnetic moment resulting from the angular momentum of the electrons). For simplicity, each spin is approximated by either of two values: $\uparrow$ (spin-up) or $\downarrow$ (spin-down). Adjacent spins tend to align. This tendency is depicted by assigning an energy $-\varsigma(a)\varsigma(b)$ to each pair of adjacent cells with states a and b, where $\varsigma(\uparrow) \triangleq 1$ and $\varsigma(\downarrow) \triangleq -1$.

A simple CA-like deterministic dynamics on the Ising model was introduced by Gérard Vichniac [82] (see e.g. [19, 80]). There, the lattice is partitioned into black and white cells, as on a chess board. At each time step, the cells in only one of the two partitions update their states. This is to remove the artifacts of synchronous updating. Thus it may be, for example, that on odd time steps, only the black cells are updated, while on even time steps, only the white cells. The spin of an updating cell is flipped (from $\uparrow$ to $\downarrow$, and vice versa) if and only if the flip does not require any energy exchange; that is, if and only if the change does not affect the total energy of the bonds in the vicinity of that cell. Figure B.1 shows few snapshots of the two-dimensional Ising CA.



(a) (b) (c)

Figure B.1: Simulation of Vichniac's dynamics on a spatially periodic configuration of the two-dimensional Ising model. Black represents $\uparrow$. White represents $\downarrow$. (a) The initial configuration. (b) The configuration at time $t = 10$. (c) The configuration at time $t = 60$.

B.1 The One-dimensional Model

Let $S \triangleq \{\uparrow, \downarrow\}$. A configuration of the one-dimensional Ising model is an element of $S^{\mathbb{Z}}$. Vichnic's dynamics is defined using two continuous mappings F_0 and F_1, which are iterated alternatingly on the configuration. For every configuration $x : \mathbb{Z} \to S$ and every cell $i \in \mathbb{Z}$, we have

$$(F_0 x)[i] \triangleq \begin{cases} \neg x[i] & \text{if } i \text{ even and } \varsigma(x[i-1]) + \varsigma(x[i+1]) = 0, \\ x[i] & \text{otherwise,} \end{cases} \tag{B.1}$$

$$(F_1 x)[i] \triangleq \begin{cases} \neg x[i] & \text{if } i \text{ odd and } \varsigma(x[i-1]) + \varsigma(x[i+1]) = 0, \\ x[i] & \text{otherwise,} \end{cases} \tag{B.2}$$

where $\neg \uparrow \triangleq \downarrow$ and $\neg \downarrow \triangleq \uparrow$, and where $\varsigma(\uparrow) \triangleq 1$ and $\varsigma(\downarrow) \triangleq -1$.

For every pattern $p : \{a, b\} \to S$ with $b = a + 1$, let $\theta(p) \triangleq -\varsigma(p[a]) \cdot \varsigma(p[b])$, and define $\theta(p) \triangleq 0$ for other patterns $p \in S^{\#}$. By construction, each of F_0 and F_1 conserves the potential difference Δ generated by θ. As we shall see, F_0 and F_1 also preserve any Gibbs measure with potential difference Δ.

For $\beta \in \mathbb{R}^+$, let $\pi \in \mathscr{G}(\beta\Delta)$ be a Gibbs measure with potential $\beta\Delta$. Equivalently, π would be a Markov measure with neighborhood $\{-1, 0, 1\}$ and conditional probabilities satisfying

$$\pi(\uparrow \mid a \sqcup b) = 2^{-\beta \cdot \Delta(a\downarrow b, a\uparrow b)} \cdot \pi(\downarrow \mid a \sqcup b) \,. \tag{B.3}$$

a	x	b	$\pi(x\|a \sqcup b)$			
			β	β=0.05	β=0.5	β=1.5
$\downarrow$	$\downarrow$	$\downarrow$	$\frac{2^{2\beta}}{2^{2\beta}+2^{-2\beta}}$	0.5346	$\frac{4}{5}$	0.9846
$\downarrow$	$\downarrow$	$\uparrow$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
$\downarrow$	$\uparrow$	$\downarrow$	$\frac{2^{-2\beta}}{2^{2\beta}+2^{-2\beta}}$	0.4654	$\frac{1}{5}$	0.0154
$\downarrow$	$\uparrow$	$\uparrow$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
$\uparrow$	$\downarrow$	$\downarrow$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
$\uparrow$	$\downarrow$	$\uparrow$	$\frac{2^{2\beta}}{2^{2\beta}+2^{-2\beta}}$	0.5346	$\frac{4}{5}$	0.9856
$\uparrow$	$\uparrow$	$\downarrow$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
$\uparrow$	$\uparrow$	$\uparrow$	$\frac{2^{-2\beta}}{2^{2\beta}+2^{-2\beta}}$	0.4654	$\frac{1}{5}$	0.0154

Table B.1: The conditional probabilities of the equilibrium measure in the one-dimensional Ising model. Parameter β represents the inverse of the temperature.

Here β is a parameter, physically interpreted as the inverse of the absolute temperature. According to Proposition 5.1 and Corollary 5.8, such a Markov measure always exists and is unique. Table B.1 shows the conditional probabilities at a few sample temperatures. Notice that the higher the temperature (the smaller the β), the closer the conditional distributions get to the uniform distribution. This is consistent with the physical situation, in which at high temperatures, the interaction between spins are undermined by the thermal motions. On the other hand, when the temperature is close to zero (i.e., as $\beta \to \infty$), every spin with probability 1 is aligned with its neighboring spins. In other words, the configuration tends to subside to the lowest energy level possible.

According to Theorem 5.7, the measure π defines a Markov chain with memory 1. Calculating the transition matrix of this Markov chain we get

$$A = \begin{bmatrix} \pi(\downarrow \mid \downarrow) & \pi(\downarrow \mid \uparrow) \\ \pi(\uparrow \mid \downarrow) & \pi(\uparrow \mid \uparrow) \end{bmatrix} = \frac{1}{2^{\beta} + 2^{-\beta}} \begin{bmatrix} 2^{\beta} & 2^{-\beta} \\ 2^{-\beta} & 2^{\beta} \end{bmatrix}. \tag{B.4}$$

For sample inverse temperature values $\beta = 0.05, 0.5, 1.5$, we get the matrices

$$A_{0.05} \approx \begin{bmatrix} 0.5173 & 0.4827 \\ 0.4827 & 0.5173 \end{bmatrix},\ A_{0.5} = \begin{bmatrix} \frac{2}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{2}{3} \end{bmatrix},\ A_{1.5} \approx \begin{bmatrix} 0.8889 & 0.1111 \\ 0.1111 & 0.8889 \end{bmatrix}. \tag{B.5}$$

Let us now verify that F_0 preserves the measure π. Let $p : [i,j] \to S$ be an arbitrary pattern, where $i, j \in \mathbb{Z}$ are both odd and $i \leq j$. Then $F_0^{-1}[p]_{[i,j]} = [q]_{[i,j]}$, where $q : [i,j] \to S$ is a pattern which agrees with p on i and j, and we have $\Delta(p,q) = 0$. Therefore,

$$\begin{aligned}
(F_0\pi)\left([p]_{[i,j]}\right) &= \pi\left([q]_{[i,j]}\right) && \text{(B.6)}\\
&= \pi\left([q]_{\{i,j\}}\right) \cdot \pi\left([q]_{(i,j)} \,|\, [q]_{\{i,j\}}\right) && \text{(B.7)}\\
&= \pi\left([q]_{\{i,j\}}\right) \cdot 2^{-\beta\cdot\Delta(p,q)} \cdot \pi\left([p]_{(i,j)} \,|\, [p]_{\{i,j\}}\right) && \text{(B.8)}\\
&= \pi\left([p]_{[i,j]}\right) \ . && \text{(B.9)}
\end{aligned}$$

Similarly, one sees that π is preserved by F_1 as well.

Let us finally remark that F_0 and F_1 can be combined to make a CA (e.g. [80]). The one-dimensional Ising CA has state set $S \times S$, neighborhood $\{-1, 0, 1\}$, and local rule

$$f\left(\begin{array}{|c|}\hline a_1\\\hline a_2\\\hline\end{array}, \begin{array}{|c|}\hline x_1\\\hline x_2\\\hline\end{array}, \begin{array}{|c|}\hline b_1\\\hline b_2\\\hline\end{array}\right) \triangleq \begin{cases} \begin{array}{|c|}\hline x_2\\\hline \neg x_1\\\hline\end{array} & \text{if } \varsigma(a_2) + \varsigma(b_2) = 0, \\ \begin{array}{|c|}\hline x_2\\\hline x_1\\\hline\end{array} & \text{otherwise.} \end{cases} \qquad \text{(B.10)}$$

A configuration of this CA can be interpreted as two Ising configuration woven into each other. At each time step, the CA applies F_0 on one thread and F_1 on the other, and then swaps the place of the two threads.

B.2 The Two-dimensional Model

A configuration of the two-dimensional Ising model is an element of $S^{\mathbb{Z}^2}$, with $S \triangleq \{\uparrow, \downarrow\}$. Vichniac's dynamics are defined as in the one-dimensional case, using Equations B.1 and B.2, where a cell $i = (i_1, i_2) \in \mathbb{Z}^2$ is called *even* (or *odd*), if $i_1 + i_2$ is even (respectively, odd). The potential difference is also defined similarly. For every pattern $p : \{a, b\} \to S$ with $\|b - a\| = 1$, let $\theta(p) \triangleq -\varsigma(p[a]) \cdot \varsigma(p[b])$, and define $\theta(p) \triangleq 0$ for other patterns $p \in S^{\#}$. Again, by construction, each of F_0 and F_1 conserves Δ.

Let π be a Markov measure with neighborhood $\{(i_1, i_2) : |i_1| + |i_2| \leq 1\}$ and conditional probabilities satisfying

$$\pi\left(\uparrow \;\middle|\; \begin{array}{ccc} & \boxed{a} & \\ \boxed{b} & \boxed{\sqcup} & \boxed{c} \\ & \boxed{d} & \end{array}\right) = 2^{-\beta\cdot\Delta\left(\begin{array}{ccc} & \boxed{a} & \\ \boxed{b} & \boxed{\downarrow} & \boxed{c} \\ & \boxed{d} & \end{array}, \begin{array}{ccc} & \boxed{a} & \\ \boxed{b} & \boxed{\uparrow} & \boxed{c} \\ & \boxed{d} & \end{array}\right)} \cdot \pi\left(\downarrow \;\middle|\; \begin{array}{ccc} & \boxed{a} & \\ \boxed{b} & \boxed{\sqcup} & \boxed{c} \\ & \boxed{d} & \end{array}\right) \ , \qquad \text{(B.11)}$$

where β represents the inverse of the temperature. Table B.2 shows the conditional probabilities.

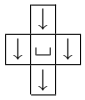
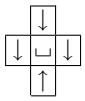
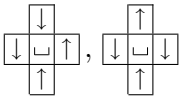
p	$\pi(\downarrow \mid p)$	$\pi(\uparrow \mid p)$
	$\frac{2^{4\beta}}{2^{4\beta}+2^{-4\beta}}$	$\frac{2^{-4\beta}}{2^{4\beta}+2^{-4\beta}}$
	$\frac{2^{2\beta}}{2^{2\beta}+2^{-2\beta}}$	$\frac{2^{-2\beta}}{2^{2\beta}+2^{-2\beta}}$
	$\frac{1}{2}$	$\frac{1}{2}$

Table B.2: The conditional probabilities of the equilibrium measure in the two-dimensional Ising model. Parameter β represents the inverse of the temperature. Symmetrically identical cases are omitted.

A Markov measure π with such specification always exists, but is not unique! In fact, there is a critical value $\beta_c = \frac{1}{2}\log(1+\sqrt{2})$ such that for $\beta < \beta_c$ (high temperatures), the above specification has a unique phase, while for $\beta > \beta_c$ (low temperatures), there are two distinct phases. See e.g. [32, 31, 78] for the proof of this fact.

Exactly as in the one-dimensional case, one can verify that each such Markov measure is preserved by F_0 and F_1.

Bibliography

[1] V. I. Arnold. *Mathematical Methods of Classical Mechanics*. Springer-Verlag, 2nd edition, 1989. English Translation.

[2] John C. Baez and James Gilliam. An algebraic approach to discrete mechanics. *Letters in Mathematical Physics*, 31:205–212, 1994.

[3] J. Banks, J. Brooks, G. Cairns, G. Davis, and P. Stacey. On Devaney's definition of chaos. *The American Mathematical Monthly*, 99(4):332–334, 1992.

[4] Heinz Bauer. *Probability Theory and Elements of Measure Theory*. Academic Press, 2nd edition, 1981. English Translation.

[5] Vincent Bernardi. *Lois de conservation sur automates cellulaires*. PhD thesis, Université de Provence, 2007.

[6] Vincent Bernardi, Bruno Durand, Enrico Formenti, and Jarkko Kari. A new dimension sensitive property for cellular automata. *Theoretical Computer Science*, 345:235–247, 2005.

[7] Patrick Billingsley. *Ergodic Theory and Information*. Wiley, 1965.

[8] A. P. Biryukov. Some algorithmic problems for finitely defined commutative semigroups. *Siberian Mathematical Journal*, 8(3):384–391, 1967.

[9] Vincent D. Blondel, Julien Cassaigne, and Codrin Nichitiu. On the presence of periodic configurations in Turing machines and in counter machines. *Theoretical Computer Science*, 289:573–590, 2002.

[10] Nino Boccara. Eventually number-conserving cellular automata. *International Journal of Modern Physics C*, 18:35–42, 2007.

[11] Nino Boccara and Henryk Fukś. Cellular automaton rules conserving the number of active sites. *Journal of Physics A: Mathematical and General*, 31(28):6007–6018, 1998.

[12] Nino Boccara and Henryk Fukś. Number-conserving cellular automaton rules. *Fundamenta Informaticae*, 52:1–13, 2002.

[13] Nino Boccara and Henryk Fukś. Motion representation of one-dimensional cellular automata rules. *International Journal of Modern Physics C*, 17:1605–1611, 2006.

[14] Tim Boykett. Towards a Noether-like conservation law theorem for one dimensional reversible cellular automata. `arXiv:nlin.CG/0312003`, 2005.

[15] Tim Boykett, Jarkko Kari, and Siamak Taati. Conservation laws in rectangular CA. *Journal of Cellular Automata*, 3(2):115–122, 2008.

[16] Timothy Boykett and Cristopher Moore. Conserved quantities in one-dimensional cellular automata. Unpublished manuscript, 1998.

[17] Mike Boyle. Open problems in symbolic dynamics. In K. Burns, D. Dolgopyat, and Y. Pesin, editors, *Geometric and Probabilistic Structures in Dynamics*, Contemporary Mathematics. American Mathematical Society, 2008.

[18] G. Cattaneo, E. Formenti, L. Margara, and J. Mazoyer. A shift-invariant metric on $S^{\mathbb{Z}}$ inducing a non-trivial topology. In I. Prívara and P. Ruzicka, editors, *Proceedings of MFCS 1997*, volume 1295 of *LNCS*, pages 179–188, 1997.

[19] Bastien Chopard and Michel Droz. *Cellular Automata Modeling of Physical Systems*. Cambridge University Press, 1998.

[20] Peter Clifford. Markov random fields in statistics. In G. Grimmett and D. Welsh, editors, *Disorder in Physical Systems*, pages 19–32. Oxford University Press, 1990.

[21] Thomas M. Cover and Joy A. Thomas. *Elements of Information Theory*. Wiley-Interscience, 1991.

[22] Robert L. Devaney. *An Introduction to Chaotic Dynamical Systems*. Addison-Wesley, 1989.

[23] James Dugundji. *Topology*. Allyn and Bacon, 1966.

[24] Bruno Durand, Enrico Formenti, and Zsuzsanna Róka. Number conserving cellular automata I: decidability. *Theoretical Computer Science*, 299:523–535, 2003.

[25] Gerald B. Folland. *Real Analysis: Modern Techniques and Their Applications*. Wiley-Interscience, 2nd edition, 1999.

[26] Enrico Formenti and Aristide Grange. Number conserving cellular automata II: dynamics. *Theoretical Computer Science*, 304:269–290, 2003.

[27] Enrico Formenti, Jarkko Kari, and Siamak Taati. The most general conservation law for a cellular automaton. In E. A. Hirsch, A. A. Razborov, A. Semenov, and A. Slissenko, editors, *Proceedings of CSR 2008*, volume 5010 of *LNCS*, pages 194–203, 2008.

[28] Enrico Formenti and Petr Kůrka. Dynamics of cellular automata in non-compact spaces. In R. Meyer, editor, *Encyclopedia of Complexity and System Science*. Springer-Verlag, 2008.

[29] Henryk Fukś. A class of cellular automata equivalent to deterministic particle systems. In S. Feng, A. T. Lawniczak, and S. R. S. Varadhan, editors, *Hydrodynamic Limits and Related Topics*, volume 27 of *Fields Institute Communications*, pages 57–69. American Mathematical Society, 2000.

[30] Felix R. Gantmacher. *The Theory of Matrices*, volume 2. Chelsea Publishing Company, 1974. English Translation.

[31] Hans-Otto Georgii. *Gibbs Measures and Phase Transitions*. Walter de Gruyter, 1988.

[32] Hans-Otto Georgii, Olle Häggström, and Christian Maes. The random geometry of equilibrium phases. In C. Domb and J. Lebowitz, editors, *Phase Transitions and Critical Phenomena*, volume 18, pages 1–142. Academic Press, 2000.

[33] Eli Glasner and Benjamin Weiss. Sensitive dependence on initial conditions. *Nonlinearity*, 6:1067–1075, 1993.

[34] J. M. Greenberg, B. D. Hassard, and S. P. Hastings. Pattern formation and periodic structures in systems modeled by reaction-diffusion equations. *Bulletin of the American Mathematical Society*, 84(6), 1978.

[35] J. M. Greenberg and S. P. Hastings. Spatial patterns for discrete models of diffusion in excitable media. *SIAM Journal on Applied Mathematics*, 34(3):515–523, 1978.

[36] James Greenberg, Curtis Greene, and Stuart Hastings. A combinatorial problem arising in the study of reaction-diffusion equations. *SIAM Journal on Algebraic and Discrete Methods*, 1(1), 1980.

[37] David Griffeath. Introduction to Markov random fields. Chapter 12 in [49].

[38] P. A. Grillet. *Semigroups: An Introduction to the Structure Theory*. Dekker, 1995.

[39] Geoffrey Grimmett. A theorem about random fields. *Bulletin of the London Mathematical Society*, 5:81–84, 1973.

[40] J. Hardy, O. de Pazzis, and Y. Pomeau. Molecular dynamics of a classical lattice gas: Transport properties and time correlation functions. *Physical Review A*, 13:1949–1961, 1976.

[41] Tetsuya Hattori and Shinji Takesue. Additive conserved quantities in discrete-time lattice dynamical systems. *Physica D*, 49:295–322, 1991.

[42] G. A. Hedlund. Endomorphisms and automorphisms of the shift dynamical system. *Mathematical System Theory*, 3:320–375, 1969.

[43] Torbjørn Helvik, Kristian Lindgren, and Mats G. Nordahl. Continuity of information transport in surjective cellular automata. *Communications in Mathematical Physics*, 272:53–74, 2007.

[44] Chris Hillman. A formal theory of information: Statics. Preprint, 1995.

[45] Jarkko Kari. Reversibility and surjectivity problems of cellular automata. *Journal of Computer and System Sciences*, 48(1):149–182, 1994.

[46] Jarkko Kari. Recent results on aperiodic Wang tilings. In *Pattern Formation in Biology, Vision and Dynamics*, pages 83–96. World Scientific, 2000.

[47] Jarkko Kari. Theory of cellular automata: A survey. *Theoretical Computer Science*, 334:3–33, 2005.

[48] Jarkko Kari and Siamak Taati. A particle displacement representation for conservation laws in two-dimensional cellular automata. In B. Durand, editor, *Proceedings of JAC 2008*, pages 65–73, 2008.

[49] John G. Kemeny, J. Laurie Snell, and Anthony W. Knapp. *Denumerable Markov Chains*. Springer-Verlag, second edition, 1976.

[50] Petr Kůrka. Languages, equicontinuity and attractors in cellular automata. *Ergodic Theory and Dynamical Systems*, 17:417–433, 1997.

[51] Petr Kůrka. Topological dynamics of cellular automata. In *Codes, Systems and Graphical Models*, pages 447–486. Springer-Verlag, 2001.

[52] Petr Kůrka. Cellular automata with vanishing particles. *Fundamenta Informaticae*, 58:1–19, 2003.

[53] Petr Kůrka. *Topological and Symbolic Dynamics*, volume 11 of *Cours Spécialisés*. Société Mathématique de France, 2003.

[54] Petr Kůrka. Cellular automata in the generic space. Manuscript, 2007.

[55] L. D. Landau and E. M. Lifshitz. *Course of Theoretical Physics: Mechanics*. Elsevier, third edition, 1976. English Translation.

[56] S. Lang. *Algebra*. Addison-Wesley, 1984.

[57] Joel L. Lebowitz. Statistical mechanics: A selective review of two central issues. *Review of Modern Physics*, 71(2), 1999.

[58] Douglas Lind and Brian Marcus. *An Introduction to Symbolic Dynamics and Coding*. Cambridge University Press, 1995.

[59] Elon Lindenstrauss. Pointwise theorems for amenable groups. *Inventiones Mathematicae*, 146:259–295, 2001.

[60] Kristian Lindgren. Correlations and random information in cellular automata. *Complex Systems*, 1:529–543, 1987.

[61] Giovanni Manzini and Luciano Margara. A complete and efficiently computable topological classification of d-dimensional linear cellular automata over $\mathbb{Z}_m$. *Theoretical Computer Science*, 221:157–177, 1999.

[62] Norman Margolus. *Physics and Computation*. PhD thesis, Massachusetts Institute of Technology, 1987.

[63] Marvin Minsky. *Computation: Finite and Infinite Machines*. Prentice-Hall, 1967.

[64] Edward F. Moore. Machine models of self-reproduction. In *Proceedings of Symposia in Applied Mathematics*, pages 17–33. AMS, 1962.

[65] Andrés Moreira. Universality and decidability of number-conserving cellular automata. *Theoretical Computer Science*, 292:711–723, 2003.

[66] Andrés Moreira, Nino Boccara, and Eric Goles. On conservative and monotone one-dimensional cellular automata and their particle representation. *Theoretical Computer Science*, 325:285–316, 2004.

[67] John Myhill. The converse of Moore's Garden-of-Eden theorem. *Proceedings of the American Mathematical Society*, 14:685–686, 1963.

[68] Masakazu Nasu. Textile systems for endomorphisms and automorphisms of the shift. *Memoirs of the American Mathematical Society*, 114(546), 1995.

[69] Amos Nevo. Pointwise ergodic theorems for actions of groups. In B. Hasselblatt and A. Katok, editors, *Handbook of Dynamical Systems*, volume 1B, chapter 13, pages 871–982. Elsevier, 2006.

[70] Nicolas Ollinger. Personal communication, 2008.

[71] John C. Oxtoby. On two theorems of Parthasarathy and Kakutani concerning the shift transformation. In Fred B. Wright, editor, *Ergodic Theory*, pages 203–215. Academic Press, 1963.

[72] Marcus Pivato. Conservation laws in cellular automata. *Nonlinearity*, 15:1781–1793, 2002.

[73] Y. Pomeau. Invariant in cellular automata. *Journal of Physics A: Mathematical and General*, 17(8):L415–L418, 1984.

[74] Christopher J. Preston. *Gibbs states on countable sets*. Cambridge University Press, 1974.

[75] Arch D. Robison. Fast computation of additive cellular automata. *Complex Systems*, 1:211–216, 1987.

[76] H. L. Royden. *Real Analysis*. Macmillan, 2nd edition, 1968.

[77] David Ruelle. *Thermodynamic Formalism*. Cambridge University Press, second edition, 2004.

[78] Ya G. Sinai. *Theory of Phase Transitions: Rigorous Results*. Pergamon Press, 1982.

[79] Shinji Takesue. Reversible cellular automata and statistical mechanics. *Physical Review Letters*, 59(22):2499–2502, 1987.

[80] Tommaso Toffoli and Norman Margolus. *Cellular Automata Machines: A New Environment for Modeling*. MIT Press, 1987.

[81] J. H. van Lint and R. M. Wilson. *A Course in Combinatorics*. Cambridge University Press, 1992.

[82] Gérard Y. Vichniac. Simulating physics with cellular automata. *Physica D*, 10:96–116, 1984.

[83] Peter Walters. *An Introduction to Ergodic Theory*. Springer-Verlag, 1982.

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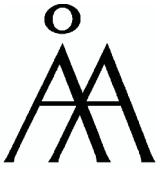

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