Relaxation Dynamics of a Lattice Spin System

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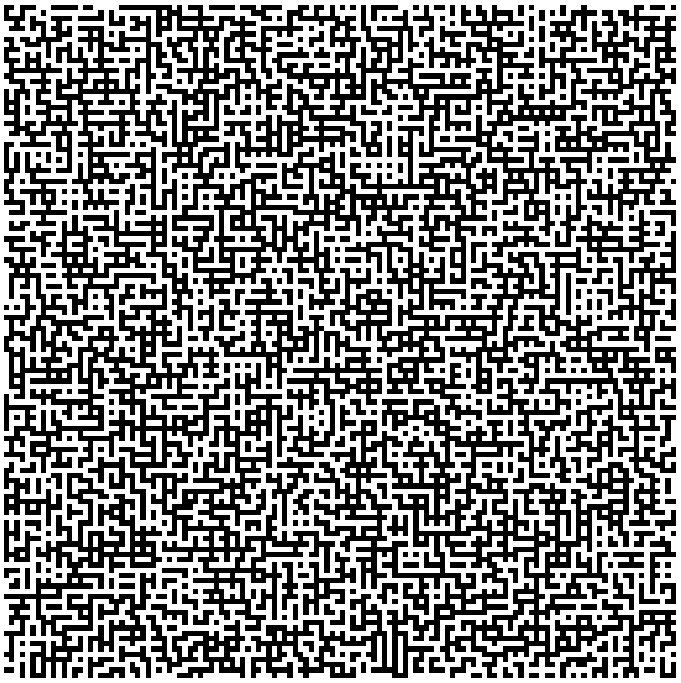
Contents

Abstract

A dynamical system, a generalization of the Ising model, is defined on two dimensional lattices with cells in one of two states. The dynamical system uses simple local rules to produce complex global behavior. Equivalence classes in the set of different rules for the system are demonstrated, and qualitative and numerical descriptions are provided for many of the rules. Finally, a localized combinatorial analysis is applied as a method of explaining the global behavior of particular rules. This analysis is useful but ultimately demonstrates the problems involved in using local information to predict global behavior.



Chapter 1

The Ising Model

1.1 Complex Systems

A unifying theme in the study of complex systems is the emergence of complex global behaviors from simple local interactions. The philosophical appeal of this phenomenon is obvious — many people believe the universe is fundamentally governed by a relatively small number of simple physical laws, and yet at the same time it supports an incredible array of complex phenomena. Even though the relationship between local rules and global behavior is manifestly interesting and important, it is not well understood.

There are many common models that capture some aspect of complexity arising out of simplicity. Cellular automata and lattice gasses use local update rules to create global behavior that models a variety of phenomena such as fluid dynamics, epidemiology, and activation spreading. Lindenmayer systems, a type of locally context-sensitive string rewriting system, have proven capable of simulating a variety of morphogenetic phenomena. Neural networks exploit a network of simple local interactions to simulate an increasingly complex set of cognitive phenomena.

All of these models share the same basic design of combining many local interactions to produce global behavior. They also share a common problem — it is very difficult to explain exactly how the global behavior emerges from the local rules. For many complex systems the only way to determine what will happen is to implement the system directly, let it run and examine the outcome. Such simulation is frequently easy to do, precisely because the rules for the model are relatively simple. But a complete analytic understanding of a complex system's global behavior is usually out of reach.

In this thesis a dynamical system is presented that uses a local update rule on a lattice to produce complex global phenomena. The model that this system is based

on, the dynamical Ising model, has been solved in several of the simpler cases. The generalization presented here produces a set of rules with widely different behaviors. First, a hierarchy of equivalence classes in the set of rules is demonstrated (chapter 3). The dynamics of representatives of the equivalence classes are then studied both statistically and qualitatively (chapters 4 and 5). Finally, a combinatorial analysis of local dynamics is applied to partially explain the global dynamics of each rule (chapter 6). This work represents one approach to studying complex systems.

1.2 The Ising Model

One complex system with a large body of analysis is the Ising model, a statistical mechanics system originally designed to simulate phase transitions in ferromagnetism. Much has been written about the Ising model since its introduction in 1925 ([Isi25]): a simple summary of the major results is available in [Cip87], and a more thorough treatment is presented in [Tho72].

The world of the Ising model is a collection of n *cells* $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_n)$. Each cell σ_i takes on a *spin*, a value either $+1$ or -1. The cells are placed on a graph with some sort of simple structure; the graph considered here is the common one where the cells are at the intersections of a two dimensional square grid, and each cell has four neighbors — one up, down, to the left, and to the right. Intuitively, this corresponds to electrons on the surface of a two dimensional crystal with a regular square structure.

Each cell can be in one of 2 states, $+1$ or -1. Therefore, an Ising model with n cells can be in a total of 2^n possible configurations, or *world states*. The Ising rule assigns to each possible world state an energy calculated by a function known as the *Hamiltonian*. For the standard Ising rule the Hamiltonian is defined as follows:

$$H(\sigma) = -E \sum_{\langle i,j \rangle} \sigma_i \sigma_j - J \sum_i \sigma_i$$

where $\sum_{\langle i,j \rangle}$ is the sum over all cells σ_i and σ_j that are adjacent in the interaction graph, and E and J are independent parameters for the system. E is the strength of the ferromagnetic interaction of two spins, and J is the strength of an external

magnetic field as applied to individual spins. There are many different systems captured in variations on E and J: for this work, the case where $J = 0$ is most relevant. The simpler Hamiltonian is then

$$H(\sigma) = -E \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

When two spins σ_i and σ_j are equal (both $+1$ or -1), their product $\sigma_i \sigma_j = +1$, and the pair contributes a negative value, $-E$, to the Hamiltonian. Pairs of opposite spins have product -1 and therefore add a positive value, $+E$, to the Hamiltonian.

The Hamiltonian is simply a sum of local pairwise spin interactions. But it has a significant global property: it is at a minimum only when *every* pair of adjacent spins are equal. There are only two world states that satisfy this requirement, the configuration where every spin is $+1$ and the configuration where every spin is -1. The Ising rule, defined entirely in terms of local spin interactions, can test for a global correlation of spins.

Most of the physics literature is concerned with the equilibrium aspects of the Ising model, in particular the *partition function:*

$$Z(\beta, E, J, n) = \sum_{\sigma_i \in \{\sigma\}} e^{-\beta H(\sigma_i)}$$

The partition function is the sum over all 2^n possible configurations σ_i of an exponential function of the Hamiltonian and $\beta = 1/kT$, where k is Boltzmann's constant and T the temperature of the model.

A major portion of the work on the Ising model is concerned with analytically solving the partition function. This function contains enough information to understand many of the equilibrium properties of the model, such as specific heat, phase transitions, etc. Solving the partition function turns out to be quite difficult, an example of the problems encountered when applying analytical techniques to complex systems. The most complete result to date is by Onsager, a solution for the two dimensional square lattice in the case when $J = 0$ (presented in [Tho72], among others). More recently, Jerrum and Sinclair have developed a probabilistic algorithm to arbitrarily approximate the partition function in polynomial time for any possible interaction graph ([JS93]).

1.3 The Dynamical Ising Model

In addition to the equilibrium properties of the Ising model, there is also a simple dynamical system that can be defined on world configurations. The Hamiltonian is usually interpreted as an energy function; physical systems generally try to *relax* to minimal energy. How might a particular world state relax to lowest energy under the Ising rule?

1.3.1 Spin Flip Dynamics

Consider the possible configurations of the world as states in a large Markov chain (with 2^n states). If the world is in a particular state σ at time t (identified with the world configuration σ), then the Markov chain defines how it can move to a new state σ' at time $t+1$. One common Markov chain defined for the Ising model is to allow only single spin flips. Two worlds are one *spin flip* apart if they are the same except for the spin at one cell in the world (ie, if the Hamming distance is 1). The Markov chain of spin flip dynamics allows transitions only when exactly one spin in σ is flipped. For example, here is a possible Ising world and a potential transition to a new state. The spin flip in the lower right middle reduces the energy by $2E$.

$$\begin{array}{ccc} -1\ -1\ +1\ +1\ +1 & & -1\ -1\ +1\ +1\ +1 \\ -1\ -1\ +1\ +1\ +1 & & -1\ -1\ +1\ +1\ +1 \\ -1\ -1\ -1\ +1\ +1 & \longrightarrow & -1\ -1\ -1\ +1\ +1 \\ -1\ -1\ -1\ \mathbf{-1}\ +1 & & -1\ -1\ -1\ \mathbf{+1}\ +1 \\ -1\ -1\ -1\ +1\ +1 & & -1\ -1\ -1\ +1\ +1 \end{array}$$

1.3.2 Transition Probabilities

Not all single spin flips are allowed with equal probability. The probability of a particular spin flip $\mathbb{P}(\sigma, \sigma')$ is a function of ΔH, the change in the Hamiltonian between σ' and σ:

$$\Delta H = H(\sigma') - H(\sigma)$$

If two worlds σ and σ' are one spin flip apart, then the probability of the transition from σ to σ' is defined in terms of ΔH and the temperature T:

$$\mathbb{P}(\sigma, \sigma') = \begin{cases} 1 & \Delta H < 0 \\ \frac{e^{-\Delta H/T}}{1+e^{-\Delta H/T}} & \Delta H \geq 0 \end{cases}$$

The spin flip dynamics with this probability function is frequently referred to as the *Glauber dynamics* [Gla63]. Note that the probability of moving between two worlds that are one spin flip apart does not depend on the particular configuration of spins in the two worlds, just on ΔH. This fact greatly simplifies the Markov chain, and will be exploited fully to understand related models where the Hamiltonian is more complicated.

The special case of this model that will be scrutinized most closely is the temperature 0 case, $T = 0$. For these models the transition probability is much simpler:

$$\mathbb{P}(\sigma, \sigma') = \begin{cases} 1 & \Delta H < 0 \\ 1/2 & \Delta H = 0 \\ 0 & \Delta H > 0 \end{cases}$$

When the temperature is 0, the only possible transitions are to configurations with equal or lower energy.

The dynamics are easily simulated by the following algorithm ([BH92], p.53):

1. Pick a random cell σ_i in the state σ.
2. Calculate ΔH for the transition from σ to the configuration $\sigma' = \sigma$ with the cell σ_i flipped.
3. Calculate the probability of the transition $\sigma \to \sigma'$ based on ΔH.
4. Simulate the probability distribution for ΔH. If the transition occurs, replace σ with σ' and repeat.

The effect of this Markov chain is to take any initial world state at high energy and slowly transform it, one spin flip at a time, to a more ordered state with lower energy. This process is known as *relaxation*, and is essentially a gradient descent method of finding minima of the Hamiltonian. Appendix A presents an example

of the relaxation process at temperature 0, showing snapshots of the world through time (states +1 and −1 are represented as white and black squares).

A major result for this dynamical Ising model is that, for any configuration on a two-dimensional grid of infinite size at temperature 0, the energy of the worlds generated by Markov chain is asymptotically $E \sim t^{-1/2}$ ([Lif62], [AC79]), and in particular $\lim_{t\to\infty} E = 0$. And the only worlds of energy 0 are those whose spins are all the same: Therefore, the dynamical process ultimately takes a random world and turns it into a configuration where every cell has spin +1 or −1.

1.3.3 Finite Size Effects

The asymptotic behavior of the dynamical Ising system is stated for worlds of infinite size. When simulating this and related dynamical systems it is impossible to represent an infinite world, so in practice one is constrained to considering worlds of finite size. The hope is that properties derived for finite systems will generalize to infinite worlds at $\lim_{n\to\infty}$.

In the two dimensional models presented here the finite size approximation will be the usual cyclic boundary conditions: connecting the left edge of the world to the right edge and the top to the bottom, producing a torus. In some cases this finite system exhibits behavior not present in the infinite limit; for example, there are instances of the Ising dynamics on finite size worlds where the energy does not go to 0 (see chapter 5). If the finite system does something that does not occur in the infinite world, that behavior will be clearly identified as a *finite size effect.*

1.4 Summary

Ising rule dynamics are defined simply and entirely locally. A function, the Hamiltonian, associates to any particular configuration an energy calculated by summing over local interactions of the individual cells. The dynamical process allows motions between nearby configurations with a certain probability that depends on the change in the Hamiltonian — in the temperature 0 case, when $\Delta H \leq 0$.

This process is governed entirely by the interaction of physically adjacent spins. And yet, at temperature 0 the end result is a global organization of spins across the entire world, not just correlation between adjacent spins. The dynamical Ising model itself is fairly simple, but it suggests a host of related models that, while still defined in terms of a simple local interaction, result in a variety of complicated and interesting global behaviors.

Chapter 2

The 2x2 Model

2.1 The Ising Model Reconsidered

The Hamiltonian for the standard Ising rule with no external magnetic field was defined as a sum over all adjacent pairs of spins:

$$H(\sigma) = -E \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

While this version of the Ising model is physically motivated, the Ising model can also be considered as a purely combinatorial system, independent of an interpretation as ferromagnetically interacting electrons.

Another way to think of the Ising rule is to consider it as a sum over all 1x2 blocks of spins: in a two dimensional square grid, two adjacent cells are always the members of a 1x2 block, oriented either horizontally or vertically. There are four possible 1x2 blocks:

$$\begin{matrix} -1 & -1 & +1 & +1 \\ -1 & +1 & -1 & +1 \end{matrix}$$

Let S denote the set of blocks whose cells have equal spin (both $+1$ or -1), and D be the set of blocks whose cells have opposite spin. For the Ising rule, members of S contribute $-E$ to the Hamiltonian, whereas members of D contribute $+E$. Therefore, the Hamiltonian can also be expressed as the sum over all blocks in S and all blocks in D:

$$H(\sigma) = \sum_{S} -E + \sum_{D} E$$

In the future, blocks will also be called "neighborhoods," borrowing the term from cellular automata literature.

Because the Hamiltonian is stated in terms of "same" and "different" blocks, instead of products of spins, there is no need for the values of the spins σ_i themselves to have any particular meaning. Instead of a world of cells of spin ± 1, the model can be stated as a collection of cells in one of two arbitrary states, state `0` and state `1`.

There are still four possible 1x2 neighborhoods, two the same and two different, and the Hamiltonian for the Ising rule can still be stated as the sum over neighborhoods in the sets S and D.

To further simplify the Hamiltonian it is helpful to eliminate negative values from the calculation. As stated, there are two energies in the Hamiltonian: $-E$, for those neighborhoods where the two states are equal, and $+E$, for those where the two states are different. Relabel these E_S and E_D.

$$H(\sigma) = \sum_S E_S + \sum_D E_D$$

When $E_S = -E$ and $E_D = +E$, the Hamiltonian is the same as the standard Ising rule. When $E_S = 0$ and $E_D = 1$, the function is essentially the same as the standard Ising rule except that the Hamiltonian is always positive. The minimum of this new Hamiltonian is $H = 0$, but still occurs only when all cells in the world are the same state. ΔH will still be the same as the standard Ising rule, up to a constant multiplier. The dynamical process is not significantly altered by this restatement.

2.2 2x2 Rules

Having stated the Ising rule in terms of 1x2 neighborhoods, a natural generalization is to consider models where the Hamiltonian is defined as sums over larger neighborhoods. The Hamiltonian for 2x2 neighborhoods is considerably more complicated than that for 1x2 neighborhoods. Each of the four cells in a neighborhood can be either `0` or `1`, resulting in $2^4 = 16$ different 2x2 neighborhoods. Give these 16 neighborhoods the arbitrary names $n_0, n_1, \ldots n_{15}$, and assign to each neighborhood an energy E_{n_i}.

Let N be the set of all 2x2 neighborhoods in the world. Note that neighborhoods overlap and that every cell is a member of 4 different neighborhoods. The Hamiltonian defined on 2x2 blocks is:

$$H(\sigma) = \sum_{N=n_0} E_{n_0} + \sum_{N=n_1} E_{n_1} + \cdots + \sum_{N=n_{15}} E_{n_{15}}$$

There is no particular physical motivation for the generalization to 2x2 blocks. A physical system that implemented this Hamiltonian would be quite unlike the ferromagnets that the Ising model simulates. Even allowing for interaction between groups of four nearby electrons, the Hamiltonian for a general 2x2 rule is not the sum over simple four-point products. For example, the product of spins in the 2x2 blocks $\begin{smallmatrix}-1&-1\\-1&-1\end{smallmatrix}$ and $\begin{smallmatrix}-1&-1\\+1&+1\end{smallmatrix}$ are both +1: they would be given the same energy by a Hamiltonian defined as a product of four spins. But the general 2x2 system can assign different energies to the corresponding neighborhoods $\begin{smallmatrix}0&0\\0&0\end{smallmatrix}$ and $\begin{smallmatrix}0&0\\1&1\end{smallmatrix}$.

The main motivation for studying this system is that it is a natural extension of the Ising rule, with enough room in the space of possible rules to have many different dynamical behaviors.

2.3 Rotational Symmetry

One feature of the general 2x2 model is that arbitrary 2x2 rules are capable of distinguishing a global property of the world: left from right, up from down. In particular, a rule can assign a different energy to $\begin{smallmatrix}1&1\\0&0\end{smallmatrix}$ than to $\begin{smallmatrix}0&0\\1&1\end{smallmatrix}$ — this amounts to global information about which direction the 'top' of the world is. Requiring that a rule assign the same energy to all rotations of a neighborhood eliminates this global information.

Definition 2.1 (Rotationally Symmetric Rule) *A 2x2 rule is rotationally symmetric if it assigns the same energy to all rotations of a neighborhood.*

There are six rotationally distinct 2x2 neighborhoods. These are:

$$\mathbf{0} = \begin{smallmatrix}0&0\\0&0\end{smallmatrix} \qquad \mathbf{1} = \begin{smallmatrix}0&0\\0&1\end{smallmatrix} \qquad \mathbf{S} = \begin{smallmatrix}0&0\\1&1\end{smallmatrix}$$

$$\mathbf{4} = \begin{smallmatrix}1&1\\1&1\end{smallmatrix} \qquad \mathbf{3} = \begin{smallmatrix}0&1\\1&1\end{smallmatrix} \qquad \mathbf{C} = \begin{smallmatrix}0&1\\1&0\end{smallmatrix}$$

The names are mnemonic. A number indicates how many 1s there are in the neighborhood. There are two distinct neighborhoods with two 1s, so they are given the names **S** for 'stripe' and **C** for 'checkerboard.'

A rotationally symmetric 2x2 rule assigns an energy to each of the six rotational classes of neighborhoods. These energies are named $E_{\mathbf{0}}, E_{\mathbf{1}}, E_{\mathbf{S}}, E_{\mathbf{C}}, E_{\mathbf{3}}$, and $E_{\mathbf{4}}$.

Each neighborhood in the world is one of the six rotational types. Let $S_{\mathbf{0}}$ be the set of all neighborhoods that are of type **0**, $S_{\mathbf{1}}$ be all neighborhoods of type **1**, etc. The rotationally symmetric rules have the following Hamiltonian:

$$H = \sum_{S_0} E_{\mathbf{0}} + \sum_{S_1} E_{\mathbf{1}} + \sum_{S_{\mathbf{S}}} E_{\mathbf{S}} + \sum_{S_{\mathbf{C}}} E_{\mathbf{C}} + \sum_{S_3} E_{\mathbf{3}} + \sum_{S_4} E_{\mathbf{4}}$$

The things being summed in the Hamiltonian are simply constants. For any neighborhood **n**, $\sum_{S_{\mathbf{n}}} E_{\mathbf{n}} = E_{\mathbf{n}} \sum_{S_{\mathbf{n}}} 1$, and the sum $\sum_{S_{\mathbf{n}}} 1$ is just a count of all neighborhoods of type **n**. As this sum is the major feature being counted in the Hamiltonian, it will be abbreviated $N_{\mathbf{n}}$ for any particular type of neighborhood **n**. Ie: $N_{\mathbf{0}} = |\{\text{neighborhoods of type } \mathbf{0}\}|$.

Definition 2.2 (Hamiltonian for Rotationally Symmetric 2x2 Rules)

$$H(\sigma) \;=\; E_{\mathbf{0}}N_{\mathbf{0}} + E_{\mathbf{1}}N_{\mathbf{1}} + E_{\mathbf{S}}N_{\mathbf{S}} + E_{\mathbf{C}}N_{\mathbf{C}} + E_{\mathbf{3}}N_{\mathbf{3}} + E_{\mathbf{4}}N_{\mathbf{4}}$$

The Ising model is one rotationally symmetric rule. The Ising rule gives energy 0 to 1x2 blocks of equal spin, and energy 1 to 1x2 blocks of opposite spin. In 2x2 terms, every pair of cells in the neighborhoods **0** and **4** are equal; therefore, in the 2x2 Ising rule **0** and **4** have energy 0. **1**, **S**, and **3** each have two pairs of cells that are different: these 2x2 neighborhoods have energy 2. Finally, in **C** every adjacent pair of cells is opposite, yielding energy 4. Assigning $E_{\mathbf{0}} = E_{\mathbf{4}} = 0$, $E_{\mathbf{1}} = E_{\mathbf{S}} = E_{\mathbf{0}} = 2$, and $E_{\mathbf{C}} = 4$, the Hamiltonian for this 2x2 rule is identical to the Ising rule on 1x2 rules, up to a constant multiplier.

2.4 A Simplification

The set of possible rotationally symmetric 2x2 rules is fairly large: each of the six energies can be any real number, yielding a six dimensional space of possible rules. To further simplify the model, the only rules considered in the future will be those where each $E_{\mathbf{n}}$ is in the set $\{0, 1\}$. These energies will be interpreted as 'allowing' or 'disallowing' certain neighborhoods.

Definition 2.3 (Allowed and Disallowed) *Neighborhoods with energy 0 are called allowed neighborhoods. Disallowed neighborhoods have energy 1.*

The Ising rule cannot be exactly expressed under this restriction. For the Ising rule on 2x2 neighborhoods, **C** has twice as many opposite pairs as **1**, and thus $E_{\mathbf{C}} = 2E_{\mathbf{1}}$. But under the restriction that all neighborhoods have only energy 0 or 1, $E_{\mathbf{C}}$ cannot be twice $E_{\mathbf{1}}$. However, the rule where $E_{\mathbf{C}} = E_{\mathbf{1}} = 1$ yields dynamics almost identical to the Ising rule (neighborhoods of type **C** do not seem to play a crucial role.) In the future, when the 'Ising rule' is mentioned it will refer to this not-quite-exact representation.

In addition to simplifying the model, the restriction of energies to $\{0, 1\}$ is motivated by related work on classes of two-dimensional string languages. Computer scientists frequently study sequences of one-dimensional symbols — sets of these strings are called "languages" [HU79]. One subset of the regular languages on one dimensional strings are the "finite complement" languages. In brief, a finite complement language is specified by a finite set of forbidden substrings. Every string that does not contain a substring in the forbidden set is in the finite complement language.

The generalization of finite complement languages to two dimensional strings is called "Local Lattice Languages" (LLLs), those languages which can be specified by forbidding certain finite blocks [LMN93]. Building a recognition machine for any particular LLL is easy — simply scan each local block to see if it is on the list of forbidden patterns.

The Hamiltonian for 2x2 rules is a machine which determines whether a world is in a given LLL. Blocks which are permitted by the LLL rule are given energy 0 ('allowed') in the Hamiltonian recognition machine, and those which are forbidden are given energy 1 ('disallowed'). The strings in the LLL are then exactly the set of world configurations σ such that $H(\sigma) = 0$, the ground states of the Hamiltonian.

The Hamiltonian is a recognition machine for LLLs; the dynamical spin-flip process suggests a way to create strings that match a certain LLL rule. Simply apply the dynamical process to a random initial world configuration. If the system

relaxes to energy 0, a string in the LLL has been generated. It will be seen that certain rules relax to energy 0 on random input and others do not. An interesting question is to what degree the outcome is predictable by simply looking at the LLL. This question is addressed in chapter 6.

2.5 Rule Space

The remainder of this thesis will be concerned with the dynamics of rotationally symmetric 2x2 rules whose energies are constrained to the set $\{0, 1\}$. There are six different neighborhoods, and thus $2^6 = 64$ different rules in this set. Each rule will be referred to by its canonical number, a number in $[0 - 63]$.

Definition 2.4 (Canonical Rule Numbering) *The canonical number N of a rotationally symmetric rule is*

$$N = E_{\mathbf{0}}2^0 + E_{\mathbf{1}}2^1 + E_{\mathbf{S}}2^2 + E_{\mathbf{C}}2^3 + E_{\mathbf{3}}2^4 + E_{\mathbf{4}}2^5$$

This numbering is simply a binary coding of the energies associated with each neighborhood. Rules will be written in boldface: "Rule **30**." Frequently, for ease of reading, the allowed neighborhoods will be listed in parenthesis next to the rule: "Rule **30** (**04**)." A complete dictionary of all rules and their corresponding allowed and disallowed neighborhoods is in Appendix B.

Each rule R defines a Hamiltonian. The Hamiltonian for R applied to a world configuration σ will be notated $H_R(\sigma)$.

2.6 The Dynamical 2x2 Model

The dynamical system for the Ising rule was defined in terms of spin flips and ΔH. Therefore, it generalizes naturally to 2x2 rules. At each time step a cell is picked in the world. If flipping its value would lower the Hamiltonian for the world ($\Delta H < 0$), then that flip is performed. At zero temperature, if flipping the cell would not change the energy ($\Delta H = 0$), then the flip happens with probability 1/2. Flips to high energy states ($\Delta H > 0$) do not happen.

The general result of this dynamical system is frequently surprising and aesthetically pleasing. The Ising rule has only two ground states and a simple dynamical behavior — shrinking domains. Any particular 2x2 rule might have a large set of interesting ground states as well as a possibly complex dynamical process. Chapter 5 gives a qualitative description of several of the rotationally symmetric rules. In addition, there are two example runs in the form of flipbooks on the corners of the pages of this thesis. Left side pages are Rule **26**, right side pages are Rule **22**. The time between each frame is not a constant, but varies according to how fast the rule acts.

As in the Ising rule, the Hamiltonian is defined by local interactions. Therefore, ΔH can again be calculated locally for any particular spin flip. Every cell in the world belongs to exactly four neighborhoods. Therefore, ΔH for any particular spin flip depends only on ΔH for the four 2x2 neighborhoods the chosen cell belongs to — a local 3x3 block.

This trick considerably shortens the amount of computation required to simulate the dynamical process. It also serves as a reminder that this system is defined locally; for any potential spin flip, only local information is necessary to decide whether to perform that flip. However the resulting dynamical behavior of repeated spin flips is a global phenomenon. As in the Ising model, the dynamical system might ultimately result in a world with correlations between far-away cells.

Chapter 3

Symmetries and Equivalent Rules

3.1 Introduction

Of the 64 rules in the set of rotationally symmetric 2x2 rules, not every rule produces a unique dynamical behavior. For example, Rule **31** (**4**) is 'equivalent', in an important sense, to Rule **62** (**0**). These two rules have exactly opposite ground states — Rule **31** allows only solid fields of `1`, whereas Rule **62** allows only solid fields of `0`. The 'meanings' of `0` and `1` are entirely arbitrary — intuitively, if `0` and `1` have no special meaning, then a configuration of all `0` is not much different from a configuration of all `1`.

For both Rule **31** and Rule **62** the Hamiltonian is simply the sum of all neighborhoods that are not exactly a block of four cells all in the same state — the only difference is which state is 'correct.' The dynamical system corresponding to these rules is identical except for the role of `0` and `1`.

Formalizing this concept, it will be seen that Rule **31** and Rule **62** *are* equivalent, at least when considered under the appropriate transformation on the world. Four different transformations on the world will be defined, and it will be shown that under these transformations the set of 64 rules can be broken up into 32 equivalence classes, each rule being a member of one of these classes.

3.2 Parity Transformation

First, formalize the notion of "two configurations are the same except for the roles of `0` and `1`":

Definition 3.1 (Parity Transformation on a World) *Application of the parity transformation P on a world configuration σ, $P(\sigma)$, results in a new configuration σ' which is the configuration σ with all* `1`*s turned into* `0`*s and all* `0`*s turned into* `1`*s.*

Definition 3.2 (Parity Equivalence of Worlds) *Two configurations σ and σ' are parity equivalent if $P(\sigma) = \sigma'$.*

Parity-equivalent configurations differ only in the roles of `0` and `1`. As the labels `0` and `1` are arbitrary, without any external meaning, this difference is not significant.

$$\begin{matrix}0&1&1&0\\0&0&1&1\\0&0&0&1\\1&0&0&0\end{matrix} \quad \text{is parity equivalent to} \quad \begin{matrix}1&0&0&1\\1&1&0&0\\1&1&1&0\\0&1&1&1\end{matrix}$$

Because the evaluation of the Hamiltonian is defined in terms of 2x2 neighborhoods, it is important to consider the action of the parity transformation just on those 2x2 neighborhoods. P turns every neighborhood into its complement: $P(\mathbf{0}) = \mathbf{4}$, $P(\mathbf{1}) = \mathbf{3}$, $P(\mathbf{S}) = \mathbf{S}$, $P(\mathbf{C}) = \mathbf{C}$, $P(\mathbf{3}) = \mathbf{1}$, and $P(\mathbf{4}) = \mathbf{0}$. The action of the parity transform will be notated:

$$\begin{aligned}\mathbf{0} &\longleftrightarrow \mathbf{4}\\ \mathbf{1} &\longleftrightarrow \mathbf{3}\end{aligned}$$

which is taken to mean "**0** and **4** switch roles, **1** and **3** switch roles, **S** and **C** remain fixed."

Now that the parity transformation is defined for worlds, it is natural to ask what rule R', when applied to the transformed configuration $\sigma' = P(\sigma)$, yields the same Hamiltonian as a rule R applied to σ.

Note that every **0** in σ is transformed into a corresponding **4** in σ'. This implies that the number of **0** neighborhoods in σ is the same as the number of **4** neighborhoods in σ':

$$N_{\mathbf{0}} = N'_{\mathbf{4}} \tag{3.1}$$

Similarly,

$$N_{\mathbf{1}} = N'_{\mathbf{3}} \quad N_{\mathbf{S}} = N'_{\mathbf{S}} \quad N_{\mathbf{C}} = N'_{\mathbf{C}} \quad N_{\mathbf{3}} = N'_{\mathbf{1}} \quad N_{\mathbf{4}} = N'_{\mathbf{0}}$$

By choosing R' with the appropriate energies E', an R' can be constructed such that $H_{R'}(\sigma') = H_R(\sigma)$.

Define R' as follows: let $E'_{\mathbf{0}} = E_{\mathbf{4}}$, $E'_{\mathbf{1}} = E_{\mathbf{3}}$, $E'_{\mathbf{S}} = E_{\mathbf{S}}$, $E'_{\mathbf{C}} = E_{\mathbf{C}}$, $E'_{\mathbf{3}} = E_{\mathbf{1}}$, and $E'_{\mathbf{4}} = E_{\mathbf{0}}$. Then:

$$\begin{aligned} H_{R'}(\sigma') &= E'_{\mathbf{0}}N'_{\mathbf{0}} + E'_{\mathbf{1}}N'_{\mathbf{1}} + E'_{\mathbf{S}}N'_{\mathbf{S}} + E'_{\mathbf{C}}N'_{\mathbf{C}} + E'_{\mathbf{3}}N'_{\mathbf{3}} + E'_{\mathbf{4}}N'_{\mathbf{4}} \\ &= E_{\mathbf{4}}N'_{\mathbf{0}} + E_{\mathbf{3}}N'_{\mathbf{1}} + E_{\mathbf{S}}N'_{\mathbf{S}} + E_{\mathbf{C}}N'_{\mathbf{C}} + E_{\mathbf{1}}N'_{\mathbf{3}} + E_{\mathbf{0}}N'_{\mathbf{4}} \\ &= E_{\mathbf{4}}N_{\mathbf{4}} + E_{\mathbf{3}}N_{\mathbf{3}} + E_{\mathbf{S}}N_{\mathbf{S}} + E_{\mathbf{C}}N_{\mathbf{C}} + E_{\mathbf{1}}N_{\mathbf{1}} + E_{\mathbf{0}}N_{\mathbf{0}} \\ &= H_R(\sigma) \end{aligned}$$

Thus for a rule R and an arbitrary configuration σ, there is a rule R' that yields the same Hamiltonian when applied to the transformed configuration σ'. The energy assignments to each neighborhood simply follows the action of the transformation on those neighborhoods.

Definition 3.3 (Parity Transformation on a Rule) *The application of P on a rule R, $P(R)$, yields a new rule R'. R' is derived from R by setting $E'_{\mathbf{0}} = E_{\mathbf{4}}$, $E'_{\mathbf{1}} = E_{\mathbf{3}}$, $E'_{\mathbf{S}} = E_{\mathbf{S}}$, $E'_{\mathbf{C}} = E_{\mathbf{C}}$, $E'_{\mathbf{3}} = E_{\mathbf{1}}$, and $E'_{\mathbf{4}} = E_{\mathbf{0}}$.*

Definition 3.4 (Parity Equivalence of Rules) *Two rules R and R' are parity equivalent if $P(R) = R'$.*

A rule R on the configuration σ has the same Hamiltonian as the parity equivalent rule R' on the parity equivalent configuration σ'. Therefore, in the dynamical system for any particular spin flip $\Delta H_R = \Delta H_{R'}$. The transition probabilities do not change, and so the the dynamical processes are the same.

Definition 3.5 (Parity Symmetric Rules) *A rule R is parity symmetric if it is parity equivalent to itself, ie: $P(R) = R$.*

Parity symmetric rules are those rules that are fixed by the parity transformation P, much as rotationally symmetric rules are those that are fixed under rotation. Parity symmetric rules have the same Hamiltonian on σ and $P(\sigma)$. They are incapable of distinguishing `0` from `1`, the parity of the world, and therefore they cannot bias the dynamical system towards a predominance of either state. One example of

a parity symmetric rule is the 2x2 version of the Ising rule, Rule **30** (**04**): under the Ising rule, the configuration where every cell is a `1` is just as probable as the configuration of all `0`.

3.3 General World Transforms

The parity transformation simply flips every bit in the world state. This is equivalent to applying the function (xor 1) to every 1x1 block in the world. One generalization of this idea is to apply a given 2x2 configuration as an xor pattern to all 2x2 blocks in the world. It will turn out that certain 2x2 xor patterns suggest other equivalences in the rule table.

Definition 3.6 (General 2x2 Transformations on Worlds) *$T(\sigma)$, the action of a transformation $T = \begin{smallmatrix} a & b \\ c & d \end{smallmatrix}$ on a world configuration σ, is defined as the application of T as an xor pattern to consecutive 2x2 blocks of σ. This action only makes sense when applied to worlds of even size.*

Note that the transformation T does not operate on every 2x2 block, as that would result would result in T being applied to each cell in the world four times — it should only be applied to each cell once.

Definition 3.7 (Canonical Transformations) *The four canonical transformations $T_{\mathbf{4}}$, $T_{\mathbf{C}}$, $T_{\mathbf{S}}$, and $T_{\mathbf{1}}$ are:*

$$
\begin{aligned}
T_{\mathbf{4}} &= \begin{smallmatrix} 1 & 1 \\ 1 & 1 \end{smallmatrix} \\
T_{\mathbf{C}} &= \begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix} \\
T_{\mathbf{S}} &= \begin{smallmatrix} 1 & 1 \\ 0 & 0 \end{smallmatrix} \\
T_{\mathbf{1}} &= \begin{smallmatrix} 0 & 0 \\ 0 & 1 \end{smallmatrix}
\end{aligned}
$$

$T_{\mathbf{4}}$ is simply P, the parity transformation, stated in terms of 2x2 blocks. $T_{\mathbf{C}}$ takes a configuration and inverts every other cell, like the black squares on a checkerboard.

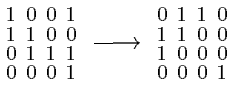


Figure 3.1: the action of T_S

$T_{\mathbf{S}}$ inverts every other line, and $T_{\mathbf{1}}$ inverts one cell out of every group of four. Figure 3.1 is an example of $T_{\mathbf{S}}$ applied to a small configuration.

Of the sixteen possible 2x2 neighborhoods, only four have been named as transformations. Rotations of these blocks are not listed as they do not produce significantly different transformations. The two other essential neighborhoods, **0** and **3** are also not in this list. $T_{\mathbf{0}}$ is the null transformation, and $T_{\mathbf{3}}$ is equivalent to $T_{\mathbf{1}}$ ($T_{\mathbf{3}} = T_{\mathbf{4}} \circ T_{\mathbf{1}}$, and it will turn out that $T_{\mathbf{3}}$ only applies when $T_{\mathbf{4}}$ does.)

The action of these various transformations on world configurations in terms of 2x2 neighborhoods can be a bit more complicated than the parity transformation. Under the parity transformation $T_{\mathbf{4}}$, there was a simple swapping of neighborhood types:

$$\begin{array}{ccc} \mathbf{0} & \longleftrightarrow & \mathbf{4} \\ \mathbf{1} & \longleftrightarrow & \mathbf{3} \end{array}$$

The simple action of $T_{\mathbf{4}}$ is largely because the neighborhood **4** itself is rotationally symmetric. When applying one of the other transformations to a given neighborhood, however, one must consider the application of that transformation to all rotations of the neighborhood. For example, consider $T_{\mathbf{S}}$ applied to all rotations of **S**:

$$T_{\mathbf{4}}\left(\begin{smallmatrix}1&1\\0&0\end{smallmatrix}\right) = \begin{smallmatrix}1&1\\0&0\end{smallmatrix} \text{ xor } \begin{smallmatrix}1&1\\0&0\end{smallmatrix} = \begin{smallmatrix}0&0\\0&0\end{smallmatrix} \quad (\mathbf{0})$$

$$T_{\mathbf{4}}\left(\begin{smallmatrix}0&1\\0&1\end{smallmatrix}\right) = \begin{smallmatrix}1&1\\0&0\end{smallmatrix} \text{ xor } \begin{smallmatrix}0&1\\0&1\end{smallmatrix} = \begin{smallmatrix}1&0\\0&1\end{smallmatrix} \quad (\mathbf{C})$$

$$T_{\mathbf{4}}\left(\begin{smallmatrix}1&0\\1&0\end{smallmatrix}\right) = \begin{smallmatrix}1&1\\0&0\end{smallmatrix} \text{ xor } \begin{smallmatrix}1&0\\1&0\end{smallmatrix} = \begin{smallmatrix}1&0\\0&1\end{smallmatrix} \quad (\mathbf{C})$$

$$T_{\mathbf{4}}\left(\begin{smallmatrix}0&0\\1&1\end{smallmatrix}\right) = \begin{smallmatrix}1&1\\0&0\end{smallmatrix} \text{ xor } \begin{smallmatrix}0&0\\1&1\end{smallmatrix} = \begin{smallmatrix}1&1\\1&1\end{smallmatrix} \quad (\mathbf{4})$$

Whereas $T_{\mathbf{4}}$ turned all **S** into **S**, $T_{\mathbf{S}}$ might turn a **S** into a **0**, **4**, or **C**. Conversely, under $T_{\mathbf{S}}$ all **0**, **4**, and **C** are transformed into **S**. In other words, **0**, **4**, and **C** get

swapped as a group with **S**. This effect is denoted

$$(\mathbf{04C}) \longleftrightarrow \mathbf{S}$$

A complete list of the application of each type of transformation is as follows:

$$\begin{array}{lrcl}
T_{\mathbf{4}} & \mathbf{0} & \longleftrightarrow & \mathbf{4} \\
 & \mathbf{1} & \longleftrightarrow & \mathbf{3} \\
 & & & \\
T_{\mathbf{C}} & (\mathbf{04}) & \longleftrightarrow & \mathbf{C} \\
 & (\mathbf{13}) & \longleftrightarrow & (\mathbf{13}) \\
 & & & \\
T_{\mathbf{S}} & (\mathbf{04C}) & \longleftrightarrow & \mathbf{S} \\
 & (\mathbf{13}) & \longleftrightarrow & (\mathbf{13}) \\
 & & & \\
T_{\mathbf{1}} & (\mathbf{04SC}) & \longleftrightarrow & (\mathbf{13})
\end{array}$$

Equation 3.1 translated the number of neighborhoods $N_{\mathbf{n}}$ to their transformed neighborhoods $N'_{\mathbf{n}}$ for $T_{\mathbf{4}}$. The analogous identities for these other transformations is more complex. For example, consider again the action of $T_{\mathbf{S}}$:

$$(\mathbf{04C}) \longleftrightarrow \mathbf{S}$$

Because each **S** in σ is mapped to exactly one of (**04C**) in σ', and every **0**, **4**, and **C** in σ is mapped to **S** in σ', the analogous identities for $T_{\mathbf{S}}$ are

$$\begin{aligned}
N'_{\mathbf{S}} &= N_{\mathbf{0}} + N_{\mathbf{4}} + N_{\mathbf{C}} \\
N'_{\mathbf{0}} + N'_{\mathbf{4}} + N'_{\mathbf{C}} &= N_{\mathbf{S}}
\end{aligned}$$

Similarly, $T_{\mathbf{S}}$ also performs

$$(\mathbf{13}) \longleftrightarrow (\mathbf{13})$$

There is a 1:1 correspondence between (**13**) in σ and (**13**) in σ', so

$$N_{\mathbf{1}} + N_{\mathbf{3}} = N'_{\mathbf{1}} + N'_{\mathbf{3}}$$

In general, under any transform T there will be an exchange of groups of neighborhoods. This exchange implies an equivalence of the number of neighborhoods in the mapping.

3.4 Equivalence of Rules under General World Transforms

Knowing the action of a general transform T on each of the possible neighborhoods suggests that it should be possible to find the rule R' such that $H_R(\sigma) = H_{R'}(\sigma')$: simply make sure the energies assigned to each neighborhood follow the neighborhood mappings. Unfortunately, the neighborhood mappings for arbitrary transforms are not as simple as for the parity transformation.

Consider trying to naively find the rule equivalent to Rule **56** (**01S**) under $T_{\mathbf{S}}$. $T_{\mathbf{S}}$ maps **0** to **S**, so $E'_{\mathbf{S}} = E_{\mathbf{0}} = 0$. However, $T_{\mathbf{S}}$ also maps **4** to **S**, so $E'_{\mathbf{S}} = E_{\mathbf{4}} = 1$, and it maps **C** to **S**, so $E'_{\mathbf{S}} = E_{\mathbf{C}} = 1$. Therefore, $E'_{\mathbf{S}} = 1$, but $E'_{\mathbf{S}} = 0$: the rule equivalent to Rule **56** would have to allow some rotations of **S** but disallow others, resulting in a non-rotationally symmetric rule.

If, however, we only try to find $T_{\mathbf{S}}$ equivalences to rules where $E_{\mathbf{0}} = E_{\mathbf{C}} = E_{\mathbf{4}}$, there is no problem: $E'_{\mathbf{S}}$ can simply be set equal to $E_{\mathbf{0}} = E_{\mathbf{C}} = E_{\mathbf{4}}$. Similarly, $T_{\mathbf{S}}$ performs $\mathbf{S} \rightarrow (\mathbf{04C})$, so $E'_{\mathbf{0}} = E'_{\mathbf{4}} = E'_{\mathbf{C}} = E_{\mathbf{S}}$. $T_{\mathbf{S}}$ also does $(\mathbf{13}) \longleftrightarrow (\mathbf{13})$ requiring $E_{\mathbf{1}} = E_{\mathbf{3}}$ in order for $T_{\mathbf{S}}$ to result in a rotationally symmetric rule. In other words,

If, in rule R, $E_{\mathbf{0}} = E_{\mathbf{C}} = E_{\mathbf{4}}$ and $E_{\mathbf{1}} = E_{\mathbf{3}}$, then there is a rule R' with $E'_{\mathbf{0}} = E_{\mathbf{S}}$, $E'_{\mathbf{1}} = E_{\mathbf{1}}$, $E'_{\mathbf{S}} = E_{\mathbf{0}}$, $E'_{\mathbf{C}} = E_{\mathbf{S}}$, $E'_{\mathbf{3}} = E_{\mathbf{1}}$, $E'_{\mathbf{4}} = E_{\mathbf{S}}$ such that $H_{R'}(T_{\mathbf{S}}(\sigma)) = H_R(\sigma)$. The proof is as follows:

$$
\begin{aligned}
H_{R'}(T_{\mathbf{S}}(\sigma)) &= E'_{\mathbf{0}}N'_{\mathbf{0}} + E'_{\mathbf{1}}N'_{\mathbf{1}} + E'_{\mathbf{S}}N'_{\mathbf{S}} + E'_{\mathbf{C}}N'_{\mathbf{C}} + E'_{\mathbf{3}}N'_{\mathbf{3}} + E'_{\mathbf{4}}N'_{\mathbf{4}} \\
&= E_{\mathbf{S}}N'_{\mathbf{0}} + E_{\mathbf{1}}N'_{\mathbf{1}} + E_{\mathbf{0}}N'_{\mathbf{S}} + E_{\mathbf{S}}N'_{\mathbf{C}} + E_{\mathbf{1}}N'_{\mathbf{3}} + E_{\mathbf{S}}N'_{\mathbf{4}} \\
&= E_{\mathbf{0}}(N'_{\mathbf{S}}) + E_{\mathbf{1}}(N'_{\mathbf{1}} + N'_{\mathbf{3}}) + E_{\mathbf{S}}(N'_{\mathbf{0}} + N'_{\mathbf{C}} + N'_{\mathbf{4}}) \\
&= E_{\mathbf{0}}(N_{\mathbf{0}} + N_{\mathbf{C}} + N_{\mathbf{4}}) + E_{\mathbf{1}}(N_{\mathbf{1}} + N_{\mathbf{3}}) + E_{\mathbf{S}}(N_{\mathbf{S}}) \\
&= E_{\mathbf{0}}N_{\mathbf{0}} + E_{\mathbf{1}}N_{\mathbf{1}} + E_{\mathbf{S}}N_{\mathbf{S}} + E_{\mathbf{0}}N_{\mathbf{C}} + E_{\mathbf{1}}N_{\mathbf{3}} + E_{\mathbf{0}}N_{\mathbf{4}} \\
&= E_{\mathbf{0}}N_{\mathbf{0}} + E_{\mathbf{1}}N_{\mathbf{1}} + E_{\mathbf{S}}N_{\mathbf{S}} + E_{\mathbf{C}}N_{\mathbf{C}} + E_{\mathbf{3}}N_{\mathbf{3}} + E_{\mathbf{4}}N_{\mathbf{4}} \\
&= H_R(\sigma)
\end{aligned}
$$

This idea can be generalized to any of the four canonical transformations.

Definition 3.8 (Transformation on a Rule) *The result of a transformation T applied to a rule R is the rule R' with the energies exchanged along the lines suggested by the action of T on 2x2 neighborhoods. This transformation is only defined if the energies of R corresponding to neighborhoods that are mapped as groups under T are equal.*

The requirement that for a transformation to be defined groups of transformed neighborhoods must have the same energy insures that the new rule assigns the same energy to every rotation of a neighborhood. Without this requirement, a transformation applied to a rule could result in a non-rotationally symmetric rule.

The proof given above for the equivalence of the Hamiltonians for R and $T_{\mathbf{S}}(R)$ generalizes to proofs for all four transformations. This generalization is conceptually trivial but the notation required is complex enough to obscure the meaning of the theorem.

The definitions of parity equivalence and parity symmetry can now also be generalized to arbitrary transformations:

Definition 3.9 (Equivalence under a Transform T) *Two rules R and R' are equivalent under T if $T(R) = R'$.*

Two rules that are equivalent under a transform have the same Hamiltonian on appropriately transformed world configurations. Therefore, ΔH for any particular spin flip on the configuration and its transformation will be the same, and so the two equivalent rules generate the same dynamical process. Any predictions a theory makes about a particular rule R will apply to any rule R' that is equivalent to R under any transformation.

Definition 3.10 (Symmetric under T) *A rule R is symmetric under a transform T if $T(R) = R$.*

Rules that are equivalent to themselves under certain transformations (or alternately, "fixed by" or "invariant under" a transformation) will play a special role in the theory.

3.5 Hierarchy of Transformations

The requirement that certain transformations are only well defined on a restricted set of rules might make the whole notion of equivalences under different transforms seem a bit suspicious. Instead, it reveals a natural hierarchy in the table of possible 2x2 rules.

Consider the conditions necessary for the $T_{\mathbf{C}}$ transformation to be defined for a particular rule: $E_{\mathbf{0}} = E_{\mathbf{4}}$ and $E_{\mathbf{1}} = E_{\mathbf{3}}$. Which rules fit those requirements? Exactly those rules which are symmetric under $T_{\mathbf{4}}$!

Similarly, $T_{\mathbf{S}}$ is only defined on those rules that are symmetric under $T_{\mathbf{C}}$, and $T_{\mathbf{1}}$ applies only to those rules that are symmetric under $T_{\mathbf{S}}$. The transformations have a hierarchy of application: a transformation is only defined for a rule that is symmetric under all of the lower transformations:

$$T_{\mathbf{4}} \longrightarrow T_{\mathbf{C}} \longrightarrow T_{\mathbf{S}} \longrightarrow T_{\mathbf{1}}$$

There are exactly two rules that are symmetric under all four transformations: Rule **0** (**01SC34**) (everything allowed) and Rule **63** () (nothing allowed). These trivial rules correspond to the Hamiltonian

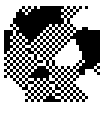
$$H = E(N_{\mathbf{0}} + N_{\mathbf{1}} + N_{\mathbf{S}} + N_{\mathbf{C}} + N_{\mathbf{3}} + N_{\mathbf{4}}) = En^2$$

where E can have either the value 0 (Rule **0**) or 1 (Rule **63**). Because the Hamiltonian is a constant, not dependent on the world state, $\Delta H = 0$ for all possible spin flips and the dynamical process is completely random. For future purposes, Rule **0** and Rule **63** will be considered equivalent.

The top level of the hierarchy of transformations is $T_{\mathbf{1}}$. Rules that are symmetric under all transforms except $T_{\mathbf{1}}$ can only distinguish the group (**04SC**) from (**13**): therefore, the Hamiltonian is:

$$H = E_{\mathbf{04SC}}(N_{\mathbf{0}} + N_{\mathbf{4}} + N_{\mathbf{S}} + N_{\mathbf{C}}) + E_{\mathbf{13}}(N_{\mathbf{1}} + N_{\mathbf{3}})$$

There are two variables in the Hamiltonian, $E_{\mathbf{04SC}}$ and $E_{\mathbf{13}}$, and so there are r rules that are symmetric under $T_{\mathbf{4}}$, $T_{\mathbf{C}}$, and $T_{\mathbf{S}}$ but not $T_{\mathbf{1}}$. Of those four rules, the



two rules where $E_{\mathbf{04SC}} = E_{\mathbf{13}}$ are symmetric under $T_{\mathbf{1}}$ and have been seen before: Rule **0** and Rule **63**. The other two rules are new, those where $E_{\mathbf{04SC}} \neq E_{\mathbf{13}}$. These are Rule **18** (**0SC4**) and Rule **45** (**13**), equivalent to each other under $T_{\mathbf{1}}$. By breaking the $T_{\mathbf{1}}$ symmetry, the number of total rules has doubled from two to four, and the number of truly unique rules has doubled from one to two.

The Hamiltonians for the rules where the first asymmetry is in $T_{\mathbf{S}}$, $T_{\mathbf{C}}$, and $T_{\mathbf{4}}$ are as follows:

$$\begin{aligned} T_{\mathbf{S}} &: H(\sigma) = E_{\mathbf{04C}}(N_{\mathbf{0}} + N_{\mathbf{4}} + N_{\mathbf{C}}) + E_{\mathbf{S}}N_{\mathbf{S}} + E_{\mathbf{13}}(N_{\mathbf{1}} + N_{\mathbf{3}}) \\ T_{\mathbf{C}} &: H(\sigma) = E_{\mathbf{04}}(N_{\mathbf{0}} + N_{\mathbf{4}}) + E_{\mathbf{C}}N_{\mathbf{C}} + E_{\mathbf{S}}N_{\mathbf{S}} + E_{\mathbf{13}}(N_{\mathbf{1}} + N_{\mathbf{3}}) \\ T_{\mathbf{4}} &: H(\sigma) = E_{\mathbf{0}}N_{\mathbf{0}} + E_{\mathbf{1}}N_{\mathbf{1}} + E_{\mathbf{S}}N_{\mathbf{S}} + E_{\mathbf{C}}N_{\mathbf{C}} + E_{\mathbf{3}}N_{\mathbf{3}} + E_{\mathbf{4}}N_{\mathbf{4}} \end{aligned}$$

Each time a symmetry is broken extra terms are added to the Hamiltonian, increasing the number of rules in that symmetry class. Breaking $T_{\mathbf{1}}$, $T_{\mathbf{S}}$, and $T_{\mathbf{C}}$ symmetries both add one extra term, doubling the total number of rules each time. Breaking $T_{\mathbf{4}}$ symmetry adds two terms, one distinguishing **0** from **4** and the other distinguishing **1** from **3**.

Each time a symmetry is broken the resulting system can then distinguish the neighborhoods associated with that transformation. When $T_{\mathbf{1}}$ symmetry is broken, the rules can distinguish (**13**) from (**04SC**). Breaking $T_{\mathbf{S}}$ symmetry allows the system to count **S** as distinct from other neighborhoods, breaking $T_{\mathbf{C}}$ singles out **C**, and breaking $T_{\mathbf{4}}$ distinguishes between **0** and **4**, as well as **1** and **3**.

3.6 Summary

For every rule R except Rule **0** and Rule **63** there is exactly one transformation under which R is equivalent to some other distinct rule. For example, if R is not symmetric under $T_{\mathbf{4}}$, then $R' = T_{\mathbf{4}}(R)$ is distinct from R, equivalent to it under $T_{\mathbf{4}}$, and equivalent to no rules under higher transformations (as they do not apply). This follows similarly for the other transformations. Therefore, $T_{\mathbf{4}}$, $T_{\mathbf{C}}$, $T_{\mathbf{S}}$, and $T_{\mathbf{1}}$ induce equivalence classes on the set of 64 rules. Each equivalence class has two members: the two rules that are equivalent under a particular transformation. In

the future, equivalent rules will be written together: Rule **30** is equivalent to Rule **55** under $T_{\mathbf{C}}$, so they will be referred to as a pair as "Rule **30/55**".

With the convention that Rule **0** is equivalent to Rule **63**, every 2x2 rule is equivalent to exactly one other distinct 2x2 rule. The number of distinct rules has been reduced from 64 to 32. Furthermore, the rules have now been placed in a hierarchy of complexity: rules that are symmetric under more transformations have simpler Hamiltonians. Appendix B contains a complete dictionary of the 64 rotationally symmetric rules, along with a listing of the action of various transformations on those rules.

The four world transformations have revealed a hidden structure in the rule table, one that cuts the number of rules that need to be studied in half. What remains to be done is to understand the global behavior of these rules and to try to explain how that behavior arises out of the local rule itself.

Chapter 4

Statistical Analysis

One common analysis performed on these types of dynamical systems is empirically calculating the behavior of energy as a function of time. The 2x2 rules are functions that define the energy of a configuration: $E(\sigma) = H_R(\sigma)$. Ideally one could solve the system itself and analytically find a solution for the expectation of energy as a function of time, $\mathbb{E}(E) = f(t)$. Unfortunately, this sort of solution is difficult to find for any particular rule.

The basic dynamical Ising model in two dimensions with spin flip dynamics (essentially Rule **30/55**) has been solved, largely by exploiting the observation that the Ising rule is driven by the curvature of the boundaries between regions ([Lif62], [AC79]). But many of the rules in these systems are not like the Ising rule in being curvature driven (as will be shown in chapter 5), and so it does not seem likely that those methods would generalize to all of the 2x2 rules. However, simulation can be used to measure the behavior of energy as a function of time.

One common class of models are those whose energy is asymptotically some power of t: $E \sim t^{\alpha}$. For example, the Ising rule goes as $E \sim t^{-1/2}$ [AC79]. There is a belief ([Bin86], [GSA84], [SB83], [RG88], etc.) that many dynamical systems fall into one of only a few *universality classes*, that there are only a few possible values of alpha, independent of the specifics of the particular dynamical process. If all models were members of only a few universality classes, it would be a very deep property about these kind of dynamical systems. The best known universality classes are $\alpha = -1/2$ and $\alpha = -1/3$. More recently, evidence has been found for an $\alpha = -1/4$ universality class [Mou85] [LC].

It will be shown that most of the seven nontrivial parity symmetric 2x2 rules are probably in the best known universality class, $\alpha = -1/2$. One rule is asymptotically faster than any power of t, and another seems to be in a new universality class, $\alpha \simeq -4/5$.

4.1 Statistical Behavior of the Parity Symmetric 2x2 Rules

At temperature 0 there is a clear division in the various 2x2 rules between those which create systems that asymptotically go to energy 0 as time gets large, and those that freeze at some higher energy. Rules that result in dynamics that freeze at high energy ("frustrated rules") are not as easy to study by simulation. Because they do not go all the way down to energy 0 it is more difficult to define their asymptotic behavior. Also, it is usually more interesting to consider frustrated rules in positive temperature contexts, as there the system can surmount the energy barriers that freeze the system at temperature 0. But at $T = 0$ the equilibrium energy is not known, so it is not clear when any relaxation process is completed. Because of these complications, the statistical behavior of rules that do not go to energy 0 will not be considered; in the set of seven non-trivial parity symmetric rules, these are Rule **18/45** and Rule **26/51**.

Of the five remaining rules, four of them have energy that is asymptotically a power of t. The one exception is Rule **8/33**, which converges extremely quickly, probably $E \sim e^{-t}$. The dynamics of Rule **8/33** are so disorganized as to be relatively uninteresting: it will not be considered further. The remaining parity symmetric rules, Rule **4/41**, Rule **12/37**, Rule **30/55**, and Rule **22/59**, all seem to fit $E \sim t^{\alpha}$.

Note that $E \sim t^{\alpha} \Rightarrow \log(E) \sim \alpha \log(t)$: rules that are a power of t will be linear in a log/log plot. The four rules listed above all appear convincingly linear on a log/log scale. Figure 4.1, for instance, is a representative graph of $\log(E)$ vs. $\log(t)$ for Rule **4/41**.

4.2 Estimation of Error

Given energy vs. time data collected over many trials of a particular run, it would seem to be a simple matter to read the exponent from the data: simply average the independent energy measurements together, fit a straight line to $\log(E)$ vs. $\log(t)$, and read the slope. Unfortunately, several potential complications in the data must be accounted for. Finite size effects yield incorrect data for predicting the behavior

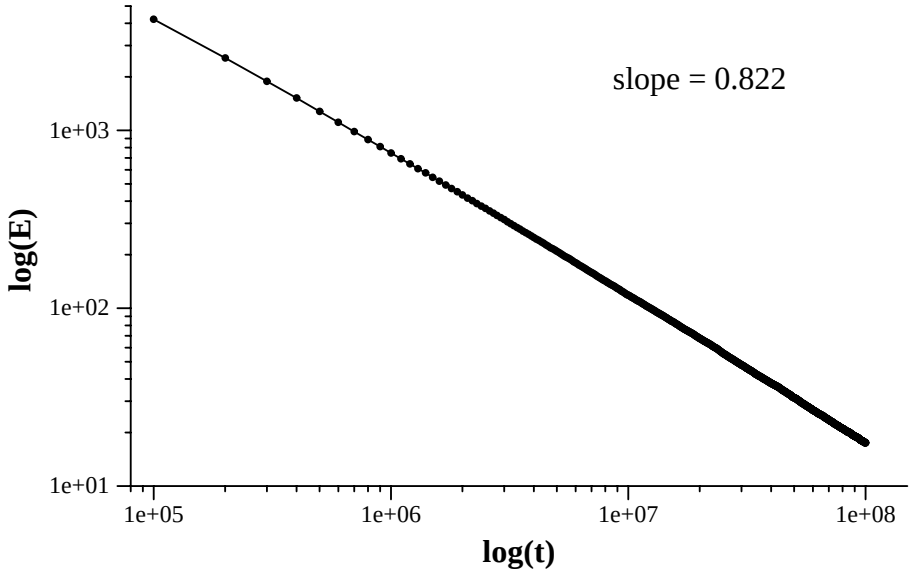


Figure 4.1: Rule **4/41**, 256x256 world, average of 200 trials.

of the model at the infinite size limit, and using a small number of random samplings yields uncertainty in the calculated exponent. These problems must be accounted for.

4.2.1 Uncertainty

For any particular simulation of the system, the measured energy has a certain *error*, the deviation from the 'true curve.' Estimating the uncertainty of the slope from the simple log/log fit of averaged data is not possible: the error in energy measurements tends to be correlated in time, making the standard estimate of error in the linear fit too optimistic. In general, the error distribution for each rule seems to be unique and difficult to model. Rule **4/41** at size 256x256 has been chosen as an example of various ways to estimate the uncertainty of the exponent. While the specific results of this error analysis might not apply to all rules, the general methodology does.

By averaging together 200 trials of Rule **4/41** at world size 256x256 and reading the slope of the log/log plot, the exponent is calculated to be -0.822 (Figure 4.1). One simple way to get a feel for the uncertainty of that figure is to calculate expo-

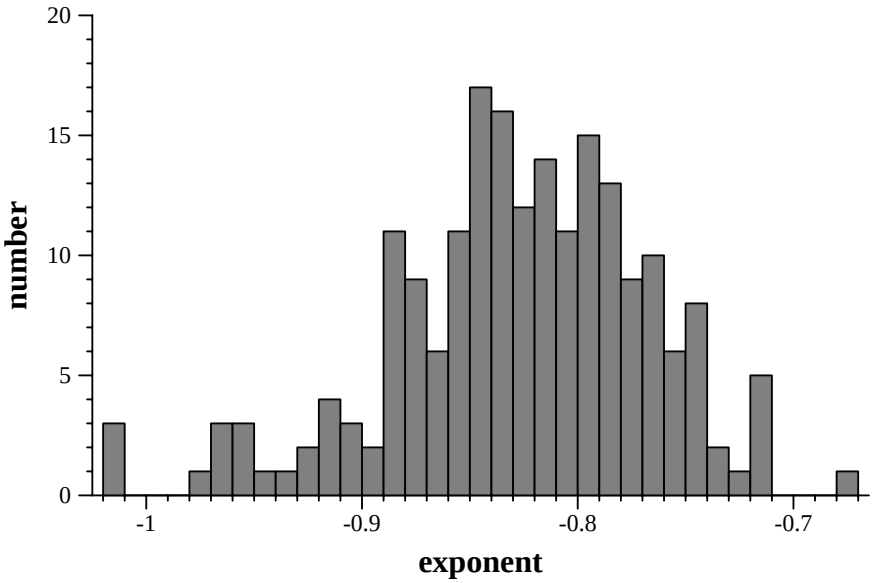


Figure 4.2: Histogram of exponents for 200 trials of Rule **4/41**, size 256x256

nents for each of the individual trials and see how the distribution falls. Figure 4.2 is a histogram of the exponents calculated for each of the 200 individual runs. Happily, the distribution tends to cluster around the mean, with a slight asymmetry towards lower exponents. The mean of this distribution is -0.822, the same exponent as calculated by the average of the runs, with a standard deviation of 0.0603.

This method estimates the uncertainty of the exponent calculated for one trial. Resampling provides a method for estimating the uncertainty in the exponent calculated by averaging together a large number of trials. The most straightforward way to estimate this uncertainty would be to do a large number of experiments, each with 200 trials, and look at the distribution of the exponents calculated from the average.

Unfortunately that many trials would take too long to perform. Instead, *bootstrapping* can be employed to produce many datasets of 200 trials averaged together [ET93]. Bootstrapping is implemented by choosing 200 trials randomly, with replacement, out of the initial pool of 200. (Note that replacement implies some trials will be duplicated in the resampling.) Each bootstrap sample yields a new dataset of size 200 from which to calculate an exponent. Perform this procedure many times,

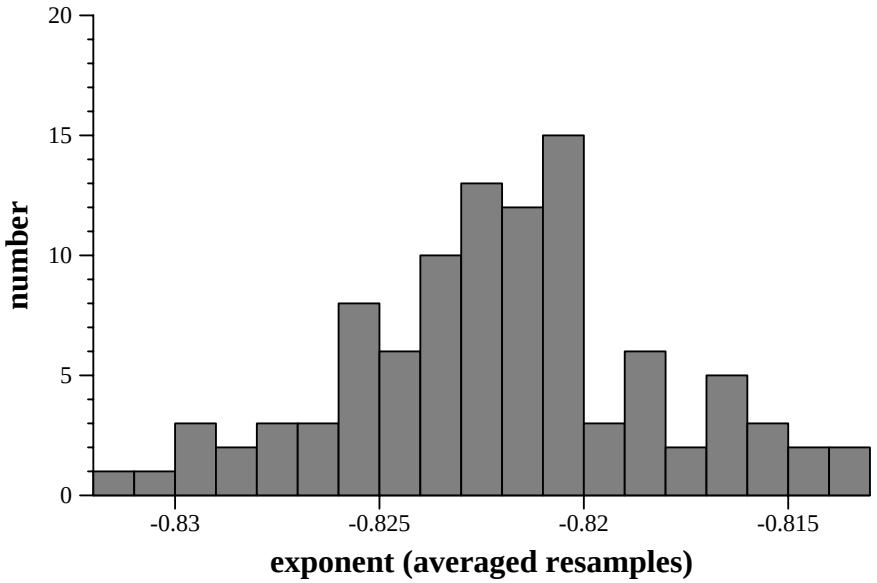


Figure 4.3: Histogram of exponents for 100 bootstrap samples of Rule **4/41**, size 256x256

and the result is a distribution of exponents of 200 trials averaged together.

Figure 4.3 is a histogram of the exponents calculated on the same dataset for 100 different bootstrap samples of the 200 runs. The exponents here are tightly clustered around the mean -0.822, with standard deviation 0.00376. Bootstrapping shows that the exponent calculated for Rule **4/41** by averaging together 200 trials is accurate to at least two significant figures.

4.2.2 Finite Size Effects

These dynamical processes are ideally taking place on an infinite plane. But numeric simulation is limited to simulating the rules on a finite lattice: some accounting must be made for the effect of world size on the calculations. Two distinct finite size effects can occur. Subtle errors can be introduced as a general effect of finite size: these will show up as a general trend in the calculated exponent at different sizes. In addition, the toroidal world topology can also introduce entirely new phenomena specific to finite size worlds (a specific example of this in the Ising rule is presented in the next chapter). To compensate for this, trials that exhibit finite

Size	α	S.D. of α
32x32	-1.039	0.0391
64x64	-0.772	0.00916
128x128	-0.819	0.0128
256x256	-0.822	0.00376
512x512	-0.805	0.00199
1024x1024	-0.805	0.00109

Figure 4.4: Exponent as a function of world size for Rule **4/41**

size-specific behavior should be thrown out.

4.2.2.1 Exponent as a Function of World Size

For Rule **4/41** the size of the world has a definite influence on the calculated exponent. Figure 4.4 presents the calculated exponents for Rule **4/41** at various world sizes (each exponent is calculated from the average of 200 runs, except the 1024x1024 world which is only 100 runs).

As the world size increases the change between exponents decreases, indicating that calculating at larger world sizes is probably helpful. Perhaps not much benefit would be derived from simulating beyond size 1024x1024; a calculation of the exponent at 2048x2048 would help verify this claim, but the computer time required to do such a calculation is prohibitive (but see Appendix C).

4.2.2.2 Uncertainty as a Function of World Size

Another phenomenon of interest is that as the world size increases, the variation in the exponents as calculated by subsampling decreases. The standard deviations in figure 4.4 are the estimated uncertainty of the measurements as calculated by the standard deviation of exponents for 100 bootstrap samples of 200 runs (except for the 1024x1024 size, which are 50 bootstrap samples of 100 runs).

Again, the indication is that calculations on larger worlds can only be better. Unfortunately, larger worlds also require more computational time, and so there is a time/accuracy tradeoff. For most rules, size 256x256 seems to be a reasonable

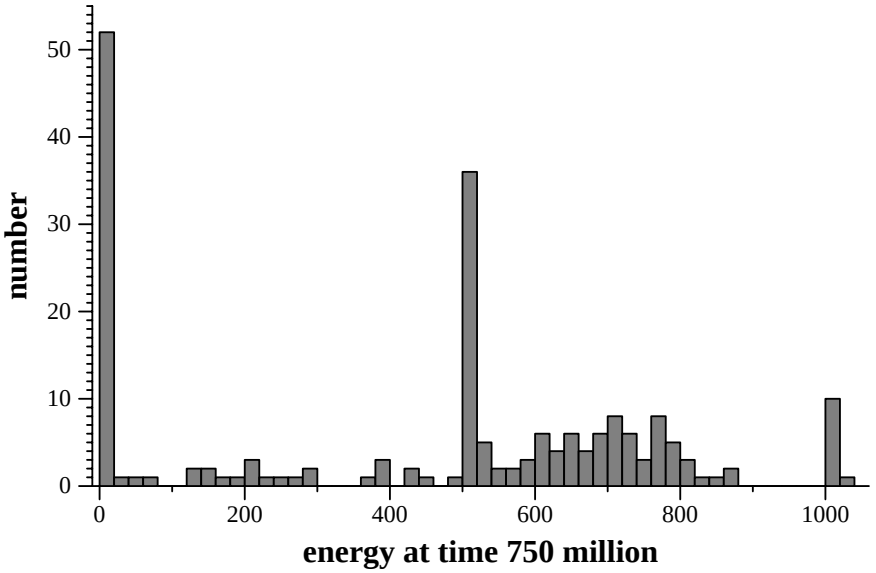


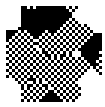
Figure 4.5: Histogram of energies for Rule **22/59**, 256x256, at time 750 million

compromise between accuracy and computation time: it should provide a useful estimate of the exponent and yet still be small enough that any one trial can be calculated in a few hours.

4.2.2.3 Artifacts Caused by Finite Size Effects

The other finite size effect that must be compensated for are behaviors introduced by the finite size world that would not be present in an infinite world. Figure 4.5, a histogram of energy at the end of a run of Rule **22/59** (an Ising-like rule with four ground states instead of two) indicates an artifact of this sort. The distribution has two large spikes, one at energy 512, one at energy 1020.

These artifacts correspond to a four-state version of a phenomenon also observed in the two-state Ising model — it is possible for the finite system to become stuck in a configuration where a large region of one type wraps around and connects to itself, creating two permanent boundaries (see chapter 5). As this structure depends on the topology of the toroidal world and is not possible in the infinite version, runs that end at energy 512 or energy 1020 are finite size effects and will be discarded. Other rules might have other finite size artifacts that are not as easy to detect: none



Rule	Size	trials	α	S.D.
4/41	512x512	200	-0.805	0.00199
12/37	256x256	200	-0.551	0.00214
30/55	256x256	193	-0.543	0.0128
22/59	256x256	153	-0.546	0.0149

Figure 4.6: Calculated exponents for various rules

have been discovered yet.

Another aspect of figure 4.5 deserves comment — for both Rule **22/59** and Rule **30/55** there is a large concentration at energy 0 at the end of the run. But another entire set of runs is still at quite high energy, around energy 700 in Figure 4.5. It is not clear whether this bimodality is some other finite size effect, or just an indication that the low-end tail of the distribution is very long but is being collected at energy 0. In either case, this phenomenon will almost certainly resulted in an estimated exponent that is too high.

4.3 Results

With the caveats about estimating the calculated exponents for the various rules, it is now possible to assert some measurements for the actual exponents themselves. Figure 4.6 presents the exponents calculated by fitting a straight line to a log/log plot of the average energy of many trials, along with their standard deviations as calculated by bootstrapping. There are less trials for Rule **30/55** and Rule **12/27** because it was necessary to throw out some data to account for the finite size effects mentioned above.

The calculated exponent for the Ising rule is .05 below the expected value of $-1/2$: whether this is a result of finite size errors or general uncertainty is not clear. Rule **22/59** seems to have an exponent exactly like Rule **30/55**: this is not entirely surprising as their dynamics are qualitatively similar (chapter 5).

Rule **12/37** and Rule **4/41** also have qualitatively similar dynamics, but dynamics that are quite different than the Ising-like Rule **30/55** and Rule **12/59** (chapter 5). It is clear from the results that Rule **4/41** belongs to a different universality

class from the Ising rule. There is a suggestion that Rule **4/41** is asymptotically $E \sim t^{-4/5}$, although more analysis is obviously needed to verify this claim.

What is surprising is that the exponent for Rule **12/37** is so close to $-1/2$, the universality class of the standard Ising rule. A solution for this rule would be particularly interesting: if its exponent is exactly $\alpha = -1/2$, then Rule **12/37** would be an example where two largely unrelated models are in the same universality class.

4.4 Summary

Statistical simulation of the different rules has various problems: uncertainties and finite size effects that obscure the 'true' behavior of the rule. However, simulation remains an effective and simple tool to estimate one global parameter. Statistical analysis has demonstrated that Rule **30/55** and Rule **22/59** are similar, but quite different from Rule **4/41**. It has also generated one hypothesis that is surprising in light of the description of the analysis that will be presented in the next chapter: that there might be some underlying connection between Rule **12/37** and the basic Ising model.

Chapter 5

Description

Statistical analysis provides one sort of information about a rule — an estimate of a global parameter that is a consequence of the local rules. Ideally, one could develop an exact solution for that parameter for every 2x2 rule, to match the solution of the Ising dynamics. A first step towards doing this is to develop an intuition about how the various rules behave. The Ising rule was characterized in the first chapter: the only ground states are solid fields of `0` or `1`, and the boundaries between homogeneous domains have high energy. Many of the other rules are very different than the Ising rule, but can also be described succinctly. Once one knows what to look for, the qualitative behavior of any particular rule is evident after watching the rule dynamics for a few minutes.

5.1 Defects

Running a rule on a random initial configuration and watching the changing lattice of `1`s and `0`s can be educational, but it can also be confusing. In particular, two rules that are equivalent under some world transformation might yield world dynamics that look quite different — our eyes cannot easily recognize the equivalence of configurations under some of the more complicated transformations.

It will frequently be useful to examine the behavior of the "hot spots" in the world, those 2x2 neighborhoods which are disallowed by the rule and thus have energy greater than 0. These 2x2 blocks are defects in the world state — the dynamical process attempts to eliminate them.

Definition 5.1 (Defects) *A defect is a 2x2 neighborhood with energy* > 0.

By the definition of rule equivalence, if rule R is equivalent to rule R' under a transformation T, then for a configuration σ and the configuration $\sigma' = T(\sigma)$,

$H_R(\sigma) = H_{R'}(\sigma')$. This equivalence is true not only for the world itself but for any smaller sub-blocks of the world — including 2x2 defect blocks. Therefore, while the transformations on the state of the world might not be obviously equivalent, the behavior of defects will be exactly the same.

For example, Rule **4** (**01C34**) is equivalent to Rule **41** (**1S3**) under $T_{\mathbf{S}}$. Under Rule **4**, every **S** neighborhood is a defect. Consider the spin flip on this example configuration:

$$\begin{array}{cccc} 1&0&1&1 \\ 0&\mathbf{1}&1&0 \\ 1&0&0&0 \\ 0&1&0&1 \end{array} \longrightarrow \begin{array}{cccc} 1&0&1&1 \\ 0&\mathbf{0}&1&0 \\ 1&0&0&0 \\ 0&1&0&1 \end{array}$$

By flipping the cell in the center, upper left, the middle **S** defect is eliminated, but a new **S** defect appears above it: in effect, the spin flip moves the **S** defect up one cell. The same spin flip on the configuration transformed by $T_{\mathbf{S}}$ produces the exact same defect motion for Rule **41**:

$$\begin{array}{cccc} 0&1&0&0 \\ 0&\mathbf{1}&1&0 \\ 0&1&1&1 \\ 0&1&0&1 \end{array} \longrightarrow \begin{array}{cccc} 0&1&0&0 \\ 0&\mathbf{0}&1&0 \\ 0&1&1&1 \\ 0&1&0&1 \end{array}$$

In Rule **41**, **C** and **4** are both defects. The spin flip makes the **4** defect disappear, only to replace it by a **C** defect above it. Just as in Rule **4**, the spin flip causes the defect to move up one cell. In general, equivalent rules will have equivalent defect structures and equivalent defect dynamics — this makes defects a convenient way to characterize rules.

5.2 Characterization of the Parity Symmetric 2x2 Rules

What follows is a qualitative description of the behavior of the eight distinct parity symmetric rules (those that are symmetric under T_4). The descriptions presented here are derived largely from directly observing the dynamics of the rules; in the next chapter, arguments will be developed for why these dynamics are implied by the rules themselves. Most rules are accompanied by example pictures — in these pictures, white and black square are states `0` and `1`, and grey is overlaid to highlight defects.

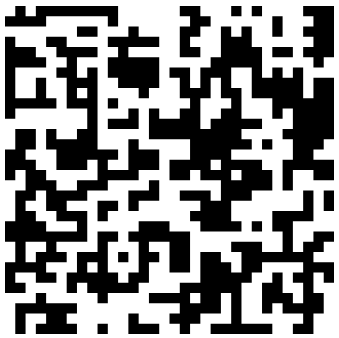


Figure 5.1: Rule **8** (**01S34**), time 2000, energy 0

5.2.1 Trivial Rules

As noted earlier, there are two rules that are absolutely trivial — Rule **0** and Rule **63**. Rule **0** allows all world configurations, and Rule **63** disallows all world configurations. Their dynamics are uninteresting: for any configuration, every possible spin flip has $\Delta H = 0$, and so the dynamical process is completely unstructured.

5.2.2 Fast Rules

The second qualitative category of rule are those that converge to energy 0 extremely quickly (Figure 5.1). Of the parity symmetric rules, there is only one unique rule of this type — Rule **8/33**, the rule which either disallows **C** or **04**. Under this rule defects in a random initial configuration disappear very quickly and the structure of the world cells changes rapidly and without any obvious order (other than disallowing the one type of disallowed neighborhood). It will be shown in the next chapter that the speed of convergence is not surprising, as defects are very easy to eliminate.

5.2.3 Slow Rules

The remaining parity symmetric rules are more interesting. The next class, slow rules, still go to energy 0 at temperature 0 but do so more slowly and with more structure than the fast Rule **8/33**. Empirical evidence in the previous chapter

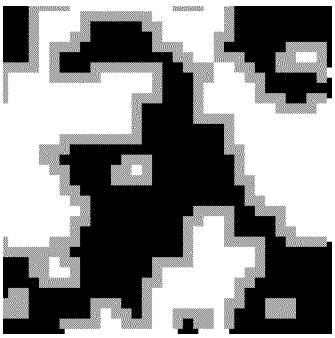


Figure 5.2: Rule **30** (**04**), time 7000, energy 257

demonstrated that all of these rules converge like $E \sim t^{\alpha}$ for some α characteristic to each rule.

5.2.3.1 Ising-like Rules

The first type of slow rules are the most familiar, the Ising-type rules. There are two of these in the parity symmetric set. Rule **30/55** is almost exactly the classical Ising rule (with a slight wrinkle about the magnitude of $E_{\mathbf{C}}$, as mentioned in chapter 2). For Rule **30** (**04**), after a quick period of initial settling down the world separates into clearly distinguishable blobs of `1`s and blobs of `0`s (Figure 5.2). The interior of these blobs has energy 0, whereas the boundary between the two types is a solid curve of defects, implying that the energy of the system is proportional to the length of the boundaries. The equivalent Rule **55** (**C**) has the exact same boundary types, but the blobs of `0` and `1` are replaced by blobs of **C** in two different phases.

Rule **22/59** is slightly more complicated — instead of two types of blobs, there are four. Rule **22** (**0C4**) allows solid `0`, `1`, and both phases of checkerboard (Figure 5.3, as well as the right-side flipbook). Rule **59** (**S**) creates blobs that are horizontal stripes in one of two phases, or vertical stripes in one of two phases. Again, the boundaries between blob types are defects, but the boundaries are more complicated because several different blob types can intersect at a point.

In both Rule **22/59** and Rule **30/55** the defect motion is basically the same: the defect boundaries are free to wiggle about, as long as the defect chain stays

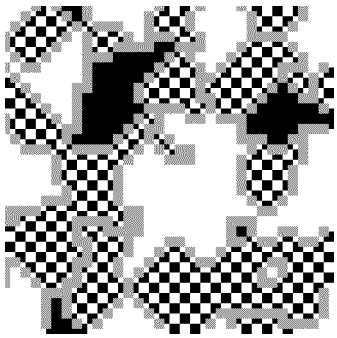


Figure 5.3: Rule **22** (**0C4**), time 9000, energy 270

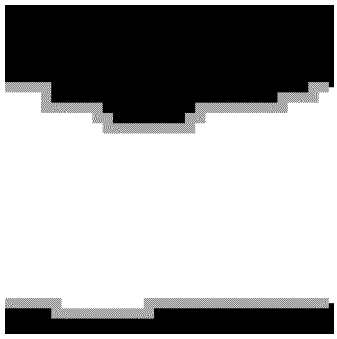


Figure 5.4: Finite size effect in Rule **30** (**04**), time 152000, energy 74

connected. Because the length of the boundary is directly proportional to the energy, the tendency is for the system to minimize the length of the boundary by gradually shrinking a blob until it disappears in a sea of the other state.

As noted in the previous chapter, there is a significant finite size effect that was seen as spikes in the energy histogram for Rule **22/59** at energy 512 and 1020. The cause of this effect is quite visible when looking at the world configurations themselves. Because the world is a torus, it is possible that at temperature 0 a permanent defect structure can be created — a blob that reaches around the world and connects with itself, making a strip (Figure 5.4). When this strip is present, the minimum energy the rule can find involves a large defect structure: to eliminate it would require going to a higher energy. This effect only occurs because the topology of a torus is radically different from an infinite plane — in the infinite sized Ising model this effect never occurs.

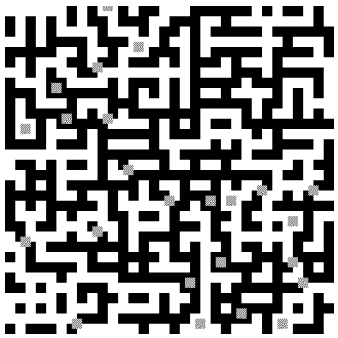


Figure 5.5: Rule **41** (**1S3**), time 9000, energy 24

5.2.3.2 Random Walk / Annihilation Rules

The other class of rules that converge slowly to energy 0 at temperature 0 are markedly different from the Ising rules. For both Rule **4/41** and Rule **12/37**, the major defect structure are isolated defects that walk randomly about the world. In both rules, isolated defects usually do not disappear: spin flips cause the defect to move around, not to be eliminated. However, when two defects collide in the appropriate fashion they both disappear, annihilating each other and lowering the energy of the world.

Annihilation seems to be the only way defects can be eliminated in Rule **4/41**. It appears that, for finite worlds, defects in Rule **4/41** come in pairs: in all runs the energy is always even. Rule **12/37** occasionally has single defects that disappear: this seems to be a secondary mechanism unrelated to the main phenomenon of annihilating pairs.

The defects in Rule **4/41** can move in both dimensions (Figure 5.5). Rule **12/37** has more complicated structure: defects are largely constrained to the boundaries between regions (Figure 5.6). The shape of these regions is more complicated than the Ising rule; in particular the formation and change in the boundaries is not obvious.

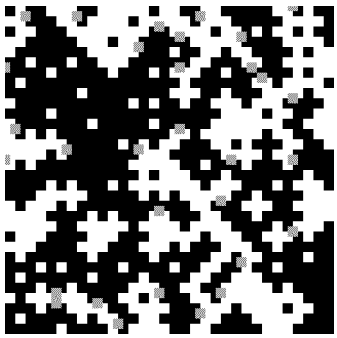


Figure 5.6: Rule **12** (**0134**), time 16000, energy 31

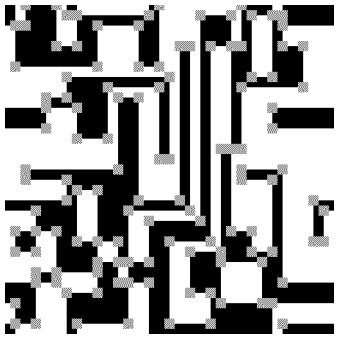


Figure 5.7: Rule **26** (**0S4**), time 30000, energy 122

5.2.4 Frustrated Rules

The last class of parity symmetric rules contains those that do not converge to energy 0 at temperature 0. Instead, these rules *freeze* at a high energy. Even though the energy is not 0, all possible transitions only raise the energy, and so the system is stuck in a local energy minimum. These systems are said to be *frustrated.*

There are two distinct rules in the parity symmetric set that exhibit this behavior — Rule **18/45** and Rule **26/51**. In both rules the major defect phenomena is isolated defects located at corners of solid rectangles (Figure 5.7, as well as the left-side flipbook). Unlike the randomly walking defect type systems, these isolated defects are *pinned*: they can neither move nor be eliminated. An important secondary structure are pairs of overlapping defects — both rules allow these pairs to travel in a random walk along one dimension.

Rules that freeze to positive energy at temperature 0 are very interesting. It

is possible that a particular defect could be locally eliminated from the world if it were possible to just temporarily raise the energy of the world slightly, to get over an *energy barrier* that is preventing the system from relaxing to a lower energy at a later time. At temperature 0 it is impossible to raise the energy, even temporarily, but positive temperature models allow energy barriers to be surmounted.

A related work hypothesizes that under certain conditions, if the energy barrier is a constant than it is still the case that $E \sim t^{\alpha}$ [SHS92]. If the energy barrier is not a constant, but rather dependent on the size of the defect, then $E \sim ln(t)$, or $E \sim ln(t)^{\alpha}$: much slower convergence.

Unfortunately, studying positive temperature models is more complicated than temperature 0. Any transition is possible in the world, not just those that move to equal or lower energies. It seems likely that all of the parity symmetric rules have only constant energy barriers, but there is evidence (not presented here) that indicates that at least one rule is $E \sim ln(t)$, contradicting the hypothesis in [SHS92]. This avenue has not been further investigated.

5.3 Summary

The set of parity symmetric, rotationally symmetric 2x2 rules contains a range of behaviors. One of the rules is almost trivial, having extremely fast dynamics and little structure. The standard Ising dynamics, boundaries between regions, exists in two forms. Two new interesting classes of behavior also occur, both marked by the importance of single defects in the lattice. In one class the defects walk randomly around the world and annihilate on collision, while in the other class the isolated defects are frozen in, resulting overall in a frustrated world. What remains is to explain why these phenomena are created by the various rules.

Chapter 6

Local Analysis

Each of the 2x2 rules defines a global dynamical process. Predicting rule behavior is difficult; for most rules, it is impossible to predict the state of any particular cell without considering the state of the entire world. In general information about the state of a particular cell can propagate arbitrary distances across the world. For example, in Rule **4/41** defects can randomly walk across the world an arbitrary distance. Therefore any particular cell in the world could potentially be influenced by any defect, given enough time.

Analysis of the 2x2 rules is difficult because of the requirement of global information. Studying the behavior of small local regions of the world is simpler than studying the entire world, but one cannot expect to be able to generalize local information to a complete solution of the global behavior.

This fact may seem somewhat surprising given that the probability of a particular spin flip event depends only on local information, and thus the rules governing the dynamical process are locally defined. In fact, the locality of individual events can be exploited to allow an analysis of the dynamics of local configurations to partially explain the global dynamics of any particular rule.

Two different analyses on small configurations will be considered as means to understand what happens to an entire world under any particular rule. One method, the *3x3 analysis*, lists all possible 3x3 world configurations and considers the result of flipping the middle cell in each configuration, thereby generating a list of possible energy transitions that can be used to infer global behavior. The other method presented, *defect analysis*, is an attempt to understand the defect phenomena that are induced by a particular rule. Like the 3x3 analysis, defect analysis also builds a list of possible configurations and considers the results of spin flips in these local environments. For defect analysis the configurations are chosen to be relevant to particular defect structures, not energy changes.

These two analyses will be applied to representative examples of the parity symmetric rules, to see how well they predict the global phenomena that the rule creates. Both analyses produce a fairly detailed accounting of the isolated events possible in the system. For the casual reader, the details of application may not be as interesting as the evaluation of the results; what is significant is the degree of success or failure of local analysis to predict global behavior.

6.1 3x3 Analysis

Individual events in the dynamical system are single spin flips: successive spin flips in time produce the global behavior. But each spin flip occurs only in a local context. The probability of flipping a particular cell depends only on the four neighborhoods of which that cell is a member, and the energy change that results from that spin flip is localized to the four neighborhoods surrounding the flipped cell (chapter 2). Therefore, the context for an event in the dynamical system is entirely local, only the 3x3 block surrounding the flipped cell. All changes in world energy ΔH are the ΔH seen by flipping the center cell in a 3x3 block; list all possible ΔH on all 3x3 blocks, and one has a list of all possible energy changes for the entire system.

Each cell in a 3x3 block is either a `0` or `1`. There are 9 cells, and so there are $2^9 = 512$ possible 3x3 blocks to consider. Each of these blocks is the union of four 2x2 neighborhoods, each with energy in $\{0, 1\}$, so every 3x3 blocks has energy in the set $\{0, 1, 2, 3, 4\}$. It is feasible to build a list of all 512 3x3 blocks, total up the change in energy that results from flipping the center cell for each of those blocks, and thereby produce an exact list of the possible energy transitions in the entire system.

Furthermore, the number of different 3x3 blocks to be considered can be made smaller than 512: because of symmetries in the rules, there are an even smaller number of truly different blocks from the rule's point of view. For example, all of the rules considered here are rotationally symmetric. Therefore, ΔH for flipping the center cell of a particular 3x3 block will be the same as ΔH for flipping the

center cell of any rotation of that 3x3 block. It is enough to examine the energy transitions possible on one representative 3x3 block: the result will be the same for its rotations.

In addition, if a rule is symmetric under a particular transformation T ($T_{\mathbf{4}}$, $T_{\mathbf{C}}$, $T_{\mathbf{S}}$, or $T_{\mathbf{1}}$), then ΔH on a 3x3 block B will be the same as ΔH on the transformed block $T(B)$. As with rotation, it is only necessary to count the energy transition on a representative block — it will be the same for any of the transformations applied to that block.

The set of operations on 3x3 blocks $\{R(\text{rotation}), T_{\mathbf{4}}, T_{\mathbf{C}}, T_{\mathbf{S}}, T_{\mathbf{1}}\}$ form an abelain group of order 32 acting on worlds: R is an element of order four, and each of the four transformations are elements of order two. For any particular rule, the subgroup generated by rotation and the set of transformations for which that rule is symmetric is the group of actions which apply to the rule. The action of that subgroup on 3x3 blocks defines a set of equivalence classes; one 3x3 block from each of the equivalence classes is representative of the energy changes possible in the entire class of 3x3 blocks.

Burnside's Lemma gives an easy way to explicitly count the number of equivalence classes for any particular subgroup ([Rob84]). Burnside's Lemma states:

$$\#\text{ classes} = \frac{1}{|G|}\sum_{\pi\in G}|\operatorname{fix}(\pi)|$$

Applying this formula to 3x3 blocks under the groups generated by any particular transformations is straightforward. For example, of the 512 3x3 blocks there are exactly 140 that are unique under rotation:

$$G = \langle R\rangle = \{e, R, RR, RRR\}$$

$$\begin{aligned} |\operatorname{fix}(e)| &= 512 \\ |\operatorname{fix}(R)| &= 8 \\ |\operatorname{fix}(RR)| &= 32 \\ |\operatorname{fix}(RRR)| &= 8 \end{aligned}$$

$$\begin{aligned} \#\text{ classes} &= \tfrac{1}{|G|}\ (|\,\mathrm{fix}(e)| + |\,\mathrm{fix}(R)| + |\,\mathrm{fix}(RR)| + |\,\mathrm{fix}(RRR)|) \\ &= 1/4 \qquad (512 + 8 + 32 + 8) \\ &= 140 \end{aligned}$$

Similar calculations find 70 unique 3x3 blocks under $\langle R, T_{\mathbf{4}} \rangle$, 38 under $\langle R, T_{\mathbf{4}}, T_{\mathbf{C}} \rangle$, 22 under $\langle R, T_{\mathbf{4}}, T_{\mathbf{C}}, T_{\mathbf{S}} \rangle$, and 14 under $\langle R, T_{\mathbf{4}}, T_{\mathbf{C}}, T_{\mathbf{S}}, T_{\mathbf{1}} \rangle$.

Given a rule and the list of representative 3x3 blocks, examining all possible energy changes on those 3x3 blocks is a simple matter of counting. For each representative block, calculate the energy of the block before and after the flip — the resulting ΔH is one possible energy transition in the entire system. The count of all ΔHs is the count of all possible energy changes in the system.

6.2 Local Defect Analysis

One important local feature of the various rules are the defects, those neighborhoods in the world that have positive energy. Many of the characterizations of the various rules in the previous chapter were descriptions of how the defects behave: what sorts of defects are possible, how those defects move, and how they are eliminated. If one understands all possible defect actions in the system, one understands the important dynamics of the system.

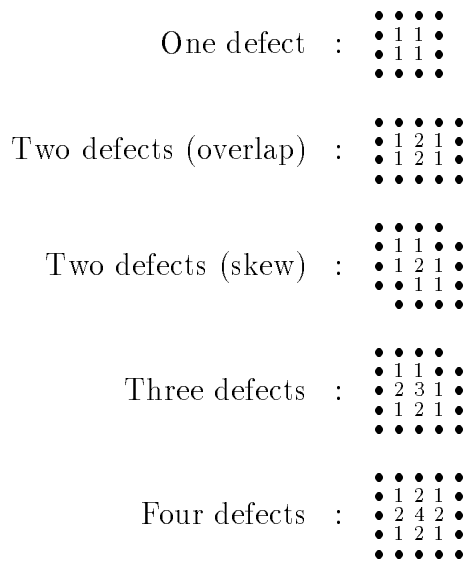
A 3x3 neighborhood does not include all of the context of an entire defect. For example, isolated defects play a large role in many of the rules. Isolated defects are a disallowed 2x2 neighborhood surrounded entirely by neighborhoods that are not defects. These features are actually 4x4 blocks: the 2x2 neighborhood in the middle and the surrounding cells. Therefore, to understand the phenomena associated with isolated defects it is necessary to consider an environment larger than 3x3 blocks. The wider environment that surrounds a particular defect phenomena is called a *defect structure*: the results of spin flips on defect structures can be counted much as spin flips in 3x3 blocks are counted.

In some rules defect structures span arbitrary distances. For example, Ising-like rules have chains of defects, long boundaries with no limit on their size. It is impossible to capture all arbitrary sized defect structures in any fixed-size window;

therefore, it is not expected that a local analysis will explain all defect phenomena. There is a limit on the power of local defect analysis, what is interesting is how useful it can be, even given the limitations.

Isolated defects and small defect interactions play a significant role most of the rules. The local defect analysis presented here will be restricted to only a small set of defect structures, those surrounding a particular cell. These structures are essentially expansions of 3x3 blocks that also take into account the relevant environment of the defect.

Any individual cell is a member of four neighborhoods, and therefore can be a member of at most four defects. There are only a small number of different defect structures that are centered on one cell. These are:



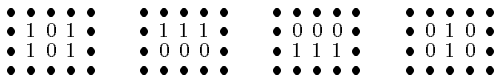
(Here, • refers to a cell that can be anything — it provides an environment for the defect. Numbers 1, 2, 3, and 4 correspond to cells that are members of that many defects.)

For any particular rule, there are only a finite number of these combinations that are defects. For example, Rule **4** (**01C34**) has only one type of defect, **S**. Therefore, all environments with one defect in the middle are rotations of single

defect environments with an **S** in its center, rotations of the small configuration

All 4x4 configurations of this type have energy at least 1, the defect in the middle. If the energy of one of these 4x4 blocks is exactly 1, then there is no other overlapping defect in the block: the defect in the middle is isolated. The set of configurations with an **S** in the middle with energy exactly 1 is exactly the set of all possible isolated defects in Rule **4**.

Similarly, there are four possible overlapping **S** – **S** interactions:



However, Rule **4** is symmetric under $T_{\mathbf{4}}$ and $T_{\mathbf{C}}$. All four of the two-defect environments are equivalent under some combination of these two transformations, so it is only necessary to examine what happens to one of these defect structures.

For a particular rule there is only a small set of possible defect structures: for Rule **4**, there is only one unique single defect structure and one unique structure with two overlapping defects. For any particular defect structure, filling in each • with a `0` or `1` generates a list of *all* possible environments in which a particular defect or defect interaction can occur. For example, there are 12 • cells in the one defect structure, and therefore $2^{12} = 4096$ possible environments for a single defect. Every 4x4 block surrounding a single defect is one of those 4096 types.

Simply counting the number of possible defect structures with a particular energy yields information about the possible defect structures in the system. For example, the set of all one defect structures with energy one is the set of all isolated defects. It will be shown that there are a significant number of isolated defects in Rule **4/41**, but none in Rule **30/55**. It was conjectured that isolated defects are the significant defect structure in Rule **4/41** but not in Rule **30/55**: counting the possible isolated defects yields a proof that isolated defects are possible in Rule **4/41** but not in Rule **30/55**.

Furthermore, as with the 3x3 analysis, it is possible to enumerate all possible energy transitions on any particular defect structure. For every configuration of a

particular defect environment, simply flip cells that are in the defect in the middle, and count the results of each spin flip. For example, enumerating the results of spin flips in single isolated defect structures counts which defect changes are possible for single isolated defects. This analysis can be used to show that, for instance, the defects in Rule **4/41** can all move in some sort of random walk, while isolated defects in Rule **18/45** are pinned, incapable of movement.

Counting what happens to single isolated defects is the simplest of the defect analyses. Multiple defect interactions can also be analyzed by considering larger structures — pairs of overlapping defects, two skewed defects, groups of three or four. The method is the same: list all instances of a particular defect structure, consider possible spin flips for cells that are members of the defect structure, and see what the resulting ΔHs are. Analysis of defect-pair interactions will be used to demonstrate the existence of defect pair annihilation in Rule **4/41**, and defect-triples will be implicated in the motion of defect boundaries in Rule **30/55**.

It should be noted that while there is a finite number of possible environments for any particular defect, there are enough that counting by hand is infeasible. For instance, the environment for a three-defect interaction contains 16 • environment cells, yielding $2^{16} = 65536$ possible three-defect environments. This can be narrowed down some by taking into account the symmetries in the rule (much as was done for the 3x3 analysis), but ultimately when counting the defect environments, the use of a computer program is invaluable. Appendix C contains a brief discussion of the software used to perform these analyses.

6.3 Local Analysis of Selected Rules

The analyses may be difficult to understand in the abstract; hopefully, by their application the method will become clearer. 3x3 analysis and local defect analysis will be applied to several of the parity symmetric rules and the success of these analyses to predict rule behavior will be evaluated. The casual reader who is uninterested in detail is invited to concentrate on the concluding paragraph of each section.

6.3.1 Fast Rules

As noted in the previous chapter, Rule **8/33** has the fastest dynamics of any of the nontrivial rule parity symmetric rules. In addition, it also has the simplest dynamics — considering Rule **33** (**1SC3**), for example, the only thing that is disallowed is solid blocks. It will be shown that this condition is very easy to satisfy.

Rule **8/33** is symmetric with respect to T_4 — therefore, when applying the 3x3 analysis it is only necessary to consider the set of 70 representative 3x3 blocks under the group $\langle R, T_4 \rangle$. The count of all possible energy transitions, as given by the 3x3 analysis, is in table 6.1.

3x3 configuration		Number that move to energy E				
Energy	Number	$E=0$	$E=1$	$E=2$	$E=3$	$E=4$
0	45	24				
1	17	13	4			
2	6	6				
3	1	1				
4	1	1				

Table 6.1: 3x3 analysis for Rule **8/33**

Each row is a tally of the 3x3 blocks with a particular energy. The "Number" column is a count of how many of the 70 possible configurations have that particular energy and the "$E = 0$," "$E = 1$," etc. columns list the number of 3x3 blocks that go to the specified energy when the center cell is flipped.

Of the 70 possible 3x3 configurations, fully 45 of them are already energy 0, already relaxed. A large proportion of 3x3 configurations are already allowed compared to, say, the Ising rule, which allows only 1 out of 70 (the solid block). This suggests that low energy configurations are common.

The count of transitions to particular energies reveals the possible ΔH in the system. All 3x3 blocks with energy greater than one can move directly to energy 0: all 6 energy 2, the one energy 3, and the one energy 4 3x3 block all go to energy 0 when the center cell is flipped. 13 of the 17 energy 1 blocks also go directly to energy 0. The remaining 4 go to some other energy 1 configuration.

The 4 energy 1 configurations that cannot be immediately resolved to energy 0 represents defects that potentially cannot be eliminated. But maybe one cell in the defect cannot be eliminated, but another can? Local defect analysis provides exactly this sort of information.

In fact, all defects are locally removable. Of the $2^{12} = 4096$ possible one defect environments, 1016 of them have energy 1: 1016 isolated defects. Table 6.2 lists the results obtained by seeing what happens when trying to flip each cell in every isolated defect:

Going	Number of structures with n moves				
to energy	$n = 0$	$n = 1$	$n = 2$	$n = 3$	$n = 4$
0	1	24	180	468	343
1	343	468	180	24	1

Table 6.2: Single defect analysis for Rule **8/33**

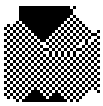
In this table, the rows tally the number of configurations that can go to a particular energy, and the columns contain the number of configurations that go to that energy in exactly n different ways. Every single defect structure has 4 cells to flip, and thus a maximum of 4 possible transitions to the given energy. Transitions to energy 0 are eliminations of the defect. Motion to energy 1 are cases where the defect is not eliminated by the spin flip, but moved.

Of the 1016 isolated defects possible in Rule **8**, 1 configuration has no transitions that bring the defect structure to energy 0, 24 configurations have only 1 transition to energy 0, 180 have 2 transitions to energy 0, 468 have 3 transitions to energy 0, and 343 have 4 transitions to energy 0. Therefore, of the 1016 defects, all but one have at least one cell that can be flipped to bring the structure to energy 0.

Furthermore, 468 of the 1016 defect environments have 1 spin flip that moves the defect environment to another energy 1 configuration. 180 of the defect environments have 2 ways to go to another 1 defect configuration, 24 have 3 ways, and one has 4 ways. Many of the isolated defects can move.

There was only one defect that could not be directly eliminated. But this defect:

```
0 1 0 1
1 1 0 0
0 0 1 1
1 0 1 0
```



actually has four different ways that it can move to another energy 1 configuration. Each of the new defect structures that are produced by spin flips on the one uneliminatable defect can be eliminated in one step.

3x3 analysis on Rule **8/33** demonstrates that most of the possible 3x3 blocks can be turned into energy 0 in one spin flips. A few energy 1 configurations might not be able to move to energy 0 directly. Looking more closely, by using defect analysis to examine the motions of isolated defects, all but 1 isolated defect can be eliminated in one spin flip. And that one configuration has an elimination in two spin flips. In other words, every possible local neighborhood can go to energy 0 in two spin flips. The combination of 3x3 analysis and defect analysis has proven, purely by counting local configurations, a global property of Rule **8/33**: that the system always relaxed to energy 0.

6.3.2 Random Walk / Annihilation Rules

Most of the other parity symmetric rules do not behave as simply. Another major class of rules identified in the previous chapter were those whose defects behaved as randomly walking, pairwise annihilating particles (Rule **4/41** and Rule **12/37**). Can local analyses account for the behavior seen in these rules?

Rule **4** (**01C34**) has only one type of defect: **S**. As noted in the previous chapter, defects in Rule **4** appear to walk randomly about the lattice and annihilate in pairs. If defects are randomly walking particles, then it must be the case that isolated defects exist, they can never disappear by themselves, but they can always move on the lattice. If pairs of defects annihilate, then there must be a way for a pair of defects to be eliminated in one spin flip.

The 3x3 analysis goes a long way towards confirming the defect annihilation hypothesis. Rule **4** is symmetric under $T_{\mathbf{4}}$ and $T_{\mathbf{C}}$, yielding 38 different 3x3 blocks. The 3x3 analysis in table 6.3 demonstrates that ΔH for this rule is always even — the only possible reductions in energy are 2 to 0, 3 to 1, or 4 to 0. Energy 1 configurations can never be eliminated: defects cannot disappear by themselves. However, many of the energy 2 configurations (7 of 9) have a single spin flip to

3x3 configuration		Number that move to energy E				
Energy	Number	$E=0$	$E=1$	$E=2$	$E=3$	$E=4$
0	14	6				
1	13		12			
2	9	7		2		
3	1		1			
4	1	1				

Table 6.3: 3x3 analysis for Rule **4/41**

energy 0, suggesting annihilation is possible. And almost all energy 1 configurations have transitions to other energy 1 configurations, and indication that defect motion is possible.

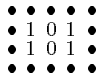
To understand the full story it is necessary to look at the more detailed defect analysis. There is only one type of defect, **S**. Of the 4096 possible single defects, 343 of these are isolated. Table 6.4 lists the results of spin flips on single defects.

Going	Number of structures with n moves				
to energy	$n=0$	$n=1$	$n=2$	$n=3$	$n=4$
0	343				
1			2	84	257

Table 6.4: Single defect analysis for Rule **4/41**

As predicted by the 3x3 analysis, no isolated defect can be eliminated in a single spin flip (all 343 have no moves to energy 0). But all isolated defects can move to other energy 1 configurations: most (257) of them in four different ways. These motions all occur as the result of one spin flip, a flip that removes the defect in the middle but creates a new defect nearby: defect motion. Local defect analysis demonstrates that all isolated defects can move. What about pairwise annihilation?

There are two types of defect-pair interactions: overlapping and skew. There is one unique type of overlapping **S** – **S** interaction:



Explicit counting of the $2^{14} = 16384$ configurations indicates that this defect pair occurs in isolation in 1042 different ways. Each of the two cells in the defect

overlap should be tested for a potential spin flip, resulting in at most two possible moves for a particular configuration.

Going to energy	Number with n moves $n=0$	$n=1$	$n=2$
0	25	288	729
1	1042		
2	729	288	25

Table 6.5: Two overlapping defect analysis for Rule **4/41**

Table 6.5 demonstrates that in Rule **4/41** there is no transition on pairs of overlapping defects that goes to energy 1: this is expected, for if there were a transition from energy 2 to energy 1 then only one defect would be eliminated in a pair, and that possibility has already been ruled out in the 3x3 analysis. All but 25 of the overlapping defect structures can go directly to energy 0 with one spin flip: an annihilation of both defects is common. Of those 25 configurations that cannot be eliminated directly, all of them have a transition to some other two defect configuration. Specifically looking at the configurations after this transition (not shown here) indicates that all of the defect pairs that cannot be eliminated in one spin flip can be eliminated in two. In most cases, when two defects meet they can annihilate. In a few instances they cannot, but in those cases they can move to another configuration that does allow annihilation.

Overlapping defects are only one of the two types of two-defect interactions. There are two distinct types of skew defects in Rule **4**:

Table 6.6 lists the transitions on the first type of skew defect. Every configuration moves from energy 2 to energy 0 when the the shared cell is flipped. Complete annihilation! However, table 6.7 shows that the other type of skew interaction is markedly different.

For the second type of skew interaction there is no possible annihilation — the only transition is to another two defect configuration. Therefore, while there is

Going	n moves	
to energy	$n = 0$	$n = 1$
0		3535
1	3535	
2	3535	

Table 6.6: Two skewed defect (type 1) analysis for Rule **4/41**

Going	n moves	
to energy	$n = 0$	$n = 1$
0	484	
1	484	
2		484

Table 6.7: Two skewed defect (type 2) analysis for Rule **4/41**

evidence that many two defect interactions allow annihilations, in some cases they do not.

Empirical evidence indicates that in Rule **4/41** all defects are eventually removed. The underlying dynamic seems to be that there are actually two different types of defect, types A and B, and the annihilation equation is $A + B \longrightarrow 0$. All isolated overlapping interactions are of heterogeneous defects (type A and type B), as are the first type of skew interaction, while the second type of skew are two defects of the same type (A and A, which cannot be eliminated). This phenomenon is observable in local defect analysis, but has not been pursued further.

Another unexplained phenomenon of Rule **4/41** is that defects seem to always come in pairs (chapter 5). The 3x3 analysis proved that if the energy is even, it remains even. It appears that in a finite world the presence of an isolated defect in the world requires that another defect exist somewhere else in the world (probably of the other type, if the two defect type hypothesis is true). However, this sister defect does not seem to have to occur within any finite distance of the first defect. In other words, "defects come in pairs" is a global property of the rule, not a local one. Because the scope of this property is not limited to a local region, no evidence can be found for it by counting local configurations.

Another interesting tangent is the possibility that there is enough information

present in the defect analysis to offer a close approximation of the dynamics of Rule **4/41**. By examining the results of spin flips on isolated defects, one can count exactly in which direction a defect can walk. From this count one could model the random walk that the defects perform. This information, coupled with the existing solutions of systems of discrete randomly walking annihilating particles [SSB90], might be the path towards a complete solution to the dynamics of Rule **4/41**.

The analysis for the other random walk / annihilation rule, Rule **12/37**, follows the same basic pattern but reveals a more complicated story. There are transitions on the world that do not keep the energy of the world even, implying that some defect elimination events are not mutual annihilation. Defects are able to move like a random walk, but the random walk seems to be constrained to one-dimensional boundaries between large regions. These boundaries are global structures, not visible in the small contexts enumerated by local defect analysis.

Local analysis explains a considerable amount of the behavior of Rule **4/41**. 3x3 analysis demonstrates that the only energy reduction possible is annihilation of pairs of defects, and defect analysis shows that all single defects can walk on the lattice. One limitation of looking at local configurations has been demonstrated — local analysis is powerless to explain the global property that in Rule **4/41**, defects come in pairs. But overall, local analysis has accounted for many of the dynamics of Rule **4/41**.

6.3.3 Frustrated Rules

The next major class of rules to be studied are Rule **18/45** and Rule **26/51**, those parity symmetric rules under which random worlds do not relax to energy 0. It will be shown that for Rule **18/45** pinned defects (defects that can neither move nor be eliminated) are implied by the rule itself. Results are similar for Rule **26/51**, but are not presented here.

Rule **18** (**0SC4**) has only two types of defects: **1** and **3**. The hypothesis from the previous chapter was that this rule had pinned defects, and that these pinned defects contributed to frustrated dynamics. There was also a secondary effect where

pairs of defects travelled in some sort of random walk. Most of these phenomena are evident in the 3x3 analysis.

3x3 configuration		Number that move to energy E				
Energy	Number	$E=0$	$E=1$	$E=2$	$E=3$	$E=4$
0	3					
1	4					
2	8			8		
3	4		4			
4	3	3				

Table 6.8: 3x3 analysis for Rule **18/45**

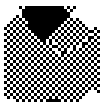
Table 6.8 shows that 3x3 configurations with energy 0 or 1 cannot be changed at all: if there are isolated defects, they will not be able to move. All of the energy 2 blocks do have possible transitions to other energy 2 configurations, and energy 3 and energy 4 configurations provide the opportunity for some energy reduction. Note that the only time a local region can go to energy 0 is when there are four defects together around the central square — complete defect elimination seems difficult.

The 3x3 analysis only indicates that if there are isolated defects, then they cannot move. A specific defect analysis on the various types of isolated defects (table 6.9 shows that there are 16 possible isolated defects. Of those 16, none of them have possible spin flips. Isolated defects cannot be changed by themselves: without another defect's influence, they are permanent features of the world.

Going	Number of structures with n moves				
to energy	$n=0$	$n=1$	$n=2$	$n=3$	$n=4$
0	16				
1	16				

Table 6.9: Single defect analysis for Rule **18/45**

Table 6.9 also demonstrates one weakness of the local defect analysis. Of the 4096 potential isolated defects, only 16 of those configurations are actually isolated defects: all other assignments to the environment of the defect structure result in other overlapping defects. The proportion of isolated defects is small enough that it



raises the question as to whether isolated defects actually occur with a reasonable probability. There is no way to estimate that probability from these tables — in general, it will be a complicated function potentially requiring global information. Observation of Rule **18/45** indicates that isolated defects are common, and local analysis then demonstrates that isolated defects are pinned, but it cannot explain why isolated defects are so common.

It was already determined by the 3x3 analysis that a pair of defects cannot be eliminated. The more detailed defect analysis provides little other useful information about defect pairs — isolated pairs of defects do exist, and when they do they can always move to other defect pair configurations. When watching the rule run it appears that the defect pairs are constrained to travelling in one dimension. This effect should be visible by examining the specific transitions of overlapping defect pairs, much like the specifics of the random walk in Rule **4/41** is, in principal, solvable by counting exactly what sort of motions are possible in each particular environment.

For Rule **18/45**, 3x3 analysis has demonstrated that transitions to lower energy are generally difficult. Defect analysis shows that isolated defects are possible, and that when they occur they are completely pinned. However, the proportion of isolated defects is small enough to make one wonder how probable they are. Observation of the dynamics suggests that isolated defects are common, but local analysis of Rule **18/45** seems unable to verify that conjecture.

6.3.4 Ising-like Rules

The final class of rules in the parity symmetric systems are the "Ising-like" rules, those where the defects are boundaries between homogeneous regions. Rule **30/55** is pretty much exactly the Ising rule, having two regions (solid `0` and solid `1` for Rule **30**), while Rule **22/59** behaves similarly but allows four types of regions, not two. Local analysis is generally not useful on these types of rules because the defect structures are potentially any size, not simple isolated single defects or pair interactions.

However, the very fact that local structures are not the dominant behavior of the rule is indicated by local analysis. In addition, some information about the possible dynamics is available. Table 6.10 shows the 3x3 analysis on Rule **30** (**04**).

3x3 configuration		Number that move to energy E				
Energy	Number	$E = 0$	$E = 1$	$E = 2$	$E = 3$	$E = 4$
0	1					
1	1					
2	6					
3	17				4	
4	45	1	1	6	13	24

Table 6.10: 3x3 analysis for Rule **30/55**

There is only one type of 3x3 block that is energy 0, blocks that are either solid `0` or `1`, the expected ground states of the Ising rule. Energy 1 and energy 2 blocks are uncommon, and when they occur they have no freedom to move. 3x3 blocks with energy 3 can sometimes move, and 3x3 blocks with energy 4 have much freedom to move, and can sometimes be eliminated.

The *only* time the energy of the world can be decreased under Rule **30** is when there are four defects together. One event that is typical for this sort of transition is:

$$\begin{array}{ccc} \begin{smallmatrix} 0&0&0\\0&1&0\\1&1&1 \end{smallmatrix} & \longrightarrow & \begin{smallmatrix} 0&0&0\\0&0&0\\1&1&1 \end{smallmatrix} \\ \text{energy } 4 & & \text{energy } 2 \end{array}$$

Flipping the center cell of the energy 4 configuration lowers the configuration to energy 2.

Unfortunately, a more general defect analysis gives very little other useful information. Counting indicates that it is impossible to have isolated groups of 1, 2, or 3 defects: as expected, isolated defects are not a factor in the Ising rule. When looking at all three and four defect interactions, not just isolated structures, one sees evidence of the motion of defect boundaries, but the resulting counts are difficult to understand.

The major feature of the Ising rule is long chains of connected defects, the boundaries between regions that are energy 0. Because these regions are arbitrarily

sized, they are not representable in the limited scope of local analysis. What can be demonstrated is that isolated defects are not present and that certain transitions of high energy regions are possible, indicating that the rule is probably not frustrated.

6.4 Summary

Analysis of spin flips on 3x3 blocks and on local defect structures is a useful tool for understanding many of the possible rules. Local regions are small enough to permit an exhaustive counting and informative enough to capture significant features of the model.

Local analyses work best for those rules where the most important defect structures are local, in particular for all rules except the Ising-like rules. Simply looking at 3x3 blocks and small defect structures predicts which rules result in processes that converge to energy 0 quickly, which are frustrated by pinned defects, and which have dynamics that appear to be random walks with annihilation.

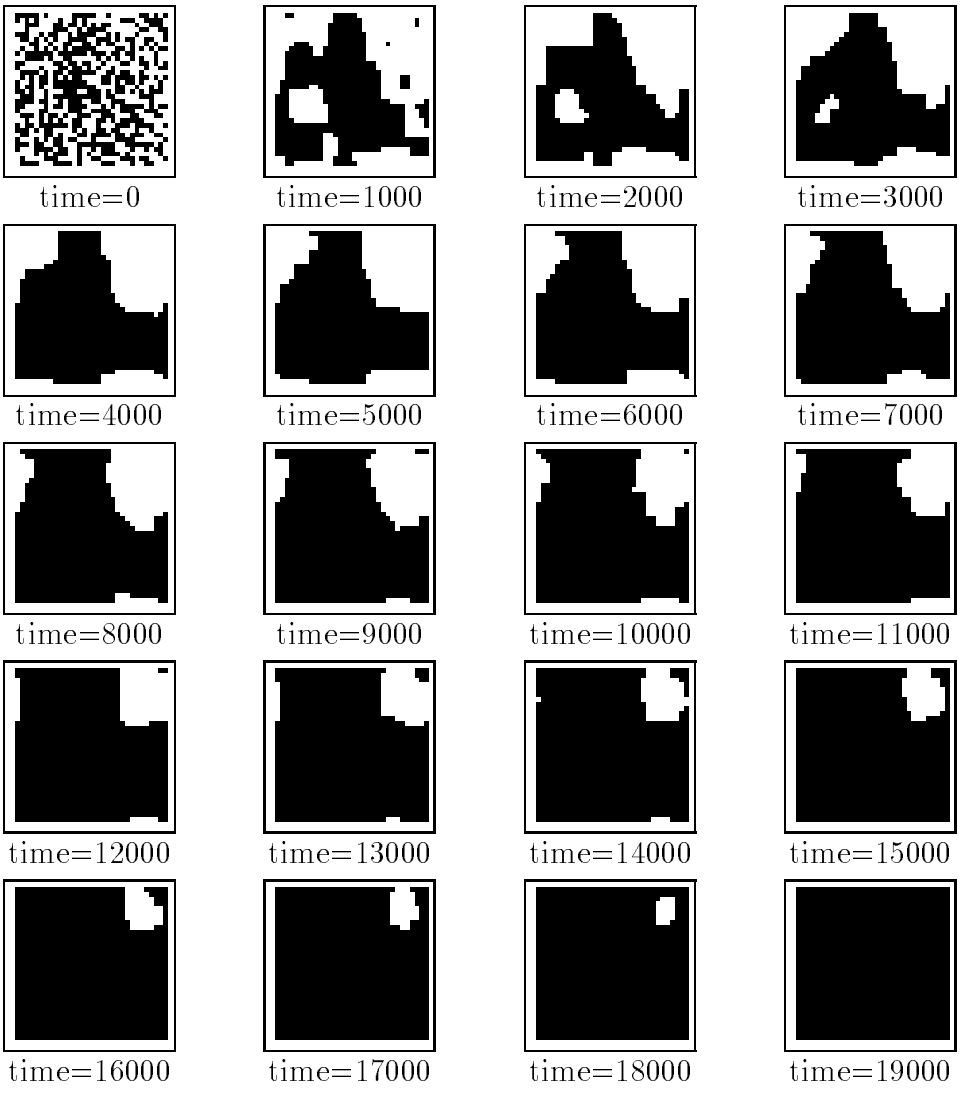
However, local analysis is ultimately incomplete. It is most successful on rules where all defect events are purely local: Rule **8/33** and Rule **4/41** in particular. Even here the analysis is somewhat lacking, for example, the inability to verify the "defects come in pairs" hypothesis for Rule **4/41**. For rules like the Ising rule where the dominant defect structure is entirely non-local, local analysis can do little more than demonstrate that global defect structures are significant.

The interplay between local and global phenomena is ultimately what is interesting in the 2x2 model. It is usually easier to focus on local aspects of a system: small configurations are easier to understand and manipulate. And when the system is defined by local rules, local analysis can be informative. But local information can be incomplete, and ultimately may not explain an entire global process. What is surprising is not that a local analysis may ultimately fail to capture every aspect of a global process, but rather that it can be so useful in predicting many of the phenomena evident in a global dynamical system.

Appendix A

Example of Rule 30/55 Dynamics

An example run of Rule **30/55** at size 32x32. Frames move from left to right, then top to bottom. Note that the system converges to energy 0, solid black, in 19000 time steps.



Appendix B

Dictionary of Rules

A table of all 64 rotationally symmetric rules. "Allowed" is a list of the neighborhoods allowed by the rule, "Forbidden" are those neighborhoods that are forbidden. The $T_{\mathbf{4}}$, $T_{\mathbf{C}}$, $T_{\mathbf{S}}$, and $T_{\mathbf{1}}$ columns list which rule is equivalent to the listed rule under that transform; an 's' means the rule is symmetric under a transformation, a blank means the transform is not applicable. The equivalence classes for each transformation can be determined by reading down the column for that transformation.

Rule	Allowed	Forbidden	$T_{\mathbf{4}}$	$T_{\mathbf{C}}$	$T_{\mathbf{S}}$	$T_{\mathbf{1}}$
0	01SC34		s	s	s	s
1	1SC34	0	32			
2	0 SC34	1	16			
3	SC34	01	48			
4	01 C34	S	s	s	41	
5	1 C34	0 S	36			
6	0 C34	1S	20			
7	C34	01S	52			
8	01S 34	C	s	33		
9	1S 34	0 C	40			
10	0 S 34	1 C	24			
11	S 34	01 C	56			
12	01 34	SC	s	37		
13	1 34	0 SC	44			
14	0 34	1SC	28			
15	34	01SC	60			
16	01SC 4	3	2			
17	1SC 4	0 3	34			
18	0 SC 4	1 3	s	s	s	45
19	SC 4	01 3	50			
20	01 C 4	S 3	6			
21	1 C 4	0 S 3	38			
22	0 C 4	1S 3	s	s	59	
23	C 4	01S 3	54			

Rule	Allowed	Forbidden	T_4	T_C	T_S	T_1
24	01S 4	C3	10			
25	1S 4	0 C3	42			
26	0 S 4	1 C3	s	51		
27	S 4	01 C3	58			
28	01 4	SC3	14			
29	1 4	0 SC3	46			
30	0 4	1SC3	s	55		
31	4	01SC3	62			
32	01SC3	4	1			
33	1SC3	0 4	s	8		
34	0 SC3	1 4	17			
35	SC3	01 4	49			
36	01 C3	S 4	5			
37	1 C3	0 S 4	s	12		
38	0 C3	1S 4	21			
39	C3	01S 4	53			
40	01S 3	C 4	9			
41	1S 3	0 C 4	s	s	4	
42	0 S 3	1 C 4	25			
43	S 3	01 C 4	57			
44	01 3	SC 4	13			
45	1 3	0 SC 4	s	s	s	18
46	0 3	1SC 4	29			
47	3	01SC 4	61			
48	01SC	34	3			
49	1SC	0 34	35			
50	0 SC	1 34	19			
51	SC	01 34	s	26		
52	01 C	S 34	7			
53	1 C	0 S 34	39			
54	0 C	1S 34	23			
55	C	01S 34	s	30		
56	01S	C34	11			
57	1S	0 C34	43			
58	0 S	1 C34	27			
59	S	01 C34	s	s	22	
60	01	SC34	15			
61	1	0 SC34	47			
62	0	1SC34	31			
63		01SC34	s	s	s	s

Appendix C

Software Tools

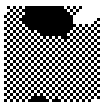
A considerable portion of this work has relied on the aid of software developed by the author. While the Ising model itself was intended to be solved analytically, it lends itself naturally to computer simulation. For the more complicated 2x2 models where analytic models are not immediately forthcoming, direct simulation remains the easiest way to study the various rules. The results obtained by simulation will hopefully develop the intuition necessary to aid analytic solutions.

In addition to simulating the model itself, other computer programs have been useful in studying the symmetries in the rule table and in performing the local analysis presented in chapter 6. Most of this thesis was done in a constant state of interaction with a computer — a particular rule was run, the behavior examined, an analytic hypothesis formed, the hypothesis implemented in a program, the program run, and the results checked against the hypothesis. This method proved to be natural and powerful.

C.1 `relax`

The simulation engine, `relax`, implements the Markov process described in chapter 2. The program takes a particular rule and a particular initial configuration (usually a random world) and directly simulates the Markov process: the output is the measured energy as a function of time.

The Markov process simulation is the simplest imaginable. At each time step, a random cell in the world is chosen and the probability of flipping that cell is calculated (based on the local ΔH). If a pseudorandom number uniformly chosen from $[0, 1)$ is lower than the probability of the flip, then the flip is performed. This process is iterated over as many time steps as needed (on the order of 500 million time steps for most rules on a 256x256 world).



If the goal of simulation is collecting lots of time series data, this algorithm is unacceptably slow. Even with a highly optimized implementation it takes several hours to do a typical 500 million time step run on a regular UNIX workstation. For all of the nontrivial rules, as the energy gets lower the time between spin flip events gets bigger — towards the end of a run there might be only one successful spin flip every million time steps. An alternate random process suggested in [SHS92] and [BH92] simulates the expected time for spin flips rather than the probability of spin flips, providing an enormous gain in speed. More serious statistical study of these rules would benefit greatly from this improved algorithm.

Fortunately, it is only necessary to run a rule for a few hundred thousand time steps to develop a basic qualitative understand of how the rule works. To aid in this sort of examination, `relax` provides a graphical display of the world changing in time. The software makes it easy to see the defect motion itself by highlighting those neighborhoods that are defects. The example pictures in chapter 5 are essentially screen captures of the program.

The importance of watching the dynamical processes for understanding the phenomena in the various rules cannot be overestimated. Many of the concepts that are difficult to describe become obvious with just a few minutes' demonstration.

C.2 `rot` and `printdict`

Two small tools, `rot` and `printdict`, automate the process of dealing with the rule table itself. `rot` simply takes the number of a rule and prints out its representation as a 16 bit string, one bit for each possible 2x2 neighborhood (in effect translating rotationally symmetric rules into the generic 2x2 framework). `printdict` produces the dictionary in appendix B — for each rule it determines what the rule 'means' as well as the effect of various transformations on it.

C.3 3x3

The analysis on all 3x3 blocks presented in chapter 6 can just barely be performed by hand — for the rules considered, there are at most 70 cases to consider. However, doing this analysis by hand is tedious and prone to error. The `3x3` program takes a rule as input, calculates a list of all unique 3x3 blocks (up to the symmetries of that rule), considers the effect of flipping the middle cell of each block, and then prints out the possible energy changes.

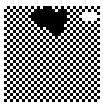
Having this tool automated makes it trivial to test the efficacy of the 3x3 analysis on arbitrary rules — the total count of all transitions for a particular rule is available almost instantaneously. It is doubtful that the 3x3 analysis would have been understood without the computer implementation.

C.4 general

The local defect analysis from chapter 6 is considerably more difficult to perform than 3x3 analysis — for most rules many hundreds of thousands of cases have to be considered. `general` (so named because it is general enough to work on all local defect structures) takes a particular rule and defect structure as input, generates a list of all possible environments for that defect, and counts the number of environments that can move from energy E to energy E' in n different ways.

This output is quite broad, capturing most information about the transitions possible on that defect structure. Various specific backends extract particular information — a list of isolated defects, counts of transitions to lower energy, simple counts of ΔH for that defect structure, etc.

Given the large number of cases considered, the need for a computer tool to implement the local defect analysis is obvious. In addition, the process of developing the tool itself was useful in understanding how the local defect analysis worked. In this, as in most of the work, the development of the computer program was coincident with the development of my understanding of the system.



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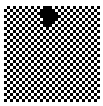

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