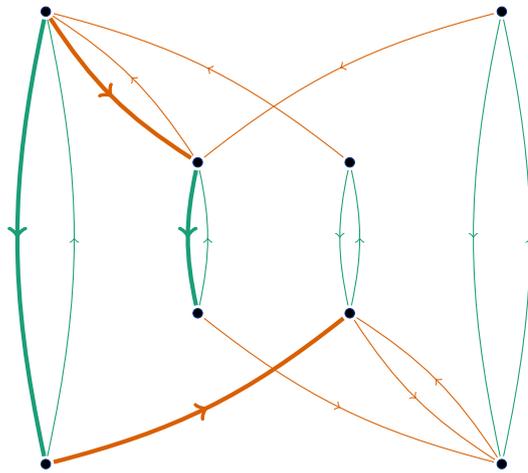




Actuating Noncommutative Deterministic Spin Systems



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Abstract

In this thesis, systems of Ising spins are approached as minimalist models for programmable mechanical metamaterials. The key motivation is to explore how complicated energy landscapes can have a response to a sequence of actuations, that depends on the order of the sequence. Examples of commutative as well as noncommutative spin systems are given. Deterministic dynamics are defined by flipping spins one by one, minimizing an energy function. Any degeneracies are lifted with quenched disorder. Consequently, the behaviour of a spin system depends on the choice of quenching constants, so fine-tuning them allows to program the dynamics. More importantly, spin systems can be programmed actively with local actuations by flipping the signs of interactions.

Depending on the quenching constants, local actuations can be commutative or noncommutative, invertible or noninvertible. An example of noncommutative invertible actuations has been found. More results are obtained by explicit computation of small spin systems.

By reformulating spin systems on cycle graphs as systems of particle-like frustrations, it is possible to reduce the complicated energy landscape of the spin system to a set of simple rules.

Two observations have been made. First, spin systems on cycles seem to reappear as subsystems on larger cycles. Secondly, quenching constants that lead to different spin systems seem to be separated by equalities which also ensure that degeneracies are lifted.

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Introduction

1.1 Motivation

Mechanical metamaterials have properties which do not so much stem from their microscopic structure as from their geometry. These materials often have an unique, sometimes unexpected, mechanical response [1]. Usually this response depends on the (geometric) state of the material. A current challenge in the design of mechanical metamaterials is that often the state is fixed during fabrication, so the material has to be redesigned and rebuilt in order to change the mechanical response [2].

To overcome this limitation, effort is being put into making metamaterials programmable. We will distinguish two types of programmability:

- I. The state can be tuned during the design process, after which the material still has to be rebuilt (e.g. [3, 4]).
- II. The fabricated material can be reconfigured such that the mechanical response changes.

Clearly, if one is interested in making multi-functional materials, type II is preferable. It could be achieved by making a material whose state depends on an external parameter (e.g. confinement [5, 6] or temperature [7]), but it would be more effective if the reconfiguration could be triggered by locally actuating the material, because then the reconfiguration would have many degrees of freedom. For example, this could be done by locally exerting a force or increasing the temperature locally [8].

Suppose we have a material that can be actuated in at least two ways, let us say A and B . We can test whether applying A first and B second to some initial state yields the same state as applying B first and then A . If

for all possible sequences of actuations the order does not matter, we call the material *commutative*. If there are any actuations A and B , such that the final state does depend on the order of their application, we call the material *noncommutative*.

One can think of actuating a commutative material as flipping a set of switches, such that the state only depends on the current position of the switches. On the other hand, actuating a noncommutative material is like pressing buttons, such that the state of the system does not only depend on which buttons are currently pressed, but also on the ordered sequence of previous button presses.

The analogy illustrates that noncommutative actuations can be combined to reconfigure a material into many more states than commuting actuations can. Thus noncommutative mechanical metamaterials can potentially be programmed to have many different mechanical responses.

The problem with relating local actuations to the state of a material is that the energy landscape of metamaterials tends to be complicated. The purpose of this thesis is to study discrete models with a finite state space, on which the state can be programmed using local actuations. The model is not defined in consideration of a particular metamaterial, but rather in a way that allows the relation of actuations and state to be characterized rigorously. Because the state space is finite, the still complicated energy landscape is manageable. That is, the model is a minimalist demonstration of type II programmability with local actuations. We will find that it is possible to completely understand the dynamics of small instances of the model and that they exhibit interesting features, such as noncommutativity of actuations.

1.2 Deterministic spin systems

The models considered in this thesis are spin systems, which consist of Ising spins pointing up or down, connected by interactions with values ± 1 . We will define dynamics on these spin systems such that the energy is lowered by flipping spins one at a time until an equilibrium state is reached, while the interactions are fixed. The energy function will be defined such that the energy is lower if positive interactions connect aligned spins and negative interactions connect spins of opposite sign.

Because we approach these systems as simplifications of mechanical materials, we do not want the dynamics to involve any kind of randomness. This is what distinguished our spin dynamics from other models involving Ising spins. This requirement causes a problem whenever

multiple equilibrium states with equal energy are accessible. Section 2.2 presents a solution to this by introducing quenched disorder on interactions. Also, once the system is in equilibrium, its state will not change until it is actuated from the outside. That is, we do not allow (e.g. thermal) fluctuations between equilibrium states.

We can locally actuate our spin systems by changing the sign of an interaction. After that, the system might not be in equilibrium, so it will again minimize its energy by single spin flips. Thus an actuation involves two steps:

1. Flip the sign of the interaction that is actuated on.
2. Lower the energy by flipping spins one by one until an equilibrium state is reached.

A more formal definition of actuations will be given in chapter 2.

Generally, we focus on the effects of actuations and sequences of actuations. As mentioned before, we need to introduce quenched disorder to make the system deterministic. Naturally, we investigate how quenched disorder influences the dynamics of the system.

This thesis contains examples of commutative and noncommutative deterministic spin systems, as well as statements on whether certain actuations are invertible. Also, there are some special cases, particularly cycles of spins, that we can characterize by reducing the complicated energy landscape to a simpler model.

Abelian sandpiles

A central effort of this thesis is to set up a rigorous definition of deterministic spin systems. Interestingly, the proposed mathematical formulation has similarities to that of abelian sandpiles [9]. Roughly, a sandpile is a distribution of “chips” on the vertices of a graph. It can be brought to equilibrium by repeatedly “toppling” vertices that have too many chips on them, that is, move a chip to each neighbour.

An important property of sandpiles is, that the final configuration is independent of the sequence in which the vertices topple. If we regard placing a single chip as a local actuation, then this implies that all actuations commute for abelian sandpiles. As we will see, this is a major difference to our spin systems.

Deterministic spin dynamics on finite graphs

2.1 Mathematical formulation of spin dynamics

Spin dynamics act on a graph $G = (V, E)$ which is finite, connected and simple (that is, undirected with no multiple edges or loops). We put a *spin* on each vertex and an *interaction* on every edge. That is, the system has *spin states* $\Omega_V = \{\pm 1\}^V$ and *interaction states* $\Omega_E = \{\pm 1\}^E$. The full state space is $\Omega = \Omega_V \times \Omega_E$. Concretely, the system in state $(S, J) \in \Omega$ is a graph where we assign to every vertex $v \in V$ a spin S_v and to every edge $j \in E$ an interaction J_j .

For $J \in \Omega_E$ and $j \in E$ we introduce the notation $J^{(j)}$ for the interaction state such that for $i \in E$

$$J_i^{(j)} = \begin{cases} -J_i & \text{if } j = i \\ J_i & \text{if } j \neq i \end{cases}$$

That is, the interaction state with the j th interaction flipped. Analogously, define for a spin state $S \in \Omega_V$ and a vertex $v \in V$

$$S_i^{(v)} = \begin{cases} -S_i & \text{if } v = i \\ S_i & \text{if } v \neq i \end{cases}$$

Single actuations

On the state space Ω , we want to define deterministic dynamics. The idea is that we can flip the sign of some interaction and then watch the sys-

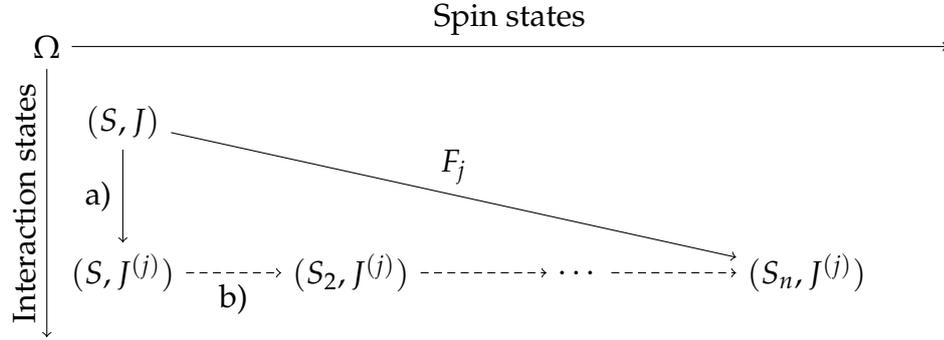


Figure 2.1: Graphic representation of a single actuation F_j acting on some state (S, J) . The final state is determined in two steps. a) The interaction j is flipped, but the spin state is unchanged. Note that the state $(S, J^{(j)})$ might not be in equilibrium. b) Each of these steps flips a spin state such that the energy is strictly lowered. This stops when an equilibrium state has been reached. The equilibrium state $F_j(S, J) = (S_n, J^{(j)})$ is the final state after the actuation.

tem evolve towards a state of minimal energy, according to some *energy function* $H : \Omega \rightarrow \mathbb{R}$. We will define H such that for positive interaction between vertices v_1 and v_2 , the energy is lowest for $S_{v_1} = S_{v_2}$, and for negative interaction for $S_{v_1} = -S_{v_2}$. Whenever the energy cannot be lowered by changing the sign of a single spin value, we say that the system is in *equilibrium*.

The dynamics are then characterized by the reactions of the system in equilibrium to *actuations*. Such an actuation starts with the flip of an interaction on a single edge. Then spins are flipped one by one, where each step strictly lowers the energy. The actuation process ends when the system has found a new equilibrium. Figure 2.1 sketches this process.

Sequences of actuations

Interesting properties of spin systems are revealed by examining how a system behaves under sequences of actuations. That is, what happens when we flip some interactions one by one. We assume that the system finds its new equilibrium state fast enough, such that it already is in equilibrium at the start of the next actuation. Figure 2.2 illustrates how a sequence of two actuations is processed by the system. It is of interest whether for example a sequence of actuations $ABCA$ produces the same final state as BC . The algebraic structure that we give to the dynamics to investigate this question is that of a semigroup.

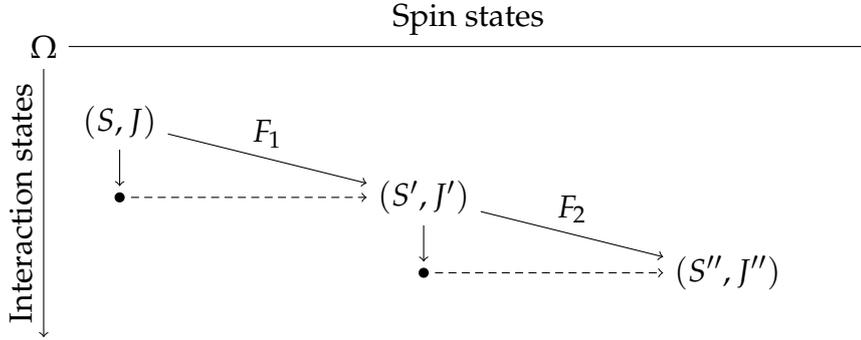


Figure 2.2: Graphic representation of the concatenation of two actuations F_1 and F_2 acting on some state. Notice that although we view F_1F_2 as a function on the set of equilibrium states, the action of F_1F_2 is still determined by the actuation processes of F_1 and F_2 in sequence.

Definition 2.1.1. A *semigroup* F is a non-empty set with a binary operation $F \times F \rightarrow F$ (denoted by multiplication $ab = c$) such that:

- For all $a, b, c \in F$ we have $(ab)c = a(bc)$. (associativity)

A semigroup F is **generated** by a subset $G \subset F$ if for each element $f \in F$ there is a finite sequence $g_1, \dots, g_n \in G$ such that $f = g_1g_2 \cdots g_n$. Notation: $F = \langle G \rangle$.

The following example of a semigroup is essential to our definition of deterministic dynamics.

Example 2.1.2. Let X be a set. The set $\text{Hom}(X, X)$ of functions from X to itself forms a semigroup under concatenation.

In particular we let X be the set of *equilibrium states*, which is

$$\Omega(H) = \{(S, J) \in \Omega : \nexists \tilde{S} \in \Omega_V : \|S - \tilde{S}\|_1 = 2 \text{ and } H(\tilde{S}, J) < H(S, J)\},$$

given an energy function $H : \Omega \rightarrow \mathbb{R}$. Then we define the dynamics as a particular subsemigroup of $\text{Hom}(\Omega(H), \Omega(H))$ that is generated by maps which correspond to the single actuations.

Definition 2.1.3. Fix a map $F : E \rightarrow \text{Hom}(\Omega(H), \Omega(H))$. If for all $(S, J) \in \Omega(H)$ and $j \in E$ there exists a $S' \in \Omega_V$ such that $F_j(S, J) = (S', J^{(j)})$, then call the subsemigroup

$$\mathbb{F}(H) := \langle \text{im } F \rangle \subset \text{Hom}(\Omega(H), \Omega(H))$$

a *(deterministic dynamical) spin system*.

Note that the notation does not include the dependence on F . That is because we will find canonical functions $F_j : \Omega(H) \rightarrow \Omega(H)$. The following condition on H ensures the existence and uniqueness of these functions along the process described in Figure 2.1.

Condition 2.1.4. *For all $j \in E$ and $(S, J) \in \Omega(H)$, there exists a sequence $S = S_1, S_2, \dots, S_n$ such that for $1 < k \leq n$, S_k is the unique element of*

$$A_k = \{\tilde{S} : \|S_{k-1} - \tilde{S}\|_1 = 2\}$$

with $H(S_k, J^{(j)}) = \min_{\tilde{S} \in A_k} H(\tilde{S}, J^{(j)})$ and the sequence is terminated by

$$(S_n, J^{(j)}) \in \Omega(H)$$

.

If condition 2.1.4 holds, then we can define the deterministic dynamical spin system $\mathbb{F}(H)$ by

$$F_j(S, J) = (S_n, J^{(j)}).$$

Indeterminism due to degeneracies

The energy function we would like to consider is the same as in Ising models with no external field:

$$H(S, J) = - \sum_{j=\{i_1, i_2\} \in E} J_j S_{i_1} S_{i_2}. \quad (2.1)$$

That condition 2.1.4 does not hold for this energy function can be seen in Fig. 2.3. From state number 4, two states (5.a and 5.b) with the same energy are accessible by a single spin flip and they both decrease the energy by the same amount. The solution that lifts degeneracies like this is making a choice for one possible spin flip in every alike situation beforehand. This can be realized by slightly modifying the energy function such that it becomes “disordered”.

2.2 Quenched disorder

In this section, we construct energy functions that are slight modifications of equation 2.1, such that no degeneracies occur. That is, for these new energy functions condition 2.1.4 holds.

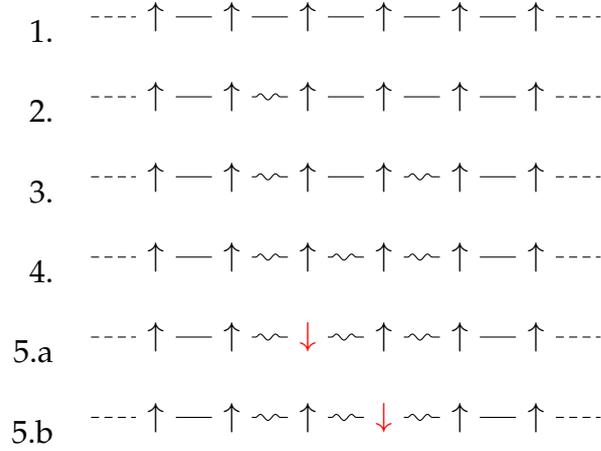


Figure 2.3: A sequence of states 1. \rightarrow 2. \rightarrow 3. \rightarrow 4. of a spin chain with $n \geq 6$ that leads to an indeterminate state. 4. is not in equilibrium. 5.a and 5.b are two possibilities to lower the energy. The arrows indicate the spin values ($\uparrow = +1, \downarrow = -1$). Straight/wavy connections mean positive/negative coupling.

The idea is to choose an order of importance of interactions. More important interactions will be satisfied first. We do this by slightly modifying the interaction values by some small *quenching constants* $\theta_j \ll 1$. This shifts the energy level of each state by a small amount. If multiple spin flips would lower the energy by the same amount originally, now one of the possibilities lowers the energy most and can thus be chosen as the successor spin state.

Theorem 2.2.1. For any connected simple finite graph $G = (V, E)$ with $\#V > 2$, $\#E = m$ and $\varepsilon < \frac{1}{2m}$, fix any quenching constants $\theta \in (0, \varepsilon)^E$ such that

$$\forall a \in \{-1, 0, 1\}^E : \sum_{j \in E} a_j \theta_j = 0 \Rightarrow a = 0. \quad (2.2)$$

Let $\Omega(H_\theta)$ be the set of equilibrium states of the energy function

$$H_\theta(S, J) = - \sum_{j=\{i_1, i_2\} \in E} J_j (1 + \theta_j) S_{i_1} S_{i_2}. \quad (2.3)$$

Then condition 2.1.4 holds.

Proof. For any edge $j \in E$ we need to show that for all states $(S, J) \in \Omega$, the energy $H_\theta(\cdot, J^{(j)})$ has an unique minimum on

$$A = \{\tilde{S} \in \Omega_V : \|\tilde{S} - S\|_1 = 2\}.$$

Then, because there are only finitely many states and the energy is lowered strictly in every step of the sequence in $S = S_1, S_2, \dots$, the sequence terminates for some $n \in \mathbb{N}$ and we have $(S_n, J^{(j)}) \in \Omega(H_\theta)$ because a local minimum has been reached.

Assume that $H(\cdot, J^{(j)})$ has two different minima $S^1, S^2 \in A$. As these spin states are nonequal, they differ on exactly two distinct vertices $x, y \in V$. Since the states have equal energy, we can calculate:

$$\begin{aligned} 0 &= H(S^1, J^{(j)}) - H(S^2, J^{(j)}) \\ &= \sum_{e=\{i_1, i_2\} \in E} \left(J_e^{(j)} (1 + \theta_e) S_{i_1}^1 S_{i_2}^1 - J_e^{(j)} (1 + \theta_e) S_{i_1}^2 S_{i_2}^2 \right) \\ &= \underbrace{\sum_{e=\{i_1, i_2\} \in E} J_e^{(j)} (S_{i_1}^1 S_{i_2}^1 - S_{i_1}^2 S_{i_2}^2)}_{\in \mathbb{Z}} + \underbrace{\sum_{e=\{i_1, i_2\} \in E} J_e^{(j)} \theta_e (S_{i_1}^1 S_{i_2}^1 - S_{i_1}^2 S_{i_2}^2)}_{\in (-2m\varepsilon, 2m\varepsilon)} \end{aligned}$$

Because $2m\varepsilon < 1$, these sums are both zero on their own. The second sum being zero is equivalent to a finite sum over the components of θ with coefficients in $\{-2, 0, 2\}$ being 0. From the independence condition of the coordinates of θ it follows that all coefficients must be 0. We assumed that $n > 2$ and G is connected, thus there is a $z \neq x, y$ such that either $\{x, z\} \in E$ or $\{y, z\} \in E$. The summand on that edge being zero implies that $S_x^1 = S_x^2$ or $S_y^1 = S_y^2$ respectively, because $S_z^1 = S_z^2$. Finally, this contradiction proves that the minimum of $H_\theta(\cdot, J^{(j)})$ over A is unique. \square

Conclusion

Fixing quenching constants allows to lift all degeneracies while keeping the central idea, that positive interactions align spins and negative interactions lead to misalignment, intact. Also, the condition 2.2 is easily realizable by randomly choosing the quenching constants, making it suitable for computer simulations.

Therefore, for the rest of this thesis, all spin systems will be defined with quenched disorder.

2.3 Homomorphisms of spin sub-systems

Sometimes it is useful to consider sequences which only consist of interactions on a subset of edges. For example, they might be especially interesting in some way or it is just not possible to comprehend the full spin system. In these situations, we need the notion of a spin sub-system.

Definition 2.3.1. Given a spin system $\mathbb{F}(H_\theta)$ on $G = (V, E)$ and a subset of edges, $\bar{E} \subset E$, we call the subsemigroup

$$\mathbb{F}(H_\theta, \bar{E}) := \langle F_j : j \in \bar{E} \rangle \subset \mathbb{F}(H_\theta)$$

generated by $F(\bar{E})$ a **spin sub-system** of $\mathbb{F}(H_\theta)$. Note that $\mathbb{F}(H_\theta) = \mathbb{F}(H_\theta, E)$, thus a spin system is a sub-system of itself.

Next, we will need a rigorous definition of whether two given spin (sub)-systems are “equal”. First we define structure preserving maps between spin sub-systems. Naturally, this also gives us the definition of an isomorphism of spin (sub)-systems.

Definition 2.3.2. Let $\mathbb{F}(H_{\theta^1}) = \langle \text{im } F^1 \rangle$ and $\mathbb{F}(H_{\theta^2}) = \langle \text{im } F^2 \rangle$ be spin systems on $G^1 = (V^1, E^1)$ and $G^2 = (V^2, E^2)$ generated by the images of F^1 and F^2 respectively. Also fix subsets of edges $\bar{E}^1 \subset E^1$ and $\bar{E}^2 \subset E^2$.

Given a map $\bar{\varphi} : \bar{E}^1 \rightarrow \bar{E}^2$, such that the map

$$\varphi : \mathbb{F}(H_{\theta^1}, \bar{E}^1) \rightarrow \mathbb{F}(H_{\theta^2}, \bar{E}^2)$$

defined by $F_j^1 \mapsto F_{\bar{\varphi}(j)}^2$ for all $j \in \bar{E}^1$ is a semigroup homomorphism, we call φ a **homomorphism of spin sub-systems**.

In the following, we take a first step towards identifying isomorphic spin systems. For example, it is intuitive that the effects of actuations on systems whose quenching constants are related by a symmetry of the graph should be equal, provided we actuate on corresponding edges.

Definition 2.3.3. The symmetry group of a graph $G = (V, E)$ is the subgroup

$$\text{Aut}(G) = \{ \sigma \in S(V) : \{v_1, v_2\} \in E \Leftrightarrow \{\sigma v_1, \sigma v_2\} \in E \}$$

of the symmetric group on its vertices, that preserves adjacency. $\text{Aut}(G)$ also acts on E by $\sigma\{v_1, v_2\} := \{\sigma v_1, \sigma v_2\}$.

It will be useful to make this idea precise in the following lemma.

Lemma 2.3.4. For a spin system $\mathbb{F}(H_\theta) = \langle \text{im } F \rangle$ on $G = (V, E)$ and a graph symmetry $\sigma \in \text{Aut}(G)$, we have

$$\mathbb{F}(H_\theta) \cong \mathbb{F}(H_{\theta \circ \sigma^{-1}}).$$

That is, permuting the quenching constants along a graph symmetry does not change the spin system.

Proof. $\text{Aut}(G)$ acts on Ω by $\sigma(S, J) := (S \circ \sigma^{-1}, J \circ \sigma^{-1})$. The equilibrium states of the new energy function are

$$\Omega(H_{\theta \circ \sigma^{-1}}) = \{\sigma(S, J) : (S, J) \in \Omega(H_\theta)\}.$$

The map $F' : E \rightarrow \text{Hom}(\Omega(H_{\theta \circ \sigma^{-1}}), \Omega(H_{\theta \circ \sigma^{-1}}))$ whose image generates $\mathbb{F}(H_{\theta \circ \sigma^{-1}})$ is given by

$$F'_j(S, J) = \sigma F_{\sigma^{-1}j}(\sigma^{-1}(S, J))$$

for any $j \in E$ and $(S, J) \in \Omega(H_{\theta \circ \sigma^{-1}})$. Now graph symmetry $\sigma : E \rightarrow E$ induces an isomorphism of spin systems

$$\begin{aligned} \varphi : \mathbb{F}(H_\theta) &\rightarrow \mathbb{F}(H_{\theta \circ \sigma^{-1}}) \\ F_j &\mapsto F'_{\sigma j} \end{aligned}$$

because $F'_{\sigma j} = \sigma F_j \sigma^{-1}$. □

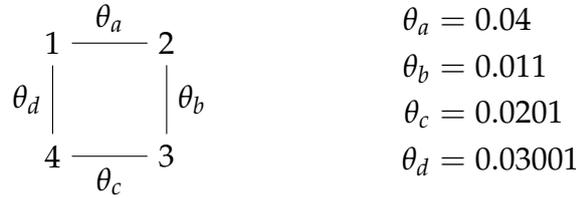
2.4 Dependence on quenched disorder

To provide a more concrete understanding of how our spin systems behave, in this section, we give some detailed examples of actuations on a cycle of 4 spins. The only distinction between our systems, figures 2.4a and 2.5a, is that the quenching constants are chosen differently. Starting from the same initial state, we will see that first actuating at a and then at b has a different effect on the systems.

First, we examine figure 2.4b more closely. The system starts with all interactions positive and all spins up. Then we actuate at the edge a , which firstly changes the sign of the interaction at a . Now, flipping the spin at 1 or 2 would lower the energy. Because $\theta_a > \theta_d > \theta_b$, slightly more energy is gained by flipping the spin at vertex 2 down. After that, the system is in equilibrium, which concludes the first actuation. Next, we actuate at b . Changing the sign of the interaction at b lowers the energy. Afterwards, the system is already in a equilibrium state. Thus the second actuation does not affect the spin state.

This reasoning already suggests that the result of an actuation depends on the quenching constants. To verify this, the constants θ' in figure 2.5 are chosen differently from those in figure 2.4. Indeed, in 2.5b, we do observe that the actuation at a yields a different result, even though the system is starting from same initial state as 2.4b. That is because a still has the

(a)



(b)

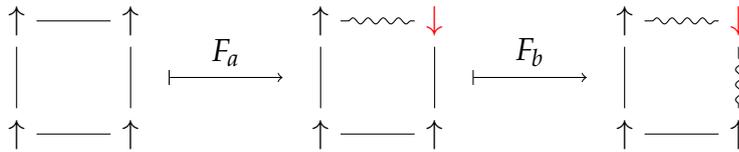
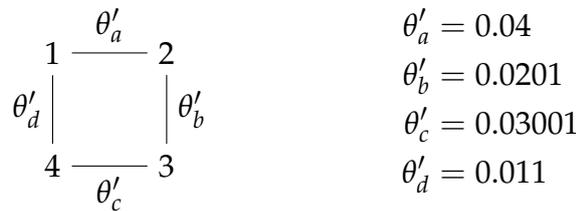
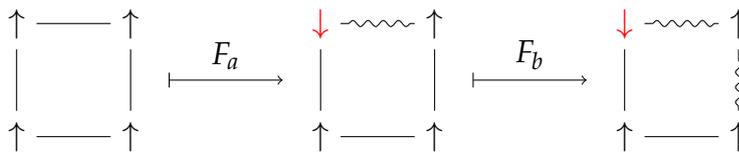


Figure 2.4: Concrete example of a deterministic dynamical spin system on a cycle of 4 vertices. **(a)** Explicit assignment of the quenching constants. **(b)** Demonstration of applying actuations to an initial state state with all interactions positive and all spins up.

(a)



(b)



(c)

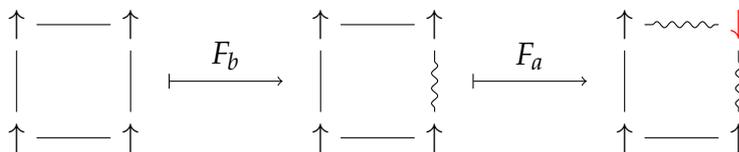


Figure 2.5: Another example of a spin system on a 4-cycle with different quenching constants than in figure 2.4. In **(b)** and **(c)**, the same initial state is actuated on the edges a and b , but in different order. Notice that changing the order changes the final state.

highest quenching constant, but now $\theta'_c < \theta'_b$. Thus, flipping the spin at 1 brings the system to an equilibrium with slightly lower energy.

The second actuation in 2.5b, at b , increases the energy, but because $\theta'_a, \theta'_c > \theta'_b$ we can flip neither the spin at 2 nor at 3. Thus the system ends in an equilibrium with quite high energy.

The conclusion is that the spin system indeed depends on the choice of quenching constants. We will start exploring how this dependence works in chapter 3. Understanding this creates the possibility of fine-tuning the quenching constants to make the spin system behave as desired. In the context of the two types of programmability of metamaterials discussed in section 1.1, fine-tuning the quenching constants would be of type I. That is, during the design process, we fix some properties (the quenching constants) to values, which result in the desired behaviour of the system. In the case of deterministic spin systems, there still is type II programmability after fixing the quenching constants, because the state can be reconfigured using local actuations.

2.5 Noncommutativity

We have not yet addressed whether the order of a sequence of actuations applied to a particular state matters, that is, whether $\mathbb{F}(H_\theta)$ is commutative. In general, spin systems are not commutative. To illustrate this, we turn to the sequences of states in 2.5b and 2.5c. Both sequences start in the same initial state and are subsequently actuated on a and b , but in different order.

In 2.5c, we first actuate at b . Because $\theta'_a, \theta'_c > \theta'_b$, the spin state is not changed. The second actuation, at a , forces the spin at 2 down and then the system is in equilibrium.

Comparing 2.5b and 2.5c, the key observation is that final state depends on the order in which the edges are actuated. Therefore the spin system $\mathbb{F}(H_{\theta'})$ is noncommutative.

In section 3.1 we will see that our first example, figure 2.4, is a commutative spin system. Showing that requires more effort, because we need to check that, for all initial equilibrium states and any two single actuations, the final state does not depend on the order, in which the actuations are applied.

As motivated in section 1.1, it is desirable that spin systems can be noncommutative. Because we have examples of commutative as well as noncommutative spin systems, we are able to study the relation between (non-)commutativity of local actuations and the complexity of a system.

Characterization of small systems

3.1 State transition diagrams

At the end of chapter 2, we have seen examples of actuations being applied to one particular initial state. However, because we want to fully characterize the system, that is, know the effects of actuations on arbitrary equilibrium states, we defined a single actuation or a sequence of actuations $F \in \mathbb{F}(H_\theta)$ as a function $F : \Omega(H_\theta) \rightarrow \Omega(H_\theta)$.

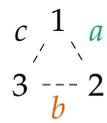
For specific examples with a small number of edges, the equilibrium states and the single actuations $F_j : \Omega(H_\theta) \rightarrow \Omega(H_\theta)$ can be computed quickly using computer algebra, but they are hard to present in a comprehensive manner. In this section, we demonstrate the structure of two actuations applied to arbitrary equilibrium states of cycles with 3 and 4 vertices. For the 4-cycle, we come back to the systems in figures 2.4a and 2.5a. But let us first consider the 3-cycle to illustrate the method.

The 3-cycle

In figure 3.1b, a table of the entire state space of a 3-cycle is shown and the equilibrium states are marked with dots. By following the arrows between the equilibrium states, we can trace the effect of actuations. The color of the arrow indicates on which edge the actuation happens. Note that we confine ourselves to two actuations, F_a and F_b , to keep the figure comprehensible. Adding the actuation on c would turn the 4 separate squares into 2 disconnected cubes.

There are two things that can be deduced from this diagram. For one thing, the actuations a and b commute. That is, no matter in which order we trace the arrows of F_a and F_b , for any initial equilibrium state, the final

(a)



$$\begin{aligned}\theta_a &= 0.03 \\ \theta_b &= 0.011 \\ \theta_c &= 0.0201\end{aligned}$$

(b)

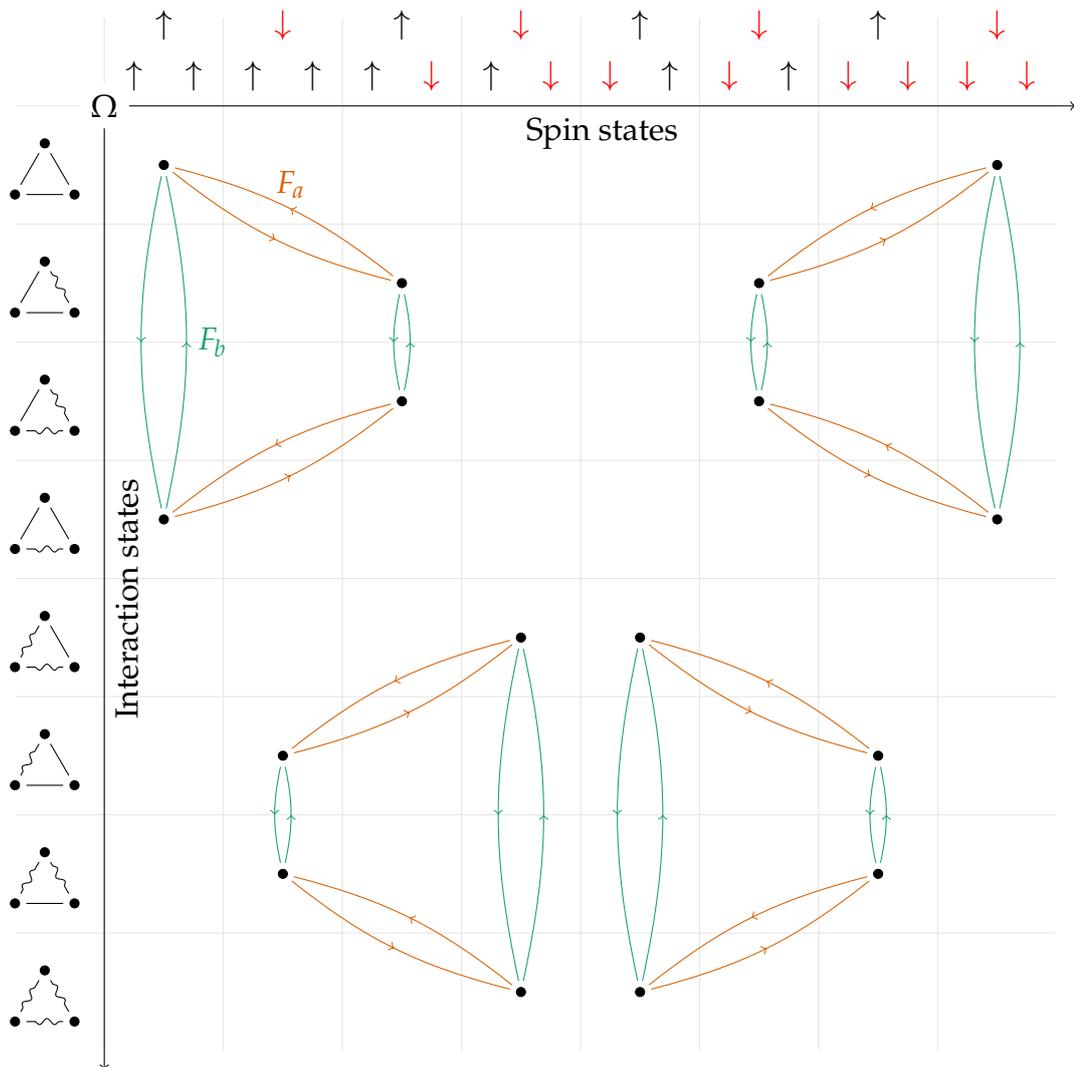


Figure 3.1: (a) A 3-cycle with given quenching constants. (b) Table of spin states (horizontally) and interaction states (vertically). The equilibrium states are marked with dots. The arrows represent the transitions between equilibrium states given by the actuations on edges a and b .

state of the system is the same. For another, applying the same actuation twice brings the system back to its initial state.

Algebraically, this means that F_a and F_b have order 2. In particular, they are invertible and generate a commutative subgroup $\langle F_a, F_b \rangle \subset \mathbb{F}(H_\theta)$ of the spin system, which is group-isomorphic to $(\mathbb{Z}/2\mathbb{Z})^2$. If we had also included F_c , it would be clear that F_c commutes with both F_a and F_b and also is its own inverse. But then $\langle F_a, F_b, F_c \rangle = \mathbb{F}(H_\theta)$ is the entire spin system. The conclusion is that this particular spin system has a group structure isomorphic to $(\mathbb{Z}/2\mathbb{Z})^3$.

The 4-cycle

Next, we consider the same type of table for a 4-cycle. In figure 3.2 we see that with the right choice of quenching constants (the same as in figure 2.4) we get equilibrium states and transitions similar to our 3-cycle. That is, repeated actuation brings back the initial state and the actuations commute. Also, it is computationally verifiable that, involving all 4 actuations, the spin system is commutative and group-isomorphic to $(\mathbb{Z}/2\mathbb{Z})^4$.

The noncommutative case, which we already encountered in figure 2.5, is shown in figure 3.3. The difference with figure 3.2 is apparent. Firstly, the number of equilibrium states is twice as high. Next, we observe that there are initial states, for which repeatedly actuating at a does not bring the system back to the initial state. Furthermore, we can clearly see that the spin system is noncommutative. Consider the magnification of the upper left corner of the table 3.3b in figure 3.4. The emphasized actuation sequences $F_b F_a$ and $F_a F_b$ acting on the initial states with all interactions positive and all spins up, as already considered in 2.5b and 2.5c, clearly have different endpoints.

Conclusion

State transition diagrams can help to fully understand the dynamics of a spin (sub-)system. The high degree of symmetry allows to focus on smaller parts of the table. Using the diagrams, we can easily tell whether actuations commute or are invertible. The downside of these diagrams is that their size increases exponentially with the size of the underlying graph. Therefore we need other methods to characterize larger systems.

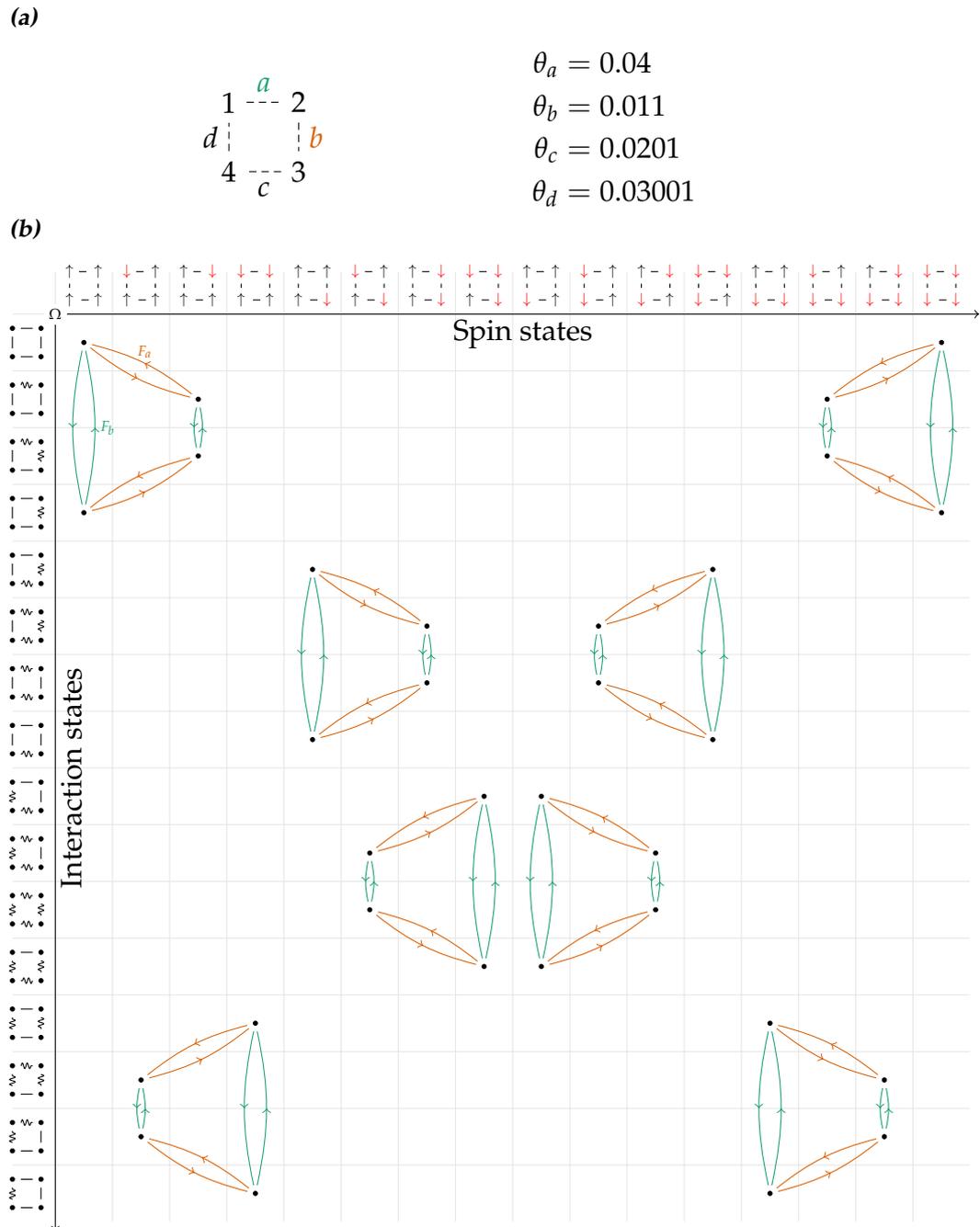
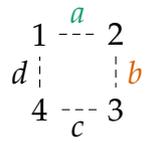


Figure 3.2: (a) A 4-cycle with quenching constants as in figure 2.4. (b) Table of spin states (horizontally) and interaction states (vertically). The equilibrium states are marked with dots. The arrows represent the transitions between equilibrium states given by the actuations on edges a and b .

(a)



$$\begin{aligned} \theta'_a &= 0.04 \\ \theta'_b &= 0.0201 \\ \theta'_c &= 0.03001 \\ \theta'_d &= 0.011 \end{aligned}$$

(b)

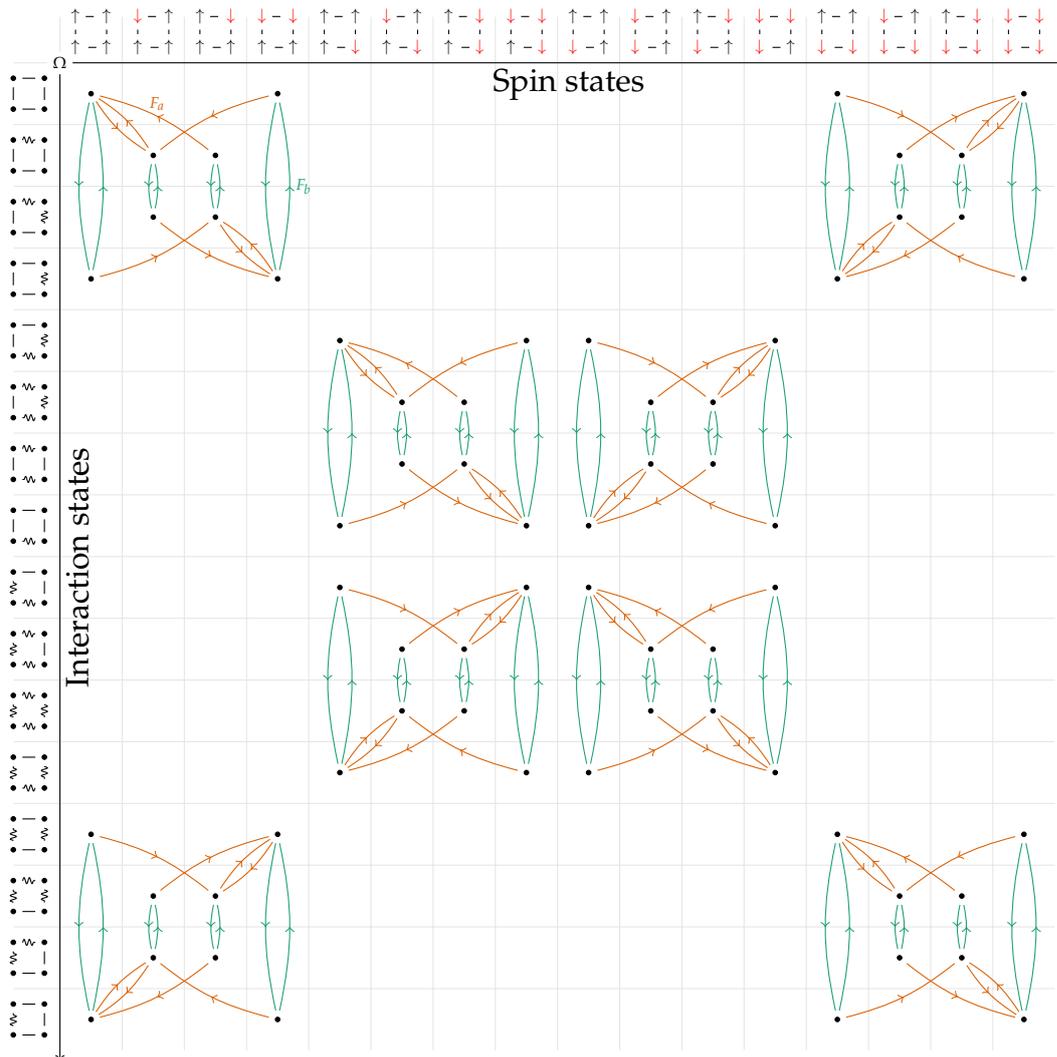


Figure 3.3: (a) A 4-cycle with quenching constants as in figure 2.5. (b) Table of spin states (horizontally) and interaction states (vertically). The equilibrium states are marked with dots. The arrows represent the transitions between equilibrium states given by the actuations on edges a and b .

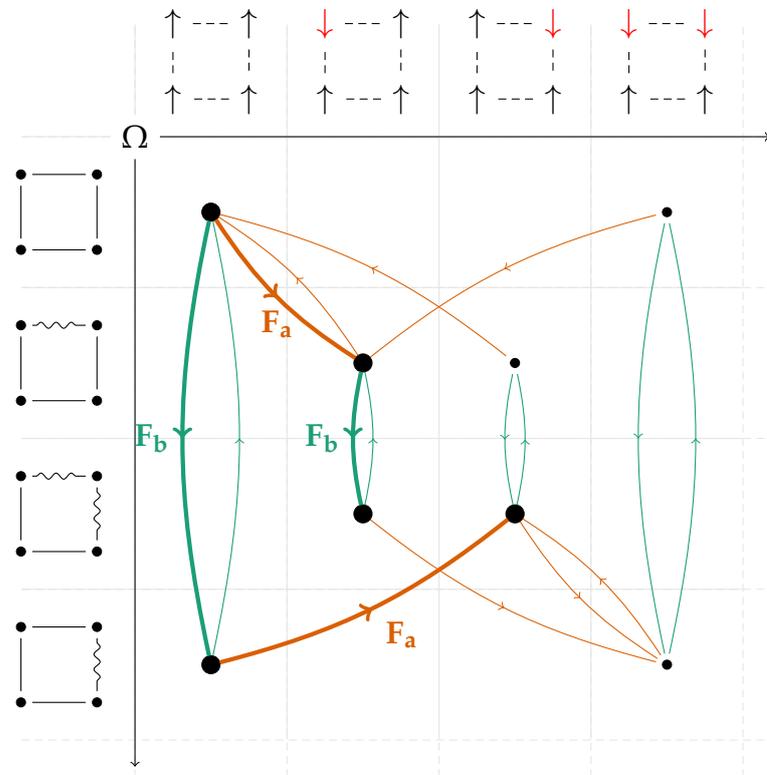


Figure 3.4: Magnification of the upper left part of figure 3.3. The sequences of actuations $F_b F_a$ and $F_a F_b$ acting on the equilibrium state with all interactions positive and all spins up are emphasized to show that they have different endpoints and thus actuation on a and b does not commute.

3.2 Small cycle graphs

In this section we determine all spin systems on cycle graphs with $3 \leq n \leq 6$ edges that quenched disorder can give. Our approach uses the following result.

Theorem 3.2.1. *On a cycle graph $C_n = (V, E)$, a spin system $\mathbb{F}(H_\theta)$ only depends on the linear ordering of the quenching constants θ .*

The proof of this proposition will be much easier after we have discussed frustrations in section 4, so we delay it until section 4.2. The theorem implies that we can use permutations of a single quenching constant to find all possible spin systems on a cycle graph. The problem can be simplified further only considering a set of permutations which is not related by graph symmetries.

n	$\frac{1}{2}(n-1)!$	$\#\mathbb{F}(H_\theta)$	$\#\Omega(H_\theta)$	commutative	$\#\{F_j \text{ invertible}\}$
3	1	8	16	yes	3
4	3	16	32	yes	4
		132	64	no	2
5	12	32	64	yes	5
		80	128	no	4
		264	128	no	3
6	60	64	128, 256	yes	6
		160	256	no	5
		160	256	no	5
		528	256	no	3
		1832	512	no	4

Figure 3.5: Exhaustive list of isomorphism classes of spin systems on cyclic graphs C_n for $3 \leq n \leq 6$. Each row corresponds to an isomorphism class. The columns give additional information about spin systems in the classes. The color indicates that a spin system is isomorphic to a spin sub-system of a larger spin system with the same color. All computations have been performed using SageMath [10].

On a cycle graph $C_n = (V, E)$, fix arbitrary initial quenching constants θ . The permutations of the quenching constants are given by $\theta \circ \sigma$ for $\sigma \in S(E)$, thus these $\theta \circ \sigma$ give all possible spin systems on C_n . We view the action of $\text{Aut}(G)$ on E in definition 2.3.3 as a group homomorphism $\varphi_n : \text{Aut}(C_n) \rightarrow S(E)$. By lemma 2.3.4, the spin systems with $\theta \circ \sigma$ are the same on right cosets $S(E)/\text{im } \varphi_n$. Therefore the aim of finding all spin systems on C_n can be reduced to computing those resulting from representatives of the cosets.

For C_n we know that the symmetry group on the edges $\text{im } \varphi_n \cong D_n$ is a dihedral group on the n edges. Note that the number of cosets, which is given by the index

$$[S(E) : D_n] = \frac{\#S(E)}{\#D_n} = \frac{n!}{2n} = \frac{1}{2}(n-1)!$$

of the dihedral group in the symmetric group is an upper bound for the number of spin systems on C_n .

For $3 \leq n \leq 6$, figure 3.5 shows the results of a computational approach to this. The rows correspond to equivalence classes of spin systems each

listing properties of the class. The following columns need additional explanation:

- $\#\mathbb{F}(H_\theta)$ is the order of the semigroup. This can be interpreted as the number of sequences of actuations for which there is no shorter sequence that has the same effect of the spin system. Therefore it is a measure for the complexity of the system.
- $\#\Omega(H_\theta)$ is the number of equilibrium states for this class of spin systems. Note that a spin system in the first isomorphism class of C_6 can have 128 or 256 equilibrium states.
- $\#\{F_j \text{ invertible}\}$ is the number of single actuations that are invertible, which are those F_j such that there is some $F \in \mathbb{F}$ such that $F \circ F_j = F_j \circ F = \text{id}_{\Omega(H_\theta)}$.

For a 3-cycle, the action of $\text{Aut}(C_3)$ on the edges $\{a, b, c\}$ given by $\varphi_3 : \text{Aut}(C_3) \rightarrow S(\{a, b, c\})$ is an isomorphism. Thus all permutations of the initial quenching constant are related by a graph symmetry. That is why we find only one isomorphism class in figure 3.5. Furthermore, the example discussed in section 3.1, figure 3.1 is the only spin system on C_3 up to isomorphism.

In section 3.1 we also found two different spin systems on C_4 : The commutative and the noncommutative case. Because $\#(S(E)/\text{im } \varphi_4) = 3$, one might wonder whether there is a third case. Figure 3.5 shows that there is not. Two of the cosets give isomorphic spin systems. Therefore we have studied all spin systems on 4-cycles through the examples in section 3.1.

Although the upper bound $\frac{1}{2}(n-1)!$ clearly is not very good, generally, we observe that with increasing cycle length more isomorphism classes of spin systems emerge. It is remarkable that, for increasing cycle length, classes of spin systems of smaller cycles reappear in a certain way. For instance, every cycle graph displayed here admits a commutative spin system.

To explain that in more detail, we first turn our attention to invertible actuations. For a spin system $\mathbb{F}(H_\theta) = \langle \text{im } F \rangle$ on $G = (V, E)$ define

$$\bar{E}(H_\theta) = \{j \in E : F_j \text{ is invertible}\}.$$

Clearly, the sub-system $\mathbb{F}(H_\theta, \bar{E}(H_\theta))$ carries a group structure. It can also be computed that for all spin systems in 3.5 the invertible single actuations are their own inverses. Therefore these spin sub-systems are group-isomorphic to $(\mathbb{Z}/2\mathbb{Z})^{\#\bar{E}(H_\theta)}$. In general, this is not true. In section 3.3 we

will see an example of a spin system on a different kind of graph whose invertible single actuations generate a noncommutative spin sub-system.

In our small cycle graphs, invertible actuations are not the interesting part of the spin system. Because an invertible actuation commutes with all the other actuations, the effect of a sequence of actuations depends only on the parity of the number of its appearances. Therefore we will now compare spin sub-systems $\mathbb{F}(H_\theta, E \setminus \bar{E}(H_\theta))$ generated by noninvertible single actuations. Computations have shown that, in addition to the commutative cases, these sub-systems are isomorphic for spin systems on cycle graphs in isomorphism classes marked with the same color in figure 3.5.

Given the small number of cycle graphs shown in the table, it can only be conjectured that they are introduced for some n and then reappear for increasing cycle size. The motivation for this is that we can add a new edge to the cycle by fitting it between two other edges and giving it a quenching constant bounded by those of its neighbours.

3.3 Invertible noncommutative actuations

In section 3.2 we found some spin sub-systems on cycle graphs that have a group structure, because all actuations are invertible. The fact that they are all commutative raises the question whether all spin sub-systems generated by invertible single actuations are commutative. In the following, we consider an example which shows that this is not the case.

Consider the graph in figure 3.6 with the given quenching constants. From the state transition diagram, which extends over the complete state space by tiling, we read that the single actuations F_b and F_e are both their own inverses, but they do not commute. Instead we have

$$F_e F_b = (F_b F_e)^3 = (F_b F_e)^{-1}.$$

In fact, the spin sub-system $\mathbb{F}(H_\theta, \{b, e\})$ is group-isomorphic to a dihedral group (the symmetry group of a square).

For the context of mechanical metamaterials, this means that if one wants to design a material with invertible actuations, it should not be necessary to give up on the advantages of noncommutativity discussed in section 1.1.

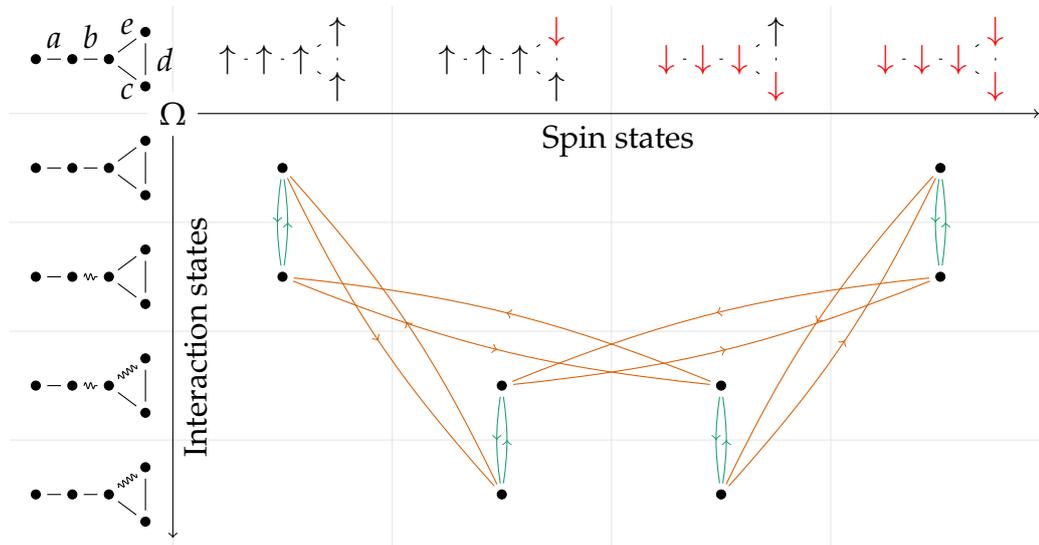


Figure 3.6: Example of a spin sub-system with invertible single actuations that is noncommutative. The quenching constants are $\theta_a = 0.002204$, $\theta_b = 0.001527$, $\theta_c = 0.004364$, $\theta_d = 0.009173$ and $\theta_e = 0.003370$. Only part of the state space is shown, but it is representative for the rest.

3.4 Spin systems on 4-edged graphs

Generally, for a graph $G = (V, E)$ that we can define a spin system on, theorem 3.2.1 does not apply. Therefore we would like to have other methods of classifying spin systems on other graphs than cycle graphs. The independence condition in theorem 2.2.1 suggests that, given quenching constants θ , inequalities of the form

$$\sum_{j \in E} a_j \theta_j > 0 \quad (3.1)$$

with $a \in \{-1, 0, 1\}^E$ should determine the isomorphism class of a spin system $\mathbb{F}(H_\theta)$.

In this section we attempt to visualize this relation for graphs with 4 edges. To do so we will make use of degrees of freedom in the choice of the quenching constant, that do not change the spin system. Namely, scalar multiplication $\theta_j \mapsto \alpha \theta_j$ and shifting all quenching constants equally $\theta_j \mapsto \theta_j + \beta$.

General invariances

The first results in this section hold for any graph $G = (V, E)$, that we can define a spin system on. For every choice of quenching constants

$$\theta \in \Theta := (0, \varepsilon)^E \setminus \left\{ \theta : \exists a \in \{-1, 0, 1\}^E : \sum_{j \in E} a_j \theta_j = 0 \right\},$$

with $\varepsilon < \frac{1}{2m}$, we have defined the spin system $\mathbb{F}(H_\theta)$. Define an equivalence relation \sim on Θ such that

$$\theta_1 \sim \theta_2 \Leftrightarrow \mathbb{F}(H_{\theta_1}) \cong \mathbb{F}(H_{\theta_2}).$$

That is, two quenching constants are equivalent if there exists an isomorphism of spin systems, as in definition 2.3.2, between the spin systems they induce.

We are interested in the number and geometry of the equivalence classes. The following theorem gives two sufficient conditions for equivalence.

Theorem 3.4.1. *Let $\theta^1, \theta^2 \in \Theta$ be quenching constants. Either of the following two properties implies $\theta^1 \sim \theta^2$.*

$$\exists \alpha \in \mathbb{R} : \theta^2 = \alpha \theta^1 \tag{3.2}$$

$$\exists \beta \in \mathbb{R} : \theta^2 = \theta^1 + (\beta, \dots, \beta) \tag{3.3}$$

Proof. For any state $(S, J) \in \Omega$, there exists a unique spin state $S' \in A$ such that

$$H_{\theta^1}(S', J) = \min_{\tilde{S} \in A} H_{\theta^1}(\tilde{S}, J)$$

where $A = \{\tilde{S} \in \Omega_V : \|\tilde{S} - S\|_1 = 2\}$. We claim that, assuming either property 3.2 or 3.3, (S', J) is also at the minimum over H_{θ^2} .

Our claim implies that $\Omega(H_{\theta^1}) = \Omega(H_{\theta^2})$. Next, the images of (S, J) under $F_j(H_{\theta^1})$ and $F_j(H_{\theta^2})$ for any $j \in E$ are determined by condition 2.1.4 by finding minima of the energy functions. These minima are equal, thus $F_j(H_{\theta^1})(S, J) = F_j(H_{\theta^2})(S, J)$. From that, we conclude $\mathbb{F}(H_{\theta^1}) = \mathbb{F}(H_{\theta^2})$. Now we proceed to prove the claim.

3.2 $\Rightarrow \theta^1 \sim \theta^2$

Without loss of generality, assume $0 < \alpha \leq 1$. Note that

$$\begin{aligned} H_{\theta^2}(S', J) &= \sum_{j=\{i_1, i_2\}} J_j(1 + \alpha\theta_j^1)S'_{i_1}S'_{i_2} \\ &= \underbrace{\sum_{j=\{i_1, i_2\}} J_jS'_{i_1}S'_{i_2}}_{\in \mathbb{Z}} + \underbrace{\sum_{j=\{i_1, i_2\}} J_j\alpha\theta_j^1S'_{i_1}S'_{i_2}}_{\in (-2m\epsilon\alpha, 2m\epsilon\alpha)}. \end{aligned}$$

As $2m\epsilon\alpha < 1$, for any other $S'' \in A$, to have $H_{\theta^2}(S'', J) < H_{\theta^2}(S', J)$, it needs to satisfy

$$\sum_{j=\{i_1, i_2\}} J_jS''_{i_1}S''_{i_2} < \sum_{j=\{i_1, i_2\}} J_jS'_{i_1}S'_{i_2}$$

or

$$\sum_{j=\{i_1, i_2\}} J_jS''_{i_1}S''_{i_2} = \sum_{j=\{i_1, i_2\}} J_jS'_{i_1}S'_{i_2} \text{ and } \sum_{j=\{i_1, i_2\}} J_j\alpha\theta_j^1S''_{i_1}S''_{i_2} < \sum_{j=\{i_1, i_2\}} J_j\alpha\theta_j^1S'_{i_1}S'_{i_2}$$

Both cases are a contradiction because they would imply $H_{\theta^1}(S'', J) < H_{\theta^1}(S', J)$. Consequently we indeed have that $H_{\theta^2}(S', J) = \min_{S \in A} H_{\theta^2}(S, J)$.

3.3 $\Rightarrow \theta^1 \sim \theta^2$

We may assume that $\beta \geq 0$. In this case we have

$$H_{\theta^2}(S', J) = \underbrace{(1 + \beta)}_{\geq 1} \underbrace{\sum_{j=\{i_1, i_2\}} J_jS'_{i_1}S'_{i_2}}_{\in \mathbb{Z}} + \underbrace{\sum_{j=\{i_1, i_2\}} J_j\theta_j^1S'_{i_1}S'_{i_2}}_{\in (-2m\epsilon, 2m\epsilon)}$$

Here we have $2m\epsilon < 1 + \beta$. Just like in the first case, if there were spin state $S'' \in A$, such that (S'', J) would make the energy lower under H_{θ^2} , that would lead to a contradiction, because it would also lower the energy under H_{θ^1} . Thus (S', J) is the minimum over H_{θ^2} . \square

4-edged graphs

Now we turn to graphs with exactly 4 edges, where Θ is a subset of \mathbb{R}^4 . Theorem 3.4.1 tells us that $\theta \mapsto \mathbb{F}(H_\theta)$ is invariant in at least two degrees of freedom. Thus it should be possible to map Θ into a 2-dimensional space without losing information. First we project into \mathbb{R}^3 by

$$p : (\theta_1, \theta_2, \theta_3, \theta_4) \mapsto \frac{1}{2} \begin{pmatrix} -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 \end{pmatrix} \cdot \begin{pmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \\ \theta_4 \end{pmatrix}$$

Because $\ker p = \langle (1, 1, 1, 1) \rangle$, the fibers satisfy 3.3, and we thus have

$$p(\theta^1) = p(\theta^2) \Rightarrow \theta^1 \sim \theta^2.$$

Note that p is a linear map, that is $p(\alpha\theta) = \alpha p(\theta)$. Hence the first property in theorem 3.4.1 allows us to normalize $p(\Theta)$, that is mapping $\Theta \rightarrow S^2$ without losing information. Concatenating stereographic projection yields a map

$$q : \Theta \rightarrow \mathbb{R}^2$$

respecting the equivalence \sim .

By associating each isomorphism class $[\mathbb{F}(H_\theta)]$ with a color, we make a geometric map of all possible spin systems. Sampling $\theta \in (0, \varepsilon)^4$ uniformly and computing the pair $(q(\theta), [\mathbb{F}(H_\theta)])$ gives a statistical approximation of this map.

Conclusion

The result of this method, applied to all possible simple connected graphs with 4 edges, is shown in figure 3.7.

Just like in section 3.2, we see that the 4-cycle has two classes of spin systems. This example also shows that regions where the quenching constants give the same spin system can be disconnected.

The maps also show projections of the hyperplanes defined by the independence condition in 2.2.1. As expected, these separate quenching constants correspond to different spin systems. This indeed suggests that the type of spin system is determined by the inequalities 3.1. While it is clear that there can only be a finite number of equivalence classes, this presumption would allow us to give an upper bound based on the number of connected components of Θ .

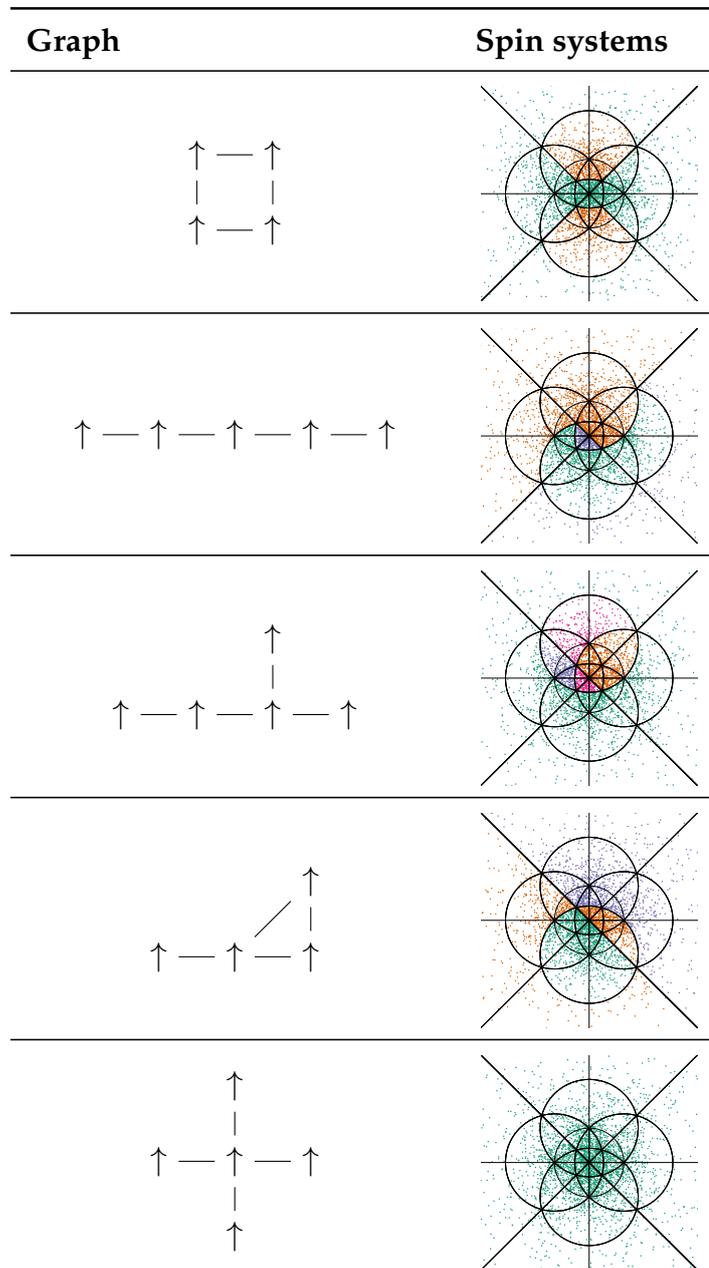


Figure 3.7: This figure lists all simple connected graphs with 4 edges. On the right, it shows approximations of 2-dimensional projections of the spaces that we can choose quenching constants from, where color indicates the isomorphism class of the spin system induced by a quenching constant. The black lines are projections of the hyperplanes given by the independence condition in theorem 2.2.1.

Frustrated edges

The time it takes to explicitly calculate spin systems increases exponentially with the size of the underlying graph, because first we need to determine which of the $2^{\#V} 2^{\#E}$ states are equilibrium states and then we still need to compute all images $F_j(S, J)$. Thus other characterizations of the system are needed for larger systems.

Definition 4.0.1. An edge $j = \{i_1, i_2\} \in E$ is *frustrated* if

$$-J_j S_{i_1} S_{i_2} > 0,$$

that is, if an edge with positive/negative interaction connects vertices with spins of opposite/equal sign.

In this chapter, we show that it is possible to understand the dynamics of spin systems on cycle graphs by studying the behaviour of frustrations.

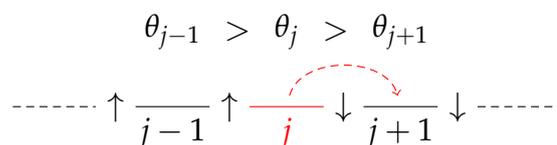


Figure 4.1: Part of a chain or cycle with a frustrated edge j . The state is not in equilibrium, because the energy can be lowered by flipping the spin at the vertex to the right of j . This is because θ is decreasing to the right. Notice that doing so will move the frustration from j to $j + 1$.

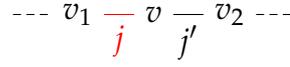


Figure 4.2: Sketching the setup in the proof of 4.1.2.

4.1 Frustrations as particles in 1-d systems

Locating the frustrated edges is useful, because their positions exhibit particle-like behaviour. In the situation of figure 4.1, j is frustrated but its neighbouring edges are not. Because $\theta_{j-1} > \theta_j > \theta_{j+1}$ the energy is lowered by flipping the spin of the right vertex of j . But then $j+1$ becomes frustrated. We can also formulate this as

“The *frustration* at j moves to $j+1$.”

by pretending the presence of a frustrated edge is a particle.

When this process moves one frustration next to another, the spin on the vertex shared by the neighbouring edges flips. That removes both frustrations. One might say, neighbouring frustrations *annihilate*. For equilibrium states, this implies a useful lemma.

Lemma 4.1.1. *In an equilibrium state $(S, J) \in \Omega(H_\theta)$ of a cycle graph, any pair of frustrated edges does not share a vertex.* \square

We have already observed that frustrations move towards lower values of θ . The following theorem shows that this is generally the case.

Theorem 4.1.2. *Let $\tilde{E} \subset E$ be the set of frustrated edges for the state $(S, J) \in \Omega$ of a cycle graph. Then the following are equivalent:*

1. (S, J) is an equilibrium state.
2. Every $j \in \tilde{E}$ is at a local minimum of θ .

Proof. First we prove 1. \Rightarrow 2. Suppose $(S, J) \in \Omega(H_\theta)$. Let any frustrated edge $j \in \tilde{E}$ and $j' \in E$ share the vertex v , where v_1 and v_2 are the other vertices of j and j' respectively, as shown in figure 4.2. We compare energies, knowing that (S, J) is in equilibrium:

$$\begin{aligned} 0 &> H(S, J) - H(S^{(v)}, J) \\ &= -J_j(1 + \theta_j)(S_{v_1}S_v - S_{v_1}^{(v)}S_v^{(v)}) - J_{j'}(1 + \theta_{j'})(S_{v_2}S_v - S_{v_2}^{(v)}S_v^{(v)}) \\ &= -J_j(1 + \theta_j) \cdot 2S_{v_1}S_v - J_{j'}(1 + \theta_{j'}) \cdot 2S_{v_2}S_v \end{aligned}$$

By lemma 4.1.1 j' is not frustrated, so

$$J_j S_{v_1} S_v = -J_{j'} S_{v_2} S_v.$$

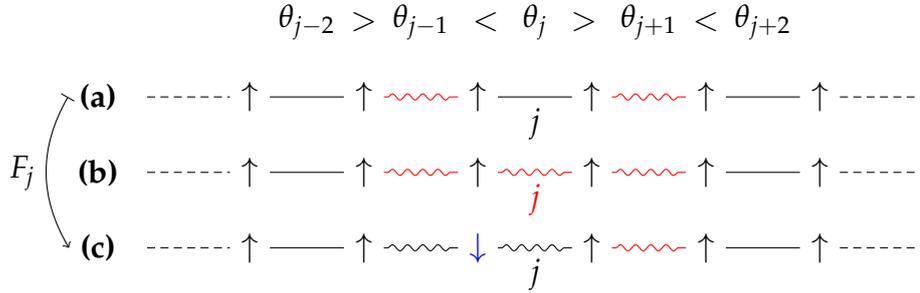


Figure 4.3: This sequence of states shows how a triplet of frustrations can appear and which pair annihilates given $\theta_{j-1} > \theta_{j+1}$. **(a)** In the initial state, there are frustrations at $j - 1$ and $j + 1$, which are local minima of θ . **(b)** Actuation at j creates a third frustration. **(c)** To minimize the energy, the spin at the vertex to the left of j flips. This annihilates the frustrations at $j - 1$ and j . The vertex to the left of j is chosen because $\theta_{j-1} > \theta_{j+1}$.

Therefore we have

$$\begin{aligned} -J_j(1 + \theta_j)S_{v_1}S_v + J_j(1 + \theta_{j'})S_{v_1}S_v &< 0 \\ -J_j\theta_jS_{v_1}S_v + J_j\theta_{j'}S_{v_1}S_v &< 0 \\ -J_jS_{v_1}S_v(\theta_j - \theta_{j'}) &< 0 \end{aligned}$$

Because j is frustrated, we conclude that $\theta_j < \theta_{j'}$.

Now we turn to 2. \Rightarrow 1. For any $v \in V$, we consider whether the energy is lowered by flipping the spin at v . This is clearly not the case if v has no incident frustrated edge. Also, by lemma 4.1.1, v can only have one incident frustrated edge. Suppose $v \in j \in \tilde{E}$ is a frustrated edge and $v \in j' \in E \setminus \tilde{E}$ is not frustrated (as in figure 4.2). Then flipping v lowers the energy only if $\theta_j > \theta_{j'}$. Yet, by the assumption, j is at a minimum of θ . Therefore it is not possible to lower the energy by flipping a single spin. This implies that (S, J) is in equilibrium. \square

While actuating a frustrated edge just removes the frustration, new frustrations are created by actuating on edges that are not frustrated. Let j be such an edge. There is a new way to explain the effect of the actuation F_j as sketched in figure 2.1:

- a. A frustration at j is created.
- b. The frustration moves until it annihilates with another frustration or it reaches a local minimum of θ .

For instance, this shows that only one frustration can move at a time. Also, there can only be one pair of neighbouring frustrations, because a first pair will already have annihilated before a second pair can be created by the movement of one frustration next to another one or the start of the next actuation. Of course, a pair immediately annihilates.

Furthermore, the only way to create a triplet of frustrations is shown in figure 4.3. A triplet is resolved as follows. The actuation at j first creates a sequence of 3 frustrations. The problem is that only one pair can annihilate and it only becomes clear which one does by comparing the disorder constant at $j - 1$ and $j + 1$. The new frustration will annihilate with the frustration at the edge with higher θ , as this will lower the energy more. Larger tuples of frustrations are not possible, because prior to their creation there would have to be more than one pair.

Conclusion

We conclude that, for the special case of cycle graphs, the locations of frustrated edges completely determine the spin dynamics by showing us which spins will be flipped in order to minimize the energy. It should be noted though, that we cannot completely reconstruct the state from the locations of frustrated edges alone, because for one we do not know the interaction state and if we did, every spin state has an opposite state with all spins pointing in the other direction, which has the same energy and frustrated edges.

Yet if we are, for example, only interested in the energy of a spin system, then tracking frustrations allows us to forget about the underlying spin state while keeping the dynamics well defined. Tracking frustrations can be interpreted as a simplification of the spin dynamics which depend on a rather complicated energy landscape to a system of particles following simple rules based on the quenching constants.

In the following section, we will see that frustrations can also be useful to obtain rigorous results in an efficient way.

4.2 Proof of theorem 3.2.1

Recall that in section 3.2 we used the following theorem to compute all spin systems on small cycles. Now that we know how to describe spin dynamics by tracking frustrations, we can apply it to the proof of this theorem.

Theorem 3.2.1. *On a cycle graph $C_n = (V, E)$, a spin system $\mathbb{F}(H_\theta)$ only depends on the linear ordering of the quenching constants θ .*

Proof. Suppose we started a single actuation on any edge from some equilibrium state and now we are minimizing the energy by single spin flips for some intermediate state. That is, we check for any vertex $v_1 \in V$ whether flipping this spin lowers the energy most.

We start by comparing incident frustrations. If there is another vertex with more incident frustrations, we do not flip the spin at v_1 . If v_1 has more incident frustrations than all other vertices, we flip at v_1 .

In the case there are other vertices with the same (maximal) number of incident frustrations, we need to compare quenching constants. Let v_2 be such a vertex. Depending on whether v_1 and v_2 are connected by an edge, we consider two cases. First, suppose they are connected by j :

$$\text{----} \cdot \frac{\text{---}}{j_1} v_1 \frac{\text{---}}{j} v_2 \frac{\text{---}}{j_2} \cdot \text{----}$$

Whether to flip the spin at v_1 depends entirely on the inequality $\theta_{j_1} > \theta_{j_2}$. If this inequality does not hold, we do not flip the spin at v_1 . If it holds, we still need to check for all other vertices with the same number of incoming frustrations, but v_1 is preferred over v_2 .

Secondly, we consider the following situation, where the middle unlabeled vertices may coincide:

$$\text{----} \cdot \text{---} v_1 \text{---} \cdot \text{----} \cdot \text{---} v_2 \text{---} \cdot \text{----}$$

The case that all four edges are frustrated does not occur, because we start the actuation from an equilibrium state, so, as explained before, there can never be more than one pair of frustrations.

The only option left is that v_1 and v_2 have one incident frustrated edge each. Because we started from an equilibrium state, where by theorem 4.1.2 all frustrations were at a local minimum, and we created at most one frustration that is not at a local minimum by flipping one interaction, we cannot have more than one frustration that is not at a local minimum of θ at the same time. Therefore at most one of the considered frustrations can move. Only if it is the frustration incident to v_1 and it would move across that vertex, we do not reject flipping the spin at v_1 .

We conclude that in all situations that can occur as an intermediate step it only depends on inequalities involving two quenching constants whether a spin $v_1 \in V$ will be flipped, that is, the linear ordering of quenching constants determines the spin system. \square

Conclusion and outlook

The purpose of this chapter is to summarize all results and relate them to the motivation in chapter 1. We also state some ideas for further exploration of the subject.

5.1 Conclusion

To define a deterministic spin system, we need a nondegenerate energy function. However, the typical energy function describing the interaction between Ising spins is degenerate. We have proved that quenched disorder can lift all degeneracies by only slightly modifying this energy function, preserving the idea that positive interactions align spins and negative interactions misalign them.

With the definition of a spin system as a semigroup generated by single actuations, we can rigorously compare the structure of spin (sub-)systems. If quenching constants are related by a graph symmetry, the spin systems are of the same type. However, in general, the spin system does depend on the choice of quenching constants.

We started by discussing two types of programmability of metamaterials (see section 1.1). Now we can relate this to our deterministic spin systems, which are programmable in both ways. Fine-tuning the quenching constants allows programmability of the type I, that is, in the design of the system. More importantly, local actuations provide type II programmability, because the state of a spin system can be reconfigured actively by locally actuating it.

It is remarkable that, depending on the quenched disorder, the effects of local actuations change. This means that we have type I programmabil-

ity setting the capabilities of type II programmability. This dependency is as significant as that the local actuations can be commutative or noncommutative, invertible or noninvertible depending on the quenching constants.

For small graphs, the dependence of properties of the spin system on quenched disorder is comprehensively visualized by state transition diagrams (section 3.1). For example, we have seen that a spin system on a 3-cycle is always commutative. Computations reveal that there are precisely two types of spin systems on a 4-cycle, the commutative and the noncommutative case. For larger cycles, the number of different spin systems increases. It looks like types of spin systems reappear as spin subsystems on larger cycles. This hypothesis is based on computations for $3 \leq n \leq 6$ in section 3.2.

In section 3.3, we have seen an example of a spin system that has invertible actuations, but is noncommutative. Therefore, for the design of metamaterials with invertible local actuations, it might still be possible to have noncommutative actuations. This can be considered positive, because invertible actuations are more predictable, while one can reach a larger part of the state space using noncommutative actuations. However, the computations in section 3.2 suggest that invertible actuations on a cycle graph do always commute.

From the geometrical map in section 3.4, which shows the relation between quenching constants and spin systems on graphs with 4 edges, it appears that quenching constants for different types of spin systems are separated by hyperplanes of the form $\sum_{j \in E} a_j \theta_j = 0$ for $a_j \in \{-1, 0, 1\}$. These also appear in the sufficient condition imposed on the independence of quenching constants, which ensures that all degeneracies are lifted. If some quenching constants lie on any of these hyperplanes, theorem 2.2.1 cannot guarantee that the spin system is well-defined.

Deterministic spin systems on cycles can be simplified by looking at frustrations. By tracking the position of frustrated edges, the spin system can be described by a few simple rules.

1. Frustrations move towards lower quenching constants.
2. If two frustrations meet, they immediately annihilate.
3. New frustrations are created by actuating unfrustrated edges.

This turns the complicated energy landscape into a system of frustrations obeying particle-like rules. While there is a lot more to be said about frustrations, this is a first step towards general statements about larger spin

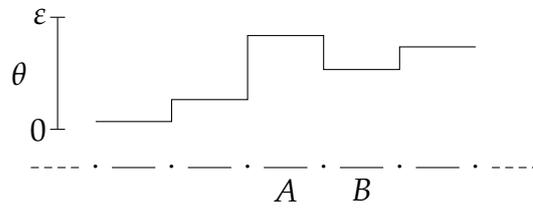


Figure 5.1: Part of a 1-dimensional spin system with noncommutative actuations on the edges A and B . The plot shows the relative quenching constants per edge.

systems without the explicit calculation of the effects of all actuations on all states.

5.2 Outlook

Reappearing spin systems on cycle graphs

Presumably, the most pressing open question of this thesis, as raised in section 3.2, is whether indeed every spin system on a cycle is isomorphic to a spin sub-system on any bigger cycle.

Also, we have observed that invertible actuations on small cycles commute, it would be interesting to know whether this holds for any size of cycle.

The class of a spin system is locally constant on Θ

From section 3.4 we learned that for 4-edged graphs, the spin systems given by quenching constants

$$\theta_1, \theta_2 \in \Theta = (0, \varepsilon)^E \setminus \left\{ \theta : \exists a \in \{-1, 0, 1\}^E : \sum_{j \in E} a_j \theta_j = 0 \right\}$$

are equal if θ_1 and θ_2 belong to the same connected components of Θ , which are separated by the aforementioned hyperplanes. In other words, under the identification $\theta \mapsto [\mathbb{F}(H_\theta)]$, the isomorphism class of the spin system is locally constant on Θ . It should be possible to prove this result in general.

Frustrations in 1-d

First, the results of section 4.1 on cycle graphs should also hold on 1-d chains. For that, consider the ends of the chain. Whenever an outermost

edge is frustrated, the frustration is immediately removed by flipping the outer spin, so frustrations just “fall off the edge”.

So far we have focused on working out the dynamics of specific situations using frustrations, but we have not yet found out how it is possible to tell whether two actuations are commutative based on frustrations. In figure 5.1 we see an example of quenching constants on a part of a 1-d system, where the actuations F_A and F_B do not commute. The situation is given by a local minimum of the quenching constant at B and a local maximum at A , such that the quenching constant to the left of A is even smaller than the minimum at B , further decreasing to the left.

Suppose we start in a state where no edge is frustrated. When we actuate at B , then we create a frustration that stays at the local minimum B . If we now actuate at A , the frustrations at A and B annihilate, so we are again in a state with no frustrations.

But if we start by first actuating at A , the new frustration will move to the left. Therefore if we now actuate at B , annihilation is not possible, because the first frustration has moved away. Thus the edge at B will stay frustrated.

So this is an example of a noncommutative 1-d system explained with frustrations, but is not clear yet whether there are other situations that induce noncommutative actuations.

Frustrations in 2-d

With the success of the application of frustrations to 1-d systems, the question arises whether they can be used to understand other geometries, for instance 2-d lattices.

First we make the following observation: For some vertex v with k incident edges, the spin at v will never flip when there are strictly more non-frustrated incident edges than frustrated ones. On the other hand, if there are more frustrated edges, the spin can flip.

If there is an equal number of frustrated and non-frustrated edges, it will depend on the quenching constants whether the spin at v will flip. If the sum of the quenching constants of the frustrated edges is higher than the sum of the quenching constants of the non-frustrated edges, the spin at v might flip. Of course, whether the spin actually flips depends on whether there are no other spin flips that can lower the energy more.

Note that with a spin flip the number of frustrations can never increase. If we flip the spin at v , all frustrated incident edges become non-frustrated and non-frustrated edges become frustrated.

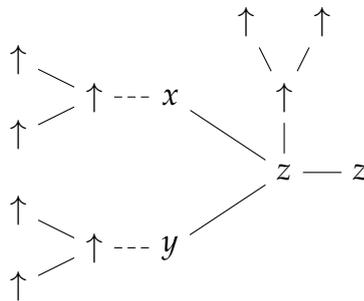


Figure 5.2: A spin system which implements an OR gate with two inputs attached. If $x = y = -1$ then also $z = -1$ because the disorder constants at $\{x, z\}$ and $\{y, z\}$ outweigh the influence of the other interactions. In any other case z will flip to 1 because of the upper attachment.

To start understanding spin systems on 2-d lattices, based in the quenching constants, one can mark at each vertex, which pairs of incident edges cause a spin flip when they are frustrated.

Logic gates in spin systems

Taking inspiration from [11], the following implementation of logic gates as spin systems has been found. Success could be interesting to explore the computational properties of metamaterials, as in [12].

First, consider a chain of positive interactions with decreasing quenching constant. When the leftmost spin is flipped, the spins to the right will sequentially assume the new position of their left neighbour. This way, a signal can propagate along a “wire”. A NOT gate can be realized by placing a negative interaction along the wire. Figure 5.2 shows the implementation of an OR gate.

With these two gates, any circuit could be built, if it were possible to split a signal into two signals. It appears that this is impossible, because there is a frustration moving along the wire and we can only create a new frustration by actuating the system. But splitting a signal would have to turn one moving frustration into two moving frustrations.

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