Metastability in the two-dimensional Ising Spin model subject to Glauber dynamics

Sharp bounds on the mean stable hitting time

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Contents

Introduction

A system in a finite volume and discrete state space and low temperature can be simplified to represent a Markov process with transition probabilities that depend on the increase (or decrease) of energy of the system.

A system is said to be in a metastable state when it remains in a state that is different from the state corresponding to the thermodynamic equilibrium, for a very long time. This state is a local minimum of the amount of energy, and the probability of escaping from this state and transition to the global minimum is small. Eventually the system reaches a critical amount of energy that makes the transition to the thermodynamic equilibrium possible. In a relatively short amount of time, the system reaches this equilibrium state, and it will stay there for a much longer time. An example are supercooled liquids that stay in the liquid state until a slight vibration causes it to freeze.

In this thesis, we study the two-dimensional Ising Spin model subject to Glauber dynamics in the low-temperature limit. The goal is to give sharp estimates on the expected hitting time of the stable configuration when the starting configuration is the metastable configuration. In this context, the metastable configuration is the configuration where, in each vertex of the two-dimensional grid, the spin is pointed downwards (it has a negative charge), in the opposite direction of the positive vectorfield, and is denoted by **-1**. The stable configuration is denoted by $\mathbf{+1}$ and is the configuration where all spins are aligned with the underlying vectorfield. Formal definitions for the Ising Spin model will be given in 1.3. The Glauber dynamics in this setting is a process that is defined as a Markov chain, a random walk on a connected graph $G(V, \mathcal{E})$ denoted by (X_t), where for each time step a vertex $v \in V$ is chosen is chosen uniformly at random, and the spin of v will change according to a probability that is dependent of the difference of the energy between the two configurations. The formal definitions of this dynamics will be given in section 1.2.

The main objects of interest to this thesis are the transition time from the metastable state to the stable state and the critical fluctuation the needed in order to perform the transition towards the equilibrium. The expected hitting time is estimated by using potential theory which reduces the analysis to a computation of Newtonian capacities. These capacities can be estimated in terms of properties of the energy landscape generated by the associated Hamiltonian in the limit of zero temperature.

There is considerable overlap between potential theory and the theory of the Laplace equation, and it is also greatly used in the theory of Markov chains. Since our system has a finite state space case, this connection can be formed by introducing an electrical network on the state space, with a resistance between vertices proportional to the inverse of the transition probabilities.

In section 1.1 some basic properties and definitions of a Markov processes will be presented. In sections 1.2 and 1.3, formal definitions for the model and the dynamics of the system studied in this thesis will be given. Since potential theory is the study of harmonic functions, definitions and some properties regarding these type of functions will be given in section 1.4.

Section 2 will associate the problem with a problem on an electrical network, starting by obtaining a formula for the equilibrium potential. Next, in section

2.2 a formula for the capacity will be derived that will be used in 2.4 for obtaining an exact formula for the mean hitting time.

In section 3.1 there will be given a formal definition of metastability, and in section 3.2 there will be some usefull definitions introduced on the energy landscape. These definitions will be used in sections 3.3 and 3.4 to reduce the problem of the estimation of the mean hitting time to a slightly easier one.

Next these results will be used to compute the specific results for the Ising spin model, subject to Glauber dynamics. First the metastable and stable states for this model will be defined in 4.1. The critical configuration will be identified in section 4.3. Next the capacity will be estimated, there will be given a lower and an upper bound in section 3.3, and these bound will be used in section 4.5 to give the main result of the paper, the sharp estimation of the mean hitting time of the stable state when starting in the metastable state.

Main theorem

The main theorem of this thesis is the following result.

Let $\Lambda \subset \mathbb{Z}^2$ be a finite set of sites, a square torus centered at the origin. Given an Ising spin model with finite state space $\Omega = \{-1, +1\}^\Lambda$, subject to Glauber dynamics, with the Hamiltonian H given by (1.2) and Gibbs measure μ associated with H given by (1.3). By the Glauber dynamics, with each $x \in \Lambda$ there is an associated spin value $\sigma(x) \in \{-1, +1\}$. Define a configuration $\sigma := \{\sigma(x) : x \in \Lambda\} \in \Omega$, and the transition probability between two configurations as (1.4). Let **-1** be the configuration where at each $x \in \Lambda$, $\sigma(x) = -1$ and **+1** be the configuration where at each $x \in \Lambda$, $\sigma(x) = +1$.

Theorem 0.1. ***(Main theorem)*** *For the expected time to reach the stable configuration* ***+1*** *when starting in the metastable configuration* ***-1****:*

$$\lim_{\beta \to \infty} e^{-\beta\Gamma} \mathbb{E}_{\boldsymbol{-1}}[\tau_{\boldsymbol{+1}}] = K \tag{0.1}$$

where K is given by:

$$\frac{3}{8(2l_c - 1)}$$

with Γ the energy of the critical droplet, and l_c the size of the critical droplet.

1 Basic notions

In this section, basic notions and notations will be given regarding the subject of the thesis.

1.1 Markov Chains

A discrete time Markov process describes a system that moves through a finite set of states S, described by a stochastic matrix P, the *one-step transition kernel*. When the system is in state $i \in S$ at time $t \geq 0$, the system will make a transition into state $j \in S$ with probability $p_t(i,j) = (P_t)_{i,j}$. The transition probability from x to any other state sum to one, i.e. they satisfy:

$$\sum_y p_t(x,y) = 1.$$

The one step transition kernel P can be seen as an operator working on a bounded, measurable function f in discrete time as

$$(Pf)(x) = \sum_{y \in S} p(x,y)f(y).$$

The generator of a discrete time Markov chain is defined as: $L = P - \mathbb{1}$. We can think of L as an operator working on f as

$$(Lf)(x) = (Pf)(x) - f(x).$$

A stochastic system $X = \{X_t, t \geq 0\}$ is a Markov process if, for each time step t and all states $x_0, \dots, x_t \in S$ it posesses the *Markov property*:

$$\mathbb{P}(X_t = x_t | X_{t-1} = x_{t-1}, \dots, X_0 = x_0) = \mathbb{P}(X_t = x_t | X_{t-1} = x_{t-1}).$$

Put into words, this means that the next state depends only on the current state and not on the path to the current state.

Definition (Hitting time)**.** The hitting time τ_D of a discrete time Markov chain $(X_t)_{t \geq 0}$ is defined as

$$\tau_A := \min_{t \in \mathbb{N}} \{X_t \in A\}$$

If the strong Markov property holds, the time t is defined as a random variable, the hitting time.

A discrete time Markov process X has *stationary transition probabilities* if the one-step transition kernel P_t at time t is independent of t, so if $\forall k \in N_{\geq 0}$:

$$\mathbb{P}(X_{s+t} = j | X_s = i) = \mathbb{P}(X_{k+t} = j | X_k = i).$$

A probability measure μ is an *invariant distribution* for X if:

$$\sum_x \mu(x)p(x,y) = \mu(y).$$

Note that this is equivalent to the condition:

$$\mu L = 0.$$

A Markov process is *reversible* if there exists a non-zero probability measure μ such that

$$\mu(x)p(x,y) = \mu(y)p(y,x) \qquad \forall x, y \in S. \tag{1.1}$$

Lemma 1.1. If μ is a reversible distribution for P, it is also an invariant distribution.

Proof. Because the probability of making a transition from x to any other state sum to one, when summing (1.1) over y it can be seen that:

$$\mu(x) = \sum_y \mu(x)p(x,y) = \sum_y \mu(y)p(y,x),$$

so that it is also invariant. □

The definitions given below are definitions regarding the classification of Markov processes.

Definition (Classification of a Markov process)**.** A Markov process X with countable state space S is said to be *irreducible* if and only if all states in the state space communicate, that is: for each $x, y \in S$ there exists a $t \in \mathbb{N}_0$ such that: $p_t(x,y) > 0$
The process is said to be *recurrent* if X is irreducible, and $\mathbb{P}(\tau_i < \infty) = 1$ for all $i \in S$ [1], and is said to be *positive recurrent* if $\mathbb{E}_i[T_i] < \infty$ for all $i \in S$.
A chain that can only return to a state in a multiple of $d > 0$ is called *periodic*, if the chain is not periodic it is called *aperiodic*.
A Markov process X is *ergodic* if it is irreducible, positive recurrent and aperiodic.

1.2 Glauber Dynamics

The state space of the Glauber Dynamics that we will study in this thesis is of the form of S^V where S is a finite set and V is the (finite) vertex set of a graph. The elements of S^V are called *configurations*, and represent the states of the nodes. It assigns a value $\sigma(v) \in S$ to each vertex $v \in V$. The state space of the system is denoted by $\Omega \subseteq S^V$. Let μ be probability distribution whose support is Ω. For the Ising Spin model, this is the gibbs measure and will be defined in (1.3), section 1.3. Single site-update *Glauber dynamics* for μ is a reversible Markov chain with state space Ω, stationary and reversible distribution μ that denotes the probability of a configuration, and transition probabilities $p(\sigma, \sigma')$ between two configurations $\sigma, \sigma' \in \Omega$ that depend on the energy of the system.

Every step in the discrete time, a vertex $v \in V$ is chosen uniformly at random. The new state is chosen according to the transition probabilities, a measure conditioned on the set of states equal to x at all vertices different from v.

1.3 Ising Spin Model

Let $\Lambda \subseteq \mathbb{Z}^2$ be a finite set of *sites*, a square torus centered at the origin which we can view as a two-dimensional grid. By the Glauber dynamics, we associate, with each site $x \in \Lambda$, a spin value $\sigma(x) \in \{-1, 1\}$. We define a configuration of the model as $\sigma := \{\sigma(x) : x \in \Lambda\} \in \Omega$ where $\Omega := \{-1, 1\}^\Lambda$ denotes the state space. The configuration space Ω is, by the Glauber dynamics, modeled as a connected non-oriented graph $(\Omega, \mathcal{E})$, with $(\sigma, \sigma') \in \mathcal{E}$ if σ' is reachable from σ by a single spin-flip.

The energy of a configuration $\sigma \in \Omega$ of the Ising Spin model is given by the *Hamiltonian* $H : S \to \mathbb{R}$, defined as:

$$H(\sigma) = -\frac{J}{2} \sum_{\substack{\{x,y\} \in \Lambda \\ ||x-y||=1}} \sigma(x)\sigma(y) - \frac{h}{2} \sum_{x \in \Lambda} \sigma(x), \tag{1.2}$$

where J is the pair potential by which the spins interact, and $h > 0$ is the external magnetic field. Assume $h \in (0, 2J)$ [1], in chapter 4.3 it will become clear why this is necessary for metastability.

The *Gibbs measure* associated with H is given by:

$$\mu(\sigma) = \frac{1}{Z_\beta} e^{-\beta H(\sigma)}, \tag{1.3}$$

where $\beta \in (0, \infty)$ is the inverse of the temperature of the system and Z_β is the normalizing partition sum [1].

We study the discrete time Markov process $(\sigma_t)_{t \in \mathbb{N}}$ with state space Λ. The transition probabilities $p(\sigma, \sigma')$ of the system between two configurations $\sigma, \sigma' \in \Omega$ are defined by the Metropolis algorithm as [1]

$$p(\sigma, \sigma') = \begin{cases} \frac{1}{|\Lambda|} e^{-\beta[H(\sigma') - H(\sigma)]_+}, & (\sigma, \sigma') \in \mathcal{E}, \\ 0, & \text{otherwise}, \end{cases} \tag{1.4}$$

where $\mathcal{E}$ denotes the set of edges between x, y, with $(x, y) \in \mathcal{E}$ if and only if $p(x, y) > 0$, so that transitions occur along edges only. This dynamics is ergodic and reversible with respect to μ_β [1],

$$\mu(\sigma)p(\sigma, \sigma') = \mu(\sigma')p(\sigma', \sigma), \qquad \forall \sigma, \sigma' \in \Omega,$$

so that μ_β is the unique equilibrium measure [3]. In this thesis, for ease of writing, μ_β will be denoted simply by μ.

1.4 Harmonic functions and Dirichlet problems

Suppose we have a discrete time Markov process X on a countable state space S with transition kernel P and generator $L = P - \mathbb{1}$. Suppose X is irreducible.

Definition (Dirichlet problem, [1])**.** Let $D \subset S$ be an open set, specify continuous functions $g : D \to \mathbb{R}$ and $\bar{g} : D^c \to \mathbb{R}$. The *Dirichlet problem* is defined as the problem of finding a continuously differentiable function $f : S \to \mathbb{R}$ such that it satisfies:

$$\begin{aligned} (-Lf)(x) &= g(x), \qquad \forall x \in D, \\ f(x) &= \bar{g}(x), \qquad \forall x \in D^c. \end{aligned} \tag{1.5}$$

In mathematics and mathematical physics, potential theory is the study of harmonic functions.

Definition (Harmonic function)**.** A function f defined on an open set $D \subset \mathbb{Z}^d$ is *harmonic* if, for all $x \in D$, it satisfies the discrete Laplace equation [3]:

$$\nabla f := \sum_{\substack{x,y \in D \\ ||x-y||=1}} (f(y) - f(x)) \equiv 0.$$

Note that by imposing the Laplace equation on the generator of the Markov chain defined in section 1.1, there is a nice property of the distribution that can be derived; because the transition probability of going from x to any other state in S sum to one, the generator can be written in the form:

$$Lf(x) := \sum_{y \in S} p(x,y)(f(y) - f(x)), \tag{1.6}$$

Therefore, the invariant measure for a Markov process is by definition a harmonic function.

Theorem 1.2 (Maximum/minimum principle, [3], p. 4)**.** *If f is harmonic and nonnegative on an open set $D \subseteq \mathbb{Z}^d$, then for all finite $K \subseteq \bar{D}$ such that f can be extended by continuity on K, $f|_k$ reaches it's maximum and it's minimum on the border of K.*

Proof. See ref [3], p.4 □

Theorem 1.2 gives the uniqueness of the solution to the Dirichlet problem.

Lemma 1.3. If there exists a continuously differentiable function f that is a solution to (1.5), then this solution is unique.

Proof. Suppose that the functions f_1, f_2 are solutions to (1.5). Define $f = f_1 - f_2$. Then f is a harmonic function with boundary conditions: $f(x) = 0,\ \forall x \in D^c$. By theorem 1.2, f is identically zero on D. Therefore $f_1 = f_2$. □

The general solution to the Dirichlet problem (1.5) is given by the following theorem:

Theorem 1.4. *Let X be a discrete time Markov process with generator L and state space S. Assume that $D \subset S$ is such that: $\mathbb{E}_x[\tau_{D^c}] < \infty,\ \forall x \in D$. If f is the unique solution to the Dirichlet problem* (1.5)*, then f is given by:*

$$f(x) = \sum_{z \in D} G_{D^c}(x,z)g(z) + \sum_{z \in D} H_{D^c}(x,z)\bar{g}(z), \qquad x \in D, \tag{1.7}$$

where

$$G_{D^c}(x,z) = \mathbb{E}_x\left[\sum_{s=0}^{\tau_{D^c}-1} \mathbb{1}_{X_s = z}\right], \qquad x, z \in D,$$

is the Green function, and

$$\begin{aligned} H_{D^c}(x,z) &= \mathbb{E}_x[\mathbb{1}_{X_{\tau_{D^c}} = z}] \\ &= \sum_{s \in \mathbb{N}_0} \mathbb{P}_x(\tau_{D^c} = s, X_s = z) \\ &= \mathbb{P}_x(X_{\tau_{D^c}} = z), \qquad x \in D, z \in D^c, \end{aligned}$$

is the Poisson kernel.

Proof. See ref [1], Chapter 7.1. □

The interpretation of the functions defined above is as follows: for a Markov process starting in $D \subset S$, the Green function $G_{D^c}(x,z)$ gives the average number of visits to $z \in D$ before exiting from D. The Poisson kernel $H_{D^c}(x,z)$ gives the probability that the process enters D^c at $z \in D^c$.

2 Electrical Networks

The discrete time Markov chain studied in this thesis has a discrete, connected state space. The transition kernel P is reversible and ergodic, and therefore denotes the transition probability matrix of a random walk on an electrical network. This is the graph with a conductance defined on each edge of the graph, proportional to the transition probabilities and densities proportional to the potentials. To any electrical network it is possible to associate an irreducible reversible Markov chain [7]. Levin, Perez and Wilmer showed that, in fact, every reversible Markov chain is a weighted random walk on a network. The study of reversible Markov chains is thus equivalent to the study of random walks on networks [5].

In this section, potential theory will be used to derive a formula for the mean hitting time, starting by obtaining a formula for the equilibrium potential. Then, in section 2.2 a formula for the capacity will be derived. In section 2.4 an exact formula for the mean hitting time will be obtained in terms of the equilibrium potential and the capacity. In section 2.3 the equilibrium potential and the capacity in the one dimensional random walk will be calculated as an illustrating example. The results are given for states denoted by $s, m \in \Omega$ for the purpose of this thesis (we want an estimation for states, after all), but these are generally true for disjoint subsets of Ω.

2.1 Potential Theory

Because of the strong Markov property, every time the system leaves the metastable state but returns to it before reaching the stable state, the probabilities of the restart. The probability of reaching some state from the starting state is equal to the probability of reaching that state when we first return to the starting state at some time in between. Therefore, to calculate the mean stable exit time, we are interested in the probability of hitting the metastable state before hitting the stable state. For configurations $x, m, s \in \Omega$ with $m \neq s$, define:

$$h_{m,s}(x) = \mathbb{P}_x(\tau_m < \tau_s). \tag{2.1}$$

Note that (2.1) is equal to 0 for $x = s$, and equal to 1 if $x = m$. By the Markov property, the probability of reaching m before s from x is equal to the probability of first making a transition into any other state in Ω and reaching m before s from this new state. This means, for a configuration $x \in \Omega$, by conditioning on the event that the process makes a transition into y, for each $y \in \Omega$, (2.1) can be written as:

$$\begin{aligned}
\mathbb{P}_x(\tau_m < \tau_s) &= \sum_{y\in\Omega} p(x,y)\mathbb{P}_y(\tau_m < \tau_s) \\
&= \sum_{y\in\Omega} p(x,y) h_{m,s}(y) \\
&= (Lh_{m,s})(x) + h_{m,s}(x).
\end{aligned} \tag{2.2}$$

For the last equality the definition of the generator is used. These conditions can be written in the form of a Dirichlet problem as:

$$\begin{aligned} (-Lh)_{m,s}(x) &= 0, \qquad x \in \Omega \setminus \{m, s\}, \\ h_{m,s}(x) &= 1, \qquad x = m, \\ h_{m,s}(x) &= 0, \qquad x = s, \end{aligned} \tag{2.3}$$

where L is the generator of the Markov chain. The solution (2.1) is called the *equilibrium potential*, and by lemma 1.3 it is the unique solution.

To derive formulas for $x = m$ and $x = s$, the known values for $h_{m,s}$ can be substituted into equation (2.1) to obtain:

$$(Lh_{m,s})(x) = \mathbb{P}_x(\tau_m < \tau_s), \qquad x = s, \tag{2.4}$$

$$\begin{aligned} (-Lh_{m,s})(x) &= 1 - \mathbb{P}_x(\tau_m < \tau_s) \\ &=: e_{m,s}(x), \qquad x = m. \end{aligned} \tag{2.5}$$

This last object, $e_{m,s}$, is the escape probability from m to s and is called the *equilibrium measure* on m.

2.2 Capacity

Definition (Capacity)**.** The *capacity* $C_{m,s}$ of a pair $m, s \in \Omega$ with $m \neq s$ on an electrical network with potential $h_{m,s}$ is defined as [1]

$$\begin{aligned} C_{m,s} :&= \mu(m)(-Lh_{m,s})(m) \\ &= \mu(m)e_{m,s}(m), \end{aligned} \tag{2.6}$$

where L is the generator of the Markov process with reversible measure μ.

We will now give a derivation of an alternative representation of the capacity. By the properties of $Lh_{m,s}$ on $\Omega \setminus \{s, m\}$, (2.6) can be written not only in terms of m but can be summed over all states in $\Omega \setminus s$, and by the properties of $h_{s,m}$, we can write the capacity as:

$$\begin{aligned} C_{m,s} &= \sum_{x \in \Omega \setminus s} \mu(x)(-Lh_{m,s})(x) \\ &= \sum_{x \in \Omega} \mu(x) h_{m,s}(x)(-Lh_{m,s})(x). \end{aligned}$$

Now using the definition of the generator, by reversibility:

$$C_{m,s} = \sum_{x,y \in \Omega} \mu(x)p(x,y)h_{m,s}(x)(h_{m,s}(x) - h_{m,s}(y)) \tag{2.7}$$

$$= \sum_{x \in \Omega} \mu(y)p(y,x)h_{m,s}(x)(h_{m,s}(x) - h_{m,s}(y)). \tag{2.8}$$

By symmetrizing between the two expressions (2.7) and (2.8), the capacity is also given by:

$$\begin{aligned} C_{m,s} &= \frac{1}{2} \sum_{x,y \in \Omega} \mu(x)p(x,y)(h_{m,s}(x) - h_{m,s}(y))^2 \\ &= \mathcal{D}(h_{m,s}, h_{m,s}). \end{aligned}$$

In the last expression, $\mathcal{D}(f,g)$ is the *Dirichlet form* given by:

$$\mathcal{D}(f,g) := \sum_{x\in\Omega} \mu(x)f(x)(-Lg)(x), \qquad f,g \in L^2(\Omega,\mu).$$

This representation gives a property that will be very useful when deriving bounds and estimating the capacity in sections 3.3 and 4.4.

Theorem 2.1 (Dirichlet principle)**.** *Let $m,s \in \Omega,\ m \neq s$. Define*

$$\mathcal{H}_{m,s} := \{h : \Omega \to [0,1] : h(m) = 1, h(s) = 0\}.$$

For potential h,

$$C_{m,s} = \min_{h\in\mathcal{H}_{m,s}} \mathcal{D}(h,h),$$

the unique minimizer is the equilibrium potential $h_{m,s}$ defined in (2.1)*.*

Proof. For any potential $f \in \mathcal{H}_{m,s}$, there exists $\varepsilon > 0$ such that $f = h + \varepsilon g$ with $h = h_{m,s}$ and $g(m) = 0,\ g(s) = 0$. By writing out, we obtain:

$$\mathcal{D}(f,f) = \mathcal{D}(h,h) + 2\varepsilon\mathcal{D}(h,g) + \varepsilon^2\mathcal{D}(g,g).$$

By reversibility of $\mathcal{D}$ and by the first condition in (2.3), the second term is zero on Ω. The last term is non-negative, therefore it follows that $\mathcal{D}(f,f) > \mathcal{D}(h,h)$ as soon as $g \not\equiv 0$, and h is a global minimum of $\mathcal{D}$ on $\mathcal{H}_{m,s}$. □

2.3 The one dimensional random walk

To illustrate the previous results, we can look at the easiest case: the one dimensional case. In this section, the equilibrium potential and capacity of a one-dimensional random walk with one step transitions will be calculated. This calculation will be useful to give a rough bound on the capacity in lemma 3.2.

We define the state space of the random walk as $a = x_0 < x_1 < \ldots < x_n = b$, with the transition probabilities are given by: $p(x_i, x_j) > 0$ if and only if $i = j \pm 1$. The random walk is reversible with respect to the measure μ,

$$\mu(x_i)p(x_i,x_j) = \mu(x_j)p(x_j,x_i).$$

We consider the equilibrium potential

$$h_{b,a}(x) = \mathbb{P}_x(\tau_b < \tau_a), \qquad a < x < b, \tag{2.9}$$

defined for all $a \neq x \neq b$ as a solution to the Dirichlet problem:

$$\begin{aligned}(-Lh)(x) &= 0,\\ h(a) &= 0,\\ h(b) &= 1.\end{aligned}$$

Equation (2.9) can be rewritten, by using the transition probabilities, as:

$$h_{b,a}(x_i) = p(x_i,x_{i+1})h_{b,a}(x_{i+1}) + p(x_i,x_{i-1})h_{a,b}(x_{i-1}). \tag{2.10}$$

Since there are only two states that can be reached from x_i,

$$p(x_i, x_{i+1}) + p(x_i, x_{i-1}) = 1,$$

therefore by writing all terms involving $p(x_i, x_{i+1})$ on the one side and all terms involving $p(x_i, x_{i-1})$ on the other side, (for ease of writing, h is used in stead of $h_{b,a}$) the following is obtained:

$$h(x_{i+1}) - h(x_i) = \frac{p(x_i, x_{i-1})}{p(x_i, x_{i+1})}(h(x_i) - h(x_{i-1})).$$

By substituting each previous equation into the next, we obtain:

$$h(x_{i+1}) - h(x_i) = \prod_{j=1}^{i-1} \frac{p(x_j, x_{j-1})}{p(x_j, x_{j+1})} h(x_1). \tag{2.11}$$

Now use reversibility with the measure μ to obtain for the righthandside:

$$\begin{aligned}\prod_{j=1}^{i-1} \frac{p(x_j, x_{j-1})}{p(x_j, x_{j+1})} h(x_1) &= \prod_{j=1}^{i-1} \frac{p(x_{j-1}, x_j)}{p(x_j, x_{j+1})} \frac{\mu(x_{j-1})}{\mu(x_j)} h(x_1) \\ &= \frac{p(x_0, x_1)}{p(x_{i-1}, x_i)} \frac{\mu(x_0)}{\mu(x_{i-1})} h(x_1). \end{aligned} \tag{2.12}$$

Add the first $i-1$ equations of (2.11), and note that if $i = 1$, then (2.12) is equal to $h(x_1)$, to obtain:

$$h(x_i) = \sum_{z=0}^{i-1} \frac{p(x_0, x_1)}{p(x_z, x_{z+1})} \frac{\mu(x_0)}{\mu(x_z)} h(x_1)$$

From the conditions, $h(b) = 1$, so that the formula of $h(x_1)$ is easily obtained. We find that the equilibrium potential $h(x) = h_{b,a}(x)$ is given by:

$$h_{b,a}(x_i) = \left(\sum_{z=0}^{i-1} \frac{1}{p(x_z, x_{z+1})\mu(x_z)} \right) \left(\sum_{z=0}^{n-1} \frac{1}{p(x_z, x_{z+1})\mu(x_z)} \right)^{-1}. \tag{2.13}$$

With formula (2.10) with $x_i = a$, and by (2.6) with (2.9), we obtain for the capacity of a and b:

$$C_{a,b} = \left(\sum_{z=0}^{n-1} \frac{1}{p(x_z, x_{z+1})\mu(x_z)} \right)^{-1}. \tag{2.14}$$

2.4 Mean Hitting Times

Now we are able to derive formulas for the mean values of hitting times τ_s for state $s \in \Omega$ for the electrical network with potential $h_{m,s}$. By the same reasoning as for (2.1), the expected value of τ_s when starting in $x \in \Omega \setminus s$ can be written as:

$$\begin{aligned}\mathbb{E}_x[\tau_s] &= \sum_{y\in\Omega} p(x,y)(\mathbb{E}_y[\tau_s]+1)\\ &= \sum_{y\in\Omega} p(x,y) + \sum_{y\in\Omega} p(x,y)\mathbb{E}_y[\tau_s]\\ &= 1 + \sum_{y\in\Omega} p(x,y)\mathbb{E}_y[\tau_s].\end{aligned}$$

It is obvious that for $x = s$, $\mathbb{E}_x[\tau_s] = 0$. These properties can be used to formulate the mean expected hitting time as the solution to a Dirichlet problem by using the definition of the generator L of the Markov process:

$$\begin{aligned}(-Lf)(x) &= 1, \qquad x \in \Omega \setminus s,\\ f(x) &= 0, \qquad x = s.\end{aligned}$$

In order to find the formula for the expected mean time, essentially the inverse operation of the generator, $(-L)^{-1}$, has to be found. By (1.7) the expected hitting time is written in the form of the general solution, so that the problem reduces to finding a formula for the Green function $G_{\Omega\setminus s}$:

$$\mathbb{E}_x[\tau_s] = \sum_{y\in\Omega\setminus s} G_{\Omega\setminus s}(x,y).$$

For $x = m$, by (2.5) and writing $h_{m,s}$ also in the form of the general solution of the dirichlet form,

$$h_{m,s}(y) = G_{\Omega\setminus s}(y,m)e_{m,s}(m).$$

Therefore, the Green function can be written in terms of the equilibrium potential and measure as

$$G_{\Omega\setminus s}(y,m) = \frac{h_{m,s}(y)}{e_{m,s}(m)}.$$

The generator L is symmetric with respect to μ. Note that the inverse is symmetric too, so that

$$G_{\Omega\setminus s}(m,y) = \frac{\mu(y)}{\mu(m)}\frac{h_{m,s}(y)}{e_{m,s}(m)}.$$

By summing this last expression over $y \in \Omega \setminus s$ (recall the boundary conditions for $h_{m,s}$), we find that the following theorem holds:

Theorem 2.2. *Let $m, s \in \Omega$ be two configurations with $m \neq s$. The mean hitting time of s when starting in m is given by*

$$\mathbb{E}_m[\tau_s] = \frac{1}{C_{m,s}} \sum_{y\in\Omega} \mu(y)h_{m,s}(y). \tag{2.15}$$

3 Metastability

In section 3.1 a general definition of metastability will be given. In section 3.2, the energy landscape will be described, by defining the optimal path and the critical increase of energy. In section 3.3, there will be given some rough bounds on the capacity, which will be used to derive some rough bounds on the potential in section 3.4. With these bounds, the sum in the equation of the mean hitting time given in theorem 2.2 can be estimated, which yields an important theorem, theorem 3.7, at the end of section 3.4.

3.1 Characterization of Metastability

Metastability is characterized by the existence of two different time scales, a short and a long one, and the partition of the state space Ω into disjoint sets $\Omega_i,\ i \in I$ such that on a short time scale it reaches some sort of local equilibrium on Ω_i, and on a long time scale it exits Ω_i and moves to Ω_j with $j \neq i$ where it again reaches some local equilibrium. The time for the system to reach a such a state when currently the system is not in an equilibrium is much shorter than the time to exit an equilibrium and to reach another equilibrium. When looking at (2.15), the following definition can be intuitively derived:

Definition (PTA-Metastable set)**.** For a Markov process X with finite state space Ω, a set $\mathscr{M} \subset \Omega$ is called a *set of metstable states* if

$$\frac{\max_{\xi \notin \mathscr{M}} \mu(\xi)/C_{\xi,\mathscr{M}}}{\min_{\xi \in \mathscr{M}} \mu(\xi)/C_{\xi,\mathscr{M}\setminus\xi}} \to 0, \qquad \text{as} \qquad \beta \to \infty. \tag{3.1}$$

Remark 1. The abbreviation 'PTA‘ stands for 'Potential Theoretic Approach', in line with the definition given in ref. [2], sec. 3.2, in order to avoid confusion with the definition of a metastable state given in section 3.2.

3.2 Energy landscape and general definitions

The *communication height*, or energy barrier, between $\sigma, \eta \in \Omega$ is the minimal energy the system takes on a path $\gamma : \sigma \to \eta$ starting in σ and ending in η,

$$\hat{H}(\sigma, \eta) := \min_{\gamma:\sigma\to\eta} \max_{\xi\in\gamma} H(\xi).$$

The *optimal path* between $\sigma, \eta \in \Omega$ is the path for which the energy does not exceed the communication height.

The *set of saddle states* $\mathscr{S}_{\sigma,\eta}$ is the set that consists of configurations that take on the highest energy on each path from σ to η,

$$\mathscr{S}_{\sigma,\eta} := \{\xi \in \Omega : \exists\gamma : \sigma \to \eta \text{ with } \xi \in \gamma, H(\xi) = \max_{\zeta\in\gamma} H(\zeta)\}.$$

Remark 2. For the system studied in this thesis, there are no edges between states within the set of saddle states. Even stronger, if $\frac{2J}{h}$ is not an integer, there will be no transitions possible between two states with the same energy. This will be proven in lemma 4.2, for now we will assume this is true.

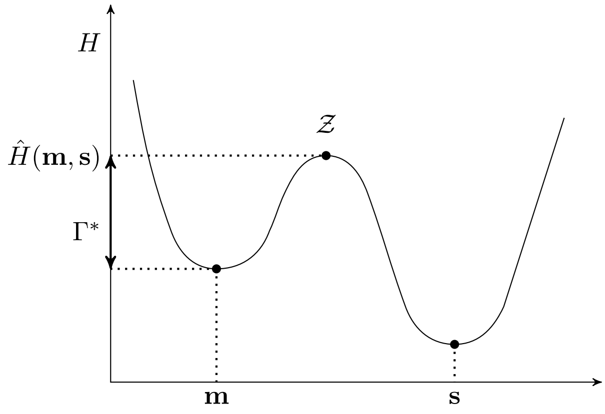

Figure 1: Optimal path.

The *communication level set* $\mathcal{Z}_{\sigma,\omega}$ between $\sigma, \eta \in \Omega$ is the set of saddle states that lies on the optimal path from σ to η,

$$\mathcal{Z}_{\sigma,\eta} := \{\xi \in \Omega : \exists \gamma : \sigma \to \eta \text{ with } \xi \in \gamma, H(\xi) = \hat{H}(\sigma, \eta)\}.$$

The *stability level* of $\sigma \in \Omega$ is the minimal increase in energy that has to be generated, when starting in σ, in order to reach states with lower energy. It will be denoted by the quantity $\Gamma(\sigma)$, defined as:

$$\Gamma(\sigma) := \hat{H}(\sigma, W_\sigma) - H(\sigma),$$

where the set W_σ is defined as:

$$W_\sigma = \{\xi \in \Omega : H(\xi) < H(\sigma)\}.$$

Definition (Stable state)**.** A *stable state* $\mathbf{s} \in \Omega$ of the system is the state for which the energy of the system has a global minimum, $H(\mathbf{s}) = \min_{\sigma \in \Omega} H(\sigma)$.

Definition (Metastable state)**.** A *metastable state* $\mathbf{m} \in \Omega$ of the system is defined as a configuration for which:

$$\Gamma(\mathbf{m}) = \max_{\sigma \in \Omega \setminus \mathbf{s}} \Gamma(\sigma). \tag{3.2}$$

The metastable state is a state with the maximal stability level. For all $\sigma \in \Omega$, $\hat{H}(\mathbf{m}, W_{\mathbf{m}}) \geq \hat{H}(\sigma, W_\sigma)$, with for each $\sigma \in \Omega$ for which equality holds, $H(\mathbf{m}) < H(\sigma)$.

Remark 3. On a general graph, there will not be a single metastable state, but for the system studied in this thesis there is an unique state that is the stable state. This claim will be proven in lemma 4.1.

Note that if there is only a single configuration for which (3.2) holds, the energy barrier between $\mathbf{m}$ and $\mathbf{s}$ is equal to

$$\Gamma^* := \Gamma(\mathbf{m}) = \hat{H}(\mathbf{m}, \mathbf{s}) - H(\mathbf{m}).$$

Lemma 3.1. For each $\sigma \in \Omega \setminus \{\mathbf{m}, \mathbf{s}\}$

$$\hat{H}(\sigma, \{\mathbf{m}, \mathbf{s}\}) - H(\sigma) < \Gamma^*.$$

Proof. Fix $\sigma \in \Omega \setminus \{\mathbf{m}\}$. Because Ω is finite, there exists an $m \in \mathbb{N}_0$ and a path $\omega : \sigma \to \mathbf{s}$, with $\omega_1, \dots, \omega_m \in \Omega \setminus \mathbf{m}$ where $\omega_m = \mathbf{s}$ such that, on this path, the energy keeps decreasing towards $\mathbf{s}$, i.e. $H(\omega_{i+1}) < H(\omega_i)$ and $\hat{H}(\omega_i, \omega_{i+1}) - H(\omega_i) < \Gamma^*$. Now

$$\hat{H}(\sigma, \mathbf{s}) - H(\sigma) \leq \max_{i=1,\dots,m} \{\hat{H}(\omega_i, \omega_{i+1}) - H(\omega_i)\} < \Gamma^*.$$

The claim follows from the fact that $\hat{H}(\mathbf{m}, \{\mathbf{m}, \mathbf{s}\}) - H(\mathbf{m}) = 0$ and from

$$\hat{H}(\sigma, \{\mathbf{m}, \mathbf{s}\}) = \min\{\hat{H}(\sigma, \mathbf{m}), \hat{H}(\sigma, \mathbf{s})\} \leq \hat{H}(\sigma, \mathbf{s}).$$

□

3.3 Bounds on the capacity

In section 2.3, the capacity was calculated for the one dimensional case. There is a nice lemma that we can derive from the one dimensional example. Suppose the states that are visited are only the states that lie on the optimal path. This path then consists of $|\Lambda| + 1$ states, including the metastable and stable states themselves. If we remove all states from the graph that are not on the path, including the edges, we can see this as a one dimensional walk. From this walk, we are able to derive a rough bound on the capacity.

Lemma 3.2. For every pair of states $\sigma, \eta \in \Omega$ with $\sigma \neq \eta$ there exist constants $0 < K_1 \leq K_2 < \infty$ such that

$$\frac{K_1}{Z_\beta} e^{-\beta \hat{H}(\sigma,\eta)} \leq C_{\sigma,\eta} \leq \frac{K_2}{Z_\beta} e^{-\beta \hat{H}(\sigma,\eta)}.$$

Proof. Let $\omega* : (\sigma \to \eta)_{opt}$ be the optimal path from σ to η. Then

$$\begin{aligned} C_{\sigma,\eta} &\geq \left(\sum_{\omega_i \in \omega*} Z|\Lambda| e^{\beta H(\omega_i)} e^{\beta(H(\omega_{i+1}) - H(\omega_i))} \right)^{-1} \\ &= \frac{1}{Z|\Lambda|} \left(\sum_{\omega_i \in \omega*} e^{\beta H(\omega_{i+1})} \right)^{-1} \\ &\geq \frac{K_1}{Z} e^{-\beta \hat{H}(\sigma,\eta)}. \end{aligned}$$

For the upper bound, set the potential to $h = \mathbb{1}_{\Phi(\sigma,\eta)}$ with $\Phi(\sigma, \eta) := \{\xi \in \Omega : \hat{H}(\xi, \sigma) \leq \hat{H}(\xi, \eta)\}$, with the Dirichlet principle 2.1 we get

$$\begin{aligned} C_{\sigma,\eta} &\leq \mathcal{D}(\mathbb{1}_{\Phi(\sigma,\eta)}, \mathbb{1}_{\Phi(\sigma,\eta)}) \\ &= \sum_{\substack{\xi \in \Phi \\ \xi' \notin \Phi}} \mu(\xi) p(\xi, \xi'). \end{aligned}$$

Now, if $\xi \in \Phi(\sigma, \eta)$ and $\xi' \notin \Phi(\sigma, \eta)$ but $(\xi, \xi') \in \mathcal{E}$, then it must be true that $H(\xi') < H(\xi)$ and $H(\xi) \geq \hat{H}(\sigma, \eta)$. We have

$$\mu(\xi)p(\xi, \xi') \leq \frac{1}{|\Lambda|Z} e^{-\beta H(\xi)} \leq \frac{1}{|\Lambda|Z} e^{-\beta \hat{H}(\sigma,\eta)},$$

such that

$$C_{\sigma,\eta} \leq \frac{K_2}{Z} e^{-\beta \hat{H}(\sigma,\eta)}.$$

By combining the upper and lower bound, we get the claim. □

Now we can show that the metastable states and stable state defined in section 3.2 are in the PTA-metastable set $\mathscr{M}$.

Lemma 3.3. The metastable state $\mathbf{m}$ and the stable state $\mathbf{s}$ are PTA-metastable.

Proof. For $\sigma \notin \{\mathbf{m}, \mathbf{s}\}$, by using the lower bound in lemma 3.2 and by using lemma 3.1, there exists a $\delta > 0$ such that:

$$\frac{e^{\beta H(\sigma)}}{Z C_{\sigma,\{\mathbf{m},\mathbf{s}\}}} \leq \frac{e^{\beta(\hat{H}(\sigma,\{\mathbf{m},\mathbf{s}\}) - H(\sigma))}}{K_1} = \frac{e^{\beta(\Gamma^* - \delta)}}{K_1},$$

and by using the upper bound of lemma 3.2, for $\sigma \in \mathscr{M}$ it is seen that:

$$\frac{e^{\beta H(\sigma)}}{Z C_{\sigma,\{\mathbf{m},\mathbf{s}\}}} \geq \frac{e^{\beta(\hat{H}(\sigma,\{\mathbf{m},\mathbf{s}\}) - H(\sigma))}}{K_2} = \frac{e^{\beta(\Gamma^*)}}{K_2},$$

so that (3.1) holds, and therefore $\mathbf{m}, \mathbf{s} \in \mathscr{M}$. □

3.4 Bounds on the potential

In order to find sharp bounds for the mean hitting time of the stable state in (2.15), some bounds on the equilibrium potential $h_{m,s}$ are needed. The lemma's in this chapter will be used to prove a useful theorem at the end of this section.

Lemma 3.4.

$$\max\{1 - \frac{C_{x,\mathbf{s}}}{C_{x,\mathbf{m}}}, 0\} \leq h_{\mathbf{m},\mathbf{s}}(x) \leq \min\{1, \frac{C_{x,\mathbf{m}}}{C_{x,\mathbf{s}}}\}. \tag{3.3}$$

Proof. For the upper bound, we can write:

$$\begin{aligned}\mathbb{P}(\tau_{\mathbf{m}} < \tau_{\mathbf{s}}) = \mathbb{P}((\tau_{\mathbf{m}} < \tau_{\mathbf{s}}) \cap (\tau_x > \tau_{\mathbf{m}\cup\mathbf{s}})) \\ + \mathbb{P}(\tau_{\mathbf{m}} < \tau_{\mathbf{s}} | \tau_x < \tau_{\mathbf{m}\cup\mathbf{s}}) \mathbb{P}(\tau_x < \tau_{\mathbf{m}\cup\mathbf{s}}).\end{aligned}$$

By using the Markov property, therefore:

$$\begin{aligned}\mathbb{P}_x(\tau_{\mathbf{m}} < \tau_{\mathbf{s}}) &= \frac{\mathbb{P}_x(\tau_{\mathbf{m}} < \tau_{\mathbf{s}\cup x})}{\mathbb{P}_x(\tau_{\mathbf{m}\cup\mathbf{s}} < \tau_x)} \leq \frac{\mathbb{P}_x(\tau_{\mathbf{m}} < \tau_x)}{\mathbb{P}_x(\tau_{\mathbf{s}} < \tau_x)} \\ &= \frac{C_{x,\mathbf{m}}}{C_{x,\mathbf{s}}}.\end{aligned}$$

The upper bound follows from the symmetry relation $h_{\mathbf{m},\mathbf{s}}(x) = 1 - h_{\mathbf{s},\mathbf{m}}(x)$. □

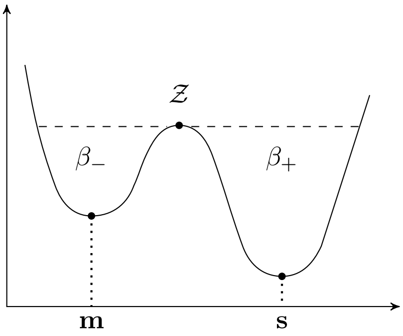

Figure 2: Optimal path. Basins of attraction.

Definition (Basin of attraction)**.** The *basin of attraction* of the metastable and stable state respectively is the set:

$$\beta_- := \{\sigma \in \Omega : \hat{H}(\sigma, \mathbf{m}) < \hat{H}(\sigma, \mathbf{s})\},$$
$$\beta_+ := \{\sigma \in \Omega : \hat{H}(\sigma, \mathbf{s}) < \hat{H}(\sigma, \mathbf{m})\}.$$

These definitions will help to define the behavior of the equilibrium potential on different parts of the path, see figure 2. Note that the optimal path from $\mathbf{m}$ to $\mathbf{s}$ starts in β_-. With each transition, the energy of the system increases, until the transition into $\mathcal{Z}$, where the system attains the maximum energy. Then it transitions into β_+, where, with each transition, the energy decreases, and finishes the path at $\mathbf{s}$, where the system attains the absolute minimal energy.

Lemma 3.5. $\exists K < \infty,\ \delta \geq 0:$

$$\min_{\xi \in \beta_-} h_{\mathbf{m},\mathbf{s}}(\xi) \geq 1 - Ke^{-\beta\delta}, \qquad \max_{\xi \in \beta_+} h_{\mathbf{m},\mathbf{s}}(\xi) \leq Ke^{-\beta\delta}.$$

Proof. Use lemma 3.4 together with lemma 3.2. □

Lemma 3.6. There exist $K < \infty,\ \delta > 0$ such that if $\sigma, \eta \in \beta_-$ or $\sigma, \eta \in \beta_+$ then

$$\max_{\sigma,\eta} |h_{\mathbf{m},\mathbf{s}}(\sigma) - h_{\mathbf{m},\mathbf{s}}(\eta)| \leq Ke^{-\beta\delta}.$$

Proof. Without loss of generality, assume $h_{\mathbf{m},\mathbf{s}}(\sigma) > h_{\mathbf{m},\mathbf{s}}(\eta)$. The equilibrium potential can be written as:

$$\begin{aligned} h_{\mathbf{m},\mathbf{s}}(\sigma) &= \mathbb{P}_\sigma(\tau_{\mathbf{m}} < \tau_{\mathbf{s}}) \\ &= \mathbb{P}_\sigma((\tau_{\mathbf{m}} < \tau_{\mathbf{s}}) \cap (\tau_{\mathbf{m}} < \tau_\eta)) + \mathbb{P}_\sigma((\tau_{\mathbf{m}} < \tau_{\mathbf{s}}) \cap (\tau_{\mathbf{m}} > \tau_\eta)). \end{aligned}$$

The first can be bounded above by:

$$\mathbb{P}_\sigma(\tau_{\mathbf{m}} < \tau_{\mathbf{s}\cup\eta}) \leq \mathbb{P}_\sigma(\tau_{\mathbf{m}} < \tau_\eta) \leq \frac{C_{\sigma,\mathbf{m}}}{C_{\sigma,\eta}} \leq Ke^{-\beta(\hat{H}(\sigma,\mathbf{m}) - \hat{H}(\sigma,\eta))} \leq Ke^{-\beta\delta}.$$

Using the Markov property when rewritten in the conditional form, the second therm can be bounded by:

$$\mathbb{P}_\eta(\tau_{\mathbf{m}} < \tau_{\mathbf{s}}) P_\sigma(\tau_{\mathbf{m}} > \tau_\eta) \leq \mathbb{P}_\eta(\tau_{\mathbf{m}} < \tau_{\mathbf{s}}) = h_{\mathbf{m},\mathbf{s}}(\eta).$$

Therefore we get that

$$h_{m,s}(\sigma) - h_{m,s}(\eta) \leq K e^{-\beta\delta}.$$

Interchange σ and β to complete the proof. □

The following theorem is an important theorem for the estimation of the mean hitting time of the stable state. This theorem, together with the bounds on the capacity that will be given in section 3.3, will prove theorem 0.1.

Theorem 3.7. *Suppose $\mathscr{M}$ is given by $\mathscr{M} = \{\boldsymbol{m}, \boldsymbol{s}\}$. The mean stable hitting time is given by*

$$\mathbb{E}_{\boldsymbol{m}}[\tau_{\boldsymbol{s}}] = \frac{\mu(\boldsymbol{m})}{C_{\boldsymbol{m},\boldsymbol{s}}}(1 + O(e^{-\beta\delta})), \tag{3.4}$$

for some $\delta > 0$, where the big O notation is used to describe the error.

Proof. By theorem 2.2, the proof consists of finding a boundary to the sum in (2.15). This can be divided into three parts, namely: β_-, β_+ and $\Omega \setminus (\beta_- \cup \beta_+)$. With lemma 3.4 and then with lemma 3.2, there exists a constant $K < \infty$ such that the capacity can be written as

$$\begin{aligned}\sum_{y\in\Omega} \mu(y) h_{\mathbf{m},\mathbf{s}}(y) &\leq \sum_{y\in\Omega} \mu(y) \frac{C_{y,\mathbf{m}}}{C_{y,\mathbf{s}}} \\ &= \sum_{y\in\Omega} \frac{1}{Z_\beta} K e^{-\beta H(y)} e^{-\beta(\hat{H}(y,\mathbf{m}) - \hat{H}(y,\mathbf{s}))}.\end{aligned}$$

Now on β_+, note that $\hat{H}(y,\mathbf{s}) \geq H(y)$, such that we can write for $y \in \beta_-$:

$$\mu(y) h_{\mathbf{m},\mathbf{s}}(y) \leq K \mu(\mathbf{m}) e^{-\beta\Gamma^*}.$$

For $y \in \Omega \setminus (\beta_- \cup \beta_+)$, it holds that $\hat{H}(y,\mathbf{m}) = \hat{H}(y,\mathbf{s})$ such that

$$H(y) + \hat{H}(y,\mathbf{m}) - \hat{H}(y,\mathbf{s}) = H(y),$$

and since $\mu(y) > \mu(\mathbf{m})$, we can write, for $y \in \Omega \setminus (\beta_- \cup \beta_+)$, for some $\delta_1 > 0$,

$$\mu(y) h_{m,s}(y) \leq \mu(\mathbf{m}) e^{-\beta\delta_1}.$$

On β_-, for $y \in \beta_- \setminus \mathbf{m}$ holds that $H(y) > H(\mathbf{m})$. Therefore, by lemma 3.5, for some $\delta_2 > 0$,

$$\mu(y) h_{\mathbf{m},\mathbf{s}}(y) = \frac{1}{Z_\beta} e^{-\beta(H(\mathbf{m})+\delta)}(1 - K e^{-\beta\delta_2}).$$

For $h_{\mathbf{m},\mathbf{s}}(\mathbf{s}) = 0$ and $h_{\mathbf{m},\mathbf{s}}(\mathbf{m}) = 1$, by combining all above, there exists a $\delta > 0$ such that the claim holds. □

4 Two Dimensional Ising Spin model

In this section, the proof of the main theorem will be finished. First the metastable and stable state of the system will be identified. Then the optimal path is identified in section 4.2. In section 4.3, the length of the droplet that will cause the system to be able to cross over to the stable configuration will be identified. This is the communication level set $\mathcal{Z}_{\mathbf{m},\mathbf{s}}$ defined in section 3.2. Finally the capacity will be estimated in section 4.4, that will yield the final result in section 4.5, the proof of theorem 0.1.

4.1 Metastable and stable states states

Denote the configuration of the Ising spin model with a positive spin on each site of Λ by $\mathbf{+1}$, and the configuration where each site of Λ has a negative spin by **-1**. This state is the only metastable state in the sense of the definition given in section 3.2.

Lemma 4.1. The metastable set is $\mathscr{M} := \{\mathbf{-1}, \mathbf{+1}\}$, where $\mathbf{+1}$ is the stable state $\mathbf{s}$ and **-1** is the metastable state $\mathbf{m}$, defined in section 3.1.

Proof. See ref. [6] thm. 4.32 □

Lemma 4.2. If $(\sigma, \eta) \in \mathcal{E}$ with $\sigma \neq \eta$, then $H(\sigma) > H(\eta)$ or $H(\sigma) < H(\eta)$.

Proof. We will use the notations of 4.1. If $H(\sigma) = H(\eta)$, then either

$$\mathcal{W}(\sigma) = \mathcal{W}(\eta) \text{ and } |\sigma| = |\eta|,$$

or

$$J(\mathcal{W}(\sigma) - \mathcal{W}(\eta)) = h(|\sigma| - |\eta|).$$

Since $\sigma \neq \eta$, $|\sigma| = |\eta| \pm 1$. We assumed $2J/h$ not to be an integer, and since every spin flip will cause $J(\mathcal{W}(\sigma)$ to change by either 2 or 4, we get the claim. □

4.2 Optimal paths

In ref [4] it was shown that small droplets are likely to disappear while large droplets are likely to grow. The system will be in the metastable state for a very long time, until eventually a *critical configuration* is formed. This leads to the system transitioning towards the state with all spins up in a relatively short time. Once the system reaches this state, it stays there for a much longer period of time.

The choice of h and J in the Hamiltonian (1.2) determines the probability at which the spins flip, and if the system will eventually transition into the configuration $\mathbf{+1}$. The difference in energy a spin flip will induce can be easily computed when writing the Hamiltonian in the form given in the proof of lemma 4.1. If a spin is -1 and one of it's neighbors is $+1$, the energy is increased by $2J - h$ if it flips to $+1$. When none of it's neighbors are positive, the flip will cause the energy to grow by $4J - h$. If there are two neighbors with a positive spin, the energy will decrease with h. The cost of adding a row of length l is equal to the cost of the first spin flip from the square (or quasi-square) which is equal to $2J - h$, and then each next spin flip in the row will cause the energy to decrease by h, see figure 3.

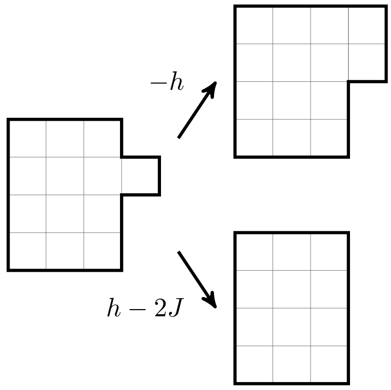

Figure 3: Cost of transitions

If $h > 4J$, any spin that is -1 will flip with probability $\frac{1}{|\Lambda|}$, independent of the value of it's neighbors, and any spin that is $+1$ will flip with a vanishing probability when $\beta \to \infty$. There is no metastability in this case.

If $h < 4J$ but $h > 2J$ and $|\Lambda|$ is large enough, the first spin flip will happen with probability $\frac{1}{|\Lambda|}e^{-\beta(4-h)}$. When the first spin has flipped to $+1$ from **-1**, with probability $\frac{1}{|\Lambda|}$ the system goes back to **-1**, and with probability $\frac{4}{|\Lambda|}$ there is a transition into a configuration with 2 neighboring spins up and with probability $\frac{|\Lambda|-5}{|\lambda|}e^{-\beta(4J-h)}$ there will be two different positive spins, which vanishes when $\beta \to \infty$. When there are two neighboring spins that are positive, one of them flips back with probability $\frac{2}{|\Lambda|}e^{-\beta(h-2J)}$ (increasing the energy by $h-2J$) which vanishes in the limit to low temperature, while their neighbors flip with a non-vanishing probability. So the configuration with two positive neighboring causes the configuration of the system to be able to become $\mathbf{+1}$ in a relatively short time.

If $2J/h$ is an integer, either the transitions where a spin flips to positive where two neighbors have a positive spin or the transitions where only one neighbor has a positive spin will not cause the energy to grow or decrease. Therefore it is unclear what happens.

See figure 3 for the increase or decrease in energy when there are neighboring spins. We will assume $h \in (0, 2J)$.

When $0 < h < 2J$, the configuration with two positive neighboring spins will no longer cause the system to tend to develop into $\mathbf{+1}$, since the spins flip back at non-vanishing probability while their neighboring spins will flip with a vanishing probability in the limit of low temperature. Nonetheless, there exists a critical configuration in this case.

The path where at each transition, the energy increase is the smallest, is the path where, after the first spin flip, one of it's neighbors flips, and then one of their neighbors, such that the positive spins will form a square or quasi-square.

4.3 Critical droplet size

The droplet of the configuration for which the system is capable of crossing over the hill is called the *critical droplet*, the length of it's sides are called the is called the *critical droplet size*. This is the length l_c that maximizes $H(\xi)-H(\mathbf{-1})$. Once the system has reached l_c, the probability of the system to make further transition towards the stable configuration is higher than the probability of that of the metastable configuration. Note that this is the configuration defined in section 3.2 as the communication level set $\mathcal{Z}_{\mathbf{-1},\mathbf{+1}}$.

To calculate the critical droplet size in the case $0 < h < 2J$, note that the number $x \in \Lambda$ with y such that $d(x, y) = 1$ where the spin of x differs from that of y in ξ is $4l$, namely: 2 for each corner, 8 in total, and $(l - 2)$ for each side, $4(l - 2)$ in total. The number of spins in ξ that differ from the spins of configuration $\mathbf{-1}$ is equal to l^2. Therefore,

$$H(\xi) - H(\mathbf{-1}) = 4Jl - hl^2,$$

differentiating yields that the maximum is at $l_c = \lceil \frac{2J}{h} \rceil$

4.4 Estimating the capacity

From theorem 3.7, it is clear that in order to provide an estimate on the mean hitting time, there is an estimate needed for the capacity. This section will provide this estimate by give an upper bound and a lower bound, such that these bounds coincide. We will denote the communication level set $\mathcal{Z}_{\mathbf{-1},\mathbf{+1}}$ simply by $\mathcal{Z}$.

4.4.1 Upper bound

By the Dirichlet principle, theorem 2.1, the minimum of the Dirichlet form is obtained when the potential between **-1** and **+1** is the equilibrium potential. Therefore, set the potential to $h|_{\beta_-} = 1$, $h|_{\beta_+} = 0$. Because we minimize the Dirichlet form, only the paths where for all transitions that increase the total energy, this increase is minimal, need to be considered. Because only one step transitions are allowed in the model such that there are no allowed transitions directly between β_- and β_+, and by lemma 4.2 there are no allowed moves within $\mathcal{Z}$. We get:

$$C_{\mathbf{-1},\mathbf{+1}} \leq \mathcal{D}(h,h) = \sum_{\substack{x\in\beta_- \\ y\in Z}} \mu(x)p(x,y)[1-h(y)]^2 + \sum_{\substack{x\in\beta_+ \\ y\in Z}} \mu(x)p(x,y)[h(y)]^2.$$

If we denote $p(x, \beta_\pm) = \sum_{y\in\beta_\pm} p(x, y)$, then by using reversibility with respect to μ we can write above as:

$$C_{\mathbf{-1},\mathbf{+1}} \leq \sum_{z\in Z} \mu(z) \left(p(z,\beta_-)[1-h(z)]^2 + p(z,\beta_+)[h(z)]^2\right).$$

By differentiating with respect to h, we find that this has a minimum for

$$h(z) = \frac{p(z,\beta_-)}{p(z,\beta_-)+p(z,\beta_+)}.$$

This minimum is given by:

$$C_{\mathbf{-1},\mathbf{+1}} \leq \sum_{z\in Z} \mu(z) \frac{p(z,\beta_-)p(z,\beta_+)}{p(z,\beta_-)+p(z,\beta_+)}.$$

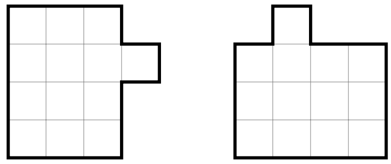

Figure 4: Orientations of the critical droplet

4.4.2 Lower bound

The lower bound comes from the one dimensional case where we remove all vertices σ with $H(\sigma) > \Gamma*$ and all edges incident to these vertices to obtain Ω^* such that the path from **-1** to **+1** becomes the optimal path. The reason that this gives a lower bound is because of the monotonicity of the Dirichlet form in the transition probabilities. This will give an error of order $\frac{1}{Z_\beta} e^{-\beta(\Gamma*+\delta)}$ for some $\delta > 0$.

Since only one spin flips at a time, there are no allowed moves between β_- and β_+. By lemma 3.6, the transitions that stay within the same basin of attraction can be put in the error. Therefore, the computation of the lower bound reduces to estimating

$$\sum_{\substack{\sigma\in\beta_- \\ \sigma\in\mathcal{Z}}} \mu(\sigma)p(\sigma,\eta)[h(\sigma)-h(\eta)]^2 + \sum_{\substack{\sigma\in\mathcal{Z} \\ \eta\in\beta_+}} \mu(\sigma)p(\sigma,\eta)[h(\sigma)-h(\eta)]^2.$$

By using the lower bound $h_{\mathbf{m},\mathbf{s}}(\sigma) = 0$ when $\sigma \in \beta_+$ and the bound from lemma 3.5 when $\sigma \in \beta_-$, the lower bound becomes

$$C_{\mathbf{-1},\mathbf{+1}} \geq \min_{h:\Omega*\to[0,1]} \Big(\sum_{\sigma\in\mathcal{Z}} \mu(\sigma)p(\sigma,\beta_-)(1-h(\sigma))^2 + \sum_{\sigma\in\mathcal{Z}} \mu(\sigma)p(\sigma,\beta_-)(h(\sigma))^2\Big).$$

where $p(\sigma, \beta_\pm)$ are defined as in the computation of the upper bound in section 4.4.1. The minimum is given by

$$C_{\mathbf{-1},\mathbf{+1}} \geq \sum_{z\in Z} \mu(z) \frac{p(z,\beta_-)p(z,\beta_+)}{p(z,\beta_-)+p(z,\beta_+)}.$$

4.5 Mean Hitting Times

Because of the definition of the saddle set, for each $z \in \mathcal{Z}$ the energy will be equal to $\hat{H}(\mathbf{-1},\mathbf{+1})$. Note that with the transitionprobabilities defined in 1.4,

$$p(x,\beta_\pm) = \frac{1}{|\Lambda|}|\{y\in\beta_\pm;(x,y)\in\mathcal{E}\}|.$$

For $z \in \mathcal{Z}$, there is one configuration in β_- that it can reach, the configuration where the protuberance flips back. The number of configurations in β_+ depends on the location of the protuberance: when it is in a corner there is one, and there are two when it is not. Since there are 8 possible ways to position the protuberance in a corner and $4(l_c - 2)$ else. There are $|\Lambda|$ ways to position the configuration, and for each position there are 2 orientations (see figure 4). Therefore we find:

$$\sum_{z\in Z} \frac{p(z,\beta_-)p(z,\beta_+)}{p(z,\beta_-)+p(z,\beta_+)} = 2(8\frac{1}{2} + 4(l_c-2)\frac{2}{3}) = \frac{8}{3}(2l_c-1). \qquad (4.1)$$

Proof. of the main theorem, 0.1
With the bounds found in 4.4.1 and 4.4.2 with formula (4.1), together with (3.4), we find that:

$$\mathbb{E}_{\mathbf{-1}}[\tau_{\mathbf{+1}}] = \frac{3}{8(2l_c - 1)Z_\beta} e^{-\beta(H(\mathbf{-1}) - \hat{H}(\mathbf{-1},\mathbf{+1})}(1 + O(e^{-\beta\delta})),$$

where $l_c = \lceil \frac{2J}{h} \rceil$. □

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