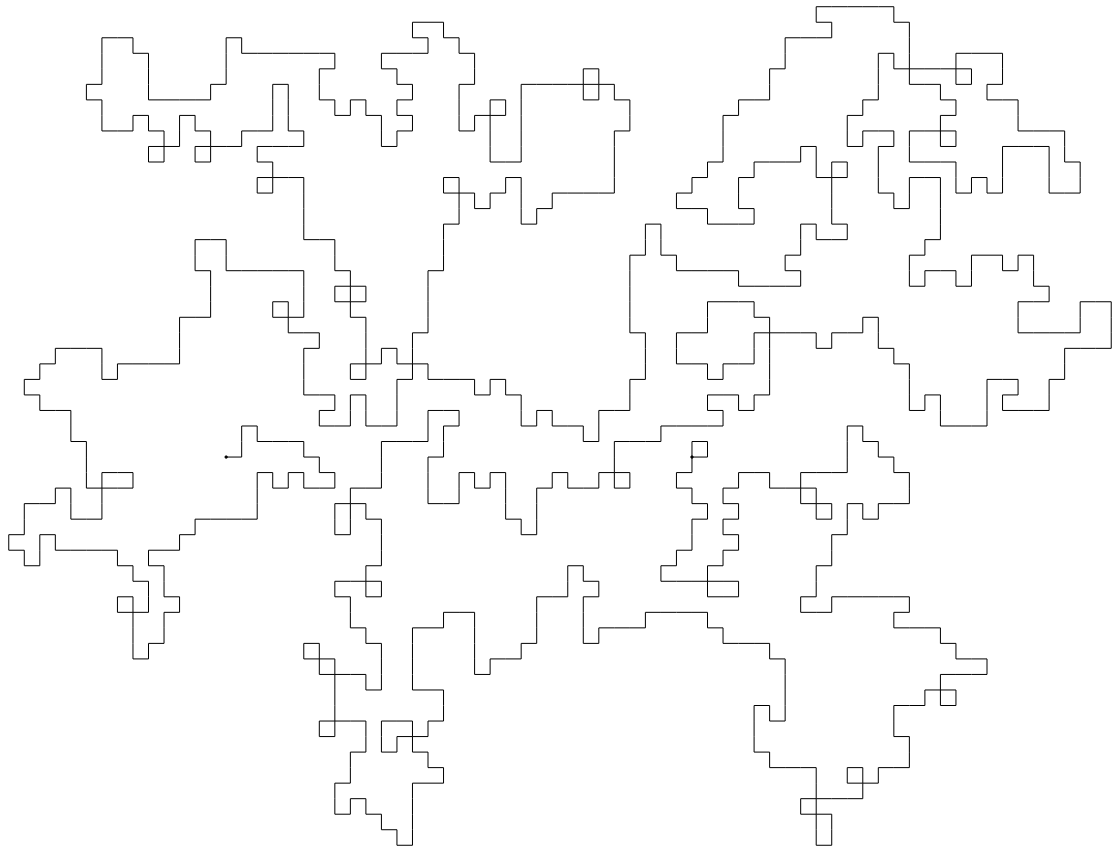




CHALMERS
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Properties of Random Connected Edge Sets on Hypercubic Lattices

Master's thesis in Engineering Mathematics and Computational Science

ANDRZEJ BRUKSMAN RZECZYCKI

DEPARTMENT OF MATHEMATICAL SCIENCES

CHALMERS UNIVERSITY OF TECHNOLOGY

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Cover: Edge set generated by sampling from our distribution μ_a with $a = 0.42$ and $l = 30$.

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Abstract

For $a > 0$, $d = 2, 3, \dots$, and $l = 0, 1, \dots$, we introduce a probability measure μ_a on a probability space $\Omega(l)$ consisting of connected edge sets in a d -dimensional hypercubic lattice, inspired by the two-point correlation function of the Ising model. We introduce a_d^* , the supremum of a such that μ_a is a well-defined probability measure. We show that a_d^* is independent of l . By means of bounding the number of elements in Ω from above, we establish the lower bound $a_d^* > \frac{1}{2d-1}$, and by means of constructing elements of Ω , we establish the upper bound $a_d^* \leq 1/d$. The parameter a in our model plays a similar role as to that of $\tanh(\beta)$ in the two-point correlation function of the Ising model. As the Ising model undergoes a phase transition at the critical inverse temperature β_d^c , we compare our bounds on a_d^* to $\tanh \beta_d^c$, using values and approximations of β_d^c found in literature. We find that $\tanh \beta_d^c$ lies within our bounds on a_d^* . We relate the edge sets in our probability space Ω to the graph theoretic concepts of walks, trails, and paths, and bound the number of edge sets of length k in Ω in terms of number of such constructs of length k . In order to visualize the distribution, we employ the Metropolis-Hastings algorithm to simulate from μ_a in two dimensions constricted to a finite lattice.

Keywords: probability theory, hypercubic lattice, edge set, trail, Ising model

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1

Introduction

In this chapter, we give a brief overview of the Ising model. In studies of the Ising model, the two-point correlation function is of interest, and serves as inspiration for the model investigated in this paper. We define our model and define a few quantities that will be useful.

1.1 The Ising model

Let $L \geq 1$. Consider the lattice $\Lambda := \{t = (t_1, t_2) \in \mathbb{Z}^2 : |t_i| \leq L, \forall i = 1, 2\}$. We call points in the lattice *sites*. With each site $i \in \Lambda$, we associate a *spin* $\sigma_i \in \{-1, 1\}$. A collection of spins in the lattice $\sigma = (\sigma_t)_{t \in \Lambda} \in \{-1, 1\}^\Lambda$ is called a *configuration*. Associate with each configuration $\sigma \in \{-1, 1\}^\Lambda$ an energy given by the Hamiltonian

$$H(\sigma) = - \sum_{x, y \in \Lambda} J(x, y) \sigma_x \sigma_y.$$

For an inverse temperature $\beta > 0$, define a probability measure on $\{-1, 1\}^\Lambda$ according to a Boltzmann distribution

$$\mathbb{P}_\beta(\sigma) = \frac{\exp(-\beta H(\sigma))}{\sum_{\sigma'} \exp(-\beta H(\sigma'))},$$

which we call the Ising model [14]. We denote by $\langle \cdot \rangle$ expectation with respect to this measure.

Define the set \mathcal{E} of edges on the lattice Λ as

$$\mathcal{E} := \left\{ \{t^1, t^2\} : t^1, t^2 \in \Lambda, \quad |t_1^1 - t_1^2| + |t_2^1 - t_2^2| = 1 \right\}.$$

A common simplification is to consider only nearest-neighbor interactions. Then we can express J in terms of edges $\{x, y\} \in \mathcal{E}$;

$$\begin{cases} J(x, y) = 0, & \text{if } \{x, y\} \notin \mathcal{E}, \\ J(x, y) = J(\{x, y\}), & \text{if } \{x, y\} \in \mathcal{E} \end{cases}$$

Making another common simplification, we set

$$J(e) = 1, \quad \forall e \in \mathcal{E}.$$

Let $\lambda : x \rightarrow y$ of length $n > 1$ be a sequence of edges (e_1, \dots, e_n) such that

$$\begin{aligned} e_i \cap e_{i+1} &\neq \emptyset, \\ e_i &\neq e_j, \quad \forall j \neq i, \\ x &\in e_1, \quad \text{and} \quad y \in e_n. \end{aligned}$$

Given a sequence $\lambda \subset \mathcal{E}$, let its *weight* be

$$w(\lambda) = \prod_{e \in \lambda} \tanh(\beta J(e))$$

For sites x, y in the lattice, a commonly asked question is: *how does σ_x and σ_y correlate?* As, for all $t \in \Lambda$, $\langle \sigma_t \rangle = 0$ by positive/negative symmetry, and

$$\langle (\sigma_t - \langle \sigma_t \rangle)^2 \rangle = \langle \sigma_t^2 \rangle - \langle \sigma_t \rangle^2 = 1,$$

we have that the correlation of σ_x and σ_y is given by

$$\langle \sigma_x \sigma_y \rangle,$$

which we call the two-point correlation function.

It can be shown that the two-point correlation function can be expressed as [10]

$$\langle \sigma_x \sigma_y \rangle = \sum_{\lambda: x \rightarrow y} w(\lambda) \frac{Z(\Lambda|\lambda)}{Z(\Lambda)},$$

for certain functions $Z(\Lambda)$ and $Z(\Lambda|\lambda)$.

For brevity, we define $a := \tanh \beta$. This gives the weight function

$$w(\lambda) = (\tanh \beta)^{|\lambda|} = a^{|\lambda|}.$$

We thus have

$$\langle \sigma_x \sigma_y \rangle = \sum_{\lambda: x \rightarrow y} a^{|\lambda|} \frac{Z(\Lambda|\lambda)}{Z(\Lambda)}. \tag{1.1}$$

Inspired by this, we will define a probability measure on connected edge sets where each edge set is weighted according to its size.

1.2 Our model

For $d = 2, 3, \dots$, let $\mathcal{E}(\mathbb{Z}^d)$ be the set of edges of the hypercubic \mathbb{Z}^d lattice. For a finite set $E \subseteq \mathcal{E}(\mathbb{Z}^d)$, we let the *boundary* of E , denoted ∂E , be the set of all vertices in \mathbb{Z}^d which are adjacent to an odd number of edges in E . We say that an edge $e \in E$ is *adjacent* to a point $x \in \mathbb{Z}^d$ if $x \in e$.

We say that an edge set E is *connected* if, for any two edges $e, f \in E$, there exists a sequence of edges $(e_i)_{i=1}^N$ such that

$$\begin{aligned} e_i &\in E, && \text{for all } i = 1, \dots, N, \\ e_1 = e, \quad e_N = f, &&& \text{and} \\ e_i \cap e_{i+1} &\neq \emptyset, && \text{for all } i = 1, \dots, N - 1. \end{aligned}$$

For $l = 0, 1, 2, \dots$, let $x = (0, \dots, 0) \in \mathbb{Z}^d$ and $y = (l, 0, \dots, 0) \in \mathbb{Z}^d$. For $l \geq 1$, let

$$\Omega(l) := \left\{ E \subseteq \mathcal{E}(\mathbb{Z}^d) : |E| < \infty, \partial E = \{x, y\}, E \text{ connected} \right\}.$$

We will frequently simply write Ω , leaving the dependence on l implicit. For $a > 0$, we will be interested in the measure $\mu_a : \Omega \rightarrow [0, 1]$ given by

$$\mu_a(\omega) := \frac{a^{|\omega|}}{Z},$$

where Z is the normalizing constant defined as

$$Z := Z(l) := \sum_{\omega \in \Omega(l)} a^{|\omega|}.$$

Although we are primarily interested in distinct x and y (that is: $l > 0$), some results will extend to the case when $x = y$, corresponding to $l = 0$. We define

$$\begin{aligned} \Omega(0) = \{E \subseteq \mathcal{E}(\mathbb{Z}^d) : \\ & |E| < \infty, \\ & \partial E = \emptyset, \\ & E \text{ connected}, \\ & \exists e \in E : e \text{ adjacent to } x\}. \end{aligned}$$

For $k = 0, 1, \dots$, and $l \geq 0$, let

$$\Omega_k(l) := \{\omega \in \Omega(l) : |\omega| = k\}.$$

Then, for any $k_1 \neq k_2$, we have $\Omega_{k_1} \cap \Omega_{k_2} = \emptyset$ and

$$\Omega = \bigcup_{k=0}^{\infty} \Omega_k.$$

This is useful, as

$$\sum_{\omega \in \Omega} a^{|\omega|} = \sum_{k=0}^{\infty} \sum_{\omega \in \Omega_k} a^{|\omega|} = \sum_{k=0}^{\infty} \sum_{\omega \in \Omega_k} a^k = \sum_{k=0}^{\infty} |\Omega_k| a^k. \quad (1.2)$$

We use this observation frequently throughout the rest of this work.

1.3 Outline

In Chapter 2, we establish some basic results about edge sets that we make use of later. In Chapter 3, we investigate for which a the probability measure μ_a is well-defined, and make a comparison with the critical temperature in the Ising model. In Chapter 4, we describe how we simulate from the distribution described by μ_a and analyze the results of the simulations.

2

Basic results

In graph theory, a *walk* is some sequence of edges $(e_i)_{i=1}^N$ such that

$$e_i \cap e_{i+1} \neq \emptyset, \quad \text{for all } i = 1, \dots, N - 1.$$

A *trail* is a walk where all edges are distinct. A *path* is a trail where all nodes are distinct.

Our first lemma describes how trails and elements of Ω relate to each other.

Lemma 1. *Any edge set $\omega \in \Omega$ can be represented as a trail; for every $\omega \in \Omega$, there exists at least one trail whose set of edges is ω and whose endpoints are x and y .*

Proof. We prove this constructively. Let $\omega \in \Omega$ and $N := |\omega| + 1$. The following procedure constructs trail, whose set of edges is ω , as represented by a node sequence n_0, \dots, n_N .

1. Let $n_0 := x$, $\omega_0 := \omega$ and $\lambda_0 := \emptyset$. Assign $i \leftarrow 0$.
2. Assign $i \leftarrow i + 1$. Take e' arbitrarily from $\{e \in \omega_{i-1} : n_{i-1} \in e\}$. Assign n_i to be the node such that $\{n_{i-1}, n_i\} = e'$. Let $\omega_i := \omega_{i-1} \setminus \{e'\}$ and $\lambda_i := \lambda_{i-1} \cup \{e'\}$.
3. If $n_i \neq y$, go to Step 2.
4. If $\omega_i = \emptyset$, terminate.
5. Assign m_0 to be an arbitrary node from

$$\{n : \exists e \in \omega_i, e' \in \lambda_i : n \in e \cap e'\}.$$

Since ω is connected, we know that such a node must exist.

6. Assign $k^* \leftarrow \max\{k : n_k = m_0\}$, $i^* \leftarrow i$ and $j \leftarrow 0$.
7. Assign $i \leftarrow i + 1$ and $j \leftarrow j + 1$. Take e' arbitrarily from $\{e \in \omega_{i-1} : m_{j-1} \in e\}$. Assign m_j to be the node such that $\{m_{j-1}, m_j\} = e'$. Let $\omega_i := \omega_{i-1} \setminus \{e'\}$ and $\lambda_i := \lambda_{i-1} \cup \{e'\}$.
8. If $m_j \neq m_0$, go to Step 7.
9. Assign

$$(n_{k^*+1}, \dots, n_i) \leftarrow (m_1, \dots, m_j, n_{k^*+1}, \dots, n_{i-j}).$$

Go to Step 4.

The idea behind the procedure is to first find some trail whose edges λ form a subset of ω . Then, for every edge $e \in \omega \setminus \lambda$ there exists a cycle in $\omega \setminus \lambda$ containing e . We find an arbitrary point m where such a cycle touches the trail, and find a trail within the cycle that goes from m back to m . This new trail we then insert into the old trail. We repeat this as many times as needed, until all edges in the edge set are part of the trail. \square

By Lemma 1, we know that for any k , the number of different trails of length k is at least $|\Omega_k|$. To expand on this, we formulate the following proposition.

Proposition 2. *Let $d \in \{2, 3, \dots\}$, and $k \in \{0, 1, \dots\}$. For $p, q \in \mathbb{Z}^d$, denote by $W_k(p, q)$ the set of walks of length k starting in p and ending in q , and by $T_k(p, q)$ and $P_k(p, q)$ the corresponding sets of trails and paths, respectively. Then we have*

$$\left| \bigcup_{q \in \mathbb{Z}^d} W_k(x, q) \right| \geq \left| \bigcup_{q \in \mathbb{Z}^d} T_k(x, q) \right| \geq |T_k(x, y)| \geq |\Omega_k| \geq |P_k(x, y)|. \quad (2.1)$$

Proof. Consider (2.1). The first inequality follows by definition, since every trail is a walk. The second inequality follows by the fact that $y \in \mathbb{Z}^d$. The third inequality is the statement of Lemma 1.

To see the final inequality of (2.1), denote by λ the edge set of an arbitrary path in $P_k(x, y)$. Then $|\lambda| = k < \infty$, $\partial\lambda = \{x, y\}$ and λ is connected; hence $\lambda \in \Omega$. This describes an injection from $P_k(x, y)_k$ to Ω_k , and hence the inequality follows. \square

The following result is very simple and has probably been shown before, but we state it here for completeness, as we shall rely on it later.

Proposition 3. *Let $l \in \{0, 1, \dots\}$. We have*

$$\begin{aligned} \bigcup_{k=1}^{\infty} \Omega_{l+2k-1}(l) &= \emptyset, \quad \text{and} \\ \bigcup_{k=1}^{\infty} \Omega_{l+2k}(l) &= \Omega(l); \end{aligned}$$

all trails between x and y have the same parity of length, which is the parity of l .

Proof. Let $d \in \{2, 3, \dots\}$. Assume $\omega \in \Omega(l)$ in d dimensions, and let $N := |\omega| + 1$. Consider a node sequence representation n_0, \dots, n_N of a trail whose edge set is ω . Such a trail must exist according to Lemma 1. Let e_1, \dots, e_d be the standard basis vectors in d dimensions. For $j = 1, \dots, d$, let

$$m_j^+ := \sum_{i=0}^{N-1} \mathbb{1}\{e_{i+1} - e_i = e_j\}, \quad \text{and} \quad m_j^- := \sum_{i=0}^{N-1} \mathbb{1}\{e_{i+1} - e_i = -e_j\}.$$

Then

$$\sum_{j=1}^d m_j^+ + m_j^- = |\omega|.$$

We have

$$l \cdot e_1 = y = n_N = \sum_{j=1}^d (m_j^+ - m_j^-) e_j.$$

Hence

$$\begin{aligned} m_1^+ - m_1^- &= l, \quad \text{and} \\ m_j^+ - m_j^- &= 0, \quad \text{for } j = 2, \dots, d. \end{aligned}$$

Thus

$$|\omega| = \sum_{j=1}^d m_j^+ + m_j^- = l + 2m_1^- + \sum_{j=2}^d 2m_j^+,$$

which proves that for any $\omega \in \Omega(l)$, the parity of $|\omega|$ is that of l . \square

Here follow a few lemmas regarding the boundary of edge sets. These results have probably been shown before, but we state them here for completeness, as we shall use them later.

Lemma 4. *For any $d = 2, 3, \dots$, let $\gamma_1, \gamma_2 \subseteq E(\mathbb{Z}^d)$ be such that $\gamma_1 \cap \gamma_2 = \emptyset$. Then*

$$\partial(\gamma_1 \cup \gamma_2) = \partial\gamma_1 \Delta \partial\gamma_2,$$

where Δ denotes symmetric set difference.

Proof. Assume $a \in \partial\gamma_1 \cap \partial\gamma_2$. Then there is an odd number of edges adjacent to a in both γ_1 and γ_2 . Since γ_1 and γ_2 are disjoint, there is an even number of edges adjacent to a in $\gamma_1 \cup \gamma_2$, so $a \notin \partial(\gamma_1 \cup \gamma_2)$.

Assume $b \in \partial\gamma_1 \setminus \partial\gamma_2$. Then there is an odd number of edges in γ_1 that are adjacent to b and an even number of such edges in γ_2 . Hence $b \in \partial(\gamma_1 \cup \gamma_2)$.

Analogously,

$$c \in \partial\gamma_2 \setminus \partial\gamma_1 \implies c \in \partial(\gamma_1 \cup \gamma_2).$$

Assume $e \notin \partial\gamma_1 \cup \partial\gamma_2$. Then there must be an even number of edges adjacent to e in both γ_1 and γ_2 . Hence $e \notin \partial(\gamma_1 \cup \gamma_2)$.

This characterizes symmetric set difference, so we are done. \square

Lemma 5. *For any $d = 2, 3, \dots$, let $\gamma_1, \gamma_2 \subseteq E(\mathbb{Z}^d)$ be such that $\gamma_1 \cap \gamma_2 = \emptyset$. Then*

$$\partial\gamma_1 \cap \partial\gamma_2 = \emptyset \iff \partial(\gamma_1 \cup \gamma_2) = \partial\gamma_1 \cup \partial\gamma_2. \quad (2.2)$$

Proof. By Lemma 4,

$$\partial(\gamma_1 \cup \gamma_2) = \partial\gamma_1 \Delta \partial\gamma_2 = (\partial\gamma_1 \cup \partial\gamma_2) \setminus (\partial\gamma_1 \cap \partial\gamma_2).$$

Now see that \implies in (2.2) follows immediately. To see \impliedby , assume

$$(\partial\gamma_1 \cup \partial\gamma_2) \setminus (\partial\gamma_1 \cap \partial\gamma_2) = \partial\gamma_1 \cup \partial\gamma_2.$$

This implies

$$(\partial\gamma_1 \cup \partial\gamma_2) \cap (\partial\gamma_1 \cap \partial\gamma_2) = \emptyset,$$

but of course

$$(\partial\gamma_1 \cap \partial\gamma_2) \subseteq (\partial\gamma_1 \cup \partial\gamma_2).$$

Hence $\partial\gamma_1 \cap \partial\gamma_2 = \emptyset$. We are done. \square

Lemma 6. *For any $d = 2, 3, \dots$, if $\omega \subset E(\mathbb{Z}^d)$ such that $|\omega| = N < \infty$, then $|\partial\omega|$ is even.*

Proof. First note that if $|A|$ and $|B|$ are even, then $|A \Delta B|$ is even. To see this, let $m = |A \setminus B|$, $n = |B \setminus A|$ and $k = |A \cap B|$. Since both $m + k$ and $n + k$ are even, all three of k , m , and n must have the same parity. Thus $|A \Delta B| = m + n$ must be even.

Denote by e_1, \dots, e_N the edges in γ . We have for all $i = 1, \dots, N$,

$$|\partial\{e_i\}| = 2,$$

which is even.

2. Basic results

Let $\omega_1 := \{e_1\}$ and

$$\omega_i := \omega_{i-1} \cup \{e_i\}, \quad \text{for } i = 2, 3, \dots, N,$$

then $\omega_N = \omega$. Note that $|\partial\omega_i|$ is even. By Lemma 4, we know that, for $i = 2, \dots, N$

$$\partial\omega_i = \partial(\omega_{i-1} \cup \{e_i\}) = \partial\omega_{i-1} \Delta \partial\{e_i\}.$$

For $i = 2$, if $|\partial\omega_{i-1}|$ is even, then

$$|\partial\omega_i| = |\partial\omega_{i-1} \Delta \partial\{e_i\}|$$

is even. We have thus proved our claim by induction. □

3

Well-definedness of μ_a

In this chapter, we investigate for which $a \in (0, 1)$ the measure μ_a is a well-defined probability measure. For μ_a to be a well-defined probability measure is equivalent to

$$\sum_{\omega \in \Omega} a^{|\omega|} < \infty. \quad (3.1)$$

We shall use the inequality (3.1) as a criterion on a to determine well-definedness of μ_a .

As the power series on the left-hand side of (3.1) is increasing in a , there must exist

$$a_d^* := \sup \left\{ a : \sum_{\omega \in \Omega(l)} a^{|\omega|} < \infty \right\}.$$

In this chapter, we will show that a^* does not depend on l , and also establish

- lower bounds L_d such that $a_d^* > L_d$ (or $a_d^* \geq L_d$) and
- upper bounds U_d such that $a_d^* < U_d$ (or $a_d^* \leq U_d$).

An important result in this chapter is the following.

Theorem 7. *For $d = 2, 3, \dots$, the constant a_d^* does not depend on l .*

With the help of Theorem 7, the results in this chapter culminate in the following result, which is a combination of the statements of Corollary 13 and Proposition 14. For $d = 2$ and $d = 3$, we give slightly better numerical lower bounds in the end of Section 3.1.

Theorem 8. *For $d = 2, 3, \dots$,*

$$\frac{1}{2d-1} < a_d^* \leq \frac{1}{d}.$$

To prove Theorem 7, we need the following lemma.

Lemma 9. *Let $l \geq 0$ and $k \geq l$. Let*

$$A_k(l) := (2 + 2k) \cdot |\Omega_{k-1}(l)| + (2 + k) \cdot |\Omega_{k+1}(l)| + (1 + k) \cdot |\Omega_{k+3}(l)|.$$

Then

$$\Omega_k(l) \leq A_k(l+1), \text{ for } l = 0, 1, 2, \dots \quad (3.2)$$

and

$$\Omega_k(l) \leq A_k(l-1), \text{ for } l = 1, 2, \dots \quad (3.3)$$

Proof. We will only prove (3.2) as (3.3) will follow analogously. Let $l \geq 0$ and $k \geq l$. We will show (3.2) by partitioning $\Omega_k(l)$ into subsets B_k^0, \dots, B_k^4 and for each such subset finding an injective mapping onto either $\Omega_{k-1}(l+1)$, $\Omega_{k+1}(l+1)$ or $\Omega_{k+3}(l+1)$. As we shall see, there exist rather simple such mappings, but some finesse is required to show that each mapping preserves connectivity. Recall that $y = (l, 0, \dots, 0) \in \mathbb{Z}^d$ and let $y' = (l+1, 0, \dots, 0) \in \mathbb{Z}^d$.

Let $\omega \in \Omega(l)$ and $\omega' \in \Omega(l+1)$. Then $\partial\omega = \{x, y\}$ and $\partial\omega' = \{x, y'\}$. Hence, any mapping from (a subset of) $\Omega(l)$ to $\Omega(l+1)$ will change the parity of the number of edges adjacent to each of y and y' . By Lemma 4, if $E \subset E(\mathbb{Z}^d)$ and $\partial E = \{y, y'\}$, then

$$\partial(\omega \Delta E) = \{x, y'\}.$$

Further, symmetric difference with respect to any set is an injective mapping. Hence, if we, given some $E \subset E(\mathbb{Z}^d)$, with $|E| < \infty$ and $\partial E = \{y, y'\}$, assert that $\omega \Delta E$ is connected, for all ω in some subset $\Omega_k^*(l)$ of $\Omega_k(l)$, then $\omega \mapsto \omega \Delta E$ is an injective mapping from $\Omega_k^*(l)$ to some subset of $\Omega(l+1)$.

Consider the plaquette with vertices $y, y', z = (l, 1, 0, \dots, 0)$ and $z' = (l+1, 1, 0, \dots, 0)$. Denote by $P(\omega)$ the edges surrounding this plaquette that are present in ω , so that

$$P(\omega) = \{\{y, y'\}, \{y, z\}, \{y', z'\}, \{z, z'\}\} \cap \omega.$$

Let

$$B_k^0(l) := \{\omega \in \Omega_k(l) : \{y, y'\} \notin \omega\},$$

$$B_k^j(l) := \{\omega \in \Omega_k(l) : \{y, y'\} \in \omega, \text{ and } |P(\omega)| = j\}, \quad \text{for } j = 1, 2, 3, 4.$$

Then $\Omega_k(l) = \cup_{j=0}^4 B_k^j$. We will bound each B_k^j to construct the bound (3.2) for $\Omega_k(l)$.

Claim: We have $|B_k^0(l)| \leq |\Omega_{k+1}(l+1)|$.

Proof: The mapping

$$\omega \mapsto \omega \cap \{\{y, y'\}\}, \quad \text{which is equivalent to } \omega \mapsto \omega \Delta \{\{y, y'\}\},$$

is clearly injective from $B_k^0 \subset \Omega_k(l)$ to $\Omega_{k+1}(l+1)$. A sketch of the procedure is shown in Figure 3.1. ■

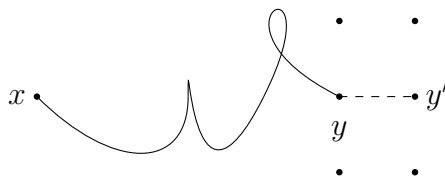


Figure 3.1: Transforming an edge set in $B_0^k = \{\omega \in \Omega_k(l) : \{y, y'\} \notin \omega\}$ to one in $\Omega_{k+1}(l+1)$.

Consider now $\omega \in \Omega_k(l)$ such that $\{y, y'\} \in \omega$. Given that that the edge $\{y, y'\}$ is present in the edge sets ω we are considering, there are eight possible $P(\omega)$. We

partition $\Omega_k(l) \setminus B_k^0$, into B_k^1, \dots, B_k^4 according to

$$B_k^i := \{\omega \in \Omega_k(l) \setminus B_k^0 : |P(\omega)| = i\}.$$

We shall also have use of partitioning B_k^3 into

$$\begin{aligned} \dot{B}_k^3 &:= \{\omega \in B_k^3 : \{\{z, z'\} \notin \omega\}\}, \quad \text{and} \\ \ddot{B}_k^3 &:= \{\omega \in B_k^3 : \{\{z, z'\} \in \omega\}\}. \end{aligned}$$

The possible states of $P(\omega)$ and the partitioning based thereupon are shown in Figure 3.2.

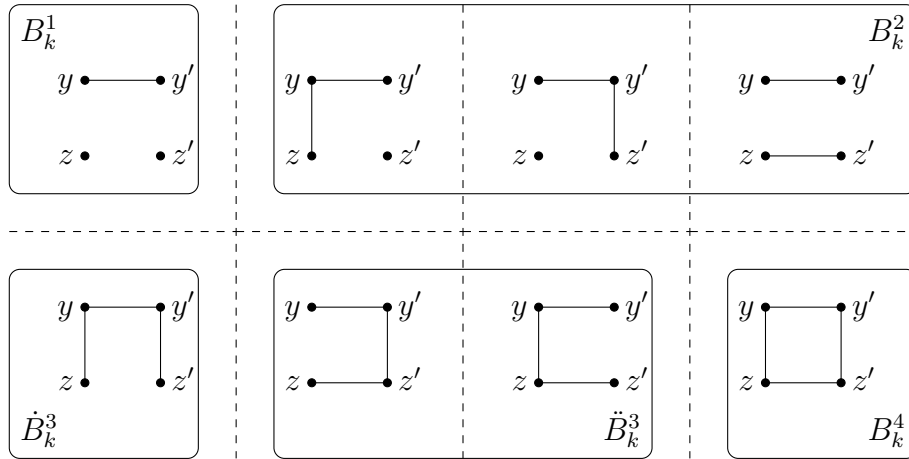


Figure 3.2: The eight possible combinations of edges in an edge set ω in a plaquette adjacent to $\{y, y'\}$, given that $\{y, y'\} \in \omega$. We show the vertical axis as increasing downwards.

Claim: We have

$$\begin{aligned} |B_k^1| &\leq |\Omega_{k+3}(l+1)|, \\ |B_k^2| &\leq |\Omega_{k+1}(l+1)|, \quad \text{and} \\ |B_k^4| &\leq |\Omega_{k-1}(l+1)|. \end{aligned}$$

Proof: Let $M := \{\{y, z\}, \{y', z'\}, \{z, z'\}\}$. Then $\partial M = \{y, y'\}$. In Figure 3.3, we display simple local modifications that illustrate the injective mappings

- from B_k^2 to $\Omega_{k+3}(l+1)$:

$$\omega \mapsto \omega \Delta M,$$

- from B_k^3 to $\Omega_{k+1}(l+1)$:

$$\omega \mapsto \omega \Delta M,$$

and

- from B_k^4 to $\Omega_{k-1}(l+1)$:

$$\omega \mapsto \omega \Delta \{\{y, y'\}\}.$$

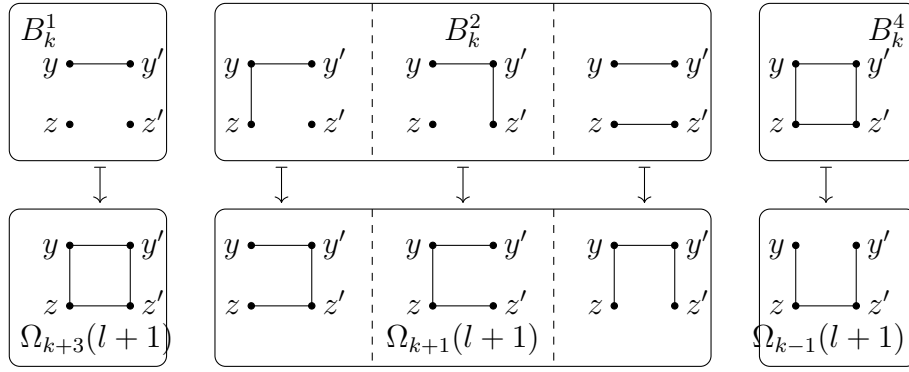


Figure 3.3: Local modifications to injectively transform edge sets in B_k^2 , B_k^3 and B_k^4 into edge sets in $\Omega(l+1)$.

As can readily be seen, these mappings are injective, preserve connectivity and change the parity of number of edges adjacent to each of y and y' . \blacksquare

Claim: We have $|\dot{B}_k^3| \leq |\Omega_{k-1}(l+1)|$.

Proof: For every $\omega \in \dot{B}_k^3$, we see that in $P(\omega)$, there are edges adjacent to y and one edge adjacent to each of z and w . Since $\partial\omega = \{x, y\}$, there must be an odd number of other edges in ω adjacent to the nodes y , z and z' , part of some subset of ω . For $i = 1, \dots, 5$, let γ_i , be maximal connected subsets of ω such that

$$\gamma_i \cap P(\omega) = \emptyset, \quad \forall i = 1, \dots, 5;$$

$$\begin{aligned} x &\in \partial\gamma_1, \\ y &\in \partial\gamma_2, \\ z &\in \partial\gamma_3, \\ z' &\in \partial\gamma_4, \text{ and} \\ \exists e \in \gamma_5 : y' &\in e \end{aligned}$$

as illustrated in Figure 3.4.

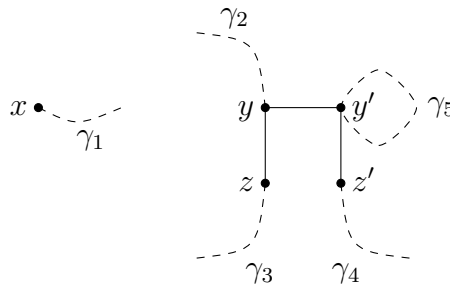


Figure 3.4: General structure of edge sets in \dot{B}_k^3 . For $i = 1, \dots, 5$, each γ_i is maximal and connected.

Let

$$\bar{\gamma} := \bigcup_{i=1}^5 \gamma_i.$$

Then

$$\omega = P(\omega) \cup \bar{\gamma}$$

and, by Lemma 4, we have

$$\partial\bar{\gamma} = \{x, y, z, z'\}, \quad \text{since} \quad \partial P(\omega) = \{z, z'\}.$$

We claim now that

$$\forall i \in \{1, 2, 3, 4\} \quad \exists j \in \mathcal{J}_i := \{1, 2, 3, 4\} \setminus \{i\} : \quad \gamma_i = \gamma_j. \quad (3.4)$$

We will prove this by contradiction; assume instead for some $i \in \{1, 2, 3, 4\}$ that

$$\partial\gamma_i \cap \partial\gamma_j = \emptyset, \quad \text{for all } j \in \mathcal{J}_i. \quad (3.5)$$

This implies that

$$\partial\gamma_i \cap \partial \bigcup_{j \in \mathcal{J}_i} \gamma_j = \emptyset.$$

Hence, by Lemma 5,

$$\{x, y, z, z'\} = \partial\gamma_i \cup \partial \bigcup_{j \in \mathcal{J}_i} \gamma_j.$$

Thus, since we, by Lemma 6, know that $|\partial\gamma_i|$ is an even number, $\partial\gamma_i$ must contain at least two elements of $\{x, y, z, z'\}$. For any $j \in \mathcal{J}_i$, $\partial\gamma_j$ contains at least one element of $\{x, y, z, z'\}$, hence our assumption (3.5) cannot hold; we realize that for every $i = 1, 2, 3, 4$, there must exist some $j \in \mathcal{J}_i$ such that $\partial\gamma_i \cap \partial\gamma_j \neq \emptyset$. Since each γ_i is maximal, this implies (3.4).

We can partition elements in \dot{B}_k^3 into a few cases;

1. if $\gamma_1 = \gamma_2$, then $\gamma_3 = \gamma_4$.
2. if $\gamma_1 \neq \gamma_2$, then either
 - $\gamma_1 = \gamma_3$ and $\gamma_2 = \gamma_4$, or
 - $\gamma_1 = \gamma_4$ and $\gamma_2 = \gamma_3$.

We can use these cases to construct an injective mapping from \dot{B}_k^3 to $\Omega_{k-1}(l+1)$, according to

$$\omega \mapsto \begin{cases} \omega \Delta \{\{y, y'\}\}, & \text{if } \gamma_1 = \gamma_2, \\ \omega \Delta M, & \text{otherwise,} \end{cases} \quad (3.6)$$

as illustrated in Figure 3.5. ■

Claim: We have

$$\ddot{B}_k^3 \leq (2 \cdot |\Omega_{k-1}(l+1)| + |\Omega_{k+1}| + |\Omega_{k+3}|) \cdot k.$$

Proof: The case \ddot{B}_k^3 needs to be handled quite differently from the previous cases. For $n = 1, 2, \dots$, let $y_n = (l, n, 0, \dots, 0)$ and $y'_n = (l+1, n, 0, \dots, 0)$. For $n = 1, 2, \dots$, let $P_n(\omega)$ be the sequence of plaquettes such that

$$P_n(\omega) = \left\{ \{y_n, y'_n\}, \{y_n, y_{n+1}\}, \{y'_n, y'_{n+1}\}, \{y_{n+1}, y'_{n+1}\} \right\} \cap \omega.$$

Let

$$N := N(\omega) := \min_n \left\{ n : |P_n(\omega)| \neq 3, \text{ or } \left\{ \{y_n, y_{n+1}\}, \{y'_n, y'_{n+1}\} \right\} \subset P_n(\omega) \right\},$$

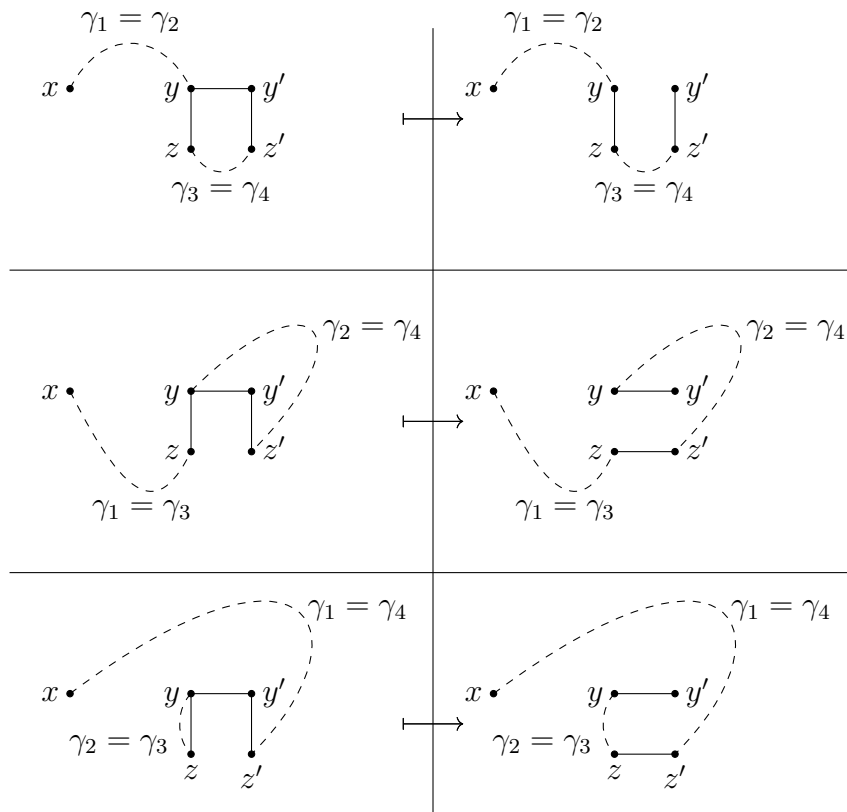


Figure 3.5: Injective mapping from \dot{B}_k^3 to $\Omega_{k-1}(l+1)$. Note that connectivity is preserved.

as illustrated in Figure 3.6. Let

$$\ddot{B}_3^{k,n} := \{\omega \in \ddot{B}_3^k : N(\omega) = n\}, \quad \forall n = 1, 2, \dots$$

For $\omega \in \ddot{B}_3^k$, we must have $N \leq k$. Hence,

$$|\ddot{B}_3^k| = \sum_{n=1}^k |\ddot{B}_3^{k,n}|. \quad (3.7)$$

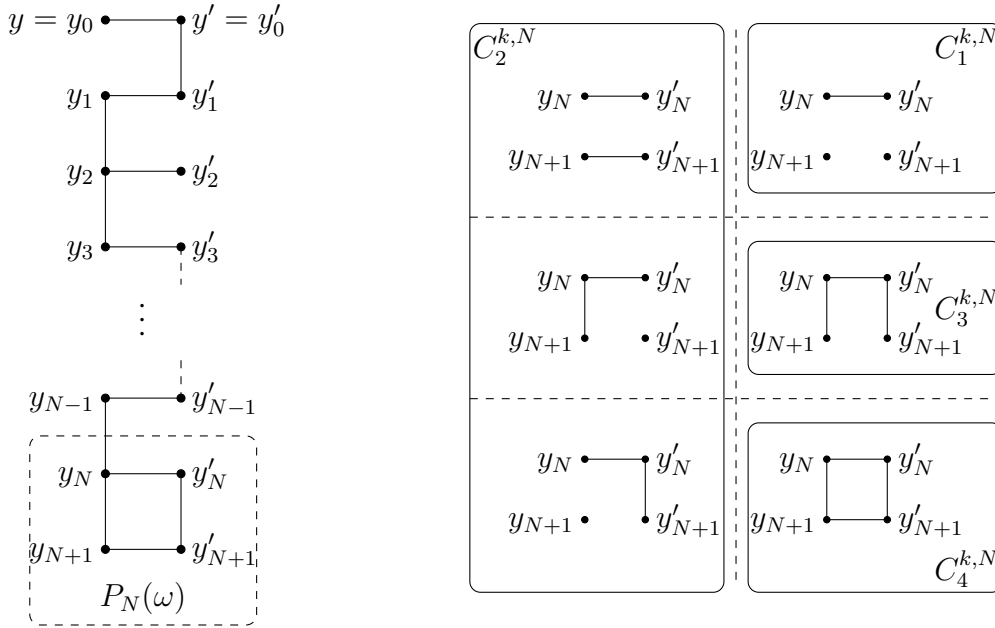


Figure 3.6: Example structure of an edge set in \ddot{B}_3^k .

Figure 3.7: The six possible combinations of edges in $P_N(\omega)$. We divide these into cases numbered 1 through 4.

For each $n = 1, 2, \dots$, we will treat each edge set ω in $\ddot{B}_3^{k,n}$ based on the size of $P_n(\omega)$. For $i = 1, 2, 3, 4$, and $n = 1, 2, \dots$, let

$$C_i^{k,n} := \{\omega \in \ddot{B}_3^{k,n} : |P_N(\omega)| = i\}.$$

For $n = 1, 2, \dots$, let

$$M_n := \{\{y_n, y_{n+1}\}, \{y'_n, y'_{n+1}\}, \{y_{n+1}, y'_{n+1}\}\}, \quad \text{and}$$

$$\xi_n := \left(\bigcup_{j=1}^n \{\{y_{j-1}, y_j\}\} \right) \cup \left(\bigcup_{j=1}^n \{\{y'_{j-1}, y'_j\}\} \right).$$

We see that $\partial(\xi_n \cup M_n) = \partial(\xi_n \cup \{\{y_n, y'_n\}\}) = \{y, y'\}$. The set ξ_n are the two lines of edges going from y and y' to y_N and y'_N , respectively. Symmetric set difference between $\omega \in \ddot{B}_3^{k,n}$ and ξ_n "mirrors" the structure between y and y'_N , as seen in Figure 3.8. This preserves connectivity and, with a suitable modification to the edges in $P_N(\omega)$, maps from $\ddot{B}_3^{k,n}$ to $\Omega(l+1)$.

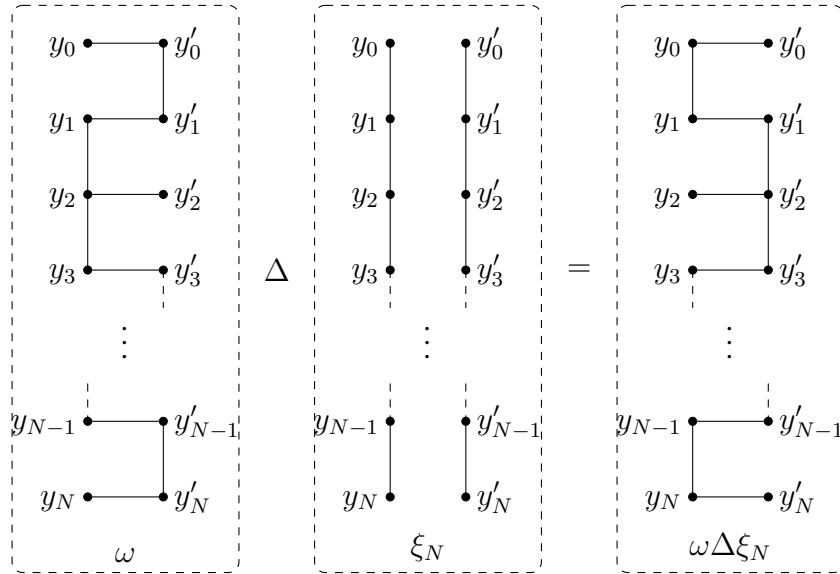


Figure 3.8: Example local structure of $\omega \in \check{B}_3^{k,N}$, and the mirroring undergone in symmetric difference with ξ_N .

The mappings

$$\begin{aligned} C_1^{k,n} \ni \omega &\mapsto \omega \Delta (\xi_n \cup M_n) \in \Omega_{k+3}(l+1), \\ C_2^{k,n} \ni \omega &\mapsto \omega \Delta (\xi_n \cup M_n) \in \Omega_{k+1}(l+1), \text{ and} \\ C_4^{k,n} \ni \omega &\mapsto \omega \Delta (\xi_n \cup \{\{y_n, y'_n\}\}) \in \Omega_{k-1}(l+1) \end{aligned}$$

are injective and preserve connectivity, for $n = 1, 2, \dots$

For $\omega \in C_3^{k,n}$, we employ a similar technique as for \check{B}_3^k . Let

$$(v, v') = \begin{cases} (y_N, y'_N), & \text{if } \{y_{N-1}, y_N\} \in \omega \\ (y'_N, y_N), & \text{otherwise.} \end{cases}$$

For $i = 1, \dots, 5$, let σ_i be maximal connected subsets of ω such that

$$\sigma_i \cap P_N(\omega) = \emptyset, \quad \forall i = 1, \dots, 5;$$

$$\begin{aligned} x &\in \partial\sigma_1, \\ v &\in \partial\sigma_2, \\ z &\in \partial\sigma_3, \\ w &\in \partial\sigma_4, \text{ and} \\ \exists e \in \sigma_5 : v' &\in e. \end{aligned}$$

Then

$$\omega \mapsto \begin{cases} \omega \Delta (\xi_n \cup \{\{y_n, y'_n\}\}), & \text{if } \sigma_1 = \sigma_2, \\ \omega \Delta (\xi_n \cup M_n), & \text{otherwise,} \end{cases} \quad (3.8)$$

is an injective mapping from $C_3^{k,n}$ to $\Omega_{k-1}(l+1)$. Hence, by (3.7), our claim follows. \blacksquare

Since

$$|\Omega_k(l)| = \sum_{i=1}^k |B_k^i|,$$

we conclude that

$$\begin{aligned} |\Omega_k(l)| &\leq (2 + 2k) \cdot |\Omega_{k-1}(l)| + \\ &\quad (2 + k) \cdot |\Omega_{k-1}(l)| + \\ &\quad (1 + k) \cdot |\Omega_{k+3}(l)|, \end{aligned}$$

which is what we set out to show. \square

Now we are ready to prove that a_d^* does not depend on l .

Proof of Theorem 7. For $l = 0, 1, \dots$, let

$$a_{d,l}^* := \sup \left\{ a : \sum_{\omega \in \Omega(l)} a^{|\omega|} < \infty \right\}.$$

By Lemma 9, we see that, for $l = 0, 1, \dots$, if $\alpha < a_{d,l+1}^*$ and $a < \alpha$,

$$\begin{aligned} \sum_{\omega \in \Omega(l)} a^{|\omega|} &= \sum_{k=1}^{\infty} |\Omega_k(l)| a^k \leq \\ &\leq \frac{1}{a} \sum_{k=1}^{\infty} (2 + 2k) \cdot |\Omega_{k+1}(l+1)| a^{k+1} + \\ &\quad + a \sum_{k=1}^{\infty} (2 + k) \cdot |\Omega_{k-1}(l+1)| a^{k-1} + \\ &\quad + \frac{1}{a^3} \sum_{k=1}^{\infty} (1 + k) \cdot |\Omega_{k+3}(l+1)| a^{k+3} < \\ &< \infty. \end{aligned}$$

Since α can be chosen arbitrarily close to $a_{d,l\pm 1}^*$ and a can be chosen arbitrarily close to α , we realize that, for $l = 0, 1, \dots$,

$$a_{d,l}^* \geq a_{d,l+1}^*.$$

Analogously, we can show that for $l = 1, 2, \dots$

$$a_{d,l}^* \geq a_{d,l-1}^*,$$

whence

$$a_{d,0}^* = a_{d,1}^* = a_{d,2}^* = \dots$$

Hence a_d^* does not depend on l . \square

3.1 Lower bounds for a_d^*

In this section, we prove, for all $k = 0, 1, \dots$, upper bounds on the number of trails of length k in $(\mathbb{Z}^d, \mathcal{E})$ starting in the origin. We thereby bound $|\Omega_k|$ from above, allowing us to find a such that

$$\sum_{k=1}^{\infty} |\Omega_k| a^k$$

must converge, thus establishing lower bounds on a_d^* .

Counting the number of walks in \mathbb{Z}^d , we can formulate a bound on a_d^* as in the following example.

Example 10. Let $d = 2, 3, \dots$. Then, by Proposition 2, we know that $|\Omega_k|$ is smaller than the number of walks starting in the origin in $(\mathbb{Z}^d, \mathcal{E})$ of length k , which is exactly $(2d)^k$. Therefore

$$\sum_{\omega \in \Omega} a^{|\omega|} \leq \sum_{k=1}^{\infty} 2da((2d-1)a)^{k-1}.$$

The sum on the right-hand side of the previous equation converges if and only if $(2d-1)a < 1$; hence μ_a is well-defined if $a < \frac{1}{2d-1}$. The result follows.

Let $d = 2, 3, \dots$. Then we have $a_d^* \geq \frac{1}{2d}$. To see this, we need to show that (3.1) is satisfied whenever $a < \frac{1}{2d}$. By (1.2), we have

$$\sum_{\omega \in \Omega} a^{|\omega|} = \sum_{k=1}^{\infty} |\Omega_k| a^k.$$

Now note that $|\Omega_k|$ is smaller than the number of walks of length k , which is $(2d)^k$. Therefore

$$\sum_{k=1}^{\infty} |\Omega_k| a^k \leq \sum_{k=1}^{\infty} (2da)^k.$$

The sum on the right-hand side of the previous equation converges if $2da < 1$, hence $a^* \geq \frac{1}{2d}$.

By the same similar principles as in Example 10, we can improve the example's lower bound on a_d^* as follows.

Proposition 11. *Let $d = 2, 3, \dots$. Then we have*

$$a_d^* \geq \frac{1}{2d-1}.$$

Proof. Let $d = 2, 3, \dots$ and $k = 0, 1, \dots$. Then, by Proposition 2, we know that $|\Omega_k|$ is smaller than the number of trails of length k in $(\mathbb{Z}^d, \mathcal{E})$ starting in the origin, which is at most $2d(2d-1)^{k-1}$, since after the first step in a trail, the trail is not allowed to double back on itself. Therefore

$$\sum_{\omega \in \Omega} a^{|\omega|} \leq \sum_{k=1}^{\infty} 2da((2d-1)a)^{k-1}.$$

The sum on the right-hand side of the previous equation converges if and only if $(2d-1)a < 1$; hence μ_a is well-defined if $a < \frac{1}{2d-1}$. The result follows. \square

Proposition 11 shows what bound for a_d^* we can attain by observing that out of the $2d$ directions a walk can turn to in each step, only at most $2d - 1$ give a trail that doesn't overlap itself. We can extend this idea by considering the number of ways there are to take several steps.

Proposition 12. *Let $a > 0$, $d \in \{2, 3, \dots\}$ and $m \in \{1, 2, \dots\}$. Assume that in d dimensions there are at most b_d^m different trails of length m . Then*

$$a_d^* \geq \sqrt[m-1]{\frac{2d}{b_d^m}}.$$

Proof. Note that any trail can be considered a concatenation of a collection of sub-trails. Let $k \in \{1, 2, 3, \dots\}$ and $m \in \{1, \dots, k\}$. Let $n(k)$ and $r(k) \in \{0, \dots, m - 2\}$ be such that $k = 1 + (m - 1)n(k) + r(k)$. Note that $n(k) = \lfloor k/m \rfloor$, and

$$\frac{n(k)}{k} \xrightarrow{k \rightarrow \infty} \frac{1}{m-1}, \quad \text{and} \quad \frac{r(k)}{k} \xrightarrow{k \rightarrow \infty} 0.$$

We realize that any trail of length k can be represented as an edge sequence

$$e_{m-1}^0, e_1^1, \dots, e_{m-1}^1, \dots, e_1^{n(k)}, \dots, e_{m-1}^{n(k)}, e'_1, \dots, e'_{r(k)}.$$

For $i = 1, \dots, n(k)$, define the trails

$$\lambda_i = (e_{m-1}^{i-1}, e_1^i, \dots, e_{m-1}^i).$$

Constructing a trail starting in the origin edge by edge, there are $2d$ ways of choosing the first edge, which we call e_{m-1}^0 . Then for each $i = 1, \dots, n(k)$ there are, by our assumption, at most

$$\frac{b_d^m}{2d}$$

ways of choosing λ_i , since the first edge is already given. For each $i = 1, \dots, r(k)$, there are at most $2d$ ways of choosing e'_i . Therefore there are at most

$$(2d)^{r(k)+1} \left(\frac{b_d^m}{2d} \right)^{n(k)}$$

different trails in d dimensions.

Hence, by Proposition 2, we can write for any k ,

$$|\Omega_k| \leq (2d)^{r(k)+1} \left(\frac{b_d^m}{2d} \right)^{n(k)}.$$

We have

$$\lim_{k \rightarrow \infty} \sqrt[k]{|\Omega_k| a^k} \leq \lim_{k \rightarrow \infty} \sqrt[k]{(2d)^{r(k)+1} \left(\frac{b_d^m}{2d} \right)^{n(k)}} a = \left(\frac{b_d^m}{2d} \right)^{m-1} a,$$

wherefore

$$\sum_{k=1}^{\infty} |\Omega_k| a^k$$

converges by the root criterion if

$$a < \sqrt[m-1]{\frac{2d}{b_d^m}},$$

which is to say that

$$a_d^* \geq \sqrt[m-1]{\frac{2d}{b_d^m}}.$$

□

Using Proposition 12, we can immediately improve on the result of Proposition 11 ever so slightly.

Corollary 13. *Let $d = 2, 3, \dots$. We have*

$$a_d^* > \frac{1}{2d-1}.$$

Proof. Let $d = 2, 3, \dots$. In d dimensions, there are

$$b_d^5 = 2d \cdot (2d-1)^4 - 4d \cdot (d-1) \tag{3.9}$$

different trails of length 5. To see this, note that there are $2d \cdot (2d-1)^4$ walks of length 5 that don't double back on themselves (compare the argument in Proposition 11. Further, the last step overlaps the first step in $4d \cdot (d-1)$ of these walks, hence (3.9).

Therefore, by Proposition 12,

$$a_d^* \geq \sqrt[4]{\frac{2d}{2d \cdot (2d-1)^4 - 4d \cdot (d-1)}} > \frac{1}{2d-1},$$

which is what we set out to show. □

The question of how many different trails there are in a lattice is called the *self-avoiding trail* problem and is of interest in statistical physics and polymer physics [4]. In the self-avoiding trail problem, one typically considers any trail starting in the origin, without any condition on its endpoint. The mean squared end-to-end displacement of trails is often investigated.

In Table 3.1, we give the number of trails in two and three dimensions, and what bound these imply for a_d^* according to Proposition 12.

Table 3.1: For $d = 2, 3$, upper bounds on number of trails of length m , and the resulting lower bound on a_d^* according to Proposition 12.

d	2	3
m	31	15
b_d^m	121 181 822 490 084 [2]	30 399 142 614 [5]
Lower bound for a_d^*	0.3553	0.2026

3.2 Upper bounds for a_d^*

In this section, we prove, by construction, for any $k = 0, 1, \dots$, lower bounds on the number of paths from x to y of length $l + 2k$. We thereby bound $|\Omega_{l+2k}|$ from below, allowing us to find a such that

$$\sum_{k=1}^{\infty} |\Omega_k| a^k$$

cannot converge, thus establishing upper bounds on a_d^* .

The main result of this section is the following proposition. We delay the proof until the end of the section, to first illustrate the ideas behind the proof in simpler examples.

Proposition 14. *Let $a > 0$. The measure μ_a is not well-defined if*

$$a \geq \frac{1}{d};$$

that is: $a_d^* \leq 1/d$.

In our first example, we construct a proof that

$$a_d^* \leq \frac{1}{\sqrt{d-1}}$$

by describing a very limited family of paths from x to y .

Example 15. Let $k = 0, 1, \dots$. We can construct paths from x to y of length $l + 2k$ as a sequence of nodes n_0, \dots, n_{l+2k} as follows. Denote by e_1, \dots, e_d the standard basis vectors in d dimensions. Take $(u_i)_{i=1}^k \in \{e_2, \dots, e_d\}^k$. We now construct a path as follows.

1. Let $n_0 = x$.
2. For $i = 1, \dots, k$, let $n_i = n_{i-1} + u_i$
3. For $i = k + 1, \dots, k + l$, let $n_i = n_{i-1} + e_1$.
4. For $i = l + k + 1, \dots, l + 2k$, let $n_i = n_{i-1} - u_{l+2k+1-i}$.

We have

$$n_{l+2k} = x + \sum_{i=1}^k u_i + l \cdot e_1 - \sum_{i=1}^k u_{l+2k+1-i} = x + l \cdot e_1 = y,$$

as required. For any $l > 1$, the path described has no overlap. For $k = 0, 1, \dots$, since there are $(d-1)^k$ choices for $(u_i)_{i=1}^k$, and each path of length $l + 2k$ corresponds to one element of Ω_{l+2k} , we have

$$|\Omega_{l+2k}| \geq (d-1)^k.$$

Hence, using Proposition 3,

$$\sum_{\omega \in \Omega} a^{|\omega|} = a^l \sum_{k=0}^{\infty} |\Omega_{l+2k}| a^{2k} \geq a^l \sum_{k=0}^{\infty} ((d-1)a^2)^k. \quad (3.10)$$

The right hand side of (3.10) does not converge if

$$a \geq \frac{1}{\sqrt{d-1}},$$

and so

$$a_d^* \leq \frac{1}{\sqrt{d-1}}.$$

In the following example, we improve on the result of the last example by allowing more freedom in the construction of the path.

Example 16. Let $k = 0, 1, \dots$. We can construct paths from x to y of length $l + 2k$ as a sequence of nodes n_0, \dots, n_{l+2k} as follows. Take $(m_j)_{j=2}^d \in \mathbb{Z}_{\geq 0}^{d-1}$ such that

$$\sum_{j=2}^d m_j = k.$$

Take $(u_i)_{i=1}^k \in \{e_2, \dots, e_d\}^k$ and, independently, $(v_i)_{i=1}^k \in \{2, \dots, d\}^k$ such that

$$\sum_{i=1}^k \mathbb{1}\{u_i = e_j\} = \sum_{i=1}^k \mathbb{1}\{v_i = e_j\} = m_j, \quad \forall j = 2, \dots, k.$$

We now construct a path as follows.

1. Let $n_0 = x$.
2. For $i = 1, \dots, k$, let $n_i = n_{i-1} + u_i$
3. For $i = k + 1, \dots, k + l$, let $n_i = n_{i-1} + e_1$.
4. For $i = l + k + 1, \dots, l + 2k$, let $n_i = n_{i-1} - v_{l+2k+1-i}$.

We have

$$\begin{aligned} n_{l+2k} &= x + \sum_{i=1}^k u_i + l \cdot e_1 - \sum_{i=1}^k v_i = x + \sum_{j=2}^d m_j e_j + l \cdot e_1 - \sum_{j=2}^d m_j e_j = \\ &= x + l \cdot e_1 = y, \end{aligned}$$

as required. For any $l > 1$, the path described has no overlap. Given m_2, \dots, m_d , there are¹,

$$\binom{k}{m_2, \dots, m_d}$$

ways of choosing $(u_i)_{i=1}^k$, and the same number of ways of choosing $(v_i)_{i=1}^k$. Hence, there are

$$\sum_{\substack{m_2, \dots, m_d = k \\ m_2, \dots, m_d \geq 0}} \binom{k}{m_2, \dots, m_d}^2$$

different paths that can be constructed in this manner.

We have [11]

$$\sum_{\substack{m_2, \dots, m_d = k \\ m_2, \dots, m_d \geq 0}} \binom{k}{m_2, \dots, m_d}^2 \sim (d-1)^{2k+(d-1)/2} (4\pi k)^{(2-d)/2},$$

wherefore

$$\lim_{k \rightarrow \infty} \sqrt[k]{|\Omega_{l+2k}|} \geq (d-1)^2 \lim_{k \rightarrow \infty} \sqrt[k]{(d-1)^{(d-1)/2} (4\pi k)^{(2-d)/2}} = (d-1)^2.$$

Hence

$$\sum_{\omega \in \Omega} a^{|\omega|} = a^l \sum_{k=0}^{\infty} |\Omega_{l+2k}| a^{2k}$$

¹For $k = k_1 + \dots + k_d$, $\binom{k}{k_1, \dots, k_d} := \frac{k!}{k_1! \dots k_d!}$ is called a multinomial coefficient.

does not converge if $a \geq \frac{1}{d-1}$, which is to say that

$$a_d^* \leq \frac{1}{d-1}.$$

Considering the case $d = 2$ in particular, Example 16 simply states $a_2^* \leq 1$, which is trivial. With this in mind, we formulate our next example, wherein we shall finally use Theorem 7.

Example 17. Let $l = 2, 3, \dots$ and $k = 0, 1, \dots$. We can construct paths from x to y of length $l+2k$ as a sequence of nodes n_0, \dots, n_{l+2k} as follows. Let q and $r = 0, \dots, l-1$ be such that $k = 1+lq+r$. Let $\mathcal{I} := \{jl : j = 1, \dots, q\} \cup \{lq, \dots, k\}$ and $\mathcal{I}^c := \{1, \dots, k\} \setminus \mathcal{I}$. Denote by e_1, \dots, e_d the standard basis vectors in d dimensions. Take

$$\begin{aligned} u_i &= e_2, \quad \text{for } i \in \mathcal{I}, \quad \text{and} \\ (u_i)_{i \in \mathcal{I}^c} &\in \{e_1, \dots, e_d\}^{(l-1)q}. \end{aligned}$$

We now construct a path as follows.

1. Let $n_0 = x$.
2. For $i = 1, \dots, k$, let $n_i = n_{i-1} + u_i$.
3. For $i = k+1, \dots, k+l$, let $n_i = n_{i-1} + e_1$.
4. For $i = l+k+1, \dots, l+2k$, let $n_i = n_{i-1} - u_{l+2k+1-i}$.

As in Example 15, we have $n_{l+2k} = y$. To see that this node sequence we have constructed actually corresponds to a path (that is: never visits a point of \mathbb{Z}^d more than once), consider the three subsequences

$$\begin{aligned} \gamma_1 &= (n_0, \dots, n_k), \\ \gamma_2 &= (n_k, \dots, n_{k+l}), \quad \text{and} \\ \gamma_3 &= (n_{l+k}, \dots, n_{l+2k}). \end{aligned}$$

As each subsequence is monotone in \mathbb{Z}^d , neither subsequence could visit a point of \mathbb{Z}^d more than once. We shall show that the subsequences have no nodes in common (except the endpoints) with each other. Clearly both γ_1 and γ_3 are separated from γ_2 in the first dimension. Now note that for all $i = 0, \dots, k$, $n_i = n_{l+2k-i} - l \cdot e_1$. Hence, if there exist $i, j \in \{0, \dots, k\}$ such that $n_i = n_{l+2k-j}$, then $n_j = n_i - l \cdot e_j$, which implies that $j = i - l$ and $u_m = e_1$ for $m = j, \dots, i+l$, which is not allowed by our construction of $(u_i)_{i=1}^k$, as $\{j, \dots, j+l\}$ contains one integer multiple of q . Therefore, the node sequence n_0, \dots, n_{l+2k} does correspond to a path from x to y .

There are

$$d^{(l-1)q}$$

ways to choose $(u_i)_{i \in \mathcal{I}}$, wherefore

$$|\Omega_{l+2k}| \geq d^{(l-1)q}.$$

Hence,

$$\sum_{\omega \in \Omega} a^{|\omega|} = a^l \sum_{k=0}^{\infty} |\Omega_{l+2k}| a^{2k} \geq a^l \sum_{k=0}^{\infty} \left(d^{(l-1)q/k} a^2 \right)^k. \quad (3.11)$$

Since

$$\frac{q}{k} \xrightarrow{k \rightarrow \infty} \frac{1}{l},$$

we see that

$$\lim_{k \rightarrow \infty} |\Omega_{l+2k}| a^{2k} \geq \lim_{k \rightarrow \infty} (d^{1-1/l} a^2)^k$$

and hence the left hand side of (3.11) does not converge if

$$a \geq \frac{d^{\frac{1}{2l}}}{\sqrt{d}}.$$

By Theorem 7, we have

$$a_d^* \leq \inf_{l=2,3,\dots} \frac{d^{\frac{1}{2l}}}{\sqrt{d}} = \frac{1}{\sqrt{d}}.$$

To close this section, we combine the techniques of Examples 16 and 17 and use Theorem 7 to prove Proposition 14.

Proof of Proposition 14. Let $l = 2, 3, \dots$ and $k = 0, 1, \dots$. We can construct paths from x to y of length $l + 2k$ as a sequence of nodes n_0, \dots, n_{l+2k} as follows. Let q and $r = 0, \dots, l - 1$ be such that $k = 1 + lq + r$. For each $p = 1, \dots, q$, take

$$(m_j^p)_{j=2}^d \in \mathbb{Z}_{\geq 0}^{d-1}, \quad \text{such that} \quad \sum_{j=2}^d m_j^p = l - 1.$$

Denote by e_1, \dots, e_d the standard basis vectors in d dimensions. For each $p = 1, \dots, q$, take

$$\begin{aligned} (u_{pl+i})_{i=1}^{l-1} &\in \{e_2, \dots, e_d\}^{l-1}, \quad \text{and independently} \\ (v_{pl+i})_{i=1}^{l-1} &\in \{e_2, \dots, e_d\}^{l-1}, \end{aligned}$$

such that

$$\sum_{i=1}^{l-1} \mathbb{1}\{u_{pl+1} = e_j\} = \sum_{i=1}^{l-1} \mathbb{1}\{v_{pl+1} = e_j\} = m_j^p, \quad \forall j = 2, \dots, k.$$

For each $i \in \{pl : p = 1, \dots, q\} \cup \{ql, \dots, k\}$, let $u_i = v_i = e_2$.

We now construct a path as follows.

1. Let $n_0 = x$.
2. For $i = 1, \dots, k$, let $n_i = n_{i-1} + u_i$
3. For $i = k + 1, \dots, k + l$, let $n_i = n_{i-1} + e_1$.
4. For $i = l + k + 1, \dots, l + 2k$, let $n_i = n_{i-1} - v_{l+2k+1-i}$.

By the same argument as in Example 17, any node sequence constructed this way corresponds in an element in Ω_{l+2k} . Let

$$B_N := \sum_{\substack{m_1 + \dots + m_d = N \\ m_1, \dots, m_d \geq 0}} \binom{N}{m_1, \dots, m_d}^2.$$

For each $p = 1, \dots, q$, there are B_{l-1} ways to choose to choose $(u_{pl+i})_{i=1}^{l-1}$ and $(v_{pl+i})_{i=1}^{l-1}$.

Hence

$$|\Omega_{l+2k}| \geq (B_{l-1})^q. \quad (3.12)$$

We make the (quite rough) estimate

$$\sum_{\substack{m_1+\dots+m_d=N \\ m_1, \dots, m_d \geq 0}} \binom{N}{m_1, \dots, m_d}^2 \geq \max_{\substack{m_1+\dots+m_d=N \\ m_1, \dots, m_d \geq 0}} \binom{N}{m_1, \dots, m_d}^2, \quad (3.13)$$

and note that

$$\max_{\substack{m_1+\dots+m_d=N \\ m_1, \dots, m_d \geq 0}} \binom{N}{m_1, \dots, m_d} = \underbrace{\max_{\substack{m_1+\dots+m_d=N \\ m_1, \dots, m_d \geq 0}} \frac{\Gamma\left(\frac{N}{d} + 1\right)^d}{m_1! \cdots m_d!}}_{(*)} \cdot \underbrace{\frac{N!}{\Gamma\left(\frac{N}{d} + 1\right)^d}}_{(**)}. \quad (3.14)$$

To bound (*), let $M := \lfloor N/d \rfloor$ and $R := N - d \cdot M$. Since Γ is increasing, we have

$$\Gamma\left(\frac{N}{d} + 1\right) \geq \Gamma(M + 1) = M!,$$

hence

$$(*) \geq \max_{\substack{m_1+\dots+m_d=N \\ m_1, \dots, m_d \geq 0}} \frac{(M!)^d}{m_1! \cdots m_d!}.$$

We also have

$$\min_{\substack{m_1+\dots+m_d=N \\ m_1, \dots, m_d \geq 0}} m_1! \cdots m_d! \leq (M!)^d (M + 1)^R,$$

wherefore

$$(*) \geq \left(\frac{1}{M + 1}\right)^R.$$

Note in particular that

$$\lim_{N \rightarrow \infty} \sqrt[N]{(*)} \geq 1.$$

To bound (**), let $n = 0, 1, \dots, d-1$ such that $N+n$ is a multiple of d . Then, since Γ is an increasing function,

$$\frac{N!}{\Gamma\left(\frac{N}{d} + 1\right)^d} \geq \frac{N!}{\Gamma\left(\frac{N+n}{d} + 1\right)^d} = \frac{N!}{\left(\frac{N+n}{d}\right)!^d}.$$

According to Robbins [12], for any non-negative integer m , we have

$$\sqrt{2\pi m} m^m e^{-m} e^{\frac{1}{12m+1}} < m! < \sqrt{2\pi m} m^m e^{-m} e^{\frac{1}{12m}}.$$

Hence,

$$\begin{aligned} (**) &\geq \frac{\sqrt{2\pi N} N^N e^{-N} e^{\frac{1}{12N+1}}}{\sqrt{2\pi \frac{N+n}{d}}^d (N+n)^{(N+n)} d^{-(N+n)} e^{-(N+n)} e^{\frac{d}{12(N+n)}}} \geq \\ &\geq d^N \left(\frac{N}{N+n}\right)^N \left(\frac{d}{N+n}\right)^n \frac{\sqrt{2\pi N}}{\sqrt{2\pi \frac{N+n}{d}}^d} \exp\left(\frac{1}{12N+1} - \frac{d}{12N} + n\right). \end{aligned}$$

Note that

$$\lim_{N \rightarrow \infty} \sqrt[N]{(**)} \geq d.$$

Thus

$$B_N \geq d^{2N} \cdot f(N), \tag{3.15}$$

where $f(N)$ is a function such that

$$\lim_{N \rightarrow \infty} \sqrt[N]{f(N)} = 1.$$

Combining the inequalities (3.12) and (3.15), we find

$$\lim_{k \rightarrow \infty} \sqrt[k]{|\Omega_{l+2k}|} \geq \lim_{k \rightarrow \infty} \left(d^{2(l-1)} \cdot f(l-1) \right)^{q/k}.$$

Since

$$\lim_{k \rightarrow \infty} \frac{q}{k} = 1/l, \quad \text{and} \quad \lim_{k \rightarrow \infty} \frac{r}{k} = 0,$$

we see that

$$\lim_{k \rightarrow \infty} \sqrt[k]{|\Omega_{l+2k}|} \geq d^{2(l-1)/l} (f(l-1))^{1/l}.$$

and so the series

$$\sum_{k=0}^{\infty} |\Omega_{l+2k}| a^{2k}$$

does not converge if

$$a \geq \frac{1}{d^{(l-1)/l}} \cdot \frac{1}{(f(l-1))^{1/2l}}.$$

Using Theorem 7, we know that

$$a_d^* \leq \inf_{l=2,3,\dots} \frac{1}{d^{(l-1)/l}} \cdot \frac{1}{(f(l-1))^{1/2l}} = \frac{1}{d},$$

which is what we set out to show. □

In the proof of Proposition 14, the estimate (3.13) is very rough, and one might wonder in if a better estimate would yield a better bound for a_d^* . Due to Richmond and Shallit [11], we have however that as $N \rightarrow \infty$,

$$\sum_{\substack{m_1+\dots+m_d=N \\ m_1,\dots,m_d \geq 0}} \binom{N}{m_1, \dots, m_d}^2 \sim d^{2N+d/2} (4\pi N)^{(1-d)/2}.$$

Taking the N th root of the right-hand side, we get

$$\lim_{N \rightarrow \infty} \sqrt[N]{d^{2N+d/2} (4\pi N)^{(1-d)/2}} = d^2,$$

which shows that a better bound than (3.13) would not be sufficient to improve the statement of Proposition 14.

3.3 Relationship between a^* and the critical temperature in the Ising model

The Ising model behaves in fundamentally different ways at high and low temperatures, corresponding to small and large inverse temperatures β , respectively. In particular, there exists a temperature, called the critical temperature, at which the Ising model undergoes a phase transition [3]. At temperatures below the critical temperature, the Ising model exhibits greater correlation between spins corresponding to sites at greater distance from each other, whereas at higher temperatures, the system is more chaotic. For $d = 2, 3, \dots$, denote by T_d^c this temperature (and by $\beta_d^c := 1/T_d^c$ the corresponding inverse temperature), leaving other parameter dependencies implicit. In this section, we comment on the relationship between β_d^c and a_d^* .

The parameter a in our model plays a role similar to that of $\tanh \beta$ in the two-point correlation function (1.1) of the Ising model. Hence, it is natural to ask whether $a_d^* = \tanh \beta_d^c$. The critical temperature for hypercubic lattices is known exactly for $d = 2$, and approximately for some higher d , including $d = 3, \dots, 7$.

In two dimensions, the critical temperature is [9]

$$T_2^c = \frac{2}{\ln(1 + \sqrt{2})}.$$

This gives

$$\tanh \beta_2^c = \tanh \frac{1}{T_2^c} \approx 0.414,$$

which is within the bounds for a_d^* given by Theorem 8, and so we can not rule out that $a_2^* = \tanh \beta_2^c$.

For $d = 3, \dots, 7$, we compare known numerical estimates $\hat{\beta}_d^c$ of β_d^c to our bounds on a_d^* . We show these values and bounds in Table 3.2. We conclude that a_d^* may be equal to β_c for all $d = 2, 3, \dots$

Table 3.2: Comparison of known approximate values for $\tanh \beta_d^c$ and the bounds on a_d^* given by Theorem 8.

d	3	4	5	6	7
$1/(2d-1)$	0.200	0.143	0.111	0.091	0.077
$\tanh \hat{\beta}_d^c$	0.218 [6]	0.149 [7]	0.113 [8]	0.092 [8]	0.078 [8]
$1/d$	0.333	0.250	0.200	0.167	0.143

As seen in Table 3.2, for $d \geq 3$, we have $\tanh \beta_d^c \approx \frac{1}{2d-1}$, in particular for $d \geq 4$. As $\tanh x \approx x$ for small x , this implies

$$T_d^c \approx 2d - 1.$$

It has been noted before [1] that T_d^c grows roughly linearly in d for $d \geq 4$.

4

Simulation

In this chapter, we describe how we can draw from a version the distribution described by μ_a constricted to edge sets on a lattice of finite size, in $d = 2$ dimensions. We will use the Metropolis-Hastings algorithm [13] to simulate a Markov chain with stationary distribution μ_a . This algorithm can be run for any number M of steps, and as the number of steps increases, it is more likely that the chain has reached higher-density regions of the stationary distribution.

4.1 Algorithm

We begin by describing the algorithm. Fix $l \in \{1, 2, \dots\}$. For $t > 0$, let

$$D(t) := \{(u, v) \in \mathbb{Z}^2 : |u - l/2| + |v| \leq t\}.$$

Then $D(t)$ is the set of points in \mathbb{Z}^2 that lie inside or on the boundary of a diagonally tilted square with diagonal length $2t$. Let

$$B(t) := \{e \in \mathcal{E}(\mathbb{Z}^2) : \exists p_1, p_2 \in D(t) : e = \{p_1, p_2\}\},$$

so that $B(t)$ is the set of edges between adjacent points in $D(t)$. Define a *plaquette* as a set of four edges in $\mathcal{E}(\mathbb{Z}^2)$ forming a square. Denote by $\mathcal{P}(\mathbb{Z}^2)$ the set of plaquettes that are subsets of $\mathcal{E}(\mathbb{Z}^2)$. Let

$$\mathcal{P}(t) = \{\pi \in \mathcal{P}(\mathbb{Z}^2) : \pi \subset B(t)\}.$$

We will refer to $\mathcal{P}(t)$ as the *proposal region*. For $t > 0$, we say that the proposal region $\mathcal{P}(t)$ has size $r = 2t$. When we simulate with proposal region $\mathcal{P}(t)$ with size r , we also say that we simulate on a lattice with size r .

For $\omega, \omega' \subset \mathcal{E}(\mathbb{Z}^2)$ and t , define the *proposal density* $q_t(\omega'|\omega)$ according to¹

$$q_t(\omega'|\omega) := \frac{1}{|\mathcal{P}(t)|} \mathbb{1}\{\exists \pi \in \mathcal{P}(t) : \omega' = \omega \Delta \pi\}.$$

Given ω and t , we simulate ω' from the proposal density by picking a plaquette π uniformly at random from $\mathcal{P}(t)$ and letting $\omega' := \omega \Delta \pi$. The construction of q_t and in particular $\mathcal{P}(t)$ might seem unnatural. This particular construction is chosen to facilitate efficient implementation in code.

¹As earlier, Δ denotes symmetric set difference.

Define the *acceptance probability* $\rho(\omega'|\omega)$ according to

$$\rho(\omega'|\omega) := \begin{cases} 0, & \text{if } \omega' \text{ is not connected,} \\ 1, & \text{if } |\omega'| \leq |\omega|, \\ a^{|\omega'|-|\omega|}, & \text{if } |\omega'| > |\omega|. \end{cases}$$

Given a proposal region size t , we will generate a sequence of samples from μ_a as follows.

1. Let $\omega_0 \in \Omega$ be the straight line from x to y .
2. For $i = 1, \dots, M$:
 Simulate ω'_i according to $q_t(\cdot|\omega_{i-1})$. Let

$$\omega_i := \begin{cases} \omega'_i, & \text{with probability } \rho(\omega'_i|\omega_{i-1}) \\ \omega_{i-1}, & \text{with probability } 1 - \rho(\omega'_i|\omega_{i-1}). \end{cases}$$

For $\omega, \omega' \in \Omega$, denote by $g(\omega'|\omega)$ the probability of transitioning from ω to ω' . For $\omega_s, \dots, \omega_t$ to be a sample of μ_a , we need, for all $i = s + 1, \dots, t$,

$$\frac{g(\omega_i|\omega_{i-1})}{g(\omega_{i-1}|\omega_i)} = \frac{\mu_a(\omega_i)}{\mu_a(\omega_{i-1})},$$

which are called the *detailed balance conditions*. We have

$$\begin{aligned} \frac{g(\omega_i|\omega_{i-1})}{g(\omega_{i-1}|\omega_i)} &= \frac{q_{r_{i-1}}(\omega_i|\omega_{i-1})\rho(\omega_i|\omega_{i-1})}{q_{r_{i-1}}(\omega_{i-1}|\omega_i)\rho(\omega_{i-1}|\omega_i)} = \frac{|\mathcal{P}(t)|}{|\mathcal{P}(t)|} \frac{a^{|\omega_i|}}{a^{|\omega_{i-1}|}} = \\ &= \frac{\mu_a(\omega_i)}{\mu_a(\omega_{i-1})}. \end{aligned}$$

Note that we defined the proposal and acceptance functions not only on $\omega \in \Omega$, but also on disconnected edge sets. What we're actually doing is simulating from a distribution on all finite subsets of $\mathcal{E}(\mathbb{Z}^2)$, with support Ω . This distribution is for our purposes indistinguishable from μ_a , and so we can use it to estimate expectations with respect to μ_a .

4.2 Results

We simulate in order to visualize. In order to pick a suitable proposal region size r for different values of a , we will investigate whether the growth of the simulated chain in any step is bounded by the lattice.

We will also, in every simulation, estimate $\mathbb{E}_{\mu_a}|\omega|$ by taking the average size of all states in the simulated chain. We denote the result of such an estimation as $X(l, a, r, M)$.

Average $X(l, a, r, m)$ over 20 simulations for $l = 1$, and $M = 10^7$, and different values of a and r are shown in Table 4.1. The proportions of the same simulations that reached the edge of the proposal region are shown in Table 4.2.

It is difficult to draw conclusions about $\mathbb{E}_{\mu_a}|\omega|$ from the data in Table 4.1. We see that when the proposal region is small, the average edge set size is smaller than for

Table 4.1: Mean $X(M, l, a, r)$ over 20 simulations. Simulations were of length $M = 10^7$ with $l = 1$ for different values of a and proposal region size r .

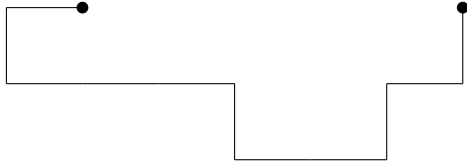
a	0.3	0.33	0.36	0.39	0.42	0.45	0.48	0.51
$r = 21$	1.90*	2.60*	4.26*	11.2*	38.7*	72.0*	94.6*	112*
$r = 41$	1.91	2.72	5.31*	44.8*	219*	331*	404*	463*
$r = 81$	2.06	2.61	4.18	28.6*	520*	1110*	1450*	1700*
$r = 161$	1.81	2.27	4.37	8.76	42.1	330	870*	1950*
$r = 241$	2.00	2.68	4.06	5.97	23.1	50.7	152	308
$r = 281$	1.97	2.41	2.99	6.03	18.04	34.3	103	181

Table 4.2: Proportion in % of 20 simulations that reached the edge of the proposal region. Simulations were of length $M = 10^7$ with $l = 1$ for different values of a and proposal region size r .

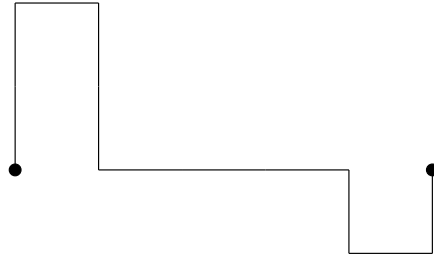
a	0.3	0.33	0.36	0.39	0.42	0.45	0.48	0.51
$r = 21$	30	70	100	100	100	100	100	100
$r = 41$	0	0	15	85	100	100	100	100
$r = 81$	0	0	0	5	100	100	100	100
$r = 161$	0	0	0	0	0	0	15	100
$r = 241$	0	0	0	0	0	0	0	0
$r = 281$	0	0	0	0	0	0	0	0

larger sizes. This could indicate that the growth of the edge set chain is limited by the size of the proposal region. For proposal region sizes that are more than sufficient to contain the edge set chain, we see that the average $X(l, a, r, M)$ is smaller than for smaller sizes, perhaps indicating that a significant proportion of iterations are consumed as proposals of disconnected edge sets, and that the chain does not have time to converge to its stationary distribution.

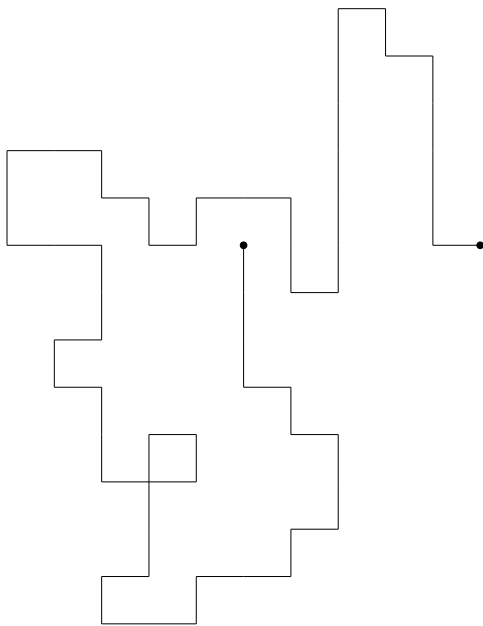
Informed by our previous conclusions in regards to suitable proposal region sizes r for different a , we generate edge sets, shown in Figure 4.1 and Figure 4.2. Each of the corresponding simulations were performed without an edge set reaching the boundary of the proposal region.



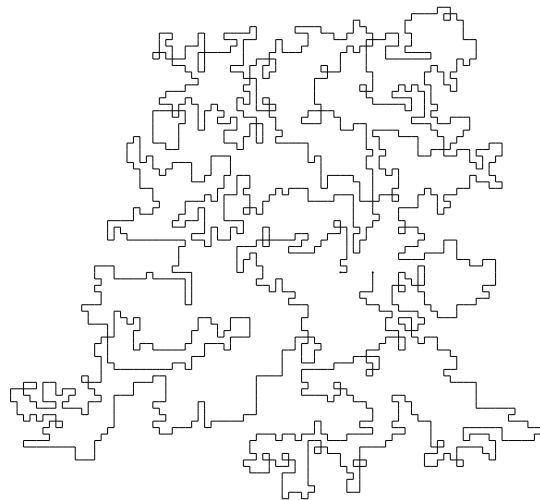
(a) With $a = 0.3$ and proposal region size 45.



(b) With $a = 0.34$ and proposal region size 45.



(c) With $a = 0.38$ and proposal region size 65.



(d) With $a = 0.42$ and proposal region size 165.

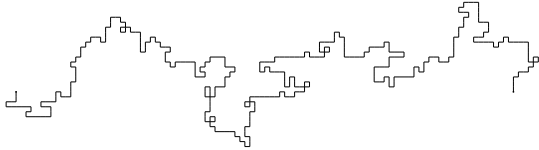
Figure 4.1: Simulated edge sets for different $l = 5$, with different a , and proposal region sizes. The edge set shown is the final edge set after 10^7 simulation steps. Proposal region sizes were tuned to prevent the simulated edge sets from reaching the edges of the proposal region.



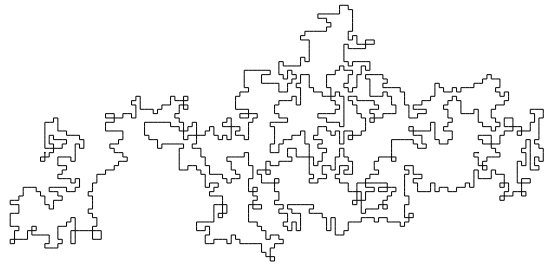
(a) With $a = 0.3$ and proposal region size 140.



(b) With $a = 0.34$ and proposal region size 140.



(c) With $a = 0.38$ and proposal region size 200.



(d) With $a = 0.42$ and proposal region size 260.

Figure 4.2: Simulated edge sets for different $l = 100$, with different a , and proposal region sizes. The edge set shown is the final edge set after 10^7 simulation steps. Proposal region sizes were tuned to prevent the simulated edge sets from reaching the edges of the proposal region.

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