이학박사 학위논문

Metastability of complex stochastic interacting systems

(복잡한 확률적 상호작용계의 메타안정성)

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이 논문을 이학박사 학위논문으로 제출함

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Metastability of complex stochastic interacting systems

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Abstract

Metastability of complex stochastic interacting systems

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In this Ph.D. thesis, we conduct quantitative analyses of the phenomenon of metastability occurring in various complex systems, such as ferromagnetic spin systems or interacting particle systems. In addition, we develop a novel approach to study metastability, the H^1-approximation method, which is particularly useful to handle non-reversible systems. The quantitative results include Eyring–Kramers formula, a sharp asymptotics of the mean metastable transition time, and Markov chain characterization of successive metastable transitions. We focus on the results on specific models in two categories. In the first part, we investigate the ferromagnetic Ising and Potts models in low temperatures and several related models. In the second part, we consider the condensing inclusion process and compare the results between reversible and non-reversible systems.

Key words: Metastability, H^1-approximation, Ising model, Potts model, inclusion process
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Chapter 1

Introduction

Metastability occurs in various dynamical systems that possess two or more locally stable states. In such cases, the dynamics spends *exponentially long time* in the initial locally stable state, until it reaches a certain *unpredictable moment*, and begins a *rapid crossover* to another locally stable state. These three characteristics are ubiquitous in systems belonging to a wide range of fields; a few examples are supercooling of water in physics, allotropic structures in chemistry, persistence of stock prices on high levels in economics, etc.

In the context of statistical physics, metastability occurs in numerous models such as small random perturbations of dynamical systems [19, 20, 21, 33, 58, 61, 62, 64, 65, 77], interacting particle systems with sticky interactions [6, 15, 56, 57, 76, 78], ferromagnetic spin systems in low temperatures [1, 9, 14, 17, 18, 22, 24, 29, 53, 54, 59, 63, 71, 72, 69], etc. These are few of the numerous important works conducted during the past few decades; for a complete list of references, refer to the monographs [16, 75].

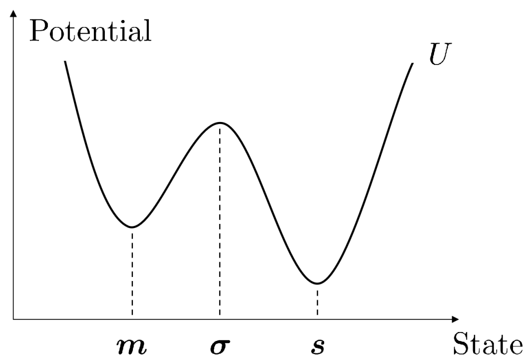


Figure 1.1: Double-well potential U with local minimum $\boldsymbol{m}$, global minimum $\boldsymbol{s}$, and critical point $\boldsymbol{\sigma}$.

1.1 Early results

One of the earliest attempts to quantify the phenomenon of metastability originates from chemical reaction rate theory in 1889, in which Arrhenius [3] proposed a formula

$$R = Ae^{-E/(kT)}, \tag{1.1}$$

known as the *Arrhenius equation*. The equation (1.1) explains that the rate constant R depends exponentially on the *inverse temperature* $1/T$, through an exponent $-E/k$ which is proportional to the *activation energy* E, along with a prefactor A which is the *amplitude*. The observation that the reaction rate depends on the three above-mentioned variables (inverse temperature, activation energy, and amplitude) turns out to be ubiquitous in most of the slow-mixing dynamical systems (cf. (1.3)).

In 1940, Kramers [49] considered the following one-dimensional (1D) diffusion equation, which is now recognized in the community as the *overdamped Langevin dynamics*:

$$dX_t = -U'(X_t)dt + \sqrt{2\epsilon}dB_t, \tag{1.2}$$

where $U : \mathbb{R} \to \mathbb{R}$ is a smooth double-well potential (see Figure 1.1), B_t

is the standard Brownian noise, and $\epsilon > 0$ is a small control parameter which corresponds to the absolute temperature of the system. In this system, a metastability scenario occurs in low temperature (small ϵ). To see this, suppose that the process starts from state $\boldsymbol{m}$, which is the local minimum of the left valley in Figure 1.1. Since ϵ is small, the behavior of (1.2) is dominated by the drift term $-U'(X_t)dt$ which consistently pushes the system to the initial state $\boldsymbol{m}$, the unique stable equilibrium point inside the left valley. However, due to the small noise term $\sqrt{2\epsilon}dB_t$, after a long random time, the process overcomes the energy barrier $U(\boldsymbol{\sigma}) - U(\boldsymbol{m})$ and eventually makes a transition through the critical point $\boldsymbol{\sigma}$ to the right valley containing the global minimum state $\boldsymbol{s}$.

More quantitatively, in this special 1D case, Kramers derived the following formula for the mean transition time from $\boldsymbol{m}$ to $\boldsymbol{s}$:

$$\mathbb{E}_{\boldsymbol{m}}[\tau_{\boldsymbol{s}}] \simeq \frac{2\pi}{\sqrt{(-U''(\boldsymbol{\sigma})) \cdot U''(\boldsymbol{m})}} \cdot e^{\frac{U(\boldsymbol{\sigma})-U(\boldsymbol{m})}{\epsilon}} \quad \text{as } \epsilon \to 0. \tag{1.3}$$

Thanks to Eyring's contributions [32] in the multi-dimensional setting, asymptotic identities as in (1.3) on the mean transition time are now widely recognized by active researchers as the *Eyring–Kramers formula*.

1.2 Freidlin–Wentzell theory and pathwise approach to metastability

In 1960s, Freidlin and Wentzell [33] established the first probabilistic methodology to characterize the metastable behavior. The idea was to apply the celebrated *large deviation theory* (e.g., [31]) to the path space of dynamical systems. Using this tool, they addressed the following dynamics, which is the d-dimensional overdamped Langevin dynamics (generalizing (1.2)):

$$dX_t = -\nabla U(X_t)dt + \sqrt{2\epsilon}dB_t, \tag{1.4}$$

where $U : \mathbb{R}^d \to \mathbb{R}$ is now a d-dimensional smooth double-well potential. They proved the following *exponential estimate* on the mean transition time from the metastable state $\boldsymbol{m}$ to the stable state $\boldsymbol{s}$:

$$\log \mathbb{E}_{\boldsymbol{m}}[\tau_{\mathcal{N}(\boldsymbol{s})}] \simeq \frac{U(\boldsymbol{\sigma}) - U(\boldsymbol{m})}{\epsilon} \quad \text{as } \epsilon \to 0,$$

where $\mathcal{N}(\boldsymbol{s})$ is a small neighborhood of $\boldsymbol{s}$. However, a further quantitative result such as (1.3) was unidentified at this point.

In 1984, Cassandro, Galves, Olivieri, and Vares [24] constructed a methodology by applying the aforementioned Freidlin–Wentzell theory to discrete systems, such as interacting particle systems or ferromagnetic spin systems. This is known as the p*athwise approach* to metastability. The main ideas of this approach, along with numerous concrete examples, are well summarized in the monograph [75] by Olivieri and Vares.

1.3 Potential-theoretic approach: Eyring–Kramers formula

A crucial breakthrough arose in the early 2000s. Bovier, Eckhoff, Gayrard, and Klein [19, 20, 21] successfully applied the well-known potential theory to provide a robust methodology to achieve quantitative metastability results, including the Eyring–Kramers formula (cf. (1.3)). The key idea was the fact that the mean transition time is closely related to the inverse of the so-called *capacity* (see Section 3.2.1 for the precise definition) between two metastable states, which can be precisely estimated using dual variational formulas known as the Dirichlet and Thomson principles (cf. Section 3.2.5). Using this approach, under suitable assumptions on the potential U, they proved that the Eyring–Kramers formula for the d-dimensional Langevin dynamics (1.4) is represented as

$$\mathbb{E}_{\boldsymbol{m}}[\tau_{\mathcal{N}(\boldsymbol{s})}] \simeq \frac{2\pi}{-\mu^{\boldsymbol{\sigma}}}\sqrt{\frac{-\det \nabla^2 U(\boldsymbol{\sigma})}{\det \nabla^2 U(\boldsymbol{m})}} \cdot e^{\frac{U(\boldsymbol{\sigma})-U(\boldsymbol{m})}{\epsilon}} \quad \text{as } \epsilon \to 0,$$

where $\mu^{\boldsymbol{\sigma}}$ is the unique negative eigenvalue of $\nabla^2 U(\boldsymbol{\sigma})$. A sketch of the gist of this approach is provided in Section 3.2. More technical details and also a summary of the main results achieved so far can be found in the monograph [16] by Bovier and den Hollander.

1.4 Martingale approach: Markov chain model reduction

About ten years later, Beltrán and Landim [5, 7, 8] introduced a new method to characterize metastability, which is the so-called *Markov chain model reduction*. They characterized the successive transitions between metastable states as Markovian *simple jumps* between the states by certain coarse-graining arguments. More precisely, the idea was to accelerate the original system by a certain time scale (which is indeed the scale of the metastable transition), and prove that the law of trajectories of this accelerated process converges, in the Skorokhod topology on the path space, to the law of a simple Markov chain which represents the macroscopic metastable transitions of the system. Details can be found in Section 3.1.2. The convergence is proved by means of the martingale characterization of Markov processes (cf. [80]); because of this feature, this method is also known as the *martingale approach* to metastability. Rich motivations and ideas of this theory are presented in the recent survey [52] by Landim.

1.5 Organization of the thesis

In Part I, we summarize the results [10, 44, 46, 47, 48] regarding the metastability phenomenon in ferromagnetic Ising and Potts models and also in some related systems. In Chapter 2, we briefly review the classic results in the Ising model with positive magnetic field. In Chapter 3, we present the first main result of this thesis, along with the outline of the general strategies used throughout. Chapters 4 and 5 are devoted to some generalized models of the model in Chapter 3. Chapter 6 deals with another model, namely the Blume–Capel model, in which we find some similar but different features of metastability in the low-temperature regime. In Chapter 7, we deal with a generalized version of the Potts model whose energy landscape has much more complex structure.

In Part II, we consider the condensing inclusion process and explain how the metastability phenomenon occurs in this interacting particle system [43, 45]. In Chapter 8, we summarize the previous results in the *reversible* case. Then, in Chapter 9, we present a result which considerably generalizes the ones presented in the previous chapter. Finally, in Chapter 10, we present yet another generalization regarding *non-reversible* inclusion processes.

Part I

Ferromagnetic Ising/Potts and related models

Here, we settle some notation and rules that are frequently used in the remainder of this thesis.

- For $a, b \in \mathbb{R}$, $[\![a, b]\!]$ denotes $[a, b] \cap \mathbb{Z}$.
- The set of natural numbers $\mathbb{N}$ includes 0.
- Written $a, b \in A$ or $\{a, b\} \subseteq A$, it is implied implicitly that a and b are different. The same holds for three or more elements.
- $C > 0$ denotes a positive constant, which does not depend on the variables (β in Part I, in particular L in Chapter 5, and N in Part II, in particular L in Sections 10.2.4 and 10.7), but may vary from line to line.
- For two functions f and g of the variable mentioned above, it is denoted as
  - $f = O(g)$ if there exists C such that $|f| \le C|g|$;
  - $f = \Theta(g)$ if $f = O(g)$ and $g = O(f)$;
  - $f = o(g)$ or $f \ll g$ if $\lim \dfrac{f}{g} = 0$ (as the variable tends to infinity);
  - $f \simeq g$ if $\lim \dfrac{f}{g} = 1$.
- For $a \in \mathbb{R}$, $\lfloor a \rfloor$ (resp. $\lceil a \rceil$) denotes the greatest (resp. least) integer less than (resp. greater than) or equal to a.

Chapter 2

Classic result: Ising model with positive external field

We fix a two-dimensional (2D) square lattice $\Lambda = \{1, 2, \ldots, L\}^2$ given periodic boundary conditions, and a collection $\Omega = \{+1, -1\}$ of plus and minus spins. Then, the spin configuration space is defined as $\mathcal{X} = \Omega^\Lambda$. For each configuration $\sigma \in \mathcal{X}$, we define the *Hamiltonian* (or *energy*) as

$$H(\sigma) = H^{\mathrm{pos}}(\sigma) := \sum_{\{x,\, y\} \subseteq \Lambda \colon x \sim y} \mathbb{1}\{\sigma(x) \neq \sigma(y)\} - h \sum_{x \in \Lambda} \mathbb{1}\{\sigma(x) = +1\},$$

where $x \sim y$ if and only if x and y are nearest neighbors. Here, $h \in (0, 1)$ is a small positive external field.

Denote by $\boxplus \in \mathcal{X}$ (resp. $\boxminus \in \mathcal{X}$) the configuration such that all spins are $+1$ (resp. -1). Then, it is easy to verify that $\boxplus$ is the unique global minimum of H and $\boxminus$ is a local minimum of H.

Definition 2.0.1 (Metropolis–Hastings dynamics)**.**

- We define a spin-flipping dynamics $\sigma_\beta^{\mathrm{MH}}(t)$, $t \geq 0$ as the continuous-time Markov chain on $\mathcal{X}$, characterized by the infinitesimal generator

$\mathcal{L}_\beta^{\mathrm{MH}}$ which acts on each function $f \in \mathbb{R}^{\mathcal{X}}$ as

$$(\mathcal{L}_\beta^{\mathrm{MH}} f)(\sigma) = \sum_{x \in \Lambda} \sum_{a \in \Omega} e^{-\beta \max\{H(\sigma^{x,a}) - H(\sigma), 0\}} (f(\sigma^{x,a}) - f(\sigma)) \tag{2.1}$$

for all $\sigma \in \mathcal{X}$, where $\sigma^{x,a}$ is obtained from σ by updating the spin at site x to spin a, and $\beta > 0$ is the inverse temperature of the system. This is a continuous-time version of the well-known *Metropolis–Hastings (MH) dynamics* (which corresponds to the superscripts MH in $\sigma_\beta^{\mathrm{MH}}$ and $\mathcal{L}_\beta^{\mathrm{MH}}$), and also known as the *Glauber dynamics*.

- Denote by $r_\beta^{\mathrm{MH}}(\cdot, \cdot)$ the jump rate of the process, i.e.,

$$r_\beta^{\mathrm{MH}}(\sigma, \sigma^{x,a}) = e^{-\beta \max\{H(\sigma^{x,a}) - H(\sigma), 0\}}, \quad r_\beta^{\mathrm{MH}}(\sigma, \zeta) = 0 \quad \text{otherwise.}$$

The jump rate to flip a spin equals 1 if the energy does not increase, and equals $e^{-\beta\Delta}$ if the energy increases by Δ. Thus, if β is large (low temperature), it is exponentially difficult to increase the energy.

According to the MH dynamics, the state $\boxminus$ is expected to be metastable. In turn, we investigate the typical behavior of the metastable transition from $\boxminus$ to the stable configuration $\boxplus$.

Definition 2.0.2 (Gibbs distribution)**.** We denote by μ_β the *Gibbs distribution* on the system:

$$\mu_\beta(\sigma) = \frac{1}{Z_\beta} e^{-\beta H(\sigma)} \quad \text{for all } \sigma \in \mathcal{X},$$

where Z_β is the normalizing constant $\sum_{\sigma \in \mathcal{X}} e^{-\beta H(\sigma)}$, known as the *partition function*, such that μ_β is indeed a probability distribution.

The following detailed balance condition holds:

$$\mu_\beta(\sigma) r_\beta^{\mathrm{MH}}(\sigma, \zeta) = \mu_\beta(\zeta) r_\beta^{\mathrm{MH}}(\zeta, \sigma) = \begin{cases} \min\{\mu_\beta(\sigma),\, \mu_\beta(\zeta)\} & \text{if } \zeta = \sigma^{x,a} \neq \sigma, \\ 0 & \text{otherwise.} \end{cases} \tag{2.2}$$

Thus, the following lemma is straightforward.

Lemma 2.0.3. *The MH dynamics* $\sigma_\beta^{\mathrm{MH}}(\cdot)$ *is reversible, and thus invariant with respect to the Gibbs distribution* μ_β*.*

Notation 2.0.4. In the remainder of the article, denote by $\mathbb{P}_\sigma$ and $\mathbb{E}_\sigma$ the law and the corresponding expectation of the dynamics starting from configuration σ. Moreover, denote by $\tau_{\mathcal{A}}$ the (random) hitting time of a collection $\mathcal{A}$ of configurations.

According to this notation, we are interested in the typical behavior of $\tau_{\boxplus}$ when the dynamics starts from $\boxminus$. The following exponential estimates were verified in [71, Theorems 2 and 3].

Theorem 2.0.5. *Define* $\Gamma = \Gamma^{\mathrm{pos}} := 4\ell_c - h[\ell_c(\ell_c - 1) + 1]$, *where* $\ell_c := \lceil 2/h \rceil$. *Then, starting from* $\boxminus$, *the following statements hold for the metastable transition of the dynamics.*

(1) $\lim_{\beta \to \infty} \beta^{-1} \log \tau_{\boxplus} = \Gamma$ *in probability.*

(2) $\lim_{\beta \to \infty} \beta^{-1} \log \mathbb{E}_{\boxminus}[\tau_{\boxplus}] = \Gamma$.

(3) $\lim_{\beta \to \infty} \tau_{\boxplus} / \mathbb{E}_{\boxminus}[\tau_{\boxplus}] = \exp(1)$ *in distribution, where* $\exp(1)$ *is a unit-mean exponential random variable.*

Remark 2.0.6. In Theorem 2.0.5, the value Γ^{pos} corresponds to the *energy barrier* of the system. More precisely, Γ^{pos} equals the minimal amount of energy to overcome among all possible transition paths from $\boxminus$ to $\boxplus$. It was further proved in [71] that this precise level Γ^{pos} is attained at configurations which contain the so-called *critical droplet* of plus spins in the sea of minus spins. The critical droplet has the form of an $(\ell_c - 1) \times \ell_c$ quasi-square plus a single protuberance on one of the longer sides. It is easy to check that this type of configuration has Hamiltonian exactly $H(\boxminus) + \Gamma^{\text{pos}}$.

This result was extended in [9, Theorem 7.36] to the same model on the three-dimensional (3D) periodic lattice, $\Lambda^{\text{3D}} = \{1, 2, \dots, L\}^3$.

Theorem 2.0.7. *Define*

$$\begin{aligned}\Gamma = \Gamma^{\text{pos-3D}} := 2m_c(m_c - \delta_c) + 2m_c(m_c - 1) + 2(m_c - \delta_c)(m_c - 1) + 4\ell_c \\ - h[m_c(m_c - \delta_c)(m_c - 1) + \ell_c(\ell_c - 1) + 1],\end{aligned}$$

where $m_c := \lceil 4/h \rceil$ *and* $\delta_c \in \{0, 1\}$ *is determined by* h*. Then, the three statements in Theorem 2.0.5 hold as well.*

Remark 2.0.8. Similarly, $\Gamma^{\text{pos-3D}}$ corresponds to the 3D energy barrier from $\boxminus$ to $\boxplus$, which is attained at 3D critical configurations. Concisely, the critical droplet has the form of a quasi-cube, plus a quasi-square attached to one of the biggest faces of the quasi-cube, plus a single protuberance on one of the longer sides of the quasi-square. Thus, one can immediately catch the inductive nature of the critical droplet, and conjecture that the d-dimensional Ising model will exhibit a similar metastable behavior characterized by critical configurations whose form consists of consecutive m-quasi-c ubes for lower dimensions $m \in [\![1, d-1]\!]$. However, proving such a result involves highly complicated analyses of the geometric nature of high-dimensional lattices, and thus the problem remains open at this point.

Focusing in particular on the second statement in Theorem 2.0.5, we may predict that the mean transition time $\mathbb{E}_{\boxminus}[\tau_{\boxplus}]$ roughly behaves like $e^{\beta\Gamma}$. Moving further, in [22], the authors obtained the corresponding Eyring–Kramers formula in both 2D and 3D models, by means of the potential-theoretic approach explained in Section 1.3.

Theorem 2.0.9 (Eyring–Kramers formula)**.**

(1) In the 2D Ising model, it holds that

$$\mathbb{E}_{\boxminus}[\tau_{\boxplus}] = (1 + o(1)) \cdot \frac{3}{4(2\ell_c - 1)L^2} \cdot e^{\beta\Gamma}.$$

(2) In the 3D Ising model, it holds that

$$\mathbb{E}_{\boxminus}[\tau_{\boxplus}] = \frac{1 + o(1)}{8(m_c - \ell_c + 1)(m_c - \ell_c - \delta_c + 1)(2\ell_c - 1)L^3} \cdot e^{\beta\Gamma}.$$

Chapter 3

Ising/Potts models with zero external fields

In this chapter, we denote by

$$\Lambda = \{1,\, 2,\, \ldots,\, K\} \times \{1,\, 2,\, \ldots,\, L\}$$

the 2D rectangular lattice with $K \le L$. For technical reasons, we assume that the lattice is sufficiently large; let $11 \le K \le L$. For simplicity, we only consider the case in which Λ is given periodic boundary conditions, so that we can write

$$\Lambda = \mathbb{T}_K \times \mathbb{T}_L, \tag{3.1}$$

where $\mathbb{T}_n := \mathbb{Z}/(n\mathbb{Z})$ represents the discrete 1D n-torus. The following arguments can also be directly applied to the same model with open boundary conditions; see Section 3.1.4 for a summary.

We denote the collection of spins as $\Omega = \{1,\, \ldots,\, q\}$, where $q = 2$ (resp. $q \ge 3$) corresponds to the Ising (resp. Potts) model. On the configuration space $\mathcal{X} = \Omega^\Lambda$, the Hamiltonian with zero external field is defined as

$$H(\sigma) = \sum_{\{x,y\}\subseteq\Lambda:\, x\sim y} \mathbb{1}\{\sigma(x) \neq \sigma(y)\}. \tag{3.2}$$

For each spin $a \in \Omega$, denote by $\boldsymbol{a}$ the configuration such that all spins are a, and collect $\mathcal{S} := \{\mathbf{1}, \ldots, \boldsymbol{q}\}$. Then,

$$\mathcal{S} = \arg\min_{\sigma\in\mathcal{X}} H(\sigma),$$

and thus the elements of $\mathcal{S}$ are called *ground states*.

Recall the Gibbs distribution from Definition 2.0.2. The next theorem asserts that μ_β is concentrated on the ground states in the low temperature regime $\beta \to \infty$.

Theorem 3.0.1. *It holds that $Z_\beta = q + O(e^{-4\beta})$. In turn,*

$$\lim_{\beta\to\infty} \mu_\beta(\mathcal{S}) = 1 \quad \textit{and} \quad \lim_{\beta\to\infty} \mu_\beta(\boldsymbol{s}) = \frac{1}{q} \quad \textit{for all } \boldsymbol{s} \in \mathcal{S}.$$

The proof is elementary, and we omit the details.

Reversible Metropolis–Hastings dynamics

As in Definitions 2.0.1 and 2.0.2, we define the spin-flipping MH dynamics $\sigma_\beta^{\mathrm{MH}}(t)$, $t \geq 0$. Then, Lemma 2.0.3 is also valid in this case, so that the μ_β is the invariant distribution of the reversible MH dynamics $\sigma_\beta^{\mathrm{MH}}(\cdot)$.

Non-reversible cyclic dynamics

We next introduce a *non-reversible* spin-flipping dynamics, also of Metropolis type, under which the spin updates occur in a cyclic manner.

Definition 3.0.2 (Cyclic dynamics)**.** First, we denote by $\tau_x\sigma \in \mathcal{X}$ the configuration obtained from σ by *rotating* the spin at x:

$$(\tau_x\sigma)(y) = \begin{cases} \sigma(x)+1 & \text{if } y = x, \\ \sigma(y) & \text{otherwise,} \end{cases}$$

where we use the convention that $q+1=1$. Then, denote by $\sigma_\beta^{\mathrm{cyc}}(t)$, $t \geq 0$ the continuous-time Markov process on $\mathcal{X}$ with its corresponding infinitesimal generator $\mathcal{L}_\beta^{\mathrm{cyc}}$ acting on functions $f \in \mathbb{R}^{\mathcal{X}}$ as

$$(\mathcal{L}_\beta^{\mathrm{cyc}} f)(\sigma) = \sum_{x\in\Lambda} e^{-\beta \max_{a\in\Omega}\{H(\sigma^{x,\,a})-H(\sigma)\}}(f(\tau_x\sigma) - f(\sigma)) \quad \text{for all } \sigma \in \mathcal{X}. \tag{3.3}$$

We call $\sigma_\beta^{\mathrm{cyc}}(\cdot)$ the *cyclic dynamics*. Later, it is verified in Proposition 3.3.1 that the Gibbs distribution μ_β is again the invariant distribution of the model. Denote by $r_\beta^{\mathrm{cyc}}(\cdot,\,\cdot)$ the transition rate of the cyclic dynamics.

For $q = 2$, that is, for the Ising model, we obtain $\sigma_\beta^{\mathrm{cyc}}(\cdot) \equiv \sigma_\beta^{\mathrm{MH}}(\cdot)$. However, for $q \geq 3$, the cyclic dynamics is *non-reversible* since a rotation of a spin cannot be reversed, and thus, the cyclic dynamics behaves in a fundamentally different manner to the reversible MH dynamics. In summary, we can regard the cyclic dynamics as a *non-reversible generalization of the standard MH dynamics of the Potts model.*

Finally, we remark that the metastability of a similar cyclic (non-reversible) dynamics for the mean-field Potts model was studied in [59, 63].

Notation for two dynamics

In the remainder of this chapter, we omit the explicit labels in $\sigma_\beta^{\mathrm{MH}}(\cdot)$ (resp. $\mathcal{L}_\beta^{\mathrm{MH}}$ and $r_\beta^{\mathrm{MH}}(\cdot,\,\cdot)$) and $\sigma_\beta^{\mathrm{cyc}}(\cdot)$ (resp. $\mathcal{L}_\beta^{\mathrm{cyc}}$ and $r_\beta^{\mathrm{cyc}}(\cdot,\,\cdot)$), and simply denote as $\sigma_\beta(\cdot)$ (resp. $\mathcal{L}_\beta$ and $r_\beta(\cdot,\,\cdot)$) for both dynamics, when no risk of confusion arises.

Other models

All metastability results that are explained in the following section for the MH/cyclic dynamics can be extended to several other interesting non-reversible models. An introduction of these models and an explanation of the corresponding main results are presented in Section 3.3 without detailed proofs.

3.1 Main results

In this section, we explain our main results of Chapter 3. To investigate the metastable behavior of the dynamical system, first one has to quantify the energy barrier between metastable sets. Since the ground states operate as metastable states in the $\beta \to \infty$ regime, we compute the energy barrier between them.

Edge structure

For $\sigma,\, \zeta \in \mathcal{X}$, we write $\sigma \sim \zeta$ if the dynamics can jump from σ to ζ or vice versa, that is,

$$r_\beta(\sigma,\, \zeta) + r_\beta(\zeta,\, \sigma) > 0. \tag{3.4}$$

Note that $\sigma \sim \zeta$ if and only if $\zeta \sim \sigma$. This relation depends on the selection of the dynamics, but not on the value of $\beta > 0$.

Height of paths

We first define *height* $H(\sigma,\, \zeta)$ between σ and ζ with $\sigma \sim \zeta$ as

$$H(\sigma,\, \zeta) = \begin{cases} \max\{H(\sigma),\, H(\zeta)\} & \text{for the MH dynamics,} \\ \max\limits_{a\in\Omega} H(\sigma^{x,\, a}), \quad \zeta = \tau_x\sigma \text{ or } \sigma = \tau_x\zeta & \text{for the cyclic dynamics.} \end{cases} \tag{3.5}$$

Note that this height is defined so that for both dynamics and for $\sigma,\,\zeta \in \mathcal{X}$ with $r_\beta(\sigma,\,\zeta) > 0$,

$$\mu_\beta(\sigma) r_\beta(\sigma,\,\zeta) = Z_\beta^{-1} e^{-\beta H(\sigma,\,\zeta)}. \tag{3.6}$$

A sequence $\omega = (\omega_n)_{n=0}^N$ of configurations is defined as a *path* from ω_0 to ω_N if $r_\beta(\omega_n,\,\omega_{n+1}) > 0$ for each $n \in [\![0,\,N-1]\!]$ (according to (3.4), this is a stronger requirement than $\omega_n \sim \omega_{n+1}$). We write $\omega : \sigma \to \zeta$ if ω is a path from σ to ζ. Subsequently, the *height* Φ_ω of a path $\omega = (\omega_n)_{n=0}^N$ is defined as

$$\Phi_\omega := \begin{cases} \max_{n \in [\![0,\,N-1]\!]} H(\omega_n,\,\omega_{n+1}) & \text{if } N \geq 1, \\ H(\omega_0) & \text{if } N = 0. \end{cases} \tag{3.7}$$

We note that, particularly in the MH dynamics, it holds that

$$\Phi_\omega = \max_{n \in [\![0,\,N-1]\!]} \max\{H(\omega_n),\,H(\omega_{n+1})\} = \max_{n \in [\![0,\,N]\!]} H(\omega_n), \tag{3.8}$$

but this result does not hold in the cyclic dynamics.

Communication height and energy barrier

For $\sigma,\,\zeta \in \mathcal{X}$ (not necessarily $\sigma \sim \zeta$), the *communication height* $\Phi(\sigma,\,\zeta)$ from σ to ζ is defined as

$$\Phi(\sigma,\,\zeta) := \min_{\omega:\sigma \to \zeta} \Phi_\omega. \tag{3.9}$$

It can be easily checked that

$$\Phi(\sigma,\,\sigma) = H(\sigma) \quad \text{for all } \sigma \in \mathcal{X}. \tag{3.10}$$

Moreover, for two disjoint subsets $\mathcal{P}$ and $\mathcal{Q}$ we define

$$\Phi(\mathcal{P},\,\mathcal{Q}) := \min_{\sigma \in \mathcal{P}} \min_{\zeta \in \mathcal{Q}} \Phi(\sigma,\,\zeta),$$

where we use the convention $\Phi(\{\sigma\},\, \mathcal{Q}) = \Phi(\sigma,\, \mathcal{Q})$ and $\Phi(\mathcal{P},\, \{\zeta\}) = \Phi(\mathcal{P},\, \zeta)$. For each $\boldsymbol{a} \in \mathcal{S}$, we write

$$\breve{\boldsymbol{a}} := \mathcal{S} \setminus \{\boldsymbol{a}\}. \tag{3.11}$$

Then, the *energy barrier* Γ between ground states is defined as

$$\Gamma := \Phi(\boldsymbol{a},\, \breve{\boldsymbol{a}}) \quad \text{for } \boldsymbol{a} \in \mathcal{S}.$$

Note that Γ does not depend on the selection of $\boldsymbol{a} \in \mathcal{S}$ owing to the symmetry of the models. The following result characterizes the energy barrier.

Theorem 3.1.1. *For all $\boldsymbol{a},\, \boldsymbol{b} \in \mathcal{S}$, it holds that*

$$\Gamma = \Phi(\boldsymbol{a},\, \boldsymbol{b}) = \begin{cases} 2K+2 & \textit{for the MH dynamics,} \\ 2K+4 & \textit{for the cyclic dynamics with } q \geq 3. \end{cases} \tag{3.12}$$

The proof of this theorem for the MH dynamics has already been obtained in [69, Theorem 2.1]. The proof for the cyclic dynamics is presented in Section 3.6.1. We note that the relation $\Gamma = \Phi(\boldsymbol{a},\, \boldsymbol{b})$ for any $\boldsymbol{a},\, \boldsymbol{b} \in \mathcal{S}$ follows directly from the symmetry of the dynamics in the case of the MH dynamics. On the other hand, this needs to be proved separately in the case of the cyclic dynamics.

3.1.1 Eyring–Kramers formula

In view of Theorem 3.0.1, when β is very large, the Gibbs distribution is concentrated on the ground states in $\mathcal{S}$, and therefore, the associated Markovian dynamics is expected to exhibit metastable behavior. More precisely, the process $\sigma_\beta(\cdot)$ starting from a ground state is expected to make a transition to another one on a large time scale. To describe this hopping dynamics among the ground states precisely, first, the mean of the transition time from one ground state to another must be calculated.

Our first main result for the metastability of the dynamics defined above is the Eyring–Kramers formula. We again emphasize that $K \le L$ is assumed. The following theorem holds for both MH and cyclic dynamics.

Theorem 3.1.2 (Eyring–Kramers formula)**.** *There exists a constant* $\kappa = \kappa(K,\, L) > 0$ *such that for all* $a,\, b \in \Omega$ *(cf.* (3.11) *and* (3.12)*),*

$$\lim_{\beta\to\infty} e^{-\Gamma\beta}\mathbb{E}_{\boldsymbol{a}}[\tau_{\check{\boldsymbol{a}}}] = \frac{\kappa}{q-1} \quad \text{and} \quad \lim_{\beta\to\infty} e^{-\Gamma\beta}\mathbb{E}_{\boldsymbol{a}}[\tau_{\boldsymbol{b}}] = \kappa. \tag{3.13}$$

Moreover, the constant κ *satisfies*

$$\kappa = \frac{\nu_0}{4} + o_K(1), \tag{3.14}$$

where $o_K(1)$ *is a term that vanishes as* $K \to \infty$*, and* ν_0 *is a constant defined as*

$$\nu_0 = \begin{cases} 1 & \text{if } K < L, \\ 1/2 & \text{if } K = L. \end{cases} \tag{3.15}$$

In the sequel, any appearance of ν_0 refers to (3.15).

We remark that in the case of $K < L$, the metastable transition occurs in only one direction of the lattice, whereas in the case of $K = L$, two possible (horizontal and vertical) directions exist. This difference induces the definition (3.15) of ν_0. Furthermore, the constants $\kappa(K,\, L)$ for the MH and cyclic dynamics differ (although their limits in the regime $K \to \infty$ are equal). Refer to Section 3.1.3 for comments on the proof of Theorem 3.1.2.

3.1.2 Markov chain model reduction

The aforementioned Eyring–Kramers formula provides a sharp estimate of the mean transition time from one ground state to another. Furthermore, since the hopping transitions between ground states occur successively, these sequential jumps need to be understood in a more systematic manner.

Approximation by trace process

Definition 3.1.3 (Trace process)**.** We define a non-decreasing random variable $T_{\mathcal{S}}$, the *local time* in $\mathcal{S}$ of the process, as

$$T_{\mathcal{S}}(t) := \int_0^t \mathbb{1}\{\eta_N(s) \in \mathcal{S}\} ds \quad \text{for } t \geq 0.$$

Let $T_{\mathcal{S}}^{-1}$ be its generalized inverse function:

$$T_{\mathcal{S}}^{-1}(s) = \sup\{t \geq 0 : T(t) \leq s\} \quad \text{for } s \geq 0.$$

Then, the *trace process* $\sigma_\beta^{\mathcal{S}}(t)$, $t \geq 0$ on $\mathcal{S}$ is defined by

$$\sigma_\beta^{\mathcal{S}}(t) = \sigma_\beta\big(T_{\mathcal{S}}^{-1}(t)\big) \quad \text{for } t \geq 0.$$

The random time $T_{\mathcal{S}}(t)$ measures the local time up to time t that the process spends in $\mathcal{S}$. Hence, the random function $T_{\mathcal{S}}^{-1}$ reconstructs the global time of the process, starting from the local time in $\mathcal{S}$. In this sense, the trace process $\sigma_\beta^{\mathcal{S}}(\cdot)$ on $\mathcal{S}$ is obtained from the original process $\sigma_\beta(\cdot)$ by turning off the clock whenever it is not in $\mathcal{S}$. Therefore, $\sigma_\beta^{\mathcal{S}}(\cdot)$ becomes a continuous-time irreducible Markov chain on $\mathcal{S}$. Rigorous proof of this fact can be found in e.g., [5, Section 6.1].

Since it can be guessed from the Eyring–Kramers formula (cf. Theorem 3.1.2) that the transitions among the ground states occur on the time scale $e^{\Gamma\beta}$, the original process first needs to be accelerated by this factor to observe the inter-ground state jumps in the ordinary time scale. Hence, we define the *accelerated* trace process

$$Y_\beta(t) = \sigma_\beta^{\mathcal{S}}(e^{\Gamma\beta}t) \quad \text{for all } t \geq 0.$$

The following estimate verifies that the accelerated original process $\sigma_\beta(e^{\Gamma\beta}\cdot)$ does not spend meaningful time outside of $\mathcal{S}$, and therefore, the accelerated trace process $Y_\beta(\cdot)$ successfully captures the inter-ground state dynamics.

Theorem 3.1.4 (Negligibility of excursions)**.** *For both dynamics, we have*

$$\lim_{\beta\to\infty} \max_{\boldsymbol{a}\in\mathcal{S}} \mathbb{E}_{\boldsymbol{a}}\Big[\int_0^T \mathbb{1}\{\sigma_\beta(e^{\Gamma\beta}u) \notin \mathcal{S}\}du\Big] = 0 \quad \text{for all } T > 0. \tag{3.16}$$

Proof. Denote by $\mathbb{P}_{\mu_\beta}$ the law of the process $\sigma_\beta(\cdot)$ starting from distribution μ_β. Then for any $u > 0$, we obtain

$$\mathbb{P}_{\boldsymbol{a}}[\sigma_\beta(u) \notin \mathcal{S}] \le \frac{1}{\mu_\beta(\boldsymbol{a})}\mathbb{P}_{\mu_\beta}[\sigma_\beta(u) \notin \mathcal{S}] = \frac{\mu_\beta(\mathcal{X}\setminus\mathcal{S})}{\mu_\beta(\boldsymbol{a})},$$

where the final identity holds because μ_β is the invariant distribution. Hence, by the Fubini theorem,

$$\mathbb{E}_{\boldsymbol{a}}\Big[\int_0^t \mathbb{1}\{\sigma_\beta(e^{\Gamma\beta}u) \notin \mathcal{S}\}du\Big] = \int_0^t \mathbb{P}_{\boldsymbol{a}}[\sigma_\beta(e^{\Gamma\beta}u) \notin \mathcal{S}]du \le t \cdot \frac{\mu_\beta(\mathcal{X}\setminus\mathcal{S})}{\mu_\beta(\boldsymbol{a})},$$

which vanishes as $\beta \to \infty$ according to Theorem 3.0.1. □

Convergence of trace process

We prove that the process $Y_\beta(\cdot)$ converges to a certain continuous-time Markov process $Y(\cdot)$ on $\mathcal{S}$. This limiting Markov chain $\{Y(t)\}_{t\ge0}$ is defined as a continuous-time Markov chain on $\mathcal{S}$ with the uniform jump rate $r_Y(\cdot,\,\cdot)$ given by

$$r_Y(\boldsymbol{a},\,\boldsymbol{b}) = \kappa^{-1} \quad \text{for all } \boldsymbol{a},\,\boldsymbol{b} \in \mathcal{S}, \tag{3.17}$$

where $\kappa = \kappa(K,\,L)$ is the constant that appears in Theorem 3.1.2. We subsequently obtain the following convergence result for both MH and cyclic dynamics.

Theorem 3.1.5 (Markov chain model reduction)**.** *Suppose that the original process $\sigma_\beta(\cdot)$ starts from $\boldsymbol{a} \in \mathcal{S}$. Then, the law of the Markov chain $Y_\beta(\cdot)$ converges to the law of the limiting Markov chain $Y(\cdot)$ starting from $\boldsymbol{a}$ as*

$\beta \to \infty$, where the convergence occurs in the sense of the usual Skorokhod topology.

By combining this result with Theorem 3.1.4, we can describe the metastable (i.e., the inter-ground state) dynamics of $\sigma_\beta(\cdot)$ on the time scale $e^{\beta\Gamma}$ using the Markovian movement expressed by $Y(\cdot)$. Therefore, the package of results in Theorems 3.1.4 and 3.1.5 is known in the literature as the Markov chain model reduction of the metastable behavior [5, 7, 8]. This method provides a powerful explanation for the metastable behavior, especially when multiple ground states exist, as in the current model.

Remark 3.1.6 (Coarse-graining effect)*.* In the cyclic dynamics, the spin can be updated in only one direction $1 \to 2 \to \cdots \to q \to 1$. However, Theorem 3.1.5 states that the macroscopic jumps among the ground states $\mathbf{1}$, $\mathbf{2}$, $\dots$, $\boldsymbol{q}$ occur in a uniform manner. Thus, it can be inferred that a *coarse-graining effect* removes the cyclic feature of the microscopic world on the macroscopic scale.

3.1.3 Comments on proof

It was demonstrated in [20] and [7] that the proof of the Eyring–Kramers formula for both reversible and non-reversible dynamics is reduced to the estimation of a potential-theoretic notion known as the *capacity*, which is defined in Section 3.2.1. The proof of the Markov chain model reduction for reversible dynamics also relies on the estimation of the capacity (cf. [5]), whereas [60] showed that the non-reversible case additionally requires the estimate of the equilibrium potential on each metastable set.

In Section 3.2, we present a novel and robust strategy to derive the estimates of the capacity as well as the equilibrium potential based on the H^1-approximation. According to this strategy, the proofs of Theorems 3.1.2 and 3.1.5 are reduced to constructions of certain *test functions*. This is a decent simplification of the already-known methodologies, in that:

(1) Classic potential-theoretic approaches (e.g., [60, 78]) require the construction of a (divergence-free) test flow, which is in general very difficult to achieve.

(2) This new method provides the estimate of the equilibrium potential as a by-product (which is crucial in the proof of the Markov chain model reduction for non-reversible dynamics).

We expect that this strategy will be applicable to a wide range of non-reversible models. The details of this method are discussed in Section 3.2.6.

Analysis of energy landscape

A deep understanding of the energy landscape as well as the behavior of the dynamics thereon is required to construct a test function to employ our strategy. The main difficulty of the zero external field model considered in this chapter lies on the complexity of the saddle structure. This structure consists of a large plateau with a high magnitude of complexity (compared to the non-zero external field model, in which the saddle structure is sharp and fully characterized by the existence of a special form of critical droplets). This is another major difficulty that we aim to overcome.

However, it is impossible to describe the saddle structure without the definition of numerous notions. Hence, we provide a detailed explanation of the saddle structure for the MH and cyclic dynamics in Sections 3.4 and 3.6, respectively. Thereafter, we construct the test functions for the MH and cyclic dynamics in Sections 3.5 and 3.7, respectively.

3.1.4 Remarks on open-boundary models

A careful investigation of our proof reveals that all results explained above can also be extended to the open-boundary model. In the open-boundary model, the energy barrier is given by

$$\Gamma = \begin{cases} K+1 & \text{for the MH dynamics,} \\ K+3 & \text{for the cyclic dynamics with } q \geq 3, \end{cases}$$

and the constant κ that appears in Theorem 3.1.2 satisfies

$$\kappa(K,\, L) = (4KL)^{-1}[\nu_0 + o_K(1)].$$

With these modifications, Theorems 3.1.1, 3.1.2, 3.1.4, and 3.1.5 also hold.

3.2 Potential theory and H^1-approximation

In this section, we first provide a brief but self-contained summary of the essential background on the potential theory of non-reversible Markov processes on discrete spaces. For more detailed explanation, we refer to [7, 34, 79]. Then, we introduce a new strategy, the *H^1-approximation method*, to prove the Eyring–Kramers formula and Markov chain model reduction. We explain our strategy in terms of the process $\sigma_\beta(\cdot)$, which is either the MH or the cyclic dynamics. Note again that we do not assume reversibility of the underlying process $\sigma_\beta(\cdot)$.

In the current section, we fix two disjoint non-empty subsets $\mathcal{P}$ and $\mathcal{Q}$ of $\mathcal{X}$.

3.2.1 Preliminaries

Equilibrium potential and capacity

The *equilibrium potential* between $\mathcal{P}$ and $\mathcal{Q}$ is the function $h_{\mathcal{P},\,\mathcal{Q}} = h^\beta_{\mathcal{P},\,\mathcal{Q}} : \mathcal{X} \to [0,\, 1]$ defined by

$$h_{\mathcal{P},\,\mathcal{Q}}(\sigma) = \mathbb{P}_\sigma[\tau_\mathcal{P} < \tau_\mathcal{Q}] \quad \text{for all } \sigma \in \mathcal{X}. \tag{3.18}$$

This function can also be characterized as the unique solution of the following equation (cf. (2.1) and (3.3)):

$$\begin{cases} h_{\mathcal{P},\,\mathcal{Q}} \equiv 1 & \text{on } \mathcal{P}, \\ h_{\mathcal{P},\,\mathcal{Q}} \equiv 0 & \text{on } \mathcal{Q}, \\ \mathcal{L}_\beta h_{\mathcal{P},\,\mathcal{Q}} \equiv 0 & \text{on } (\mathcal{P} \cup \mathcal{Q})^c. \end{cases} \tag{3.19}$$

Denote by $D_\beta(\cdot)$ the *Dirichlet form* associated with the process $\sigma_\beta(\cdot)$; i.e., for each $f : \mathcal{X} \to \mathbb{R}$,

$$D_\beta(f) := \langle f,\, -\mathcal{L}_\beta f \rangle_{\mu_\beta} = \frac{1}{2} \sum_{\sigma,\,\zeta \in \mathcal{X}} \mu_\beta(\sigma) r_\beta(\sigma,\, \zeta) [f(\zeta) - f(\sigma)]^2, \tag{3.20}$$

where $\langle \cdot,\, \cdot \rangle_{\mu_\beta}$ denotes the $L^2(\mu_\beta)$-inner product defined by

$$\langle f,\, g \rangle_{\mu_\beta} := \sum_{\sigma \in \mathcal{X}} f(\sigma) g(\sigma) \mu_\beta(\sigma).$$

Especially, according to the second representation, the Dirichlet form gives an H^1*-seminorm structure* to $L^2(\mu_\beta)$. In particular, it holds that

$$\sqrt{D_\beta(f+g)} \le \sqrt{D_\beta(f)} + \sqrt{D_\beta(g)} \quad \text{for all } f,\, g : \mathcal{X} \to \mathbb{R}. \tag{3.21}$$

The *capacity* between $\mathcal{P}$ and $\mathcal{Q}$ is then defined as

$$\mathrm{Cap}_\beta(\mathcal{P},\, \mathcal{Q}) := D_\beta(h_{\mathcal{P},\,\mathcal{Q}}). \tag{3.22}$$

Adjoint dynamics

We denote by $r_\beta^*(\cdot,\, \cdot)$ the adjoint transition rate with respect to the original transition rate $r_\beta(\cdot,\, \cdot)$; i.e., for all $\sigma,\, \zeta \in \mathcal{X}$,

$$r_\beta^*(\sigma,\, \zeta) := \frac{\mu_\beta(\zeta) r_\beta(\zeta,\, \sigma)}{\mu_\beta(\sigma)}. \tag{3.23}$$

The adjoint dynamics $\{\sigma_\beta^*(t)\}_{t\geq 0}$ is the continuous-time Markov process on $\mathcal{X}$ with jump rate $r_\beta^*(\cdot,\,\cdot)$. The process $\sigma_\beta^*(\cdot)$ also admits μ_β as its unique invariant distribution (cf. [34, Section 2]). Note that if the process $\sigma_\beta(\cdot)$ is reversible, we have $r_\beta^*(\cdot,\,\cdot) \equiv r_\beta(\cdot,\,\cdot)$ by the detailed balance condition, and hence it holds that $\sigma_\beta(\cdot) \equiv \sigma_\beta^*(\cdot)$.

We can define the equilibrium potential $h^*_{\mathcal{P},\,\mathcal{Q}}$ and the capacity $\mathrm{Cap}^*_\beta(\mathcal{P},\,\mathcal{Q})$ with respect to the adjoint dynamics $\sigma_\beta^*(\cdot)$ in the same manner as above. It is well known, see e.g. [34, display (2.4)], that $\mathrm{Cap}_\beta(\mathcal{P},\,\mathcal{Q}) = \mathrm{Cap}^*_\beta(\mathcal{P},\,\mathcal{Q})$.

3.2.2 Reduction to potential-theoretic estimates

In this subsection, we explain the relation between the potential-theoretic notions explained above and our main theorems (namely, the Eyring–Kramers formula and the Markov chain model reduction).

General strategy for Eyring–Kramers formula

The proof of the Eyring–Kramers formula relies on the so-called magic formula discovered for the reversible case in [20] and then extended to the non-reversible case in [7, Proposition A.2]. This formula asserts that for $\boldsymbol{a} \in \mathcal{S}$ and $\mathcal{Q} \subseteq \breve{\boldsymbol{a}}$ (cf. (3.11)), we have the following expression for the mean transition time:

$$\mathbb{E}_{\boldsymbol{a}}[\tau_{\mathcal{Q}}] = \frac{1}{\mathrm{Cap}_\beta(\boldsymbol{a},\,\mathcal{Q})} \sum_{\zeta\in\mathcal{X}} \mu_\beta(\zeta) h^*_{\boldsymbol{a},\,\mathcal{Q}}(\zeta). \tag{3.24}$$

By Theorem 3.0.1 and a trivial bound $0 \leq h^*_{\boldsymbol{a},\,\mathcal{Q}} \leq 1$ (cf. (3.18)), we have

$$0 \leq \sum_{\zeta\in\mathcal{X}\setminus\mathcal{S}} \mu_\beta(\zeta) h^*_{\boldsymbol{a},\,\mathcal{Q}}(\zeta) \leq \mu_\beta(\mathcal{X}\setminus\mathcal{S}) = o(1).$$

Inserting this to (3.24) and applying Theorem 3.0.1 again, we obtain

$$\mathbb{E}_{\boldsymbol{a}}[\tau_{\mathcal{Q}}] = \frac{1}{\mathrm{Cap}_\beta(\boldsymbol{a},\,\mathcal{Q})} \Big[\sum_{\boldsymbol{s}\in\mathcal{S}} \frac{1}{q} h^*_{\boldsymbol{a},\,\mathcal{Q}}(\boldsymbol{s}) + o(1) \Big]. \tag{3.25}$$

Therefore, in order to prove the Eyring–Kramers formula, *it suffices to deduce sharp asymptotics of* $\mathrm{Cap}_\beta(\boldsymbol{a},\, \mathcal{Q})$ *and* $h^*_{\boldsymbol{a},\, \mathcal{Q}}(\boldsymbol{s})$ *for each* $\boldsymbol{s} \in \mathcal{S}$.

General strategy for Markov chain model reduction

Denote by $r_{Y_\beta}(\cdot,\, \cdot) : \mathcal{S} \times \mathcal{S} \to [0,\, \infty)$ the jump rate of the accelerated trace process $Y_\beta(\cdot)$. Then, to prove the convergence of $Y_\beta(\cdot)$ to the process $Y(\cdot)$ with jump rate (3.17), it suffices to prove conditions **(H0)** and **(H1)** in [7, Theorem 2.1]. In the specific cases when the metastable sets are singletons, such as in our case, condition **(H1)** is trivial and we are left to verify condition **(H0)**, which is according to our notation,

$$\lim_{\beta \to \infty} r_{Y_\beta}(\boldsymbol{a},\, \boldsymbol{b}) = \frac{1}{\kappa}. \tag{3.26}$$

It has been discovered in [7, 60] that

$$r_{Y_\beta}(\boldsymbol{a},\, \boldsymbol{b}) = e^{\beta\Gamma} \frac{\mathrm{Cap}_\beta(\boldsymbol{a},\, \breve{\boldsymbol{a}})}{\mu_\beta(\boldsymbol{a})} h_{\boldsymbol{b},\, \mathcal{S} \setminus \{\boldsymbol{a},\, \boldsymbol{b}\}}(\boldsymbol{a}) \quad \text{for } \boldsymbol{a},\, \boldsymbol{b} \in \mathcal{S}. \tag{3.27}$$

Thus, in view of Theorem 3.0.1, to prove (3.26), *it suffices to estimate* $\mathrm{Cap}_\beta(\boldsymbol{a},\, \breve{\boldsymbol{a}})$ *and* $h_{\boldsymbol{b},\, \mathcal{S} \setminus \{\boldsymbol{a},\, \boldsymbol{b}\}}(\boldsymbol{a})$ *for* $\boldsymbol{a},\, \boldsymbol{b} \in \mathcal{S}$.

Summing up, we can observe that Theorems 3.1.2 and 3.1.5 are consequences of sharp estimates of $\mathrm{Cap}_\beta(\mathcal{P},\, \mathcal{Q})$, $h_{\mathcal{P},\, \mathcal{Q}}(\boldsymbol{s})$, and $h^*_{\mathcal{P},\, \mathcal{Q}}(\boldsymbol{s})$ for disjoint non-empty subsets $\mathcal{P},\, \mathcal{Q} \subseteq \mathcal{S}$ and $\boldsymbol{s} \in \mathcal{S}$. These estimates will be established in the next subsection (cf. Theorems 3.2.3 and 3.2.4).

Remark 3.2.1. We remark that in the reversible case, it is possible to calculate the transition rate of the trace process in terms of capacities only. Indeed, according to [5, Lemma 6.8], it holds that for $\boldsymbol{a},\, \boldsymbol{b} \in \mathcal{S}$,

$$\mu_\beta(\boldsymbol{a}) r_{Y_\beta}(\boldsymbol{a},\, \boldsymbol{b}) = \frac{1}{2}\big[\mathrm{Cap}_\beta(\boldsymbol{a},\, \breve{\boldsymbol{a}}) + \mathrm{Cap}_\beta(\boldsymbol{b},\, \breve{\boldsymbol{b}}) - \mathrm{Cap}_\beta(\{\boldsymbol{a},\, \boldsymbol{b}\},\, \mathcal{S} \setminus \{\boldsymbol{a},\, \boldsymbol{b}\})\big]. \tag{3.28}$$

According to this strategy, in the reversible case, it suffices to estimate

$\mathrm{Cap}_\beta(\mathcal{A}, \mathcal{S} \setminus \mathcal{A})$ for $\mathcal{A} \subseteq \mathcal{S}$. However, to pursue the complete level of generality also for non-reversible dynamics, we focus on the former strategy based on (3.27).

3.2.3 Estimates of capacity and equilibrium potential

Auxiliary constants

To state the main estimates, we first need to introduce the bulk and edge constants, which stand for the bulk and edge parts, respectively, of the saddle structure.

The *bulk constant* $\mathfrak{b} = \mathfrak{b}(K, L)$ is defined by (cf. (3.15))

$$\mathfrak{b} := \begin{cases} \nu_0 \dfrac{(K+2)(L-4)}{4KL} & \text{for the MH dynamics,} \\ \nu_0 \dfrac{(K-2)(L-4)}{4KL} & \text{for the cyclic dynamics with } q \geq 3, \end{cases} \tag{3.29}$$

while the *edge constant* $\mathfrak{e} = \mathfrak{e}(K, L)$ is defined by

$$\mathfrak{e} := \frac{\nu_0}{L} \mathfrak{e}_0, \tag{3.30}$$

where a complicated expression for the constant $\mathfrak{e}_0$ will be given in (3.64) and (3.104) for the MH and cyclic dynamics, respectively. Finally, the constant κ that appears in Theorem 3.1.2 is defined by

$$\kappa := \mathfrak{b} + 2\mathfrak{e}. \tag{3.31}$$

Lemma 3.2.2. *The constant κ satisfies* (3.14).

Proof. By Propositions 3.4.23 and 3.6.14, we have $0 < \mathfrak{e} \leq \frac{1}{L}$ and $0 < \mathfrak{e} < \frac{2}{L}$ for the MH and cyclic dynamics, respectively. Thus, $\mathfrak{e} = o_K(1)$ and therefore the conclusion of the lemma follows immediately from the expression (3.29) of the bulk constant. □

Main estimates

We start from the capacity estimate.

Theorem 3.2.3. *If* $\mathcal{P}$ *and* $\mathcal{Q}$ *are disjoint non-empty subsets of* $\mathcal{S}$*, it holds that*

$$\mathrm{Cap}_\beta(\mathcal{P},\ \mathcal{Q}) = (1+o(1)) \cdot c_0(\mathcal{P},\ \mathcal{Q}) e^{-\Gamma\beta}, \tag{3.32}$$

where $c_0(\mathcal{P},\ \mathcal{Q}) := \dfrac{|\mathcal{P}||\mathcal{Q}|}{\kappa(|\mathcal{P}|+|\mathcal{Q}|)}$.

Next, we state the estimate of equilibrium potentials.

Theorem 3.2.4. *If* $\mathcal{P}$ *and* $\mathcal{Q}$ *are disjoint non-empty subsets of* $\mathcal{S}$ *and* $\boldsymbol{s} \in \mathcal{S} \setminus (\mathcal{P} \cup \mathcal{Q})$*, it holds that*

$$h_{\mathcal{P},\,\mathcal{Q}}(\boldsymbol{s}),\ h^*_{\mathcal{P},\,\mathcal{Q}}(\boldsymbol{s}) = (1+o(1)) \cdot \frac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|}.$$

Up to this point, we followed a standard argument from the study of metastability. The main difficulty in this approach lies on the proof of these two theorems, especially when the dynamics is non-reversible.

3.2.4 Proof of the main results

Before proceeding to the proof of Theorems 3.2.3 and 3.2.4, we assume that these theorems hold and then prove the main results.

Proof of Theorem 3.1.2. We fix $\boldsymbol{a} \in \mathcal{S}$ and $\mathcal{Q} \subseteq \breve{\boldsymbol{a}}$, so that the estimate (3.25) on $\mathbb{E}_{\boldsymbol{a}}[\tau_{\mathcal{Q}}]$ holds. Applying Theorems 3.2.3 and 3.2.4 to this estimate, we obtain

$$\mathbb{E}_{\boldsymbol{a}}[\tau_{\mathcal{Q}}] = (1+o(1)) \cdot \frac{\kappa}{|\mathcal{Q}|} e^{\Gamma\beta}.$$

Inserting $\mathcal{Q} = \breve{\boldsymbol{a}}$ or $\{\boldsymbol{b}\}$ completes the proof. □

Proof of Theorem 3.1.5. Applying Theorems 3.0.1, 3.2.3 and 3.2.4 to the expression (3.27) of the jump rate $r_{Y_\beta}(\cdot,\,\cdot)$ yields that, for all $\boldsymbol{a},\,\boldsymbol{b}\in\mathcal{S}$,

$$r_{Y_\beta}(\boldsymbol{a},\,\boldsymbol{b})=e^{\Gamma\beta}\cdot\frac{(1+o(1))\cdot\frac{1\cdot(q-1)}{\kappa(1+(q-1))}e^{-\Gamma\beta}}{\frac{1}{q}+o(1)}\cdot\Big(\frac{1}{q-1}+o(1)\Big)=\frac{1}{\kappa}+o(1).$$

This completes the proof. □

We remark that particularly in the reversible case, we may alternatively apply the stategy explained in Remark 3.2.1. Namely, for all $\boldsymbol{a},\,\boldsymbol{b}\in\mathcal{S}$,

$$r_{Y_\beta}(\boldsymbol{a},\,\boldsymbol{b})=\frac{\mathrm{Cap}_\beta(\boldsymbol{a},\,\breve{\boldsymbol{a}})+\mathrm{Cap}_\beta(\boldsymbol{b},\,\breve{\boldsymbol{b}})-\mathrm{Cap}_\beta(\{\boldsymbol{a},\,\boldsymbol{b}\},\,\mathcal{S}\setminus\{\boldsymbol{a},\,\boldsymbol{b}\})}{2\mu_\beta(\boldsymbol{a})}.$$

Hence, by Theorems 3.2.3 and 3.0.1, we obtain the desired result.

3.2.5 Classic strategy: Dirichlet and Thomson principles

In this subsection, we explain two classic variational principles to estimate the capacity.

Dirichlet principle: reversible case

First, we establish the minimization principle for $\mathrm{Cap}_\beta(\mathcal{P},\,\mathcal{Q})$ when the process is reversible. We define

$$\mathfrak{C}_{a,\,b}(\mathcal{P},\,\mathcal{Q}):=\{f\in\mathbb{R}^{\mathcal{X}}:f=a\text{ on }\mathcal{P}\text{ and }f=b\text{ on }\mathcal{Q}\}.\tag{3.33}$$

Theorem 3.2.5 (Dirichlet principle, reversible case)**.** *If the process is reversible, we have*

$$\mathrm{Cap}_\beta(\mathcal{P},\,\mathcal{Q})=\min_{f\in\mathfrak{C}_{1,\,0}(\mathcal{P},\,\mathcal{Q})}D_\beta(f).$$

Moreover, the equilibrium potential $h_{\mathcal{P},\,\mathcal{Q}}$ is the unique optimizer of the minimization problem.

For the proof of this well-known principle, we refer to [16, Chapter 7]. We remark that this principle holds for the process $\sigma_\beta^{\mathrm{MH}}(\cdot)$ since the MH dynamics is reversible, whereas it does not necessarily hold for $\sigma_\beta^{\mathrm{cyc}}(\cdot)$ since the cyclic dynamics is irreversible for $q \geq 3$.

Thomson principle: reversible case

In order to explain the maximization problem for capacities, we introduce the flow structure.

Definition 3.2.6 (Flow structure)**.**

- A function $\phi : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is called a *flow* on $\mathcal{X}$ associated with the Markov process $\sigma_\beta(\cdot)$, if it is anti-symmetric in the sense that $\phi(\sigma,\,\zeta) = -\phi(\zeta,\,\sigma)$ for all $\sigma,\,\zeta \in \mathcal{X}$, and satisfies $\phi(\sigma,\,\zeta) \neq 0$ only if $\sigma \sim \zeta$ (cf. (3.4)).
- For each flow ϕ, we define the *norm* and *divergence* of the flow ϕ by

$$
\begin{aligned}
\|\phi\|^2 &:= \frac{1}{2} \sum_{\sigma,\,\zeta \in \mathcal{X}:\, \sigma \sim \zeta} \frac{\phi(\sigma,\,\zeta)^2}{\mu_\beta(\sigma) r_\beta(\sigma,\,\zeta)},\\
(\operatorname{div}\phi)(\sigma) &:= \sum_{\zeta \in \mathcal{X}} \phi(\sigma,\,\zeta) = \sum_{\zeta \in \mathcal{X}:\, \sigma \sim \zeta} \phi(\sigma,\,\zeta),\\
(\operatorname{div}\phi)(\mathcal{P}) &:= \sum_{\sigma \in \mathcal{P}} (\operatorname{div}\phi)(\sigma).
\end{aligned}
$$

- A flow ϕ is called a *unit flow* from $\mathcal{P}$ to $\mathcal{Q}$ if $(\operatorname{div}\phi)(\mathcal{P}) = 1$, $(\operatorname{div}\phi)(\mathcal{Q}) = -1$, and

$$
(\operatorname{div}\phi)(\sigma) = 0 \quad \text{for all } \sigma \in (\mathcal{P} \cup \mathcal{Q})^c.
$$

Then, the following Thomson principle holds, which is a natural counterpart to the Dirichlet principle.

Theorem 3.2.7 (Thomson principle, reversible case)**.** *If the process is reversible, we have*

$$\mathrm{Cap}_\beta(\mathcal{P},\ \mathcal{Q}) = \max_{\phi:\ \textit{unit flow from } \mathcal{P} \textit{ to } \mathcal{Q}} \frac{1}{\|\phi\|^2}.$$

Moreover, the harmonic flow

$$\varphi_{\mathcal{P},\,\mathcal{Q}}(\sigma,\,\zeta) := \mu_\beta(\sigma) r_\beta(\sigma,\,\zeta)[h_{\mathcal{P},\,\mathcal{Q}}(\sigma) - h_{\mathcal{P},\,\mathcal{Q}}(\zeta)] \tag{3.34}$$

is the unique optimizer of the maximization problem.

For the moment, assume that the process is reversible. Combining Theorems 3.2.5 and 3.2.7, if we find suitable test objects f_{test} and ϕ_{test}, approximating the equilibrium potential $h_{\mathcal{P},\,\mathcal{Q}}$ and the harmonic flow $\varphi_{\mathcal{P},\,\mathcal{Q}}$, respectively, we obtain the bounds

$$\frac{1}{\|\phi_{\text{test}}\|^2} \le \mathrm{Cap}_\beta(\mathcal{P},\ \mathcal{Q}) \le D_\beta(f_{\text{test}}).$$

If the asymptotic limits of the upper and lower bounds match, then we may conclude that the asymptotic limit of the capacity is also the same.

Generalized Dirichlet and Thomson principles

Next, we state a generalized version of the previous variational principles in the non-reversible setting, established in [34, 79, 78]. For a function $f : \mathcal{X} \to \mathbb{R}$ we define flows Φ_f and Φ_f^* as

$$\begin{aligned} \Phi_f(\sigma,\,\zeta) &:= f(\sigma)\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta) - f(\zeta)\mu_\beta(\zeta)r_\beta(\zeta,\,\sigma). \\ \Phi_f^*(\sigma,\,\zeta) &:= f(\sigma)\mu_\beta(\zeta)r_\beta(\zeta,\,\sigma) - f(\zeta)\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta). \end{aligned} \tag{3.35}$$

One can easily verify that Φ_f and Φ_f^* are indeed flows. Moreover, if the process is reversible, it is straightforward that $\Phi_f \equiv \Phi_f^*$. Notice that the harmonic flow $\varphi_{\mathcal{P},\,\mathcal{Q}}$ defined in (3.34) in the reversible case is exactly $\Phi_{h_{\mathcal{P},\,\mathcal{Q}}}$.

Theorem 3.2.8 (Generalized Dirichlet–Thomson principle [78, Theorem 5.3])**.**

(1) (Generalized Dirichlet principle) For $f \in \mathfrak{C}_{1,0}(\mathcal{P},\, \mathcal{Q})$ *and flow* ϕ*,*

$$\mathrm{Cap}_\beta(\mathcal{P},\, \mathcal{Q}) \le \|\Phi_f - \phi\|^2 + 2\sum_{\sigma\in\mathcal{X}} h_{\mathcal{P},\,\mathcal{Q}}(\sigma)(\mathrm{div}\,\phi)(\sigma). \tag{3.36}$$

Equality holds if and only if

$$(f,\, \phi) = \Big(\frac{h_{\mathcal{P},\,\mathcal{Q}} + h^*_{\mathcal{P},\,\mathcal{Q}}}{2},\, \frac{\Phi_{h^*_{\mathcal{P},\,\mathcal{Q}}} - \Phi^*_{h_{\mathcal{P},\,\mathcal{Q}}}}{2}\Big).$$

(2) (Generalized Thomson principle) For $g \in \mathfrak{C}_{0,0}(\mathcal{P},\, \mathcal{Q})$ *and flow* ψ*,*

$$\mathrm{Cap}_\beta(\mathcal{P},\, \mathcal{Q}) \ge \frac{1}{\|\Phi_g - \psi\|^2}\Big[\sum_{\sigma\in\mathcal{X}} h_{\mathcal{P},\,\mathcal{Q}}(\sigma)(\mathrm{div}\,\psi)(\sigma)\Big]^2. \tag{3.37}$$

Equality holds if and only if

$$(g,\, \psi) = \Big(\frac{h^*_{\mathcal{P},\,\mathcal{Q}} - h_{\mathcal{P},\,\mathcal{Q}}}{2\mathrm{Cap}_\beta(\mathcal{P},\, \mathcal{Q})},\, \frac{\Phi_{h^*_{\mathcal{P},\,\mathcal{Q}}} + \Phi^*_{h_{\mathcal{P},\,\mathcal{Q}}}}{2\mathrm{Cap}_\beta(\mathcal{P},\, \mathcal{Q})}\Big).$$

Thus, the strategy remains the same as in the reversible case; we intend to find suitable test objects f_{test}, ϕ_{test}, g_{test}, and ψ_{test} such that the right-hand sides of (3.36) and (3.37) give the same asymptotic limit as $\beta \to \infty$. However, one can easily notice that it becomes a far more demanding task than it was in the reversible case.

3.2.6 New strategy based on H^1-approximation

In this subsection, we now explain our new strategy, the H^1-approximation method, to prove Theorems 3.2.3 and 3.2.4.

H^1-approximation of equilibrium potentials

In view of the expression (3.22), the natural first step to estimate the capacity is to find good approximations of the equilibrium potentials $h_{\mathcal{P},\,\mathcal{Q}}$ and $h^*_{\mathcal{P},\,\mathcal{Q}}$. Since the Dirichlet form $D_\beta(f)$ can be regarded as the square of an H^1-seminorm (cf. (3.21)), the approximation is carried out in the sense of this seminorm.

Proposition 3.2.9. *In the setting of Theorems 3.2.3 and 3.2.4, there exist* $\widetilde{h} = \widetilde{h}_{\mathcal{P},\,\mathcal{Q}}$ *and* $\widetilde{h}^* = \widetilde{h}^*_{\mathcal{P},\,\mathcal{Q}}$ *such that all of the following properties hold.*

(1) Two functions $\widetilde{h}$ *and* $\widetilde{h}^*$ *approximate* $h_{\mathcal{P},\,\mathcal{Q}}$ *and* $h^*_{\mathcal{P},\,\mathcal{Q}}$ *in the sense that*

$$D_\beta(h_{\mathcal{P},\,\mathcal{Q}} - \widetilde{h}),\ D_\beta(h^*_{\mathcal{P},\,\mathcal{Q}} - \widetilde{h}^*) = o(e^{-\beta\Gamma}). \tag{3.38}$$

(2) We have

$$D_\beta(\widetilde{h}),\ D_\beta(\widetilde{h}^*) = (1 + o(1)) \cdot c_0(\mathcal{P},\ \mathcal{Q})e^{-\Gamma\beta}, \tag{3.39}$$

where $c_0(\mathcal{P},\ \mathcal{Q})$ *is the constant that appears in Theorem 3.2.3.*

(3) The values of $\widetilde{h}$ *and* $\widetilde{h}^*$ *on the set* $\mathcal{S}$ *of ground states are given as*

$$\widetilde{h}(\boldsymbol{s}) = \widetilde{h}^*(\boldsymbol{s}) = \begin{cases} 1 & \text{if } \boldsymbol{s} \in \mathcal{P}, \\ 0 & \text{if } \boldsymbol{s} \in \mathcal{Q}, \\ \dfrac{|\mathcal{P}|}{|\mathcal{P}| + |\mathcal{Q}|} & \text{if } \boldsymbol{s} \in \mathcal{S} \setminus (\mathcal{P} \cup \mathcal{Q}). \end{cases} \tag{3.40}$$

The proof of this proposition, i.e., the construction of $\widetilde{h}$ and $\widetilde{h}^*$ satisfying all properties above will be given in Sections 3.5 and 3.7 for the MH and cyclic dynamics, respectively. We note that the properties (3.39) and (3.40) are inspired from Theorems 3.2.3 and 3.2.4, respectively.

We now conclude this section by explaining the general strategy to derive Theorems 3.2.3 and 3.2.4 from Proposition 3.2.9. We abbreviate $h = h_{\mathcal{P},\,\mathcal{Q}}$ and $h^* = h^*_{\mathcal{P},\,\mathcal{Q}}$. Let us first look at Theorem 3.2.3.

Proof of Theorem 3.2.3. In principle, the estimate of $\mathrm{Cap}_\beta(\mathcal{P},\,\mathcal{Q}) = D_\beta(h)$ should follow from that of $D_\beta(h-\widetilde{h})$ and $D_\beta(\widetilde{h})$ obtained in (3.38) and (3.39), respectively, since $D_\beta(\cdot)^{1/2}$ defines a seminorm. Indeed, by (3.21), we have

$$D_\beta(\widetilde{h})^{1/2} - D_\beta(h-\widetilde{h})^{1/2} \le D_\beta(h)^{1/2} \le D_\beta(\widetilde{h})^{1/2} + D_\beta(h-\widetilde{h})^{1/2},$$

and thus by (3.38) and (3.39), we obtain

$$D_\beta(h) = (1+o(1)) \cdot c_0(\mathcal{P},\,\mathcal{Q})e^{-\Gamma\beta}.$$

This completes the proof since $\mathrm{Cap}_\beta(\mathcal{P},\,\mathcal{Q}) = D_\beta(h)$. □

Remark 3.2.10. It should be emphasized here that Proposition 3.2.9-(3) is not used in the proof of the capacity estimate. It will only be used in the proof of Theorem 3.2.4.

Next, we explain the robust proof of Theorem 3.2.4. It should be remarked that there was no robust method known in the literature to estimate the equilibrium potential.

Proof of Theorem 3.2.4. We only prove the theorem for $h = h_{\mathcal{P},\,\mathcal{Q}}$ since the proof for h^* is identical. Let us fix $\boldsymbol{s} \in \mathcal{S} \setminus (\mathcal{P} \cup \mathcal{Q})$. Write

$$\delta(\boldsymbol{s}) := h(\boldsymbol{s}) - \widetilde{h}(\boldsymbol{s}) = h(\boldsymbol{s}) - \frac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|},$$

so that we wish to prove $\delta(\boldsymbol{s}) = o(1)$. Note that there is nothing to prove if $\delta(\boldsymbol{s}) = 0$. Otherwise, write

$$G(\sigma) = \frac{1}{\delta(\boldsymbol{s})}\big[h(\sigma) - \widetilde{h}(\sigma)\big] \quad \text{for } \sigma \in \mathcal{X}.$$

By (3.38), we have

$$D_\beta(G) = \frac{1}{\delta(\boldsymbol{s})^2} D_\beta(h-\widetilde{h}) = \frac{1}{\delta(\boldsymbol{s})^2} o(e^{-\beta\Gamma}).$$

Therefore, it suffices to prove that there exists a constant $C > 0$ independent of β such that $D_\beta(G) \geq Ce^{-\beta\Gamma}$. This follows from the fact that $G(\boldsymbol{s}) = 1$, $G(\sigma) = 0$ for all $\sigma \in \mathcal{P} \cup \mathcal{Q}$, and the next lemma. $\square$

Lemma 3.2.11. *Let $\boldsymbol{s} \in \mathcal{S} \setminus (\mathcal{P} \cup \mathcal{Q})$. Then, there exists a constant $C > 0$ such that*

$$D_\beta(F) \geq Ce^{-\beta\Gamma} \tag{3.41}$$

for all $F \in \mathfrak{C}_{1,0}(\boldsymbol{s}, \mathcal{P} \cup \mathcal{Q})$ (cf .(3.33)).

Now, we finally discuss the proof of Lemma 3.2.11 which is the last ingredient in our robust argument. First, we present few standard strategies regarding the proof of Lemma 3.2.11.

(1) If $\sigma_\beta(\cdot)$ is reversible (e.g., the MH dynamics), by the Dirichlet principle for reversible Markov chains (cf. Theorem 3.2.5), we have $D_\beta(F) \geq \mathrm{Cap}_\beta(\boldsymbol{s}, \mathcal{P} \cup \mathcal{Q})$. Thus, the lemma is a direct consequence of our capacity estimate, i.e., Theorem 3.2.3.

(2) If $\sigma_\beta(\cdot)$ is non-reversible, we can define the symmetrized dynamics $\sigma_\beta^s(\cdot)$ with jump rate $\frac{1}{2}(r_\beta + r_\beta^*)(\cdot, \cdot)$. This dynamics is reversible with respect to μ_β. Denote by $\mathrm{Cap}_\beta^s(\cdot, \cdot)$ the capacity with respect to $\sigma_\beta^s(\cdot)$. Since the Dirichlet form associated with the process $\sigma_\beta^s(\cdot)$ is again $D_\beta(\cdot)$, by the Dirichlet principle for reversible Markov chains (cf. Theorem 3.2.5), we have

$$D_\beta(F) \geq \mathrm{Cap}_\beta^s(\boldsymbol{s}, \mathcal{P} \cup \mathcal{Q}). \tag{3.42}$$

Hence, it suffices to estimate $\mathrm{Cap}_\beta^s(\boldsymbol{s}, \mathcal{P} \cup \mathcal{Q})$.

(2-1) Since the capacity estimate of reversible dynamics cannot be more difficult than non-reversible ones, we can readily derive a result similar to Theorem 3.2.3 for $\mathrm{Cap}_\beta^s(\cdot, \cdot)$ (of course, the constant $c_0(\mathcal{P}, \mathcal{Q})$ in the right-hand side must be modified). Such a result, along with (3.42), directly implies (3.41).

(2-2) On the other hand if, for all $\beta > 0$, the process $\sigma_\beta(\cdot)$ satisfies the so-called *sector condition* (cf. [34, Section 2]) with a certain constant $C_0 > 0$ independent of β, then by [34, Lemma 2.6],

$$C_0 \mathrm{Cap}_\beta^s(\boldsymbol{s},\, \mathcal{P} \cup \mathcal{Q}) \geq \mathrm{Cap}_\beta(\boldsymbol{s},\, \mathcal{P} \cup \mathcal{Q}).$$

Thus, in this case Theorem 3.2.3, along with (3.42), immediately implies (3.41).

In our model, it is possible to use strategy **(2-2)** since an elementary computation reveals that the cyclic dynamics satisfies the sector condition with constant $C_0 = q^2$. However, instead of explaining this tedious detail, we provide another simple proof computing $D_\beta(F)$ directly, which is also suitable for our model.

Proof of Lemma 3.2.11. Let us take $\boldsymbol{a} \in \mathcal{P} \cup \mathcal{Q}$. By Theorem 3.1.1, there exists a path $\omega = (\omega_n)_{n=0}^N$ from $\boldsymbol{a}$ to $\boldsymbol{s}$ such that $H(\omega_n,\, \omega_{n+1}) \leq \Gamma$ for all $n \in [\![0,\, N-1]\!]$. Note that this path, and thus N, is independent of the inverse temperature β.

Since $r_\beta(\omega_n,\, \omega_{n+1}) > 0$ and $H(\omega_n,\, \omega_{n+1}) \leq \Gamma$, it holds from Theorem 3.0.1 and (3.6) that

$$\mu_\beta(\omega_n) r_\beta(\omega_n,\, \omega_{n+1}) = \frac{1}{Z_\beta} e^{-\beta H(\omega_n, \omega_{n+1})} \geq c e^{-\beta \Gamma}$$

for some $c > 0$. Therefore, by (3.38) and the formula (3.20) for the Dirichlet form, it holds that

$$\begin{aligned} D_\beta(F) &\geq \frac{1}{2} \sum_{n=0}^{N-1} \mu_\beta(\omega_n) r_\beta(\omega_n,\, \omega_{n+1}) [F(\omega_{n+1}) - F(\omega_n)]^2 \\ &\geq \frac{c}{2} e^{-\beta\Gamma} \sum_{n=0}^{N-1} [F(\omega_{n+1}) - F(\omega_n)]^2. \end{aligned}$$

Since $F(\omega_N) = F(\boldsymbol{s}) = 1$ and $F(\omega_0) = F(\boldsymbol{a}) = 0$, by the Cauchy–Schwarz inequality, the last summation is bounded from below by N^{-1}. This completes the proof. □

3.2.7 Concluding remark

The idea of finding proxies of equilibrium potentials is not novel. Such proxies already played a significant role in the previous potential-theoretic approach to metastability as well, since they provide approximations of the optimizers of the Dirichlet and Thomson principles. The point here is that the new method suggested above looks at these proxies in a completely different point of view, and in turn provides much more straightforward way to handle non-reversible situations and also the equilibrium potential. We refer to Remark 3.7.1 for more detail.

3.3 Other non-reversible models

Before proceeding to the analysis of the energy landscape and construction of the test functions, we explain some other interesting *non-reversible* dynamics associated with the Ising and Potts models that fall into the framework of Section 3.2. Proofs of the Eyring–Kramers formula and Markov chain model reduction for these models are similar with that of the cyclic model, and thus we will omit repetition of the proof.

3.3.1 Generalized cyclic dynamics on the Potts model

In the cyclic dynamics defined in Definition 3.0.2, a spin can only be rotated in the increasing order $(1 \to 2 \to \cdots)$. One can also imagine a model for which the spin can rotate in the opposite direction as well. To introduce this model, let us define an operator $\tau_x^{-1} : \mathcal{X} \to \mathcal{X}$ by

$$(\tau_x^{-1}\sigma)(y) = \begin{cases} \sigma(x) - 1 & \text{if } y = x, \\ \sigma(y) & \text{otherwise,} \end{cases}$$

where we use the convention $1 - 1 = q$. Then, for $p \in [0, 1]$, define the jump rate $r_{\beta,p}(\cdot, \cdot)$ on $\mathcal{X} \times \mathcal{X}$ as

$$r_{\beta,p}(\sigma, \zeta) = \begin{cases} pr_\beta^{\text{cyc}}(\sigma, \tau_x\sigma) & \text{if } \zeta = \tau_x\sigma \text{ and } x \in \Lambda, \\ (1-p)r_\beta^{\text{cyc}}(\sigma, \tau_x\sigma) & \text{if } \zeta = \tau_x^{-1}\sigma \text{ and } x \in \Lambda, \\ 0 & \text{otherwise.} \end{cases}$$

We denote by *p-cyclic dynamics* the continuous-time Markov process with jump rate $r_{\beta,p}(\cdot, \cdot)$. Note that the original cyclic dynamics corresponds to the 1-cyclic dynamics (i.e., $p = 1$).

Proposition 3.3.1. *For all $p \in [0, 1]$, the unique invariant distribution of the p-cyclic dynamics is the Gibbs distribution μ_β.*

Proof. Since it is clear that the p-cyclic dynamics is irreducible, a unique invariant distribution exists. In order to show that this is indeed μ_β, it suffices to check that for all $\sigma \in \mathcal{X}$,

$$\sum_{x\in\Lambda} \mu_\beta(\sigma) r_{\beta,p}(\sigma, \tau_x^{\pm1}\sigma) = \sum_{x\in\Lambda} \mu_\beta(\tau_x^{\pm1}\sigma) r_{\beta,p}(\tau_x^{\pm1}\sigma, \sigma). \tag{3.43}$$

By a direct computation based on the explicit formula for μ_β and $r_{\beta,p}$, we can check that both sides equal

$$\frac{1}{Z_\beta} \sum_{x\in\Lambda} \exp\big\{ -\beta \max_{a\in\Omega} H(\sigma^{x,a})\big\},$$

and therefore the proof is completed. □

Suppose from now on that $q \geq 3$, so that the p-cyclic dynamics is not the MH dynamics. Then, one can readily check that the p-cyclic dynamics is reversible if and only if $p = 1/2$, and the symmetrization (cf. strategy **(2-1)** after Lemma 3.2.11) of any p-cyclic dynamics is the $1/2$-cyclic dynamics. All results for the cyclic dynamics can be extended to the p-cyclic dynamics as follows.

Theorem 3.3.2. *For all $p \in [0,\, 1]$, the following statements hold for the p-cyclic dynamics.*

(1) The energy barrier is $\Gamma = 2K + 4$.

(2) (Eyring–Kramers formula) There exist constants $\kappa_i = \kappa_i(K,\, L,\, p) > 0$, $i \in [\![1,\, q-1]\!]$, such that

$$\lim_{\beta\to\infty} e^{-\Gamma\beta}\mathbb{E}_{\boldsymbol{a}}[\tau_{\breve{\boldsymbol{a}}}] = \frac{1}{\kappa_1^{-1} + \cdots + \kappa_{q-1}^{-1}} \quad \text{and} \quad \lim_{\beta\to\infty} e^{-\Gamma\beta}\mathbb{E}_{\boldsymbol{a}}[\tau_{\boldsymbol{b}}] = \kappa_{|b-a|} \tag{3.44}$$

for all $a,\, b \in \Omega$. The constants $(\kappa_i)_{i=1}^{q-1}$ satisfy $\kappa_i = \kappa_{q-i}$ for each $i \in [\![1,\, q-1]\!]$ and

$$\kappa_i(K,\, L,\, p) = \nu_0 \frac{(1+\hat{p})(1+\cdots+\hat{p}^{i-1})(1+\cdots+\hat{p}^{q-i-1})}{4(1+\cdots+\hat{p}^{q-1})} + o_K(1), \tag{3.45}$$

where ν_0 is the constant defined in (3.15) and

$$\hat{p} = \min\{p,\, 1-p\}/\max\{p,\, 1-p\}.$$

(3) (Markov chain model reduction) Theorems 3.1.4 and 3.1.5 hold with limiting Markov chain $Y(\cdot)$ defined by the jump rate $r_Y(\boldsymbol{a},\, \boldsymbol{b}) = \kappa_{|b-a|}^{-1}$.

Remark 3.3.3 (Comparison of transition rates). By an elementary computation, we can verify that the fraction in the right-hand side of (3.45) is increasing in $p \in [0,\, 1/2]$ and decreasing in $p \in [1/2,\, 1]$. Therefore, in view of the Eyring–Kramers formula (3.44), we can observe that the speed of transition becomes slower if p approaches to $1/2$, i.e., to reversibility. We can draw the same conclusion when we investigate the Markov chain model reduction. *This verifies a widely-believed fact that a non-reversible dynamics runs faster than the symmetrized reversible dynamics.*

3.3.2 Directed dynamics on the Ising model

One can readily observe that the p-cyclic dynamics defined above is identical to the reversible MH dynamics if $q = 2$. Therefore, so far we did not consider non-reversible dynamics associated with the Ising model. Here, we introduce such a non-reversible dynamics, first constructed in [38], for which the analysis of metastable behavior can be done in a similar manner.

Suppose from now on that $q = 2$, so that $\Omega = \{1, 2\}$. For each edge $e = \{x, y\}$ in Λ (i.e., with $x \sim y$), write

$$H_e(\sigma) := \mathbb{1}\{\sigma(x) \neq \sigma(y)\},$$

so that by definition we can write $H(\sigma) = \sum_{e\colon \text{edge of } \Lambda} H_e(\sigma)$.

For $\sigma \in \mathcal{X}$, we denote by σ^x, $x \in \Lambda$, the configuration obtained from σ by flipping the spin at site x. Then for $p \in [0, 1]$, the *p-directed dynamics* $\{\sigma^{\text{dir}}_{\beta,p}(t)\}_{t\geq 0}$ is defined as the continuous-time Markov process with jump rate $r^{\text{dir}}_{\beta,p}(\cdot, \cdot)$ defined by

$$r^{\text{dir}}_{\beta,p}(\sigma, \zeta) = \begin{cases} \exp\big\{ -\beta\Delta_p(\sigma, \zeta)\big\} & \text{if } \zeta = \sigma^x \text{ and } x \in \Lambda, \\ 0 & \text{otherwise,} \end{cases}$$

where

$$\begin{aligned} \Delta_p(\sigma, \sigma^x) := p\big[&H_{e_x}(\sigma^x) - H_{e_x}(\sigma) + H_{n_x}(\sigma^x) - H_{n_x}(\sigma)\big] \\ &+ (1-p)\big[H_{w_x}(\sigma^x) - H_{w_x}(\sigma) + H_{s_x}(\sigma^x) - H_{s_x}(\sigma)\big]. \end{aligned}$$

Here, e_x, n_x, w_x, and s_x denote four edges emanating from x towards eastern, northern, western and southern directions, respectively.

Note that $\Delta_{1/2}(\sigma, \sigma^x) = [H(\sigma^x) - H(\sigma)]/2$ and therefore for $p = 1/2$, the dynamics is reduced to the well-known reversible heat-bath Glauber dynamics. On the other hand, for $p \neq 1/2$, the dynamics puts different masses on the north/east edges and on the south/west edges, and thereby exhibits a *spatial non-reversibility*. It is verified in [38, Section 3.3] that μ_β is the unique invariant distribution of the p-directed dynamics for all $p \in [0, 1]$.

We can also analyze metastability of the p-directed model, and thus deduce the following results.

Theorem 3.3.4. *For all $p \in [0, 1]$, the following statements hold for the p-directed model.*

(1) The energy barrier is $\Gamma = 2K + 4\min\{p, 1-p\}$.

(2) (Eyring–Kramers formula) There exists a constant $\kappa_0 = \kappa_0(K, L, p) > 0$ such that

$$\lim_{\beta\to\infty} e^{-\Gamma\beta}\mathbb{E}_{\mathbf{1}}[\tau_{\mathbf{2}}] = \lim_{\beta\to\infty} e^{-\Gamma\beta}\mathbb{E}_{\mathbf{2}}[\tau_{\mathbf{1}}] = \kappa_0.$$

The constant κ_0 satisfies $\kappa_0(K, L, p) = \nu_0 + o_K(1)$.

(3) (Markov chain model reduction) Theorems 3.1.4 and 3.1.5 hold with limiting Markov chain $Y(\cdot)$ defined by the jump rate $r_Y(\mathbf{1}, \mathbf{2}) = r_Y(\mathbf{2}, \mathbf{1}) = \kappa_0^{-1}$.

We remark that the analysis of the p-directed dynamics is valid only under periodic boundary conditions.

3.4 Energy landscape analysis: Metropolis–Hastings dynamics

In this section, we investigate the energy landscape subjected to the MH dynamics, and in the next section, we construct the test functions to complete the proof of Proposition 3.2.9 for the MH dynamics.

Notation. In Sections 3.4 and 3.5 where we consider the MH dynamics, we use Greek letters η and ξ to denote the spin configurations. On the other hand, in Sections 3.6 and 3.7 where we consider the cyclic dynamics, we alternatively use Greek letters σ and ζ to denote the spin configurations.

Remark 3.4.1. The following remarks are important in the upcoming sections.

(1) In Sections 3.4 and 3.5, we always consider the *MH dynamics*. In particular, we have $\Gamma = 2K + 2$ and we know from [69, Theorem 2.1] that this Γ is indeed the energy barrier, i.e., Theorem 3.1.1 holds.

(2) In order to focus on the explanation of the saddle structure, which is quite complicated, we postpone detailed combinatorial proofs of the technical results to Section 3.9.

3.4.1 Neighborhoods

In the analysis of the energy landscape, the following notions are importantly used.

Definition 3.4.2 (Neighborhood of configurations)**.** For $\eta \in \mathcal{X}$, we define the neighborhoods of η as

$$\mathcal{N}(\eta) := \{\xi \in \mathcal{X} : \Phi(\eta, \xi) < \Gamma\} \quad \text{and} \quad \widehat{\mathcal{N}}(\eta) := \{\xi \in \mathcal{X} : \Phi(\eta, \xi) \le \Gamma\}.$$

Then, for $\mathcal{P} \subseteq \mathcal{X}$, we define

$$\mathcal{N}(\mathcal{P}) := \bigcup_{\eta \in \mathcal{P}} \mathcal{N}(\eta) \quad \text{and} \quad \widehat{\mathcal{N}}(\mathcal{P}) := \bigcup_{\eta \in \mathcal{P}} \widehat{\mathcal{N}}(\eta).$$

Remark 3.4.3. The following statements hold for neighborhoods.

(1) By (3.10), the set $\mathcal{N}(\eta)$ (resp. $\widehat{\mathcal{N}}(\eta)$) does not contain η provided that $H(\eta) \geq \Gamma$ (resp. $H(\eta) > \Gamma$).

(2) By (3.8) and (3.9), each configuration $\xi \in \mathcal{N}(\eta)$ (resp. $\widehat{\mathcal{N}}(\eta)$) satisfies $H(\xi) < \Gamma$ (resp. $H(\xi) \leq \Gamma$).

With this notation, the fact that Γ is the energy barrier can be reformulated in the following manner.

Notation 3.4.4. We say that a path ω is a *c-path* if $\Phi_\omega \leq c$. Moreover, a path $\omega = (\omega_n)_{n=0}^N$ is called a path in $\mathcal{P}$ if $\omega_n \in \mathcal{P}$ for all $n \in [\![0,\, N]\!]$.

Proposition 3.4.5. *For any* $\boldsymbol{a}, \boldsymbol{b} \in \mathcal{S}$*, we have* $\mathcal{N}(\boldsymbol{a}) \cap \mathcal{N}(\boldsymbol{b}) = \emptyset$ *and* $\widehat{\mathcal{N}}(\boldsymbol{a}) = \widehat{\mathcal{N}}(\boldsymbol{b})$.

Proof. By [69, Theorem 2.1-(i)], any path connecting $\boldsymbol{a}$ and $\boldsymbol{b}$ has height at least Γ, and there indeed exists a Γ-path from $\boldsymbol{a}$ to $\boldsymbol{b}$. The first assertion indicates by contradiction that $\mathcal{N}(\boldsymbol{a}) \cap \mathcal{N}(\boldsymbol{b}) = \emptyset$, while the second one implies that $\widehat{\mathcal{N}}(\boldsymbol{a}) = \widehat{\mathcal{N}}(\boldsymbol{b})$. □

We will now investigate what happens on the boundary of the set $\widehat{\mathcal{N}}(\eta)$.

Lemma 3.4.6. *Let* $\eta \in \mathcal{X}$ *and let* $\xi_1 \in \widehat{\mathcal{N}}(\eta)$*,* $\xi_2 \notin \widehat{\mathcal{N}}(\eta)$*, and* $\xi_1 \sim \xi_2$*. Then,* $H(\xi_2) > \Gamma$.

Proof. Since $\xi_1 \in \widehat{\mathcal{N}}(\eta)$, there exists a path $\omega : \eta \to \xi_1$ such that $\Phi_\omega \leq \Gamma$. Suppose to the contrary that $H(\xi_2) \leq \Gamma$. Then, we can concatenate the directed edge $(\xi_1,\, \xi_2)$ at the end of the path ω to form a new path $\widetilde{\omega} : \eta \to \xi_2$ satisfying $\Phi_{\widetilde{\omega}} \leq \Gamma$. This contradicts the assumption that $\xi_2 \notin \widehat{\mathcal{N}}(\eta)$. □

The following notion is also important in our investigation.

Definition 3.4.7 (Restricted neighborhood)**.** Let $\mathcal{Q} \subseteq \mathcal{X}$. For $\eta \in \mathcal{X} \setminus \mathcal{Q}$, we define

$$\widehat{\mathcal{N}}(\eta;\, \mathcal{Q}) := \{\xi \in \mathcal{X} : \exists \omega : \eta \to \xi \text{ in } \mathcal{Q}^c \text{ such that } \Phi_\omega \le \Gamma\}.$$

For $\mathcal{P} \subseteq \mathcal{X}$ disjoint with $\mathcal{Q}$, we define $\widehat{\mathcal{N}}(\mathcal{P};\, \mathcal{Q}) := \bigcup_{\eta \in \mathcal{P}} \widehat{\mathcal{N}}(\eta;\, \mathcal{Q})$.

By definition, the following lemma is immediate.

Lemma 3.4.8. *For all $\mathcal{P} \subseteq \mathcal{X}$, it holds that*

$$\widehat{\mathcal{N}}(\mathcal{P}) = \widehat{\mathcal{N}}(\mathcal{P};\, \emptyset).$$

3.4.2 Canonical configurations

First, we introduce the special form of configurations which will be called *canonical configurations*. These configurations are inspired by the expansion algorithm given in [69, Proposition 2.3]. We note that we shall consistently refer to Figure 3.1 for illustrations of the configurations introduced in the following definition. In the figures of this article, each square corresponds to a site (or vertex) of the lattice Λ.

Definition 3.4.9 (Pre-canonical and pre-regular configurations)**.** We fix $a,\, b \in \Omega$ and construct pre-canonical and pre-regular configurations between two ground states $\boldsymbol{a}$ and $\boldsymbol{b}$. We remark that k and ℓ are used throughout to represent elements of $\mathbb{T}_K$ and $\mathbb{T}_L$, respectively. In addition, v and h are used to denote vertical and horizontal lengths, respectively.

- For $\ell \in \mathbb{T}_L$ and $v \in [\![0,\, L]\!]$, we denote by $\xi_{\ell,\, v}^{a,\, b} \in \mathcal{X}$ the spin configuration whose spins are b on the sites in

$$\mathbb{T}_K \times \{\ell + n \in \mathbb{T}_L : n \in [\![0,\, v-1]\!] \subseteq \mathbb{Z}\}$$

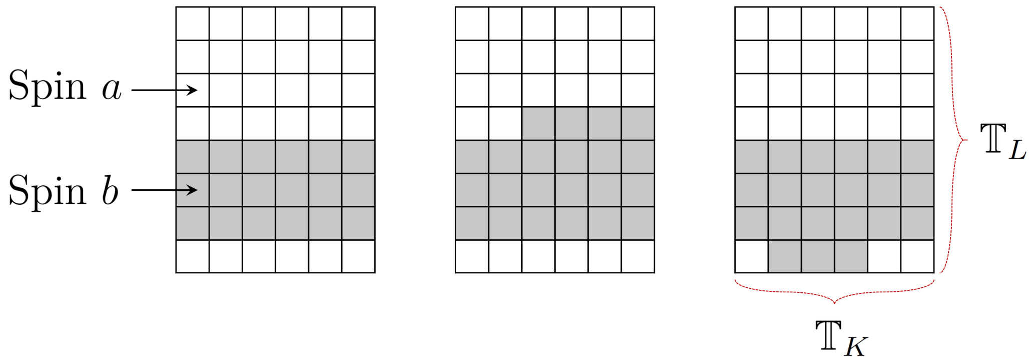


Figure 3.1: Canonical configurations for the case $(K,\, L) = (6,\, 8)$. These configurations illustrate $\xi^{a,\,b}_{2,\,3}$ (left), $\xi^{a,\,b,\,+}_{2,\,3;\,3,\,4}$ (middle), and $\xi^{a,\,b,\,-}_{2,\,3;\,2,\,3}$ (right), respectively (see Definition 3.4.9). Notice that our labeling of coordinates follows the two-dimensional coordinate system, instead of the matrix system.

and a on the remainder. Hence, we have $\xi^{a,\,b}_{\ell,\,0} = \boldsymbol{a}$ and $\xi^{a,\,b}_{\ell,\,L} = \boldsymbol{b}$ for all $\ell \in \mathbb{T}_L$. The configurations $\xi^{a,\,b}_{\ell,\,v}$ are called *pre-regular configurations*.

- For $\ell \in \mathbb{T}_L$, $v \in [\![0,\, L-1]\!]$, $k \in \mathbb{T}_K$ and $h \in [\![0,\, K]\!]$, we denote by $\xi^{a,\,b,\,+}_{\ell,\,v;\,k,\,h} \in \mathcal{X}$ the configuration whose spins are b on the sites in

$$\big\{x \in \Lambda : \xi^{a,\,b}_{\ell,\,v}(x) = b\big\} \cup \big[\{k+n \in \mathbb{T}_K : n \in [\![0,\, h-1]\!] \subseteq \mathbb{Z}\} \times \{\ell + v\}\big]$$

and a on the remainder. Similarly, we denote by $\xi^{a,\,b,\,-}_{\ell,\,v;\,k,\,h} \in \mathcal{X}$ whose spins are b on the sites in

$$\big\{x \in \Lambda : \xi^{a,\,b}_{\ell,\,v}(x) = b\big\} \cup \big[\{k+n \in \mathbb{T}_K : n \in [\![0,\, h-1]\!] \subseteq \mathbb{Z}\} \times \{\ell - 1\}\big]$$

and a on the remainder. Namely, we obtain $\xi^{a,\,b,\,+}_{\ell,\,v;\,k,\,h}$ (resp. $\xi^{a,\,b,\,-}_{\ell,\,v;\,k,\,h}$) from $\xi^{a,\,b}_{\ell,\,v}$ by attaching a protuberance of spins b of size h at its upper (resp. lower) side of the cluster of spin b starting from the k-th location. It is clear that $\xi^{a,\,b,\,+}_{\ell,\,v;\,k,\,0} = \xi^{a,\,b,\,-}_{\ell,\,v;\,k,\,0} = \xi^{a,\,b}_{\ell,\,v}$, $\xi^{a,\,b,\,+}_{\ell,\,v;\,k,\,K} = \xi^{a,\,b}_{\ell,\,v+1}$ and $\xi^{a,\,b,\,-}_{\ell,\,v;\,k,\,K} = \xi^{a,\,b}_{\ell-1,\,v+1}$.

Now, we are ready to define the canonical configurations of $\mathcal{X}$.

Definition 3.4.10 (Canonical and regular configurations)**.** The definition of canonical configurations differs between the cases of $K < L$ and $K = L$. Indeed, this is the main reason why the prefactor of the Eyring–Kramers formula given in Theorem 3.1.2 differs between these two cases.

- **(Case** $K < L$**)** For $a,\, b \in \Omega$, we define the collection $\mathcal{C}^{a,\,b}$ of *canonical configurations* between $\boldsymbol{a}$ and $\boldsymbol{b}$ as

$$\mathcal{C}^{a,\,b} := \bigcup_{\ell\in\mathbb{T}_L} \bigcup_{v\in[\![0,\,L]\!]} \{\xi_{\ell,\,v}^{a,\,b}\} \cup \bigcup_{\ell\in\mathbb{T}_L} \bigcup_{v\in[\![0,\,L-1]\!]} \bigcup_{k\in\mathbb{T}_K} \bigcup_{h\in[\![1,\,K-1]\!]} \{\xi_{\ell,\,v;\,k,\,h}^{a,\,b,\,+},\, \xi_{\ell,\,v;\,k,\,h}^{a,\,b,\,-}\}.$$

One can easily see that the right-hand side is a decomposition of $\mathcal{C}^{a,\,b}$. Then, we define the collection $\mathcal{C}$ of *canonical configurations* as

$$\mathcal{C} := \bigcup_{a,\,b\in\Omega} \mathcal{C}^{a,\,b}. \tag{3.46}$$

Similarly, we define

$$\mathcal{R}_v^{a,\,b} := \bigcup_{\ell\in\mathbb{T}_L} \{\xi_{\ell,\,v}^{a,\,b}\} \quad \text{and} \quad \mathcal{Q}_v^{a,\,b} := \bigcup_{\ell\in\mathbb{T}_L} \bigcup_{k\in\mathbb{T}_K} \bigcup_{h\in[\![1,\,K-1]\!]} \{\xi_{\ell,\,v;\,k,\,h}^{a,\,b,\,\pm}\},$$

and then define $\mathcal{R}_v$ and $\mathcal{Q}_v$ as in (3.46). A configuration belonging to $\mathcal{R}_v$ for some $v \in [\![0,\, L]\!]$ is called a *regular configuration*.

- **(Case** $K = L$**)** For $a,\, b \in \Omega$, we temporarily denote by $\widetilde{\mathcal{C}}^{a,\,b}$, $\widetilde{\mathcal{R}}_v^{a,\,b}$ and $\widetilde{\mathcal{Q}}_v^{a,\,b}$ the collections $\mathcal{C}^{a,\,b}$, $\mathcal{R}_v^{a,\,b}$ and $\mathcal{Q}_v^{a,\,b}$ defined in the previous case of $K < L$. Define a transpose operator $\Theta : \mathcal{X} \to \mathcal{X}$ by

$$(\Theta(\sigma))(k,\, \ell) = \sigma(\ell,\, k) \quad \text{for } k \in \mathbb{T}_K \text{ and } \ell \in \mathbb{T}_L. \tag{3.47}$$

Then, we define $\mathcal{A} = \widetilde{\mathcal{A}} \cup \Theta(\mathcal{A})$ where $\mathcal{A} = \mathcal{C}^{a,\,b}$, $\mathcal{R}_v^{a,\,b}$ or $\mathcal{Q}_v^{a,\,b}$. The sets $\mathcal{C}$, $\mathcal{R}_v$ and $\mathcal{Q}_v$ are defined as in (3.46). These modified definitions for the case of $K = L$ reflect the fact that the transitions can occur in both horizontal and vertical directions of the lattice.

We can readily verify from the definition of the Hamiltonian H that $H(\eta) \le \Gamma$ for all $\eta \in \mathcal{C}^{a,\,b}$, and moreover for $a,\, b \in \Omega$,

$$H(\eta) = \begin{cases} \Gamma - 2 & \text{if } \eta \in \mathcal{R}_v^{a,\,b} \text{ for } v \in [\![1,\, L-1]\!], \\ \Gamma & \text{if } \eta \in \mathcal{Q}_v^{a,\,b} \text{ for } v \in [\![1,\, L-2]\!]. \end{cases} \tag{3.48}$$

We stress that the definition of canonical configurations is not symmetric between rows and columns if $K < L$, as they play different roles. Indeed, the roles are fundamentally different in the metastable transitions, and that leads to the fact that the energy barrier Γ depends only on K, not on L.

The following notation will be used throughout.

Notation 3.4.11. Suppose that $N \ge 2$ is a positive integer.

- Define $\mathfrak{S}_N$ as the collection of connected subsets of $\mathbb{T}_N$, including the empty set.
- For $P,\, P' \in \mathfrak{S}_N$, we write $P \prec P'$ if $P \subseteq P'$ and $|P'| = |P| + 1$.
- A sequence $(P_m)_{m=0}^N$ of sets in $\mathfrak{S}_N$ is called an *increasing sequence* if it satisfies
$$\emptyset = P_0 \prec P_1 \prec \cdots \prec P_N = \mathbb{T}_N,$$
so that $|P_m| = m$ for all $m \in [\![0,\, N]\!]$.

Now, we construct the so-called canonical paths between two ground states.

Definition 3.4.12 (Canonical paths)**.**

(1) We first introduce a *standard sequence* of subsets of Λ connecting the empty set $\emptyset$ and the full set Λ.

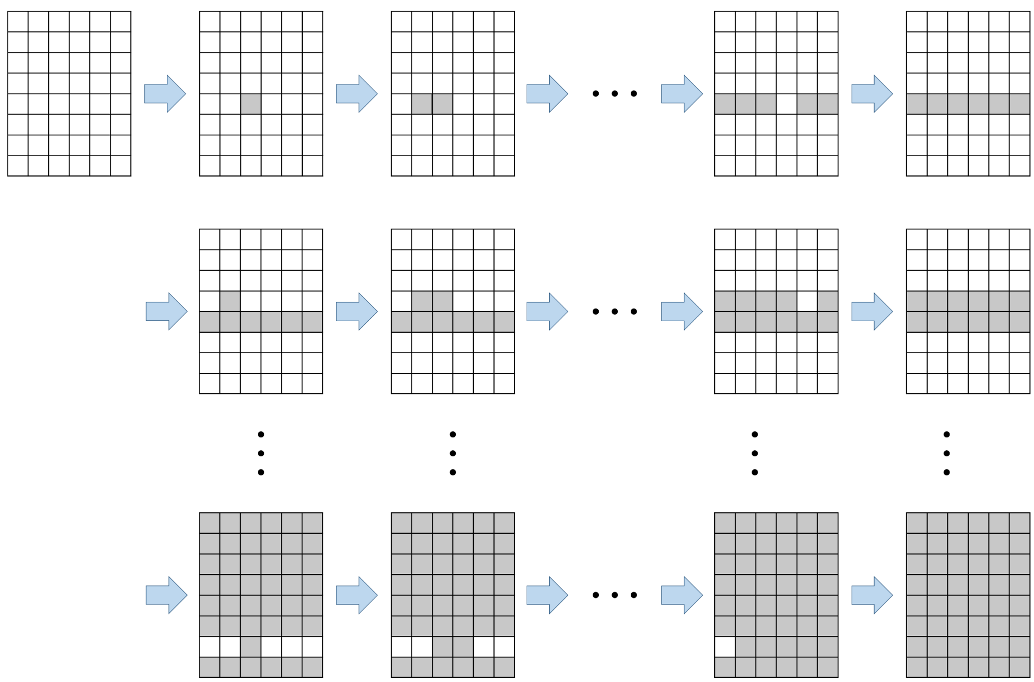


Figure 3.2: Example of a canonical path for the case of $(K,\ L) = (6,\ 8)$.

(a) First, for $P,\ P' \in \mathfrak{S}_L$ with $P \prec P'$, we say that a sequence $(A_h)_{h=0}^{K}$ of subsets of Λ is a standard sequence connecting $\mathbb{T}_K \times P$ and $\mathbb{T}_K \times P'$ if there exists an increasing sequence $(Q_h)_{h=0}^{K}$ in $\mathfrak{S}_K$ such that

$$A_h = (\mathbb{T}_K \times P) \cup \left[Q_h \times (P' \setminus P)\right] \quad \text{for all } h \in [\![0,\ K]\!].$$

(b) Now, a sequence $(A_m)_{m=0}^{KL}$ of subsets of Λ is a standard sequence connecting $\emptyset$ and Λ if there exists an increasing sequence $(P_v)_{v=0}^{L}$ in $\mathfrak{S}_L$ such that $A_{Kv} = \mathbb{T}_K \times P_v$ for all $v \in [\![0,\ L]\!]$, and furthermore for each $v \in [\![0,\ L-1]\!]$ the subsequence $(A_h)_{h=Kv}^{K(v+1)}$ is a standard sequence connecting $\mathbb{T}_K \times P_v$ and $\mathbb{T}_K \times P_{v+1}$.

(2) For $a,\ b \in \Omega$, a sequence of configurations $\omega = (\omega_m)_{m=0}^{KL}$ in $\mathcal{X}$ is called a *pre-canonical path* (between $\boldsymbol{a}$ and $\boldsymbol{b}$) if there exists a standard sequence $(A_m)_{m=0}^{KL}$ connecting $\emptyset$ and Λ such that

$$\omega_m(x) = \begin{cases} a & \text{if } x \notin A_m, \\ b & \text{if } x \in A_m. \end{cases}$$

It is easy to verify that indeed, ω is a path connecting $\omega_0 = \boldsymbol{a}$ and $\omega_{KL} = \boldsymbol{b}$.

(3) Moreover, $(\omega_m)_{m=0}^{KL}$ in $\mathcal{X}$ is called a *canonical path* connecting $\boldsymbol{a}$ and $\boldsymbol{b}$ (i.e., $\omega_0 = \boldsymbol{a}$ and $\omega_{KL} = \boldsymbol{b}$) if there exists a pre-canonical path $(\widetilde{\omega}_m)_{m=0}^{KL}$ such that

(a) **(Case $K < L$)** $\omega_m = \widetilde{\omega}_m$ for all $m \in [\![0,\ KL]\!]$,

(b) **(Case $K = L$)** $\omega_m = \widetilde{\omega}_m$ for all $m \in [\![0,\ KL]\!]$ or $\omega_m = \Theta(\widetilde{\omega}_m)$ for all $m \in [\![0,\ KL]\!]$.

An example of a canonical path is given in Figure 3.2. It is direct from the construction that a canonical path consists of canonical configurations only.

In particular, the following properties are immediate from the construction.

Lemma 3.4.13. *For any canonical path* $(\omega_m)_{m=0}^{KL}$ *connecting* $\boldsymbol{a}$ *and* $\boldsymbol{b}$*, the following statements hold.*

(1) For all $v \in [\![0,\, L]\!]$*, we have* $\omega_{Kv} \in \mathcal{R}_v^{a,\,b}$*.*

(2) For all $v \in [\![0,\, L-1]\!]$ *and* $h \in [\![1,\, K-1]\!]$*, we have* $\omega_{Kv+h} \in \mathcal{Q}_v^{a,\,b}$*.*

(3) It holds that $\Phi_\omega = \Gamma$*.*

In view of part (3) of the previous lemma, a canonical path between $\boldsymbol{a}$ and $\boldsymbol{b}$ is an optimal path that achieves the communication height Γ.

3.4.3 Typical configurations

Let us now define typical configurations which are extensions of canonical configurations and indeed the main ingredient in the explanation of the saddle structure. The definition is complicated, but its meaning will become clear later. We refer to Figure 3.3 for an illustration of typical configurations.

Definition 3.4.14 (Typical configurations)**.**

- For $a,\, b \in \Omega$, define the collection of *bulk typical configurations* (between $\boldsymbol{a}$ and $\boldsymbol{b}$) by

$$\mathcal{B}^{a,\,b} = \bigcup_{v\in[\![2,\,L-2]\!]} \mathcal{R}_v^{a,\,b} \cup \bigcup_{v\in[\![2,\,L-3]\!]} \mathcal{Q}_v^{a,\,b}. \tag{3.49}$$

  One can easily notice that $\mathcal{B}^{a,\,b} = \mathcal{B}^{b,\,a}$. Then, we define $\mathcal{B} = \bigcup_{a,\,b\in\Omega} \mathcal{B}^{a,\,b}$.

- Define

$$\mathcal{B}_\Gamma^{a,\,b} = \bigcup_{v\in[\![2,\,L-3]\!]} \mathcal{Q}_v^{a,\,b} = \{\eta \in \mathcal{B}^{a,\,b} : H(\eta) = \Gamma\}.$$

  Then, we define

$$\mathcal{B}_\Gamma := \bigcup_{a,\,b\in\Omega} \mathcal{B}_\Gamma^{a,\,b} = \bigcup_{a,\,b\in\Omega} \bigcup_{v\in[\![2,\,L-3]\!]} \mathcal{Q}_v^{a,\,b}.$$

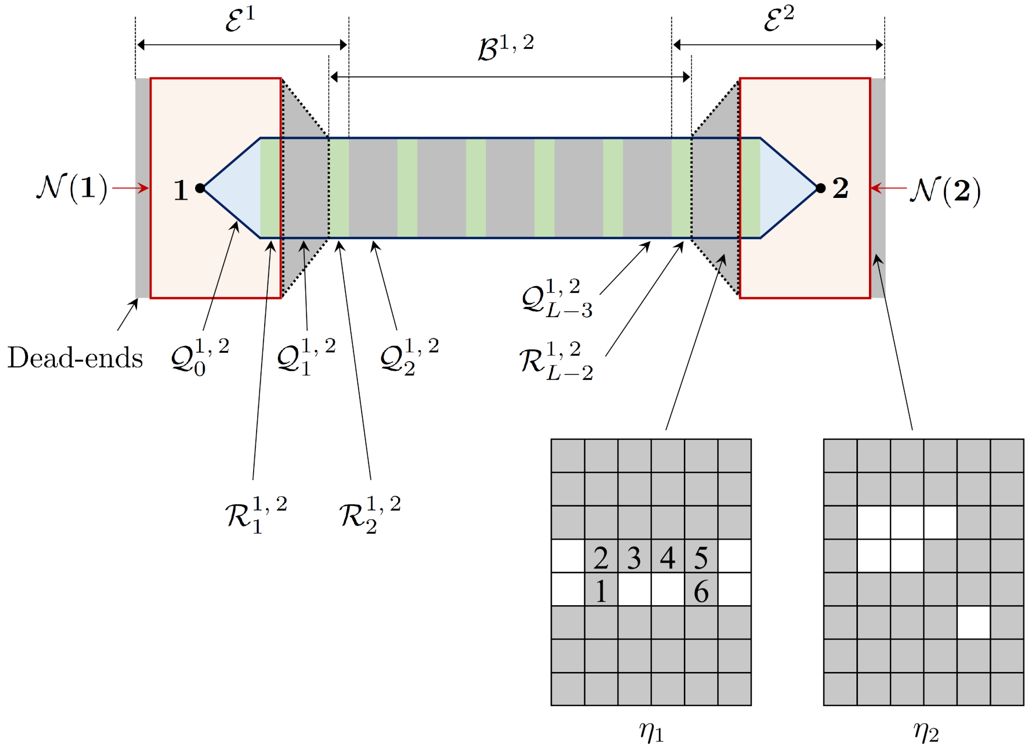


Figure 3.3: Typical configurations for the Ising model. This figure illustrates the structure of $\widehat{\mathcal{N}}(\mathcal{S})$ in the case of $q = 2$. We can notice from the figure that as verified in Proposition 3.4.17, $\widehat{\mathcal{N}}(\mathcal{S}) = \mathcal{E}^1 \cup \mathcal{B}^{1,2} \cup \mathcal{E}^2$, $\mathcal{R}_2^{1,2} = \mathcal{E}^1 \cap \mathcal{B}^{1,2}$ and $\mathcal{R}_{L-2}^{1,2} = \mathcal{B}^{1,2} \cap \mathcal{E}^2$. Regions consisting of configurations with energy $\Gamma = 2K+2$ are colored gray. The hexagonal region at the center of the figure enclosed by the blue line denotes the set $\mathcal{C} = \mathcal{C}^{1,2}$ of canonical configurations between $\mathbf{1}$ and $\mathbf{2}$. Since the MH dynamics cannot escape from $\widehat{\mathcal{N}}(\mathcal{S})$ during the transition from $\mathbf{1}$ to $\mathbf{2}$ (with dominating probability), the dynamics must path through the $\mathcal{B}^{1,2}$-part of the canonical configurations. The set $\mathcal{E}^2$ of edge typical configurations near $\mathbf{2}$ consists of four regions. The first one is the neighborhood $\mathcal{N}(\mathbf{2})$ denoted by the red-enclosed box. The second one is the region consisting of configurations with energy Γ which is connected to $\mathcal{R}_{L-2}^{1,2}$ via a Γ-path in $\mathcal{X} \setminus \mathcal{B}_\Gamma$. This region will be denoted by $\mathcal{Z}^{2,1}$ in Section 3.4.4 (cf. Figure 3.4). An example of a configuration belonging to this region is η_1. In particular, we can connect η_1 with a configuration in $\mathcal{R}_{L-2}^{1,2}$ via a Γ-path by updating six gray boxes in the order indicated in the figure (cf. Proposition 3.4.18). The third region consists of dead-ends (cf. (3.55)). An example of a dead-end is η_2, which has energy $14 = 2 \times 6 + 2 = 2K + 2$. The fourth region is $\mathcal{R}_{L-2}^{1,2}$. A similar decomposition holds for $\mathcal{E}^1$ as well.

- For $a \in \Omega$, the collection of *edge typical configurations* with respect to $\boldsymbol{a}$ is defined as
$$\mathcal{E}^a = \widehat{\mathcal{N}}(\boldsymbol{a};\, \mathcal{B}_\Gamma). \tag{3.50}$$
Finally, we set $\mathcal{E} = \bigcup_{a \in \Omega} \mathcal{E}^a$.

A configuration belonging to $\mathcal{B} \cup \mathcal{E}$ is called a *typical configuration*.

At first glance, the definition of typical configurations may look weird. However, the meaning of this will become clear after investigating their properties. In particular, in Proposition 3.4.17, we shall demonstrate that $\mathcal{E}^a$, $a \in \Omega$ are mutually disjoint, and that typical configurations are exactly the configurations which can be reached from ground states via Γ-paths. Hence, they form the collection of configurations relevant to the transitions between the ground states in $\mathcal{S}$.

Remark 3.4.15 (Tube of typical trajectories)*.* Later in Proposition 3.4.17, we will show that
$$\mathcal{E} \cup \mathcal{B} = \widehat{\mathcal{N}}(\mathcal{S}).$$
From the viewpoint of the pathwise approach to metastability, $\widehat{\mathcal{N}}(\mathcal{S})$ is exactly the *tube of typical trajectories* [73, 74] of the metastable transitions between the ground states in $\mathcal{S}$. In this sense, we demonstrate in Proposition 3.4.17 that $\mathcal{B} \cup \mathcal{E}$ is exactly the tube of typical trajectories of the metastable transitions. We also remark here that this is also the case in the cyclic dynamics as well; see Proposition 3.6.12.

Remark 3.4.16 (Classification of typical configurations)*.* We decompose typical configurations into the bulk and edge ones, since the patterns of transitions therein are qualitatively different. We refer to Figure 3.3 for a detailed explanation. Roughly speaking, to make a transition from $\boldsymbol{a}$ to $\boldsymbol{b}$ (without touching the energy level higher than Γ, i.e., without escaping from $\widehat{\mathcal{N}}(\mathcal{S})$), the dynamics has to pass through $\mathcal{E}^a$ first to arrive at $\mathcal{B}^{a,b}$. Then, it goes through $\mathcal{B}^{a,b}$ along the canonical path to arrive at $\mathcal{E}^b$, and then finally it reaches $\boldsymbol{b}$. The behavior of the dynamics on $\mathcal{E}^a$ and $\mathcal{E}^b$ is somewhat complicated and is explained by an auxiliary Markov chain defined in Definition 3.4.21, which can be regarded as a random walk on the space of sub-trees of a ladder graph (cf. Proposition 3.4.18).

The next proposition demonstrates the relations between bulk and edge typical configurations rigorously.

Proposition 3.4.17. *The following properties hold for the typical configurations.*

(1) For spins $a, b \in \Omega$*, we have* $\mathcal{E}^a \cap \mathcal{E}^b = \emptyset$.

(2) For spins $a, b \in \Omega$*, we have* $\mathcal{E}^a \cap \mathcal{B}^{a,b} = \mathcal{R}_2^{a,b}$.

(3) For three spins $a, b, c \in \Omega$*, we have* $\mathcal{E}^a \cap \mathcal{B}^{b,c} = \emptyset$.

(4) We have $\mathcal{E} \cup \mathcal{B} = \widehat{\mathcal{N}}(\mathcal{S})$.

We prove this proposition in Section 3.9.2. The bulk typical configurations have a clear structure and we do not need a further investigation on this set. On the other hand, the structure of edge typical configurations is quite complicated and possesses one of the main difficulties of the current problem. This structure will be explained in the remainder of the current section.

3.4.4 Classification of edge typical configurations

We fix a spin $a \in \Omega$ and focus on the classification of the configurations in the set $\mathcal{E}^a$. We refer to Figure 3.4 for an illustration of the definition given here.

For another spin $b \neq a$, we define a set $\mathcal{Z}^{a,b}$ as

$$\mathcal{Z}^{a,b} := \{\eta \in \mathcal{X} : \exists \text{a path } (\omega_n)_{n=0}^N \text{ in } \mathcal{X} \setminus \mathcal{B}_\Gamma \text{ such that} \\ \omega_0 \in \mathcal{R}_2^{a,b},\ \omega_N = \eta,\ \text{and } H(\omega_n) = \Gamma \text{ for all } n \in [\![1, N]\!]\}. \tag{3.51}$$

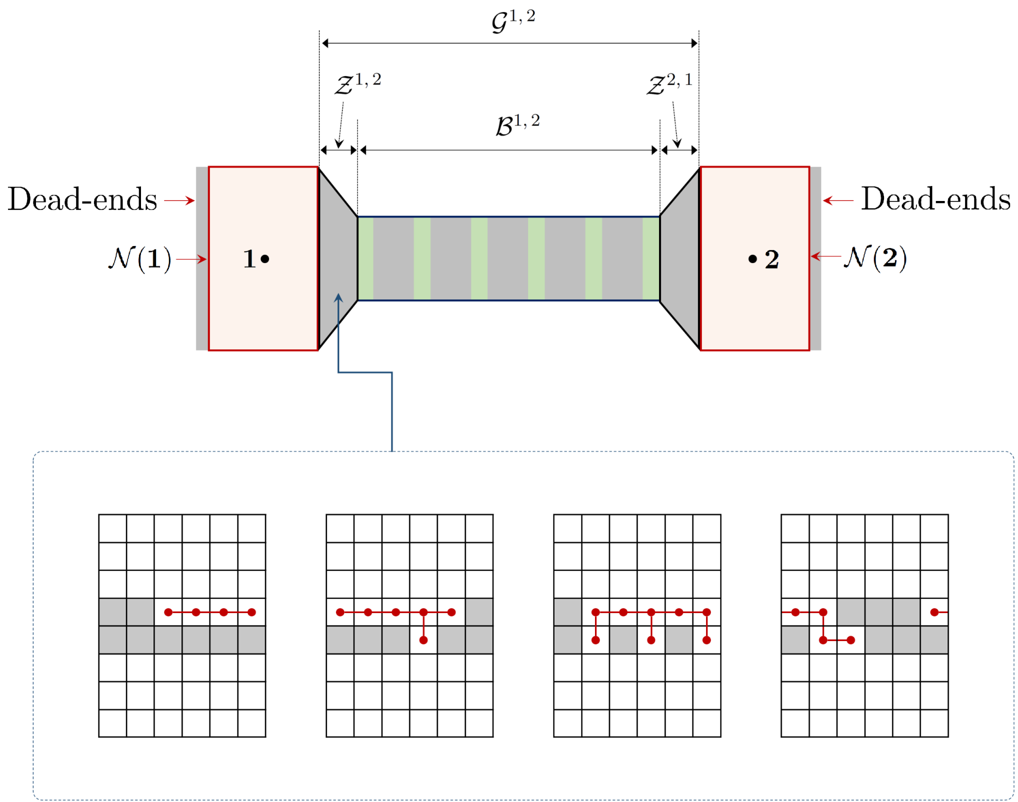


Figure 3.4: Edge typical configurations. The configurations belonging to gray regions have energy Γ. Green regions denote the sets of the form $\mathcal{R}_v^{1,2}$, $v \in [\![2, L-2]\!]$. We can notice from this figure that the set $\mathcal{N}(\mathbf{1})$ and the bulk typical configurations in $\mathcal{B}^{1,2}$ are connected through the configurations in $\mathcal{Z}^{1,2}$. Below the energy landscape, we give four examples of highly non-trivial configurations belonging to $\mathcal{Z}^{1,2}$. Indeed, as indicated in the figures, the sites with spin 1 within the strip form sub-trees. These configurations have energy Γ and do not belong to the dead-ends since each one of them can be connected to $\mathcal{R}_2^{1,2}$ by a Γ-path in $\mathcal{X} \setminus \mathcal{N}(\mathbf{1})$.

Note that $\mathcal{Z}^{a,b} \neq \mathcal{Z}^{b,a}$. Write

$$\mathcal{Z}^a := \bigcup_{b \in \Omega \setminus \{a\}} \mathcal{Z}^{a,b} \quad \text{and} \quad \mathcal{R}^a := \bigcup_{b \in \Omega \setminus \{a\}} \mathcal{R}_2^{a,b}.$$

Then, by (3.51) and Proposition 3.4.17 we have that

$$\mathcal{Z}^a \subseteq \mathcal{E}^a \quad \text{and} \quad \mathcal{R}^a \subseteq \mathcal{E}^a. \tag{3.52}$$

Properties of $\mathcal{Z}^{a,b}$

For a configuration $\eta \in \mathcal{X}$ and a spin $a \in \Omega$, we denote by $P_a(\eta)$ the set of sites of spin a with respect to σ, i.e.,

$$P_a(\eta) := \{x \in \Lambda : \eta(x) = a\}. \tag{3.53}$$

The next proposition verifies that each configuration in $\mathcal{Z}^{a,b}$ can be matched with *a sub-tree of a ladder graph* (cf. Figure 3.4).

Proposition 3.4.18. *For $a, b \in \Omega$ and $\eta \in \mathcal{X}$, it holds that $\eta \in \mathcal{Z}^{a,b}$ if and only if the following three conditions hold simultaneously.*

- **[Z1]** *For all $x \in \Lambda$, we have $\eta(x) \in \{a, b\}$.*
- **[Z2]** *There exists $\ell \in \mathbb{T}_L$ such that $P_b(\eta) \subseteq \mathbb{T}_K \times \{\ell, \ell+1\}$ (or $\{\ell, \ell+1\} \times \mathbb{T}_K$ if $K = L$).*
- **[Z3]** *Define $G_a(\eta) := P_a(\eta) \cap [\mathbb{T}_K \times \{\ell, \ell+1\}]$ (or $P_a(\eta) \cap [\{\ell, \ell+1\} \times \mathbb{T}_K]$ if $K = L$). Then, the set $G_a(\eta)$ consists of vertices of a sub-tree[1] of the ladder graph $\mathbb{T}_K \times \{\ell, \ell+1\}$ (or $\{\ell, \ell+1\} \times \mathbb{T}_K$ if $K = L$).*

We prove this statement in Section 3.9.3.

[1] We regard that the empty set is not a tree.

Definition 3.4.19. Fix $a, b \in \Omega$. For each $\xi_{\ell,2}^{a,b} \in \mathcal{R}_2^{a,b}$, $\ell \in \mathbb{T}_L$ (and also $\Theta(\xi_{\ell,2}^{a,b}) \in \mathcal{R}_2^{a,b}$ if $K = L$), Proposition 3.4.18 implies that there exists a subset of configurations in $\mathcal{Z}^{a,b}$ connected to $\xi_{\ell,2}^{a,b}$ with tree structures on $\mathbb{T}_K \times \{\ell, \ell+1\}$ (or $\{\ell, \ell+1\} \times \mathbb{T}_K$ for the case of $\Theta(\xi_{\ell,2}^{a,b}) \in \mathcal{R}_2^{a,b}$). We will denote this subset by $\mathcal{Z}_\ell^{a,b} \subseteq \mathcal{Z}^{a,b}$ (or $\Theta(\mathcal{Z}_\ell^{a,b}) \subseteq \mathcal{Z}^{a,b}$ for the case of $\Theta(\xi_{\ell,2}^{a,b}) \in \mathcal{R}_2^{a,b}$). Thus, we have the following decomposition of $\mathcal{Z}^{a,b}$:

$$\mathcal{Z}^{a,b} = \begin{cases} \bigcup_{\ell \in \mathbb{T}_L} \mathcal{Z}_\ell^{a,b} & \text{if } K < L, \\ \bigcup_{\ell \in \mathbb{T}_L} \mathcal{Z}_\ell^{a,b} \cup \bigcup_{\ell \in \mathbb{T}_L} \Theta(\mathcal{Z}_\ell^{a,b}) & \text{if } K = L. \end{cases} \tag{3.54}$$

Moreover, it is clear that each copy of $\mathcal{Z}_\ell^{a,b}$ (or $\Theta(\mathcal{Z}_\ell^{a,b})$ if $K = L$) has the same structure. This structure will be further investigated in the next subsection.

Decomposition of $\mathcal{E}^a$

We write

$$\mathcal{D}^a := \widehat{\mathcal{N}}(\boldsymbol{a};\, \mathcal{Z}^a), \tag{3.55}$$

where $\mathcal{D}$ stands for dead-ends. Indeed, the set $\mathcal{D}^a \setminus \mathcal{N}(\boldsymbol{a})$ consists of the dead-end configurations with energy Γ (cf. caption of Figure 3.3). We now classify the edge typical configurations.

Proposition 3.4.20. *For $a \in \Omega$, we have the following decomposition of $\mathcal{E}^a$:*

$$\mathcal{E}^a = \mathcal{D}^a \cup \mathcal{Z}^a \cup \mathcal{R}^a. \tag{3.56}$$

This proposition is also proved in Section 3.9.3.

3.4.5 Graph structure of edge typical configurations

We consistently refer to Figure 3.5 for an illustration of the notions constructed in this subsection.

Fix a spin $a \in \Omega$. The decomposition given in Proposition 3.4.20 can be alternatively expressed as

$$\mathcal{E}^a = \mathcal{D}^a \cup \bigcup_{b \in \Omega \setminus \{a\}} [\mathcal{Z}^{a,\,b} \cup \mathcal{R}_2^{a,\,b}]. \tag{3.57}$$

Moreover, according to (3.54), $\mathcal{E}^a$ can be further expressed as

$$\begin{cases} \mathcal{D}^a \cup \bigcup_{b \neq a} \bigcup_{\ell \in \mathbb{T}_L} [\mathcal{Z}_\ell^{a,\,b} \cup \{\xi_{\ell,\,2}^{a,\,b}\}] & \text{if } K < L, \\ \mathcal{D}^a \cup \bigcup_{b \neq a} \bigcup_{\ell \in \mathbb{T}_L} [\mathcal{Z}_\ell^{a,\,b} \cup \{\xi_{\ell,\,2}^{a,\,b}\}] \cup \bigcup_{b \neq a} \bigcup_{\ell \in \mathbb{T}_L} [\Theta(\mathcal{Z}_\ell^{a,\,b}) \cup \{\Theta(\xi_{\ell,\,2}^{a,\,b})\}] & \text{if } K = L. \end{cases} \tag{3.58}$$

We now construct a graph and a Markov chain describing the behavior of the MH dynamics on $\mathcal{E}^a$.

Definition 3.4.21. We introduce a graph structure and a Markov chain thereon. Fix $b \neq a$, $\ell \in \mathbb{T}_L$ and consider the set $\mathcal{N}(\boldsymbol{a}) \cup \mathcal{Z}_\ell^{a,\,b} \cup \{\xi_{\ell,\,2}^{a,\,b}\}$.

- **(Graph)** The vertex set $\mathscr{V}_\ell^{a,\,b}$ is given by

$$\mathscr{V}_\ell^{a,\,b} := \{\boldsymbol{a}\} \cup \mathcal{Z}_\ell^{a,\,b} \cup \{\xi_{\ell,\,2}^{a,\,b}\}. \tag{3.59}$$

  Then, the edge set $\mathscr{E}_\ell^{a,\,b}$ is defined as follows: $\{\eta,\,\eta'\} \in \mathscr{E}_\ell^{a,\,b}$ for $\eta,\,\eta' \in \mathscr{V}_\ell^{a,\,b}$ if and only if either $\eta,\,\eta' \neq \boldsymbol{a}$ and $\eta \sim \eta'$, or $\eta \in \mathcal{Z}_\ell^{a,\,b}$, $\eta' = \boldsymbol{a}$ and $\eta \sim \xi$ for some $\xi \in \mathcal{N}(\boldsymbol{a})$. By definition, we can understand $\boldsymbol{a} \in \mathscr{V}_\ell^{a,\,b}$ as a collapsed state representing the neighborhood $\mathcal{N}(\boldsymbol{a})$. By symmetry, the graph structure $\mathscr{G}_\ell^{a,\,b} := (\mathscr{V}_\ell^{a,\,b},\,\mathscr{E}_\ell^{a,\,b})$ does not depend on $a \in \Omega$, $b \neq a$ and $\ell \in \mathbb{T}_L$ (or even for the collection $\{\boldsymbol{a}\} \cup \Theta(\mathcal{Z}_\ell^{a,\,b}) \cup \{\Theta(\xi_{\ell,\,2}^{a,\,b})\}$ if $K = L$). Thus, if there is no risk of confusion, we may omit the

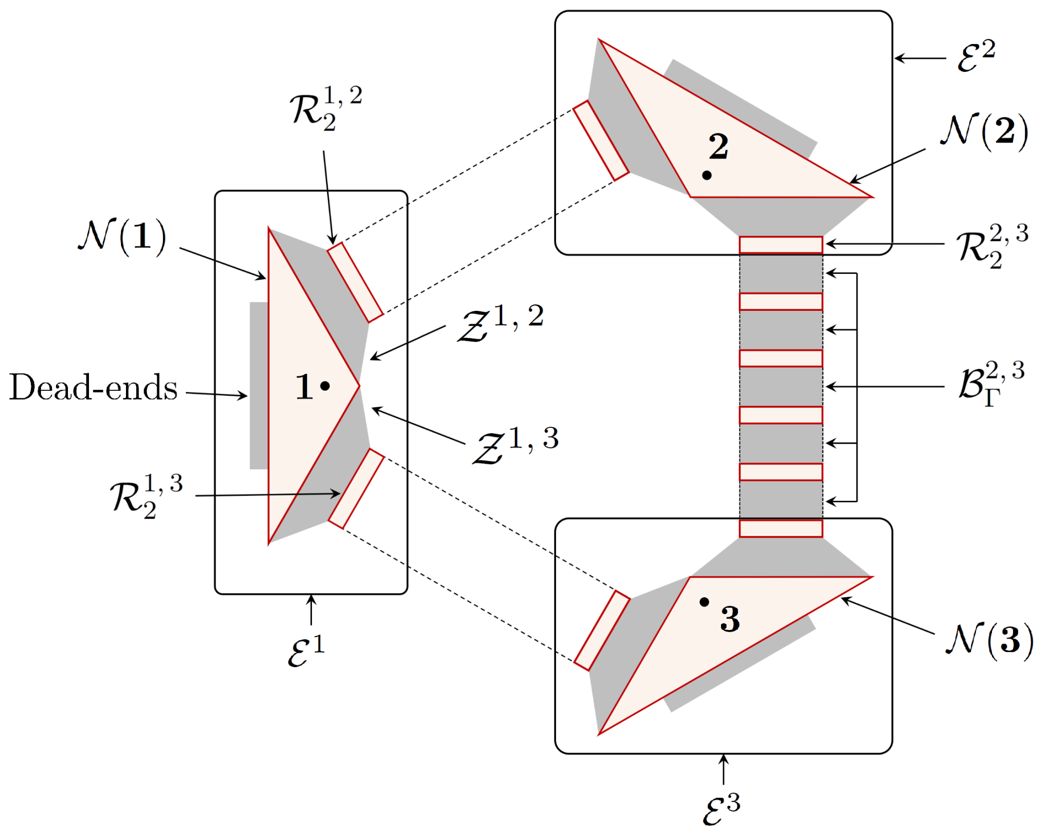


Figure 3.5: Structure of edge typical configurations. Let $S = \{1, 2, 3\}$ and $K < L$. Note that the set $\mathcal{E}^1$ consists of six parts: $\mathcal{N}(\mathbf{1})$, the dead-ends attached to $\mathcal{N}(\mathbf{1})$ (cf. caption of Figure 3.3), $\mathcal{R}_2^{1,2}$, $\mathcal{Z}^{1,2}$ (gray region of equilateral-trapezoid shape), and finally two more similar collections $\mathcal{R}_2^{1,3}$ and $\mathcal{Z}^{1,3}$.

subscript and superscript so that we simply write $\mathscr{G} = (\mathscr{V},\, \mathscr{E})$.

- **(Markov chain)** Define $\mathfrak{r} : \mathscr{V} \times \mathscr{V} \to [0,\, \infty)$ by setting

$$\mathfrak{r}(\eta,\, \eta') := \begin{cases} 1 & \text{if } \eta,\, \eta' \neq \boldsymbol{a}, \\ |\{\xi \in \mathcal{N}(\boldsymbol{a}) : \xi \sim \eta'\}| & \text{if } \eta = \boldsymbol{a} \text{ and } \eta' \in \mathscr{Z}^{a,\,b}, \\ |\{\xi \in \mathcal{N}(\boldsymbol{a}) : \xi \sim \eta\}| & \text{if } \eta \in \mathscr{Z}^{a,\,b} \text{ and } \eta' = \boldsymbol{a}, \end{cases} \tag{3.60}$$

for $\{\eta,\, \eta'\} \in \mathscr{E}$, and by setting $\mathfrak{r}(\eta,\, \eta') = 0$ otherwise. Define $\{\mathfrak{Z}(t)\}_{t \geq 0}$ as the continuous-time Markov chain on $\mathscr{V}$ with rate $\mathfrak{r}(\cdot,\, \cdot)$. Since the rate function $\mathfrak{r}(\cdot,\, \cdot)$ is symmetric by its definition, the Markov chain $\mathfrak{Z}(\cdot)$ is reversible with respect to its invariant distribution, which is the uniform distribution on $\mathscr{V}$.

We next argue that the process $\mathfrak{Z}(\cdot)$ defined above approximates the MH dynamics on the subset $\mathcal{N}(\boldsymbol{a}) \cup \mathscr{Z}_\ell^{a,\,b} \cup \{\xi_{\ell,\,2}^{a,\,b}\}$ for each selection $b \in \Omega \setminus \{a\}$ and $\ell \in \mathbb{T}_L$.

Proposition 3.4.22. *For each $b \neq a$ and $\ell \in \mathbb{T}_L$, define a projection map $\Pi_\ell^{a,\,b} : \mathcal{N}(\boldsymbol{a}) \cup \mathscr{Z}_\ell^{a,\,b} \cup \{\xi_{\ell,\,2}^{a,\,b}\} \to \mathscr{V}$ by*

$$\Pi_\ell^{a,\,b}(\eta) = \begin{cases} \boldsymbol{a} & \text{if } \eta \in \mathcal{N}(\boldsymbol{a}), \\ \eta & \text{if } \eta \in \mathscr{Z}_\ell^{a,\,b} \cup \{\xi_{\ell,\,2}^{a,\,b}\}. \end{cases}$$

(1) For $\eta_1,\, \eta_2 \neq \boldsymbol{a}$, we have

$$\frac{1}{q} e^{-\Gamma\beta} \mathfrak{r}(\Pi_\ell^{a,\,b}(\eta_1),\, \Pi_\ell^{a,\,b}(\eta_2)) = (1 + o(1)) \cdot \mu_\beta(\eta_1) r_\beta(\eta_1,\, \eta_2). \tag{3.61}$$

(2) For $\eta_1 \neq \boldsymbol{a}$, we have

$$\frac{1}{q} e^{-\Gamma\beta} \mathfrak{r}(\Pi_\ell^{a,\,b}(\eta_1),\, \boldsymbol{a}) = (1 + o(1)) \cdot \sum_{\xi \in \mathcal{N}(\boldsymbol{a})} \mu_\beta(\eta_1) r_\beta(\eta_1,\, \xi). \tag{3.62}$$

In the case of $K = L$, *we define* $\Theta(\Pi_\ell^{a,b}) : \mathcal{N}(\boldsymbol{a}) \cup \Theta(\mathcal{Z}_\ell^{a,b}) \cup \{\Theta(\xi_{\ell,2}^{a,b})\} \to \mathscr{V}$ *in a similar way. Then, the same results hold as well.*

We prove this approximation statement in Section 3.9.4.

In view of the previous proposition, we can construct a test function on $\mathcal{E}^a$ in terms of the process $\mathfrak{Z}(\cdot)$. To this end, we have to investigate the potential-theoretic objects of the process $\mathfrak{Z}(\cdot)$. Denote by $\mathfrak{f}_{\cdot,\cdot}(\cdot)$, $\mathfrak{cap}(\cdot,\,\cdot)$ and $\mathfrak{D}(\cdot)$ the equilibrium potential, capacity and Dirichlet form with respect to the Markov chain $\mathfrak{Z}(\cdot)$, respectively (we define them in the same way as in Section 3.2.1). We also denote by $\mathfrak{L}$ the infinitesimal generator associated with the process $\mathfrak{Z}(\cdot)$ which acts on functions $F : \mathscr{V} \to \mathbb{R}$ as

$$(\mathfrak{L}F)(\eta) = \sum_{\eta' \in \mathscr{V} :\, \{\eta,\,\eta'\} \in \mathscr{E}} \mathfrak{r}(\eta,\,\eta')\{F(\eta') - F(\eta)\}. \tag{3.63}$$

Then, the constant $\mathfrak{e}_0$ that appears in (3.30) for the MH dynamics is defined by

$$\mathfrak{e}_0 := \frac{1}{|\mathscr{V}| \cdot \mathfrak{cap}(\boldsymbol{a},\, \xi_{\ell,2}^{a,b})}. \tag{3.64}$$

By the symmetry of the model, this constant $\mathfrak{e}_0$ does not depend on a, b or ℓ. We emphasize that this constant appears in the capacity estimate because the equilibrium potential

$$\mathfrak{f} := \mathfrak{f}_{\boldsymbol{a},\,\xi_{\ell,2}^{a,b}} \tag{3.65}$$

approximates that of the MH dynamics in $\mathcal{E}^a$ (cf. Proposition 3.4.22). Indeed, this function plays a significant role in the construction of the test function in Section 3.5.

We conclude this section by showing that $\mathfrak{e}_0$ is indeed small, so that asymptotically (in K) this constant has a negligible effect on the constant κ that appears in the Eyring–Kramers formula.

Proposition 3.4.23. *It holds that* $\mathfrak{e}_0 \leq 1$.

Again, we give a nice proof in Section 3.9.4.

Remark 3.4.24. In fact, with a more refined argument, we can verify that there exist two constants C_1, $C_2 > 0$ such that $\frac{C_1}{K} \le \mathfrak{e}_0 \le \frac{C_2}{K}$. However, this level of precision is unnecessary in our logical structure and thus we omit the proof.

3.5 Test functions: Metropolis–Hastings dynamics

Throughout the section, we will again consider the MH dynamics and fix two disjoint, non-empty subsets $\mathcal{P}$ and $\mathcal{Q}$ of $\mathcal{S}$. The purpose of this section is to construct the test function $\widetilde{h} = \widetilde{h}_{\mathcal{P},\mathcal{Q}} : \mathcal{X} \to \mathbb{R}$ and verify three conditions (3.38), (3.39) and (3.40) for this test function. This will provide the proof of Proposition 3.2.9 and thus conclude our analysis given in Section 3.2 for the MH dynamics. Note that in this case, the dynamics is reversible and thus we do not need to construct $\widetilde{h}^*$.

Notation 3.5.1. Throughout this section, we always use the alphabets a, b, c to represent the spins subjected to $\boldsymbol{a} \in \mathcal{P}$, $\boldsymbol{b} \in \mathcal{Q}$, and $\boldsymbol{c} \in \mathcal{S} \setminus (\mathcal{P} \cup \mathcal{Q})$, respectively. If necessary, we also use a', b', c' to represent $\boldsymbol{a'} \in \mathcal{P}$, $\boldsymbol{b'} \in \mathcal{Q}$, and $\boldsymbol{c'} \in \mathcal{S} \setminus (\mathcal{P} \cup \mathcal{Q})$.

3.5.1 Construction of $\widetilde{h}$

In this subsection, we construct the desired test function $\widetilde{h} : \mathcal{X} \to \mathbb{R}$. Before the explicit construction, we briefly explain the nature behind such a description. On edge typical configurations, we let $\widetilde{h}$ be a proper rescaled function of $\mathfrak{f}$, which is the equilibrium potential of the auxiliary dynamics defined in (3.65). This construction is natural because Proposition 3.4.22 ensures us that the auxiliary process successfully characterizes the behavior of the original process on the collection $\mathcal{E}$ of edge typical configurations. Next, on bulk typical configurations, we define $\widetilde{h}$ as a proper rescaling of the equilibrium potential of the symmetric simple random walk on an one-dimensional line. This is because the dynamics on the collection of bulk typical configurations is approximately one-dimensional with symmetric simple transition rates due to the simple geometry.

Definition 3.5.2 (Test function)**.** We construct $\widetilde{h}:\mathcal{X}\to[0,\,1]$ on $\mathcal{E}$, $\mathcal{B}$ and $\mathcal{X}\setminus(\mathcal{E}\cup\mathcal{B})$ separately. Recall the constants defined in (3.29) and (3.30). Note that we always use Notation 3.5.1.

(1) **Construction on** $\mathcal{E}=\bigcup_{\boldsymbol{a}\in\mathcal{P}}\mathcal{E}^{a}\cup\bigcup_{\boldsymbol{b}\in\mathcal{Q}}\mathcal{E}^{b}\cup\bigcup_{\boldsymbol{c}\in\mathcal{S}\setminus(\mathcal{P}\cup\mathcal{Q})}\mathcal{E}^{c}$**.**

- For $\eta\in\mathcal{E}^{a}$, we recall the decomposition (3.57) of $\mathcal{E}^{a}$. We define $\widetilde{h}(\eta)$ as

$$\begin{cases}1 & \text{if } \eta\in\mathcal{D}^{a}\cup\mathcal{Z}^{a,\,a'}\cup\mathcal{R}_{2}^{a,\,a'},\;\; a'\neq a,\\ 1-\dfrac{\mathfrak{e}}{\kappa}(1-\mathfrak{f}(\eta)) & \text{if } \eta\in\mathcal{Z}^{a,\,b}\cup\mathcal{R}_{2}^{a,\,b},\\ 1-\dfrac{|\mathcal{Q}|}{|\mathcal{P}|+|\mathcal{Q}|}\dfrac{\mathfrak{e}}{\kappa}(1-\mathfrak{f}(\eta)) & \text{if } \eta\in\mathcal{Z}^{a,\,c}\cup\mathcal{R}_{2}^{a,\,c}.\end{cases} \tag{3.66}$$

- For $\eta\in\mathcal{E}^{b}$, define $\widetilde{h}(\eta)$ as

$$\begin{cases}0 & \text{if } \eta\in\mathcal{D}^{b}\cup\mathcal{Z}^{b,\,b'}\cup\mathcal{R}_{2}^{b,\,b'},\;\; b'\neq b,\\ \dfrac{\mathfrak{e}}{\kappa}(1-\mathfrak{f}(\eta)) & \text{if } \eta\in\mathcal{Z}^{b,\,a}\cup\mathcal{R}_{2}^{b,\,a},\\ \dfrac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|}\dfrac{\mathfrak{e}}{\kappa}(1-\mathfrak{f}(\eta)) & \text{if } \eta\in\mathcal{Z}^{b,\,c}\cup\mathcal{R}_{2}^{b,\,c}.\end{cases} \tag{3.67}$$

- For $\eta \in \mathcal{E}^c$, define $\widetilde{h}(\eta)$ as

$$\begin{cases} \dfrac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|} & \text{in } \mathcal{D}^c \cup \mathcal{Z}^{c,\,c'} \cup \mathcal{R}_2^{c,\,c'}, \\ \dfrac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|} + \dfrac{|\mathcal{Q}|}{|\mathcal{P}|+|\mathcal{Q}|} \dfrac{\mathfrak{e}}{\kappa}(1-\mathfrak{f}(\eta)) & \text{in } \mathcal{Z}^{c,\,a} \cup \mathcal{R}_2^{c,\,a}, \\ \dfrac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|} - \dfrac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|} \dfrac{\mathfrak{e}}{\kappa}(1-\mathfrak{f}(\eta)) & \text{in } \mathcal{Z}^{c,\,b} \cup \mathcal{R}_2^{c,\,b}. \end{cases} \tag{3.68}$$

(2) **Construction on $\mathcal{B}$.** Recall the decomposition (3.49).

- We set $\widetilde{h} \equiv 1$ on $\mathcal{B}^{a,\,a'}$, $\widetilde{h} \equiv 0$ on $\mathcal{B}^{b,\,b'}$ and $\widetilde{h} \equiv \dfrac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|}$ on $\mathcal{B}^{c,\,c'}$.
- For $\eta \in \mathcal{R}_v^{a,\,b}$ with $v \in [\![2,\, L-2]\!]$, we set

$$\widetilde{h}(\eta) := \frac{1}{\kappa}\Big[\frac{L-2-v}{L-4}\mathfrak{b} + \mathfrak{e}\Big]. \tag{3.69}$$

For $\eta \in \mathcal{Q}_v^{a,\,b}$ with $v \in [\![2,\, L-3]\!]$, we can write $\eta = \xi_{\ell,\,v;\,k,\,h}^{a,\,b,\,\pm}$ (or $\Theta(\xi_{\ell,\,v;\,k,\,h}^{a,\,b,\,\pm})$ if $K=L$) for some $\ell \in \mathbb{T}_L$, $k \in \mathbb{T}_K$, and $h \in [\![1,\, K-1]\!]$. For such η, we set

$$\widetilde{h}(\eta) := \frac{1}{\kappa}\Big[\frac{(K+2)(L-2-v)-(h+1)}{(K+2)(L-4)}\mathfrak{b} + \mathfrak{e}\Big]. \tag{3.70}$$

- For $\eta \in \mathcal{R}_v^{a,\,c}$, $v \in [\![2,\, L-2]\!]$,

$$\widetilde{h}(\eta) := \frac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|} + \frac{|\mathcal{Q}|}{|\mathcal{P}|+|\mathcal{Q}|}\frac{1}{\kappa}\Big[\frac{L-2-v}{L-4}\mathfrak{b} + \mathfrak{e}\Big].$$

For $\eta \in \mathcal{Q}_v^{a,\,c}$, $v \in [\![2,\, L-3]\!]$, similarly $\eta = \xi_{\ell,\,v;\,k,\,h}^{a,\,c,\,\pm}$ (or $\Theta(\xi_{\ell,\,v;\,k,\,h}^{a,\,c,\,\pm})$ if $K=L$) for some ℓ, k and h. For such η, we set $\widetilde{h}(\eta)$ as

$$\frac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|} + \frac{|\mathcal{Q}|}{|\mathcal{P}|+|\mathcal{Q}|}\frac{1}{\kappa}\Big[\frac{(K+2)(L-2-v)-(h+1)}{(K+2)(L-4)}\mathfrak{b} + \mathfrak{e}\Big].$$

- For $\eta \in \mathcal{R}_v^{c,b}$, $v \in [\![2,\, L-2]\!]$,

$$\widetilde{h}(\eta) := \frac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|}\frac{1}{\kappa}\Big[\frac{L-2-v}{L-4}\mathfrak{b}+\mathfrak{e}\Big].$$

  For $\eta \in \mathcal{Q}_v^{c,b}$, $v \in [\![2,\, L-3]\!]$, again, $\eta = \xi_{\ell,\,v;\,k,\,h}^{c,\,b,\,\pm}$ (or $\Theta(\xi_{\ell,\,v;\,k,\,h}^{c,\,b,\,\pm})$ if $K=L$) for some ℓ, k and h. We set

$$\widetilde{h}(\eta) := \frac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|}\frac{1}{\kappa}\Big[\frac{(K+2)(L-2-v)-(h+1)}{(K+2)(L-4)}\mathfrak{b}+\mathfrak{e}\Big].$$

(3) **Construction on $\mathcal{X} \setminus (\mathcal{E} \cup \mathcal{B})$.** We define $\widetilde{h} \equiv 1$ on this set.

Remark 3.5.3. Since $\mathcal{E} \cap \mathcal{B} = \mathcal{R}_2$ by Proposition 3.4.17-(2), we need to check that the constructions of $\widetilde{h}$ on $\mathcal{E}$ and on $\mathcal{B}$ agree with each other on this intersection. This is immediate from our definition.

Remark 3.5.4. According to Definition 3.5.2, it is inferred that

- $\widetilde{h}(\eta) = 1$ for all $\eta \in \mathcal{D}^a$, $\boldsymbol{a} \in \mathcal{P}$,
- $\widetilde{h}(\eta) = 0$ for all $\eta \in \mathcal{D}^b$, $\boldsymbol{b} \in \mathcal{Q}$,
- $\widetilde{h}(\eta) = \dfrac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|}$ for all $\eta \in \mathcal{D}^c$, $\boldsymbol{c} \in \mathcal{S} \setminus (\mathcal{P} \cup \mathcal{Q})$.

Remark 3.5.5. It is clear from our definition that the test function $\widetilde{h}$ fulfills the requirement (3.40). Hence, it remains to check (3.38) and (3.39).

3.5.2 Dirichlet energy of the test function

We first check (3.39).

Proposition 3.5.6. *The function $\widetilde{h}$ constructed in Definition 3.5.2 satisfies* (3.39)*, i.e.,*

$$D_\beta(\widetilde{h}) = (1+o(1)) \cdot \frac{|\mathcal{P}||\mathcal{Q}|}{\kappa(|\mathcal{P}|+|\mathcal{Q}|)}e^{-\Gamma\beta}.$$

Proof. Let us divide the Dirichlet form $D_\beta(\widetilde{h})$ into three parts as

$$\Big[\sum_{\{\eta,\,\xi\}\subseteq\mathcal{X}\setminus(\mathcal{E}\cup\mathcal{B})}+\sum_{\eta\in\mathcal{E}\cup\mathcal{B},\,\xi\in\mathcal{X}\setminus(\mathcal{E}\cup\mathcal{B})}+\sum_{\{\eta,\,\xi\}\subseteq\mathcal{E}\cup\mathcal{B}}\Big]\mu_\beta(\eta)r_\beta(\eta,\,\xi)\{\widetilde{h}(\xi)-\widetilde{h}(\eta)\}^2, \tag{3.71}$$

where all summations are carried out for two connected configurations η and ξ, i.e., $\eta\sim\xi$. Note that the first summation is 0 by part (3) of Definition 3.5.2.

For the second summation, we recall from part (4) of Proposition 3.4.17 that $\mathcal{E}\cup\mathcal{B}=\widehat{\mathcal{N}}(\mathcal{S})$. Hence, by Lemma 3.4.6, we have $H(\xi)\ge\Gamma+1$. Since $H(\eta)\le\Gamma$, by Theorem 3.0.1 and (2.2),

$$\mu_\beta(\eta)r_\beta(\eta,\,\xi)=\mu_\beta(\xi)=\frac{1}{Z_\beta}e^{-\beta H(\xi)}=O(e^{-(\Gamma+1)\beta}).$$

Since $\widetilde{h}:\mathcal{X}\to[0,\,1]$, we can conclude that the second summation of (3.71) is $O(e^{-(\Gamma+1)\beta})$.

It remains to estimate the third summation of (3.71), which is indeed the main constituent of the Dirichlet form. For each subset $\mathcal{P}\subseteq\mathcal{X}$, we write

$$E(\mathcal{P})=\big\{\{\sigma,\,\zeta\}\subseteq\mathcal{P}:\sigma\sim\zeta\big\}. \tag{3.72}$$

Then, we can observe from Proposition 3.4.17 that we can decompose $E(\mathcal{E}\cup\mathcal{B})$ as

$$E(\mathcal{E}\cup\mathcal{B})=E(\mathcal{B})\cup E(\mathcal{E}), \tag{3.73}$$

and thus we can rewrite the first summation of (3.71) as

$$\Big[\sum_{\{\eta,\,\xi\}\in E(\mathcal{B})}+\sum_{\{\eta,\,\xi\}\in E(\mathcal{E})}\Big]\mu_\beta(\eta)r_\beta(\eta,\,\xi)\{\widetilde{h}(\xi)-\widetilde{h}(\eta)\}^2. \tag{3.74}$$

Now, we divide the estimate of these summations into two cases: $K<L$ or $K=L$.

(Case $K < L$) We start by calculating the first summation of (3.74). Note that $\mathcal{B}$ can be decomposed as (cf. Notation 3.5.1)

$$\bigcup_{\boldsymbol{a}\neq\boldsymbol{a'}} \mathcal{B}^{a,\,a'} \cup \bigcup_{\boldsymbol{b}\neq\boldsymbol{b'}} \mathcal{B}^{b,\,b'} \cup \bigcup_{\boldsymbol{c}\neq\boldsymbol{c'}} \mathcal{B}^{c,\,c'} \cup \bigcup_{\boldsymbol{a},\,\boldsymbol{b}} \mathcal{B}^{a,\,b} \cup \bigcup_{\boldsymbol{a},\,\boldsymbol{c}} \mathcal{B}^{a,\,c} \cup \bigcup_{\boldsymbol{b},\,\boldsymbol{c}} \mathcal{B}^{c,\,b}.$$

Moreover, note that the summations with respect to $\bigcup_{\boldsymbol{a}\neq\boldsymbol{a'}} \mathcal{B}^{a,\,a'}$, $\bigcup_{\boldsymbol{b}\neq\boldsymbol{b'}} \mathcal{B}^{b,\,b'}$ and $\bigcup_{\boldsymbol{c}\neq\boldsymbol{c'}} \mathcal{B}^{c,\,c'}$ vanish by part (2) of Definition 3.5.2. Thus, we can divide the first summation of (3.74) as

$$\sum_{\boldsymbol{a},\,\boldsymbol{b}} \sum_{\{\eta,\,\xi\}\in E(\mathcal{B}^{a,\,b})} + \sum_{\boldsymbol{a},\,\boldsymbol{c}} \sum_{\{\eta,\,\xi\}\in E(\mathcal{B}^{a,\,c})} + \sum_{\boldsymbol{b},\,\boldsymbol{c}} \sum_{\{\eta,\,\xi\}\in E(\mathcal{B}^{c,\,b})} . \tag{3.75}$$

Since

$$E(\mathcal{B}^{a,\,b}) = \bigcup_{v\in[\![2,\,L-3]\!]} E(\mathcal{R}_v^{a,\,b} \cup \mathcal{Q}_v^{a,\,b} \cup \mathcal{R}_{v+1}^{a,\,b}), \tag{3.76}$$

the first double summation of (3.75) equals

$$\sum_{\boldsymbol{a},\,\boldsymbol{b}} \sum_{v\in[\![2,\,L-3]\!]} \sum_{\{\eta,\,\xi\}\in E(\mathcal{R}_v^{a,\,b}\cup\mathcal{Q}_v^{a,\,b}\cup\mathcal{R}_{v+1}^{a,\,b})} \mu_\beta(\eta) r_\beta(\eta,\,\xi)\{\widetilde{h}(\xi) - \widetilde{h}(\eta)\}^2.$$

Fixing $\boldsymbol{a} \in \mathcal{P}$ and $\boldsymbol{b} \in \mathcal{Q}$, which is possible because of symmetry, the last display can be written as

$$|\mathcal{P}||\mathcal{Q}| \sum_{v\in[\![2,\,L-3]\!]} \sum_{\{\eta,\,\xi\}\in E(\mathcal{R}_v^{a,\,b}\cup\mathcal{Q}_v^{a,\,b}\cup\mathcal{R}_{v+1}^{a,\,b})} \mu_\beta(\eta) r_\beta(\eta,\,\xi)\{\widetilde{h}(\xi) - \widetilde{h}(\eta)\}^2. \tag{3.77}$$

The last summation in $\{\eta,\, \xi\}$ can be written as $\sum_{\ell\in\mathbb{T}_L}\sum_{k\in\mathbb{T}_K}$ of

$$\begin{aligned}
&\mu_\beta(\xi^{a,\,b}_{\ell,\,v})r_\beta(\xi^{a,\,b}_{\ell,\,v},\, \xi^{a,\,b,\,\pm}_{\ell,\,v;\,k,\,1})\{\widetilde{h}(\xi^{a,\,b,\,\pm}_{\ell,\,v;\,k,\,1})-\widetilde{h}(\xi^{a,\,b}_{\ell,\,v})\}^2\\
&+\sum_{h\in[\![1,\,K-2]\!]}\mu_\beta(\xi^{a,\,b,\,\pm}_{\ell,\,v;\,k,\,h})r_\beta(\xi^{a,\,b,\,\pm}_{\ell,\,v;\,k,\,h},\, \xi^{a,\,b,\,\pm}_{\ell,\,v;\,k,\,h+1})\{\widetilde{h}(\xi^{a,\,b,\,\pm}_{\ell,\,v;\,k,\,h+1})-\widetilde{h}(\xi^{a,\,b,\,\pm}_{\ell,\,v;\,k,\,h})\}^2\\
&+\sum_{h\in[\![1,\,K-2]\!]}\mu_\beta(\xi^{a,\,b,\,\pm}_{\ell,\,v;\,k,\,h})r_\beta(\xi^{a,\,b,\,\pm}_{\ell,\,v;\,k,\,h},\, \xi^{a,\,b,\,\pm}_{\ell,\,v;\,k-1,\,h+1})\{\widetilde{h}(\xi^{a,\,b,\,\pm}_{\ell,\,v;\,k-1,\,h+1})-\widetilde{h}(\xi^{a,\,b,\,\pm}_{\ell,\,v;\,k,\,h})\}^2\\
&+\mu_\beta(\xi^{a,\,b,\,+}_{\ell,\,v;\,k,\,K-1})r_\beta(\xi^{a,\,b,\,+}_{\ell,\,v;\,k,\,K-1},\, \xi^{a,\,b}_{\ell,\,v+1})\{\widetilde{h}(\xi^{a,\,b}_{\ell,\,v+1})-\widetilde{h}(\xi^{a,\,b,\,+}_{\ell,\,v;\,k,\,K-1})\}^2\\
&+\mu_\beta(\xi^{a,\,b,\,-}_{\ell,\,v;\,k,\,K-1})r_\beta(\xi^{a,\,b,\,-}_{\ell,\,v;\,k,\,K-1},\, \xi^{a,\,b}_{\ell-1,\,v+1})\{\widetilde{h}(\xi^{a,\,b}_{\ell-1,\,v+1})-\widetilde{h}(\xi^{a,\,b,\,-}_{\ell,\,v;\,k,\,K-1})\}^2.
\end{aligned}$$

By (2.2), (3.69), and (3.70), this equals $2\sum_{\ell\in\mathbb{T}_L}\sum_{k\in\mathbb{T}_K}$ (where 2 is multiplied since $+$ and $-$ in $\pm$ give us the same computation) of

$$\begin{aligned}
&\frac{e^{-\Gamma\beta}}{Z_\beta}\cdot\frac{4\mathfrak{b}^2}{[\kappa(K+2)(L-4)]^2}+\sum_{h\in[\![1,\,K-2]\!]}\frac{e^{-\Gamma\beta}}{Z_\beta}\cdot\frac{\mathfrak{b}^2}{[\kappa(K+2)(L-4)]^2}\\
&\quad+\sum_{h\in[\![1,\,K-2]\!]}\frac{e^{-\Gamma\beta}}{Z_\beta}\cdot\frac{\mathfrak{b}^2}{[\kappa(K+2)(L-4)]^2}+\frac{e^{-\Gamma\beta}}{Z_\beta}\cdot\frac{4\mathfrak{b}^2}{[\kappa(K+2)(L-4)]^2}.
\end{aligned}$$

By Theorem 3.0.1, this is further simplified as

$$(1+o(1))\cdot\frac{e^{-\Gamma\beta}}{q}\cdot\frac{(2K+4)\mathfrak{b}^2}{(K+2)^2(L-4)^2\kappa^2}=(1+o(1))\cdot\frac{2\mathfrak{b}^2}{q(K+2)(L-4)^2\kappa^2}e^{-\Gamma\beta}.$$

Therefore by (3.29), we can conclude that

$$\begin{aligned}
&\sum_{\boldsymbol{a},\,\boldsymbol{b}}\sum_{\{\eta,\,\xi\}\in E(\mathcal{B}^{a,\,b})}\mu_\beta(\eta)r_\beta(\eta,\,\xi)\{\widetilde{h}(\xi)-\widetilde{h}(\eta)\}^2\\
&=(1+o(1))\cdot|\mathcal{P}||\mathcal{Q}|\cdot\sum_{v\in[\![2,\,L-3]\!]}2\sum_{\ell\in\mathbb{T}_L}\sum_{k\in\mathbb{T}_K}\frac{2\mathfrak{b}^2}{q(K+2)(L-4)^2\kappa^2}e^{-\Gamma\beta}\\
&=(1+o(1))\cdot|\mathcal{P}||\mathcal{Q}|\frac{4KL(L-4)\mathfrak{b}^2}{q(K+2)(L-4)^2\kappa^2}e^{-\Gamma\beta}=(1+o(1))\cdot\frac{|\mathcal{P}||\mathcal{Q}|\mathfrak{b}}{q\kappa^2}e^{-\Gamma\beta}.
\end{aligned}$$

The second and third summations of (3.75) can be dealt with in the same way (but with suitable constants multiplied), so that the second and the third summations have limits in $\beta \to \infty$ as

$$\frac{|\mathcal{Q}|^2|\mathcal{P}|(q-|\mathcal{P}|-|\mathcal{Q}|)\mathfrak{b}}{(|\mathcal{P}|+|\mathcal{Q}|)^2 q\kappa^2}e^{-\Gamma\beta} \quad \text{and} \quad \frac{|\mathcal{P}|^2|\mathcal{Q}|(q-|\mathcal{P}|-|\mathcal{Q}|)\mathfrak{b}}{(|\mathcal{P}|+|\mathcal{Q}|)^2 q\kappa^2}e^{-\Gamma\beta},$$

respectively. Summing up the last two displays, we obtain

$$\sum_{\{\eta,\,\xi\}\in E(\mathcal{B})} \mu_\beta(\eta) r_\beta(\eta,\,\xi)\{\widetilde{h}(\xi)-\widetilde{h}(\eta)\}^2 = (1+o(1))\cdot\frac{|\mathcal{P}||\mathcal{Q}|\mathfrak{b}}{(|\mathcal{P}|+|\mathcal{Q}|)\kappa^2}e^{-\Gamma\beta}. \tag{3.78}$$

Next, we calculate the second summation of (3.74). We may decompose $E(\mathcal{E})$ as

$$E(\mathcal{E}) = \bigcup_{\boldsymbol{a}} E(\mathcal{E}^a) \cup \bigcup_{\boldsymbol{b}} E(\mathcal{E}^b) \cup \bigcup_{\boldsymbol{c}} E(\mathcal{E}^c).$$

First, consider the summation in $\bigcup_{\boldsymbol{a}} E(\mathcal{E}^a)$. By (3.57), Definition (3.5.2)-(1) and Remark 3.5.4, we may rewrite it as

$$\begin{aligned}
&\sum_{\boldsymbol{a},\,\boldsymbol{b}}\sum_{\ell\in\mathbb{T}_L}\sum_{\{\eta_1,\,\eta_2\}\subseteq\mathcal{Z}_\ell^{a,\,b}\cup\{\xi_{\ell,\,2}^{a,\,b}\}} \mu_\beta(\eta_1)r_\beta(\eta_1,\,\eta_2)\{\widetilde{h}(\eta_2)-\widetilde{h}(\eta_1)\}^2\\
&+\sum_{\boldsymbol{a},\,\boldsymbol{b}}\sum_{\ell\in\mathbb{T}_L}\sum_{\eta_1\in\mathcal{Z}^{a,\,b}\cup\{\xi_{\ell,\,2}^{a,\,b}\}}\sum_{\xi\in\mathcal{N}(\boldsymbol{a})} \mu_\beta(\eta_1)r_\beta(\eta_1,\,\xi)\{\widetilde{h}(\xi)-\widetilde{h}(\eta_1)\}^2\\
&+\sum_{\boldsymbol{a},\,\boldsymbol{c}}\sum_{\ell\in\mathbb{T}_L}\sum_{\{\eta_1,\,\eta_2\}\subseteq\mathcal{Z}_\ell^{a,\,c}\cup\{\xi_{\ell,\,2}^{a,\,c}\}} \mu_\beta(\eta_1)r_\beta(\eta_1,\,\eta_2)\{\widetilde{h}(\eta_2)-\widetilde{h}(\eta_1)\}^2\\
&+\sum_{\boldsymbol{a},\,\boldsymbol{c}}\sum_{\ell\in\mathbb{T}_L}\sum_{\eta_1\in\mathcal{Z}^{a,\,c}\cup\{\xi_{\ell,\,2}^{a,\,c}\}}\sum_{\xi\in\mathcal{N}(\boldsymbol{a})} \mu_\beta(\eta_1)r_\beta(\eta_1,\,\xi)\{\widetilde{h}(\xi)-\widetilde{h}(\eta_1)\}^2.
\end{aligned}$$

By Proposition 3.4.22, taking into advantage the model symmetry, this equals

$$|\mathcal{P}||\mathcal{Q}|\cdot L(1+o(1))\cdot\Big[\sum_{\{\eta_1,\,\eta_2\}\subseteq\mathcal{Z}_\ell^{a,\,b}\cup\{\xi_{\ell,\,2}^{a,\,b}\}}+\sum_{\eta_1\in\mathcal{Z}^{a,\,b}\cup\{\xi_{\ell,\,2}^{a,\,b}\},\,\eta_2=\boldsymbol{a}}\Big]$$
$$+|\mathcal{P}|(q-|\mathcal{P}|-|\mathcal{Q}|)\cdot L(1+o(1))\cdot\Big[\sum_{\{\eta_1,\,\eta_2\}\subseteq\mathcal{Z}_\ell^{a,\,c}\cup\{\xi_{\ell,\,2}^{a,\,c}\}}+\sum_{\eta_1\in\mathcal{Z}^{a,\,c}\cup\{\xi_{\ell,\,2}^{a,\,c}\},\,\eta_2=\boldsymbol{a}}\Big]\tag{3.79}$$

applied to the summand $q^{-1}e^{-\Gamma\beta}\mathfrak{r}(\eta_1,\,\eta_2)\{\widetilde{h}(\eta_2)-\widetilde{h}(\eta_1)\}^2$. By (3.66), this becomes

$$|\mathcal{P}||\mathcal{Q}|\cdot L(1+o(1))\cdot\frac{\mathfrak{e}^2}{\kappa^2}\sum_{\{\eta_1,\,\eta_2\}\in\mathscr{E}}$$
$$+|\mathcal{P}|(q-|\mathcal{P}|-|\mathcal{Q}|)\cdot L(1+o(1))\cdot\frac{|\mathcal{Q}|^2}{(|\mathcal{P}|+|\mathcal{Q}|)^2}\frac{\mathfrak{e}^2}{\kappa^2}\sum_{\{\eta_1,\,\eta_2\}\in\mathscr{E}}$$

applied to the summand $q^{-1}e^{-\Gamma\beta}\mathfrak{r}(\eta_1,\,\eta_2)\{\mathfrak{f}(\eta_2)-\mathfrak{f}(\eta_1)\}^2$. Noting the definition of capacities (cf. (3.22)), this is equal to

$$\Big[1+\frac{(q-|\mathcal{P}|-|\mathcal{Q}|)|\mathcal{Q}|}{(|\mathcal{P}|+|\mathcal{Q}|)^2}\Big]\cdot|\mathcal{P}||\mathcal{Q}|\cdot L(1+o(1))\cdot\frac{e^{-\Gamma\beta}\mathfrak{e}^2}{\kappa^2 q}|\mathscr{V}|\mathfrak{cap}(\boldsymbol{a},\,\mathcal{R}_2^{a,\,b})$$
$$=\Big[1+\frac{(q-|\mathcal{P}|-|\mathcal{Q}|)|\mathcal{Q}|}{(|\mathcal{P}|+|\mathcal{Q}|)^2}\Big]\cdot\frac{|\mathcal{P}||\mathcal{Q}|\mathfrak{e}(1+o(1))}{\kappa^2 q}e^{-\Gamma\beta},$$

where in the equality we used (3.30) and (3.64). Employing the same arguments to the summations in $\bigcup_{\boldsymbol{b}}E(\mathcal{E}^b)$ and $\bigcup_{\boldsymbol{c}}E(\mathcal{E}^c)$ in the second summation of (3.74), we obtain that the summations in $\bigcup_{\boldsymbol{b}}E(\mathcal{E}^b)$ equals

$$\Big[1+\frac{|\mathcal{P}|(q-|\mathcal{P}|-|\mathcal{Q}|)}{(|\mathcal{P}|+|\mathcal{Q}|)^2}\Big]\cdot\frac{|\mathcal{P}||\mathcal{Q}|\mathfrak{e}(1+o(1))}{\kappa^2 q}e^{-\Gamma\beta},$$

and the summation in $\bigcup_{c} E(\mathcal{E}^c)$ becomes

$$\Big[\frac{(q-|\mathcal{P}|-|\mathcal{Q}|)|\mathcal{Q}|}{(|\mathcal{P}|+|\mathcal{Q}|)^2}+\frac{|\mathcal{P}|(q-|\mathcal{P}|-|\mathcal{Q}|)}{(|\mathcal{P}|+|\mathcal{Q}|)^2}\Big]\cdot\frac{|\mathcal{P}||\mathcal{Q}|\mathfrak{e}(1+o(1))}{\kappa^2 q}e^{-\Gamma\beta}.$$

Therefore, summing up the last three displays, we conclude that

$$\sum_{\{\eta,\,\xi\}\in E(\mathcal{E})}\mu_\beta(\eta)r_\beta(\eta,\,\xi)\{\widetilde{h}(\xi)-\widetilde{h}(\eta)\}^2=\frac{2|\mathcal{P}||\mathcal{Q}|}{|\mathcal{P}|+|\mathcal{Q}|}\cdot\frac{\mathfrak{e}(1+o(1))}{\kappa^2}e^{-\Gamma\beta}. \quad (3.80)$$

Therefore, by (3.74), (3.78), and (3.80), we conclude that the third summation of (3.71) equals $1+o(1)$ times

$$\frac{|\mathcal{P}||\mathcal{Q}|}{|\mathcal{P}|+|\mathcal{Q}|}\cdot\frac{\mathfrak{b}+2\mathfrak{e}}{\kappa^2}e^{-\Gamma\beta}=\frac{|\mathcal{P}||\mathcal{Q}|}{\kappa(|\mathcal{P}|+|\mathcal{Q}|)}e^{-\Gamma\beta},$$

as desired.

(Case $K=L$**)** This case is analogous to the previous case. The only difference is the fact that (3.74) must be counted twice. This fact is reflected in the definition of the constants $\mathfrak{b}$ and $\mathfrak{e}$ in (3.29) and (3.30) through the constant ν_0. □

Remark 3.5.7. The estimates (3.78) and (3.80) are the reason that we call $\mathfrak{b}$ and $\mathfrak{e}$ the bulk and edge constants, respectively.

3.5.3 Proof of H^1-approximation

In this subsection, we prove (3.38) to complete the proof of Proposition 3.2.9 for the MH dynamics. To prove (3.38), we first expand

$$\begin{aligned}D_\beta(h_{\mathcal{P},\,\mathcal{Q}}-\widetilde{h})&=\langle h_{\mathcal{P},\,\mathcal{Q}}-\widetilde{h},\,-\mathcal{L}_\beta(h_{\mathcal{P},\,\mathcal{Q}}-\widetilde{h})\rangle_{\mu_\beta}\\&=D_\beta(h_{\mathcal{P},\,\mathcal{Q}})+D_\beta(\widetilde{h})-\langle h_{\mathcal{P},\,\mathcal{Q}},\,-\mathcal{L}_\beta\widetilde{h}\rangle_{\mu_\beta}-\langle\widetilde{h},\,-\mathcal{L}_\beta h_{\mathcal{P},\,\mathcal{Q}}\rangle_{\mu_\beta}.\end{aligned} \quad (3.81)$$

Since $\widetilde{h} \equiv 1$ on $\mathcal{P}$, $\widetilde{h} \equiv 0$ on $\mathcal{Q}$ (cf. Remark 3.5.5), and since $\mathcal{L}_\beta h_{\mathcal{P},\,\mathcal{Q}} \equiv 0$ on $(\mathcal{P} \cup \mathcal{Q})^c$ (cf. (3.19)), we have

$$\begin{aligned}\langle \widetilde{h},\, -\mathcal{L}_\beta h_{\mathcal{P},\,\mathcal{Q}} \rangle_{\mu_\beta} &= \sum_{\boldsymbol{a} \in \mathcal{P}} \widetilde{h}(\boldsymbol{a})(-\mathcal{L}_\beta h_{\mathcal{P},\,\mathcal{Q}})(\boldsymbol{a})\mu_\beta(\boldsymbol{a}) \\ &= \sum_{\boldsymbol{a} \in \mathcal{P}} h_{\mathcal{P},\,\mathcal{Q}}(\boldsymbol{a})(-\mathcal{L}_\beta h_{\mathcal{P},\,\mathcal{Q}})(\boldsymbol{a})\mu_\beta(\boldsymbol{a}) = D_\beta(h_{\mathcal{P},\,\mathcal{Q}}).\end{aligned}$$

In the second equality, we used that $h_{\mathcal{P},\,\mathcal{Q}} \equiv \widetilde{h} \equiv 1$ on $\mathcal{P}$. Inserting this into (3.81) and expanding the first inner product in the right-hand side, we obtain

$$D_\beta(h_{\mathcal{P},\,\mathcal{Q}} - \widetilde{h}) = D_\beta(\widetilde{h}) - \sum_{\eta \in \mathcal{X}} h_{\mathcal{P},\,\mathcal{Q}}(\eta)(-\mathcal{L}_\beta \widetilde{h})(\eta)\mu_\beta(\eta). \tag{3.82}$$

By the definition of $\mathcal{L}_\beta$ (cf. (2.1)) and Proposition 3.5.6, it suffices to prove that

$$\sum_{\eta \in \mathcal{X}} h_{\mathcal{P},\,\mathcal{Q}}(\eta) \sum_{\xi \in \mathcal{X}} \mu_\beta(\eta) r_\beta(\eta,\,\xi)[\widetilde{h}(\eta) - \widetilde{h}(\xi)] = (1 + o(1)) \cdot \frac{|\mathcal{P}||\mathcal{Q}|}{\kappa(|\mathcal{P}| + |\mathcal{Q}|)} e^{-\Gamma\beta}. \tag{3.83}$$

Before proving this identity, we present a simple lemma which states that the equilibrium potential $h_{\mathcal{P},\,\mathcal{Q}}$ is asymptotically constant on each neighborhood $\mathcal{N}(\boldsymbol{s})$ for $\boldsymbol{s} \in \mathcal{S}$.

Lemma 3.5.8. *For all $\boldsymbol{s} \in \mathcal{S}$, we have* $\max_{\eta \in \mathcal{N}(\boldsymbol{s})} \left| h_{\mathcal{P},\,\mathcal{Q}}(\eta) - h_{\mathcal{P},\,\mathcal{Q}}(\boldsymbol{s}) \right| = o(1)$.

Proof. We first recall from [70, Theorem 3.2-(iii)] that, for all $\boldsymbol{s} \in \mathcal{S}$, we have

$$\max_{\eta \in \mathcal{N}(\boldsymbol{s})} \mathbb{P}_\eta[\tau_{\mathcal{X} \setminus \mathcal{N}(\boldsymbol{s})} < \tau_{\boldsymbol{s}}] = o(1). \tag{3.84}$$

We first assume that $\boldsymbol{s} \in \mathcal{Q}$, so that $h_{\mathcal{P},\,\mathcal{Q}}(\boldsymbol{s}) = 0$. For $\eta \in \mathcal{N}(\boldsymbol{s})$, we can bound

$$|h_{\mathcal{P},\,\mathcal{Q}}(\eta) - h_{\mathcal{P},\,\mathcal{Q}}(\boldsymbol{s})| = h_{\mathcal{P},\,\mathcal{Q}}(\eta) = \mathbb{P}_\eta[\tau_{\mathcal{P}} < \tau_{\mathcal{Q}}] \le \mathbb{P}_\eta[\tau_{\mathcal{X} \setminus \mathcal{N}(\boldsymbol{s})} < \tau_{\boldsymbol{s}}].$$

Thus, the proof is completed by (3.84). We can handle the case $\boldsymbol{s} \in \mathcal{P}$ by an entirely same manner.

Let us finally consider the case $\boldsymbol{s} \in \mathcal{S} \setminus (\mathcal{P} \cup \mathcal{Q})$. By the Markov property, for $\eta \in \mathcal{N}(\boldsymbol{s})$,

$$h_{\mathcal{P},\,\mathcal{Q}}(\eta) = \mathbb{P}_\eta[\tau_{\boldsymbol{s}} < \tau_{\mathcal{X}\setminus\mathcal{N}(\boldsymbol{s})}]\mathbb{P}_{\boldsymbol{s}}[\tau_{\mathcal{P}} < \tau_{\mathcal{Q}}] + \mathbb{P}_\eta[\tau_{\boldsymbol{s}} > \tau_{\mathcal{X}\setminus\mathcal{N}(\boldsymbol{s})},\, \tau_{\mathcal{P}} < \tau_{\mathcal{Q}}].$$

From this, we obtain

$$|h_{\mathcal{P},\,\mathcal{Q}}(\eta) - h_{\mathcal{P},\,\mathcal{Q}}(\boldsymbol{s})| \le 2\mathbb{P}_\eta[\tau_{\boldsymbol{s}} > \tau_{\mathcal{X}\setminus\mathcal{N}(\boldsymbol{s})}]$$

and thus the proof of this case is also completed by (3.84). □

Remark 3.5.9. We can also prove this lemma by using a capacity bound on the equilibrium potential (cf. [16, Lemma 8.4]), and then applying the Dirichlet–Thomson principle.

Now, we begin to prove (3.83). Write

$$\phi(\eta) := \sum_{\xi\in\mathcal{X}} \mu_\beta(\eta) r_\beta(\eta,\, \xi)[\widetilde{h}(\eta) - \widetilde{h}(\xi)], \tag{3.85}$$

so that our claim (3.83) can be simply rewritten as

$$\sum_{\eta\in\mathcal{X}} h_{\mathcal{P},\,\mathcal{Q}}(\eta)\phi(\eta) = (1 + o(1)) \cdot \frac{|\mathcal{P}||\mathcal{Q}|}{\kappa(|\mathcal{P}| + |\mathcal{Q}|)} e^{-\Gamma\beta}. \tag{3.86}$$

First, we deduce that ϕ is negligible outside $\widehat{\mathcal{N}}(\mathcal{S})$.

Lemma 3.5.10. *For all $\eta \in \mathcal{X} \setminus \widehat{\mathcal{N}}(\mathcal{S})$, we have $\phi(\eta) = o(e^{-\Gamma\beta})$.*

Proof. Since $\widetilde{h}$ is defined as constant outside $\widehat{\mathcal{N}}(\mathcal{S})$, we may only consider $\eta \in \mathcal{X} \setminus \widehat{\mathcal{N}}(\mathcal{S})$ which is connected to at least one configuration in $\widehat{\mathcal{N}}(\mathcal{S})$. Then, by Lemma 3.4.6, we have $H(\eta) \ge \Gamma + 1$, and thus by (2.2), it holds for $\xi \in \widehat{\mathcal{N}}(\mathcal{S})$ with $\eta \sim \xi$ that

$$0 \le \mu_\beta(\eta) r_\beta(\eta,\, \xi) = \min\{\mu_\beta(\eta),\, \mu_\beta(\xi)\} = \mu_\beta(\eta) = O(e^{-\beta(\Gamma+1)}).$$

This completes the proof since $\widetilde{h} : \mathcal{X} \to [0,\, 1]$. □

Next, we deal with $\phi(\eta)$ where $\eta \in \widehat{\mathcal{N}}(\mathcal{S})$. We decompose $\phi(\eta) = \phi_1(\eta) + \phi_2(\eta)$ where

$$\phi_1(\eta) = \sum_{\xi \in \widehat{\mathcal{N}}(\mathcal{S})} \mu_\beta(\eta) r_\beta(\eta,\, \xi)[\widetilde{h}(\eta) - \widetilde{h}(\xi)],$$

$$\phi_2(\eta) = \sum_{\xi \notin \widehat{\mathcal{N}}(\mathcal{S})} \mu_\beta(\eta) r_\beta(\eta,\, \xi)[\widetilde{h}(\eta) - \widetilde{h}(\xi)].$$

The first claim is that $\phi_2(\eta)$ is negligible for all $\eta \in \widehat{\mathcal{N}}(\mathcal{S})$.

Lemma 3.5.11. *Suppose that $\eta \in \widehat{\mathcal{N}}(\mathcal{S})$. Then, $\phi_2(\eta) = o(e^{-\Gamma\beta})$.*

Proof. If $\xi \notin \widehat{\mathcal{N}}(\mathcal{S})$ with $\eta \sim \xi$, then

$$\mu_\beta(\eta) r_\beta(\eta,\, \xi) = \min\{\mu_\beta(\eta),\, \mu_\beta(\xi)\} = \mu_\beta(\xi) = O(e^{-\beta(\Gamma+1)})$$

by (2.2), Proposition 3.4.17-(4), Lemma 3.4.6 and Theorem 3.0.1. Thus, since $0 \le \widetilde{h} \le 1$,

$$|\phi_2(\eta)| \le \sum_{\xi \notin \widehat{\mathcal{N}}(\mathcal{S}):\, \xi \sim \eta} \mu_\beta(\eta) r_\beta(\eta,\, \xi) = O(e^{-\beta(\Gamma+1)}),$$

which is $o(e^{-\beta\Gamma})$ as desired. □

Summing up, instead of (3.86), it suffices to show that

$$\sum_{\eta \in \widehat{\mathcal{N}}(\mathcal{S})} h_{\mathcal{P},\, \mathcal{Q}}(\eta)\phi_1(\eta) = (1 + o(1)) \cdot \frac{|\mathcal{P}||\mathcal{Q}|}{\kappa(|\mathcal{P}| + |\mathcal{Q}|)} e^{-\Gamma\beta}. \tag{3.87}$$

Let us now investigate ϕ_1. We start with the set $\mathcal{B} \setminus \mathcal{E}$.

Lemma 3.5.12. *It holds that* $\phi_1(\eta) = 0$ *for all* $\eta \in \mathcal{B} \setminus \mathcal{E}$.

Proof. By construction of the function $\widetilde{h}$ on $\mathcal{B}$, it suffices to deal with the cases $\eta \in \mathcal{B}^{a,b} \setminus \mathcal{E}$, $\eta \in \mathcal{B}^{a,c} \setminus \mathcal{E}$ and $\eta \in \mathcal{B}^{c,b} \setminus \mathcal{E}$ where $\boldsymbol{a} \in \mathcal{P}$, $\boldsymbol{b} \in \mathcal{Q}$ and $\boldsymbol{c} \in \mathcal{S} \setminus (\mathcal{P} \cup \mathcal{Q})$. We start with the case $\eta \in \mathcal{B}^{a,b} \setminus \mathcal{E}$.

We first consider the case $K < L$. If $\eta = \xi_{\ell,v}^{a,b}$ for some $\ell \in \mathbb{T}_L$ and $v \in [\![3,\, L-3]\!]$, by simple inspection, $\phi_1(\eta)$ equals

$$\sum_{k \in \mathbb{T}_K} \sum_{\xi \in \{\xi_{\ell,v;k,1}^{a,b,+},\, \xi_{\ell,v;k,1}^{a,b,-},\, \xi_{\ell,v-1;k,K-1}^{a,b,+},\, \xi_{\ell+1,v-1;k,K-1}^{a,b,-}\}} \mu_\beta(\eta) r_\beta(\eta,\, \xi)[\widetilde{h}(\eta) - \widetilde{h}(\xi)].$$

Substituting the exact values from Definition 3.5.2 and noting (2.2), this becomes

$$\frac{e^{-\beta\Gamma}}{Z_\beta} \sum_{k \in \mathbb{T}_K} \frac{2\mathfrak{b}}{\kappa(K+2)(L-4)}[1+1-1-1],$$

which is zero. If $\eta = \xi_{\ell,v;k,h}^{a,b,+}$ for some $\ell \in \mathbb{T}_L$, $v \in [\![2,\, L-3]\!]$, $k \in \mathbb{T}_K$ and $h \in [\![1,\, K-1]\!]$, then $\phi_1(\eta)$ equals

$$\begin{aligned}&\sum_{\xi \in \{\xi_{\ell,v;k,h+1}^{a,b,+},\, \xi_{\ell,v;k-1,h+1}^{a,b,+},\, \xi_{\ell,v;k,h-1}^{a,b,+},\, \xi_{\ell,v;k+1,h-1}^{a,b,+}\}} \mu_\beta(\eta) r_\beta(\eta,\, \xi)[\widetilde{h}(\eta) - \widetilde{h}(\xi)] \\ &= \frac{e^{-\Gamma\beta}}{Z_\beta} \cdot \frac{\mathfrak{b}}{\kappa(K+2)(L-4)}[1+1-1-1],\end{aligned}$$

which is again zero. The case of $\eta = \xi_{\ell,v;k,h}^{a,b,-}$ can be handled similarly. Therefore, we conclude the case $\eta \in \mathcal{B}^{a,b} \setminus \mathcal{E}$ under the assumption $K < L$. If $K = L$, then there are twice more possibilities obtained by transposing the above configurations. However, this case can be dealt with identically as above.

Finally, note that the structure of $\widetilde{h}$ on $\mathcal{B}^{a,c}$ and $\mathcal{B}^{c,b}$ are the same as the structure on $\mathcal{B}^{a,b}$, except for linear transformations. Thus, we can repeat the same calculations to obtain the same result that $\phi_1(\eta) = 0$. □

Next, we show that ϕ_1 is also zero on $\mathcal{R}_2$ and $\mathcal{R}_{L-2}$.

Lemma 3.5.13. *It holds that* $\phi_1(\eta) = 0$ *for all* $\eta \in \mathcal{R}_2 \cup \mathcal{R}_{L-2}$.

Proof. We have $\mathcal{R}_2 = \mathcal{R}_{L-2}$ by Definition 3.4.10 and thus we only focus on $\mathcal{R}_2$. By Definition 3.5.2, we only need to consider $\eta \in \mathcal{R}_2^{a,\,b} \cup \mathcal{R}_2^{a,\,c} \cup \mathcal{R}_2^{c,\,b}$ for $\boldsymbol{a} \in \mathcal{P}$, $\boldsymbol{b} \in \mathcal{Q}$ and $\boldsymbol{c} \in \mathcal{S} \setminus (\mathcal{P} \cup \mathcal{Q})$. First consider $\eta \in \mathcal{R}_2^{a,\,b}$. Without loss of generality, we assume $\eta = \xi_{\ell,\,2}^{a,\,b}$, since we can deal with the case of $\eta = \Theta(\xi_{\ell,\,2}^{a,\,b})$ in the same way. Recall that $\mathfrak{f} = \mathfrak{f}_{\boldsymbol{a},\,\xi_{\ell,\,2}^{a,\,b}}$ from (3.65) and recall the generator $\mathfrak{L}$ from (3.63). Then, since the uniform measure on $\mathscr{V}$ is the invariant measure for the process $\mathfrak{Z}(\cdot)$, by the property of capacities (e.g., [16, (7.1.39)]), we can write

$$\frac{1}{|\mathscr{V}|} \sum_{\xi \in \mathscr{V} \setminus \{\xi_{\ell,\,2}^{a,\,b}\}} \mathfrak{r}(\xi_{\ell,\,2}^{a,\,b},\,\xi)[\mathfrak{f}(\xi_{\ell,\,2}^{a,\,b}) - \mathfrak{f}(\xi)] = -\frac{1}{|\mathscr{V}|}(\mathfrak{L}\mathfrak{f})(\xi_{\ell,\,2}^{a,\,b}) = -\mathfrak{cap}(\boldsymbol{a},\,\xi_{\ell,\,2}^{a,\,b}).$$

On the other hand, by the definition of $\widetilde{h}$, we can write

$$\begin{aligned} &\sum_{\xi \in \mathcal{E}^a} \mu_\beta(\xi_{\ell,\,2}^{a,\,b}) r_\beta(\xi_{\ell,\,2}^{a,\,b},\,\xi)[\widetilde{h}(\xi_{\ell,\,2}^{a,\,b}) - \widetilde{h}(\xi)] \\ &= \frac{1}{Z_\beta} e^{-\beta\Gamma} \frac{\mathfrak{e}}{\kappa} \sum_{\xi \in \mathscr{V} \setminus \{\xi_{\ell,\,2}^{a,\,b}\}} \mathfrak{r}(\xi_{\ell,\,2}^{a,\,b},\,\xi)\{\mathfrak{f}(\xi_{\ell,\,2}^{a,\,b}) - \mathfrak{f}(\xi)\}. \end{aligned}$$

Summing up the computations above, we get

$$\begin{aligned} &\sum_{\xi \in \mathcal{E}^a} \mu_\beta(\xi_{\ell,\,2}^{a,\,b}) r_\beta(\xi_{\ell,\,2}^{a,\,b},\,\xi)[\widetilde{h}(\xi_{\ell,\,2}^{a,\,b}) - \widetilde{h}(\xi)] \\ &= -\frac{1}{Z_\beta} e^{-\beta\Gamma} \frac{\mathfrak{e}}{\kappa} \times |\mathscr{V}| \mathfrak{cap}(\boldsymbol{a},\,\xi_{\ell,\,2}^{a,\,b}) = -\nu_0 \frac{e^{-\beta\Gamma}}{Z_\beta \kappa L}, \end{aligned} \tag{3.88}$$

where the second identity is a consequence of the definitions of $\mathfrak{e}$ and $\mathfrak{e}_0$ given in (3.30) and (3.64), respectively. On the other hand, by the definition of $\mathfrak{b}$,

$$\begin{aligned}&\sum_{\xi\in\mathcal{B}^{a,\,b}}\mu_\beta(\xi_{\ell,\,2}^{a,\,b})r_\beta(\xi_{\ell,\,2}^{a,\,b},\,\xi)[\widetilde{h}(\xi_{\ell,\,2}^{a,\,b})-\widetilde{h}(\xi)]\\&=\frac{1}{Z_\beta}e^{-\beta\Gamma}\cdot 2K\cdot\frac{2\mathfrak{b}}{\kappa(K+2)(L-4)}=\nu_0\frac{e^{-\beta\Gamma}}{Z_\beta\kappa L}.\end{aligned}\tag{3.89}$$

By adding (3.88) and (3.89), we obtain

$$\phi_1(\xi_{\ell,\,2}^{a,\,b})=-\nu_0\frac{e^{-\beta\Gamma}}{Z_\beta\kappa L}+\nu_0\frac{e^{-\beta\Gamma}}{Z_\beta\kappa L}=0.$$

The same computations can be done with the remaining cases $\eta\in\mathcal{R}_2^{a,\,c}$ and $\eta\in\mathcal{R}_2^{c,\,b}$, just by multiplying constants to each term. Thus, we do not repeat the proof. □

Next, we show that $\phi_1(\eta)=0$ for $\eta\in\mathcal{Z}^{a,\,b}\cup\mathcal{Z}^{a,\,c}\cup\mathcal{Z}^{c,\,b}$, $\boldsymbol{a}\in\mathcal{P}$, $\boldsymbol{b}\in\mathcal{Q}$ and $\boldsymbol{c}\in\mathcal{S}\setminus(\mathcal{P}\cup\mathcal{Q})$.

Lemma 3.5.14. *It holds that $\phi_1(\eta)=0$ for all $\eta\in\mathcal{Z}^{a,\,b}\cup\mathcal{Z}^{a,\,c}\cup\mathcal{Z}^{c,\,b}$.*

Proof. We consider only the case $\eta\in\mathcal{Z}^{a,\,b}$, since the structure is identical in the other cases (with constants multiplied). Recall $\mathfrak{L}$ from (3.63). Then for each $\eta\in\mathcal{Z}^{a,\,b}$, we can write

$$\phi_1(\eta)=\frac{1}{Z_\beta}e^{-\Gamma\beta}\frac{\mathfrak{e}}{\kappa}\times(\mathfrak{L}\mathfrak{f})(\eta).\tag{3.90}$$

By the elementary property of equilibrium potentials (e.g., [16, (7.1.21)]), we can easily conclude from (3.90) that $\phi_1(\eta)=0$. □

All it remains is to consider the configurations in $\mathcal{D}^s$ for all $s\in S$. This is the content of the following two lemmas.

Lemma 3.5.15. *For any $\boldsymbol{s}\in\mathcal{S}$ and $\eta\in\mathcal{D}^s\setminus\mathcal{N}(\boldsymbol{s})$, we have $\phi_1(\eta)=0$.*

Proof. Recall from Definition 3.5.2-(1) that $\widetilde{h}$ is defined to be constant on $\mathcal{D}^s$, and thus for all $\eta \in \mathcal{D}^s \setminus \mathcal{N}(\boldsymbol{s})$,

$$\phi_1(\eta) = \sum_{\xi \in \widehat{\mathcal{N}}(\mathcal{S}) :\, \xi \sim \eta} \mu_\beta(\eta) r_\beta(\eta,\, \xi)[\widetilde{h}(\eta) - \widetilde{h}(\xi)] = 0.$$

This concludes the proof. □

Lemma 3.5.16. *For $\boldsymbol{a} \in \mathcal{P}$, $\boldsymbol{b} \in \mathcal{Q}$, and $\boldsymbol{c} \in \mathcal{S} \setminus (\mathcal{P} \cup \mathcal{Q})$, it holds that*

$$\sum_{\eta \in \mathcal{N}(\boldsymbol{a})} \phi_1(\eta) = (1 + o(1)) \cdot \frac{|\mathcal{Q}|}{\kappa(|\mathcal{P}| + |\mathcal{Q}|)} e^{-\Gamma\beta}, \tag{3.91}$$

$$\sum_{\eta \in \mathcal{N}(\boldsymbol{b})} \phi_1(\eta) = -(1 + o(1)) \cdot \frac{|\mathcal{P}|}{\kappa(|\mathcal{P}| + |\mathcal{Q}|)} e^{-\Gamma\beta}, \tag{3.92}$$

$$\sum_{\eta \in \mathcal{N}(\boldsymbol{c})} \phi_1(\eta) = o(e^{-\Gamma\beta}). \tag{3.93}$$

Moreover, there exists $C > 0$ independent of β such that for all $\eta \in \mathcal{N}(\boldsymbol{a}) \cup \mathcal{N}(\boldsymbol{b}) \cup \mathcal{N}(\boldsymbol{c})$, $|\phi_1(\eta)| \le Ce^{-\Gamma\beta}$.

Proof. To start, we prove the first identity which is

$$\sum_{\eta \in \mathcal{N}(\boldsymbol{a})} \sum_{\xi \in \widehat{\mathcal{N}}(\mathcal{S}) :\, \xi \sim \eta} \mu_\beta(\eta) r_\beta(\eta,\, \xi)[\widetilde{h}(\eta) - \widetilde{h}(\xi)] = (1 + o(1)) \cdot \frac{|\mathcal{Q}||}{\kappa(|\mathcal{P}| + |\mathcal{Q}|)} e^{-\Gamma\beta}. \tag{3.94}$$

The left-hand side can be written as

$$- \sum_{\eta \in \mathcal{N}(\boldsymbol{a})} \sum_{\boldsymbol{b} \in \mathcal{Q}} |\mathcal{R}_2^{a,\, b}| \sum_{\xi \in \mathcal{Z}_\ell^{a,\, b} :\, \xi \sim \eta} \frac{e^{-\Gamma\beta}}{Z_\beta} \frac{\mathfrak{e}}{\kappa} [\mathfrak{f}(\xi) - \mathfrak{f}(\boldsymbol{a})]$$
$$- \sum_{\eta \in \mathcal{N}(\boldsymbol{a})} \sum_{\boldsymbol{c} \in \mathcal{S} \setminus (\mathcal{P} \cup \mathcal{Q})} |\mathcal{R}_2^{a,\, c}| \sum_{\xi \in \mathcal{Z}_\ell^{a,\, c} :\, \xi \sim \eta} \frac{e^{-\Gamma\beta}}{Z_\beta} \frac{|\mathcal{Q}|}{|\mathcal{P}| + |\mathcal{Q}|} \frac{\mathfrak{e}}{\kappa} [\mathfrak{f}(\xi) - \mathfrak{f}(\boldsymbol{a})].$$

This can be rewritten as

$$
\begin{aligned}
&-\frac{e^{-\Gamma\beta}}{Z_\beta}\frac{\mathfrak{e}}{\kappa}\sum_{\boldsymbol{b}\in\mathcal{Q}}|\mathcal{R}_2^{a,\,b}|\sum_{\xi\in\mathcal{Z}_\ell^{a,\,b}:\,\{\xi,\,\boldsymbol{a}\}\in\mathscr{E}}\mathfrak{r}(\boldsymbol{a},\,\xi)[\mathfrak{f}(\xi)-\mathfrak{f}(\boldsymbol{a})]\\
&-\frac{e^{-\Gamma\beta}}{Z_\beta}\frac{|\mathcal{Q}|}{|\mathcal{P}|+|\mathcal{Q}|}\frac{\mathfrak{e}}{\kappa}\sum_{\boldsymbol{c}\in\mathcal{S}\setminus(\mathcal{P}\cup\mathcal{Q})}|\mathcal{R}_2^{a,\,c}|\sum_{\xi\in\mathcal{Z}_\ell^{a,\,c}:\,\{\xi,\,\boldsymbol{a}\}\in\mathscr{E}}\mathfrak{r}(\boldsymbol{a},\,\xi)[\mathfrak{f}(\xi)-\mathfrak{f}(\boldsymbol{a})].
\end{aligned}
$$

By the property of capacities (e.g., [16, (7.1.39)]), the last display equals

$$
\begin{aligned}
&-\frac{e^{-\Gamma\beta}}{Z_\beta}\frac{\mathfrak{e}}{\kappa}\Big[\sum_{\boldsymbol{b}\in\mathcal{Q}}|\mathcal{R}_2^{a,\,b}|\times(\mathfrak{L}\mathfrak{f})(\boldsymbol{a})+\frac{|\mathcal{Q}|}{|\mathcal{P}|+|\mathcal{Q}|}\sum_{\boldsymbol{c}\in\mathcal{S}\setminus(\mathcal{P}\cup\mathcal{Q})}|\mathcal{R}_2^{a,\,c}|\times(\mathfrak{L}\mathfrak{f})(\boldsymbol{a})\Big]\\
&=\frac{e^{-\Gamma\beta}}{Z_\beta}\frac{\mathfrak{e}}{\kappa}\Big[|\mathcal{Q}|\times\frac{1}{\mathfrak{e}}+(q-|\mathcal{P}|-|\mathcal{Q}|)\times\frac{|\mathcal{Q}|}{|\mathcal{P}|+|\mathcal{Q}|}\frac{1}{\mathfrak{e}}\Big]=\frac{qe^{-\Gamma\beta}}{Z_\beta\kappa}\frac{|\mathcal{Q}|}{|\mathcal{P}|+|\mathcal{Q}|}.
\end{aligned}
$$

By Theorem 3.0.1, we can verify (3.94). The second and third identities of the lemma can be proved in the exact same way and thus we omit the detail.

Finally, take $\eta\in\mathcal{N}(\boldsymbol{a})\cup\mathcal{N}(\boldsymbol{b})\cup\mathcal{N}(\boldsymbol{c})$. By Definition 3.5.2, if $\xi\in\widehat{\mathcal{N}}(\mathcal{S})$ with $\xi\sim\eta$, we know that $\widetilde{h}(\eta)\neq\widetilde{h}(\xi)$ only if $\min\{H(\eta),\,H(\xi)\}\geq\Gamma$. This implies that

$$
|\phi_1(\eta)|\leq\sum_{\xi\in\widehat{\mathcal{N}}(\mathcal{S}):\,\xi\sim\eta}\mu_\beta(\eta)r_\beta(\eta,\,\xi)|\widetilde{h}(\eta)-\widetilde{h}(\xi)|\leq\frac{C}{Z_\beta}e^{-\Gamma\beta}.
$$

The inequality holds by (2.2) and the fact that $0\leq\widetilde{h}\leq1$. Since $Z_\beta=q+o(1)$ by Theorem 3.0.1, we conclude the proof. □

Now, we have all ingredients to prove (3.38). Thus, we are ready to complete the proof of Proposition 3.2.9 for the MH dynamics.

Proof of Proposition 3.2.9 for the MH dynamics. By Remark 3.5.5 and Proposition 3.5.6, it suffices to verify (3.38). As we have discussed earlier, proving (3.38) is reduced to proving (3.87). This has been verified in Lemmas 3.5.8

and 3.5.12-3.5.16. More precisely, by Lemmas 3.5.12-3.5.15, we obtain

$$\sum_{\eta\in\widehat{\mathcal{N}}(\mathcal{S})} h_{\mathcal{P},\,\mathcal{Q}}(\eta)\phi_1(\eta) = \sum_{\boldsymbol{s}\in\mathcal{S}}\sum_{\eta\in\mathcal{N}(\boldsymbol{s})} h_{\mathcal{P},\,\mathcal{Q}}(\eta)\phi_1(\eta) = o(e^{-\Gamma\beta})$$
$$= o(e^{-\Gamma\beta}) + \sum_{\boldsymbol{s}\in\mathcal{S}}\Big[h_{\mathcal{P},\,\mathcal{Q}}(\boldsymbol{s})\sum_{\eta\in\mathcal{N}(\boldsymbol{s})}\phi_1(\eta)\Big],$$

where the second identity follows from Lemma 3.5.8 and the last part of Lemma 3.5.16. Inserting (3.91), (3.92) and (3.93) at the right-hand side, we obtain (3.87) and thus the proof is completed. □

3.6 Energy landscape analysis: cyclic dynamics

In the current and the following sections, we always assume that the process is the cyclic dynamics with $q \geq 3$.

3.6.1 Energy barrier: proof of Theorem 3.1.1

We denote by $\Gamma = \Gamma^{\mathrm{cyc}}$ the energy barrier of the cyclic dynamics. In this subsection, we prove Theorem 3.1.1, i.e., $\Gamma = 2K + 4$.

We first need to modify the canonical path of the MH dynamics defined in Definition 3.4.12 to get a corresponding object with respect to the cyclic dynamics, since the spin updates for the cyclic dynamics are more restrictive compared to that for the MH dynamics. To this end, we fix two spins $a,\, b \in \Omega$ and define the canonical paths from $\boldsymbol{a} \in \mathcal{S}$ to $\boldsymbol{b} \in \mathcal{S}$.

Definition 3.6.1 (Canonical paths of cyclic dynamics)**.** We denote by $r \in [\![1,\, q-1]\!]$ the unique integer which makes $b - a - r$ a multiple of q[2]. Then, a sequence of configurations $(\omega_n)_{n=0}^{rKL}$ is called a *canonical path* from $\boldsymbol{a}$ to $\boldsymbol{b}$

[2]Indeed, $r = b - a$ if $a < b$ and $r = q + b - a$ if $a > b$.

if there exists a backbone canonical path $(\widetilde{\omega}_m)_{m=0}^{KL}$ of the MH dynamics from $\boldsymbol{a}$ to $\boldsymbol{b}$ such that for each $m \in [\![0,\, KL-1]\!]$ and $i \in [\![0,\, r]\!]$,

$$\omega_{rm+i} = \tau_{x_m}^i \widetilde{\omega}_m,$$

where $\tau_x^i \sigma$ denotes the configuration obtained from σ by applying τ_x for i times, and where $x_m \in \Lambda$ is the site on which the spin update $\widetilde{\omega}_m \to \widetilde{\omega}_{m+1}$ occurs in the MH dynamics (i.e., $\widetilde{\omega}_{m+1} = \widetilde{\omega}_m^{x_m,\, b}$).

Remark 3.6.2. We note that the sequence $(\omega_n)_{n=0}^{rKL}$ is well defined. To this end, we need to verify that the definition agrees on each ω_{rm} for $m \in [\![1,\, KL-1]\!]$. Indeed, this is the case since

$$\omega_{rm} = \widetilde{\omega}_m = \tau_{x_{m-1}}^r \widetilde{\omega}_{m-1},$$

where the second identity holds since $\widetilde{\omega}_m = \widetilde{\omega}_{m-1}^{x_{m-1},\, b}$ and r is exactly the number of $\tau_{x_{m-1}}$ needed to be applied to $\widetilde{\omega}_{m-1}$ to obtain $\widetilde{\omega}_m$.

Now, we verify that a canonical path is indeed a path in the sense of the cyclic dynamics, and that it indeed achieves the desired energy level $2K+4$.

Lemma 3.6.3. *Suppose that $\omega = (\omega_n)_{n=0}^{rKL}$ is a canonical path from $\boldsymbol{a}$ to $\boldsymbol{b}$, where $r \in [\![1,\, q-1]\!]$ is as defined in Definition 3.6.1.*

(1) The sequence ω is indeed a path.

(2) Recall (3.7)*. Then, it holds that $\Phi_\omega = 2K+4$.*

Proof. We recall the notation of Definition 3.6.1 so that $(\widetilde{\omega}_m)_{m=0}^{KL}$ denotes the backbone MH-canonical path associated with the path ω with $\widetilde{\omega}_{m+1} = \widetilde{\omega}_m^{x_m,\, b}$.

(1) By definition, for each $m \in [\![0,\, KL-1]\!]$ and $i \in [\![0,\, r-1]\!]$, we can write $\omega_{rm+i} = \tau_{x_m}^i \widetilde{\omega}_m$ and $\omega_{rm+i+1} = \tau_{x_m}^{i+1} \widetilde{\omega}_m$. Thus, we have $\omega_{rm+i+1} = \tau_{x_m} \omega_{rm+i}$ which implies $r_\beta(\omega_{rm+i},\, \omega_{rm+i+1}) > 0$. This concludes the proof of part (1).

(2) We continue the notation of part (1), so that ω is induced from an MH-canonical path $(\widetilde{\omega}_m)_{m=0}^{KL}$. Recall from (3.5) and (3.7) that

$$\begin{aligned}\Phi_\omega &= \max_{n\in[\![0,\,rKL-1]\!]} H(\omega_n,\,\omega_{n+1})\\ &= \max_{m\in[\![0,\,KL-1]\!]}\max_{i\in[\![0,\,r-1]\!]} H(\omega_{rm+i},\,\omega_{rm+i+1}) = \max_{m\in[\![0,\,KL-1]\!]}\max_{c\in\Omega} H(\widetilde{\omega}_m^{x_m,\,c}).\end{aligned} \tag{3.95}$$

Then, by an elementary computation, we can explicitly calculate $\max_{c\in\Omega} H(\widetilde{\omega}_m^{x_m,\,c})$. Namely,

$$\max_{c\in\Omega} H(\widetilde{\omega}_m^{x_m,\,c}) = \begin{cases} 4 & \text{if } m=0 \text{ or } KL-1,\\ 2m+5 & \text{if } m\in[\![1,\,K-2]\!],\\ 2K+2 & \text{if } m=K-1 \text{ or } K(L-1),\\ 2K+3 & \text{if } m=Kv \text{ or } K(v+1)-1,\\ 2K+4 & \text{if } m\in[\![Kv+1,\,K(v+1)-2]\!],\\ 2KL-2m+3 & \text{if } m\in[\![K(L-1)+1,\,KL-2]\!],\end{cases} \tag{3.96}$$

where $v\in[\![1,\,L-2]\!]$. Here, the condition $q\geq 3$ is used in the fact that there always exists a third spin which is neither 1 nor 2. Therefore, by (3.95), we have $\Phi_\omega = 2K+4$ and thus conclude the proof. □

Now, we are ready to present the upper bound of the energy barrier.

Proposition 3.6.4. *For all $\boldsymbol{a}$, $\boldsymbol{b}\in\mathcal{S}$, we have $\Phi(\boldsymbol{a},\,\boldsymbol{b})\leq 2K+4$.*

Proof. The statement is direct from part (2) of Lemma 3.6.3. □

A combinatorial proof of the next result is postponed to Section 3.11.1.

Proposition 3.6.5. *For any path $\omega=(\omega_n)_{n=0}^{N}$ from $\boldsymbol{a}$ to $\breve{\boldsymbol{a}}$, we have $\Phi_\omega\geq 2K+4$.*

Finally, we are ready to prove Theorem 3.1.1.

Proof of Theorem 3.1.1. Let $\boldsymbol{a}, \boldsymbol{b} \in \mathcal{S}$. Proposition 3.6.4 implies that $\Phi(\boldsymbol{a}, \breve{\boldsymbol{a}}) \le \Phi(\boldsymbol{a}, \boldsymbol{b}) \le 2K+4$. On the other hand, Proposition 3.6.5 implies that $\Phi(\boldsymbol{a}, \breve{\boldsymbol{a}}) \ge 2K+4$. Combining this two, we obtain that $\Phi(\boldsymbol{a}, \breve{\boldsymbol{a}}) = \Phi(\boldsymbol{a}, \boldsymbol{b}) = 2K+4$. □

3.6.2 Neighborhoods

In this subsection, we explain the neighborhoods for the cyclic dynamics. Before proceeding to define them, we first check the following lemma which was obvious for the MH dynamics but not quite so for the cyclic dynamics.

Lemma 3.6.6. *For all $\sigma, \zeta \in \mathcal{X}$, we have $\Phi(\sigma, \zeta) = \Phi(\zeta, \sigma)$.*

Proof. Let $\omega = (\omega_n)_{n=0}^N : \sigma \to \zeta$ be an optimal path satisfying $\Phi_\omega = \Phi(\sigma, \zeta)$. Note that the reversed sequence $(\omega_N, \omega_{N-1}, \dots, \omega_0)$ is no longer a path with respect to the cyclic dynamics. However, since $\omega_{n+1} = \tau_x \omega_n$ for some $x \in \Lambda$, we can write $\omega_n = \tau_x^{q-1} \omega_{n+1}$ where $\tau_x^i \sigma$ denotes the configuration obtained from σ by applying τ_x for i times. Thus, we can replace (ω_{n+1}, ω_n) with

$$(\omega_{n+1}, \tau_x \omega_{n+1}, \tau_x^2 \omega_{n+1}, \dots, \tau_x^{q-1} \omega_{n+1}). \tag{3.97}$$

Replacing each (ω_{n+1}, ω_n) in $(\omega_N, \omega_{N-1}, \dots, \omega_0)$ in this manner, we get a path $\widetilde{\omega}$ (with respect to the cyclic dynamics) from ζ to σ. Since

$$H(\omega_{n+1}, \tau_x \omega_{n+1}) = \cdots = H(\tau_x^{q-2} \omega_{n+1}, \tau_x^{q-1} \omega_{n+1}) = H(\omega_n, \omega_{n+1}),$$

we immediately have that $\Phi_{\widetilde{\omega}} = \Phi_\omega = \Phi(\sigma, \zeta)$. Thus we have $\Phi(\zeta, \sigma) \le \Phi(\sigma, \zeta)$. Replacing the roles of σ and ζ, we also obtain the reversed inequality $\Phi(\zeta, \sigma) \ge \Phi(\sigma, \zeta)$ and thus we complete the proof. □

Next, we define the neighborhood $\mathcal{N}(\sigma)$, $\widehat{\mathcal{N}}(\sigma)$, $\mathcal{N}(\mathcal{P})$, and $\widehat{\mathcal{N}}(\mathcal{P})$ in the same manner with Definition 3.4.2. Then, since we also know that Γ is the energy barrier, Proposition 3.4.5 also holds for the cyclic dynamics. On the other hand, we now have to modify Lemma 3.4.6 in the following way.

Lemma 3.6.7. *Let $\sigma \in \mathcal{X}$ and let $\zeta_1 \in \widehat{\mathcal{N}}(\sigma)$, $\zeta_2 \notin \widehat{\mathcal{N}}(\sigma)$ and $\zeta_1 \sim \zeta_2$. Then, $H(\zeta_1,\, \zeta_2) > \Gamma$.*

Proof. Suppose to the contrary that $H(\zeta_1,\, \zeta_2) \le \Gamma$. Since $\zeta_1 \sim \zeta_2$, we have either $r_\beta(\zeta_1,\, \zeta_2) > 0$ or $r_\beta(\zeta_2,\, \zeta_1) > 0$. For the former case, we first find a path $\omega : \sigma \to \zeta_1$ such that $\Phi_\omega \le \Gamma$ (such a path exists since $\zeta_1 \in \widehat{\mathcal{N}}(\sigma)$). Then, we can concatenate the directed edge $(\zeta_1,\, \zeta_2)$ at the end of the path ω to form a path $\omega' : \sigma \to \zeta_2$ satisfying $\Phi_{\omega'} \le \Gamma$. This contradicts $\zeta_2 \notin \widehat{\mathcal{N}}(\sigma)$.

On the other hand, for the latter case, i.e., the case $r_\beta(\zeta_2,\, \zeta_1) > 0$, we find a path $\omega : \zeta_1 \to \sigma$ such that $\Phi_\omega \le \Gamma$, where such a path exists since $\Phi(\zeta_1,\, \sigma) = \Phi(\sigma,\, \zeta_1) \le \Gamma$ thanks to Lemma 3.6.6. Then, we concatenate the directed edge $(\zeta_2,\, \zeta_1)$ at the front of the path ω to form a path $\omega'' : \zeta_2 \to \sigma$ satisfying $\Phi_{\omega''} \le \Gamma$. Thus, we have $\Phi(\zeta_2,\, \sigma) \le \Gamma$ and again by Lemma 3.6.6 we obtain $\Phi(\sigma,\, \zeta_2) \le \Gamma$. This again contradicts $\zeta_2 \notin \widehat{\mathcal{N}}(\sigma)$. □

In turn, we modify the definition of the restricted neighborhoods given in Definition 3.4.7.

Definition 3.6.8 (Restricted neighborhood of cyclic dynamics)**.** Let $\mathcal{Q} \subseteq \mathcal{X}$. For $\sigma \in \mathcal{X} \setminus \mathcal{Q}$, we define $\widehat{\mathcal{N}}(\sigma;\, \mathcal{Q})$ as the collection of all ζ with $H(\zeta) \le \Gamma$ such that there exist $\omega_0,\, \omega_1,\, \dots,\, \omega_N \in \mathcal{X} \setminus \mathcal{Q}$ satisfying $\omega_0 = \sigma$, $\omega_N = \zeta$ and

$$\omega_n \sim \omega_{n+1} \text{ with } H(\omega_n,\, \omega_{n+1}) \le \Gamma \quad \text{for all } n \in [\![0,\, N-1]\!].$$

For $\mathcal{P} \subseteq \mathcal{X}$ disjoint with $\mathcal{Q}$, we define $\widehat{\mathcal{N}}(\mathcal{P};\, \mathcal{Q}) := \bigcup_{\sigma \in \mathcal{P}} \widehat{\mathcal{N}}(\sigma;\, \mathcal{Q})$.

Then, as we did in the analysis of the MH dynamics, we formulate the following lemma.

Lemma 3.6.9. *For all $\mathcal{P} \subseteq \mathcal{X}$, we have*

$$\widehat{\mathcal{N}}(\mathcal{P}) = \widehat{\mathcal{N}}(\mathcal{P};\, \emptyset).$$

Proof. One can notice that this identity is not as trivial as in the MH dynamics, since in Definition 3.6.8 ω_n and ω_{n+1} satisfy $\omega_n \sim \omega_{n+1}$ instead of $r_\beta(\omega_n, \omega_{n+1}) > 0$. Naturally, the proof presented here overcomes this difference.

We fix $\sigma \in \mathcal{P}$ and prove that $\widehat{\mathcal{N}}(\sigma) = \widehat{\mathcal{N}}(\sigma; \emptyset)$. Since $r_\beta(\zeta_1, \zeta_2) > 0$ implies $\zeta_1 \sim \zeta_2$ for any $\zeta_1, \zeta_2 \in \mathcal{X}$, and since $H(\zeta) \le \Gamma$ for all $\zeta \in \widehat{\mathcal{N}}(\sigma)$, it is immediate that $\widehat{\mathcal{N}}(\sigma) \subseteq \widehat{\mathcal{N}}(\sigma; \emptyset)$. Thus, it suffices to demonstrate that

$$\widehat{\mathcal{N}}(\sigma) \supseteq \widehat{\mathcal{N}}(\sigma; \emptyset).$$

Take an arbitrary $\zeta \in \widehat{\mathcal{N}}(\sigma; \emptyset)$, so that $H(\zeta) \le \Gamma$ and there exist $\omega_0, \ldots, \omega_N \in \mathcal{X}$ which satisfy $\omega_0 = \sigma$, $\omega_N = \zeta$, $\omega_n \sim \omega_{n+1}$ and $H(\omega_n, \omega_{n+1}) \le \Gamma$. We claim that for every $n \in [\![0, N]\!]$, there exists a path $\widetilde{\omega}^{(n)} : \omega_0 \to \omega_n$ such that $\Phi_{\widetilde{\omega}^{(n)}} \le \Gamma$. This claim concludes the proof by simply substituting $n = N$ and noting that $\omega_0 = \sigma$ and $\omega_N = \zeta$, which would then imply that $\zeta \in \widehat{\mathcal{N}}(\sigma)$ as desired.

It remains to prove the claim. We inductively construct a path $\widetilde{\omega}^{(n)} : \sigma = \omega_0 \to \omega_n$ as follows. First, set $\widetilde{\omega}_0 = \omega_0 = \sigma$ which immediately proves the case $n = 0$. Then, for each $n \in [\![0, N-1]\!]$ suppose that $\widetilde{\omega}^{(n)} : \omega_0 \to \omega_n$ is constructed. Note that $r_\beta(\omega_n, \omega_{n+1}) > 0$ or $r_\beta(\omega_{n+1}, \omega_n) > 0$. If the former case holds, then we simply define $\widetilde{\omega}^{(n+1)}$ by concatenating $\omega' = (\omega_n, \omega_{n+1})$ at the end of $\widetilde{\omega}^{(n)}$. If the latter case holds, we concatenate a detour path ω' of length $q-1$, as explained in (3.97), at the end of $\widetilde{\omega}^{(n)}$. In any case, $\widetilde{\omega}^{(n+1)}$ is indeed a path from ω_0 to ω_{n+1}, and moreover

$$\Phi_{\widetilde{\omega}^{(n+1)}} = \max\{\Phi_{\widetilde{\omega}^{(n)}}, \Phi_{\omega'}\} \le \Gamma,$$

where the inequality holds by the induction hypothesis and the fact that $\Phi_{\omega'} = H(\omega_n, \omega_{n+1}) \le \Gamma$ in both cases. Therefore, we conclude the proof of the lemma. $\square$

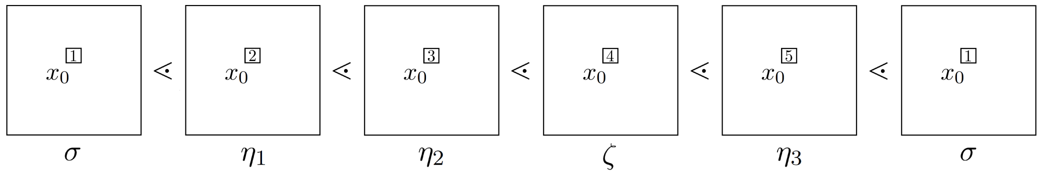


Figure 3.6: Example of an orbit. Here, $q = 5$. Suppose that $\zeta = \tau_{x_0}^3 \sigma$ with $\sigma(x_0) = 1$ and $\zeta(x_0) = 4$ as in the figure. Then, the orbit $\mathfrak{O}_{x_0}(\sigma) = \mathfrak{O}(\sigma, \zeta)$ consists of the presented five configurations. Note that $\sigma \lessdot \eta_1 \lessdot \eta_2 \lessdot \zeta \lessdot \eta_3 \lessdot \sigma$.

3.6.3 Orbits and typical configurations

Definition 3.6.10 (Orbits)**.** We refer to Figure 3.6.

(1) For $\sigma \in \mathcal{X}$ and $x \in \Lambda$, the *orbit* $\mathfrak{O}_x(\sigma)$ consists of q configurations which have same spin values with σ on $\Lambda \setminus \{x\}$, namely,

$$\mathfrak{O}_x(\sigma) := \{\sigma,\, \tau_x \sigma,\, \dots,\, \tau_x^{q-1}\sigma\}.$$

Note that for all $\zeta_1,\, \zeta_2 \in \mathfrak{O}_x(\sigma)$, we have $r_\beta^{\mathrm{MH}}(\zeta_1,\, \zeta_2) > 0$ where $r_\beta^{\mathrm{MH}}(\cdot,\, \cdot)$ denotes the transition rate of the MH dynamics.

(2) Fix $\sigma,\, \zeta \in \mathcal{X}$ such that $\zeta = \tau_{x_0}^i \sigma$ for some $x_0 \in \Lambda$ and $i \in [\![1,\, q-1]\!]$ (i.e., such that $r_\beta^{\mathrm{MH}}(\sigma,\, \zeta) > 0$). The *orbit* $\mathfrak{O}(\sigma,\, \zeta)$ containing σ and ζ is defined as

$$\mathfrak{O}(\sigma,\, \zeta) := \mathfrak{O}_{x_0}(\sigma) = \{\sigma,\, \tau_{x_0}\sigma,\, \dots,\, \tau_{x_0}^{q-1}\sigma\}.$$

It is clear that $\sigma,\, \zeta \in \mathfrak{O}(\sigma,\, \zeta)$, and that $\mathfrak{O}(\sigma,\, \zeta) = \mathfrak{O}(\zeta,\, \sigma)$.

(3) Following the above notation, for $\eta \in \mathfrak{O}(\sigma,\, \zeta) \setminus \{\sigma,\, \zeta\}$ so that $\eta = \tau_{x_0}^j \sigma$ with $j \in [\![1,\, q-1]\!] \setminus \{i\}$, we write $\sigma \lessdot \eta \lessdot \zeta$ if $j \in [\![1,\, i-1]\!]$ and $\zeta \lessdot \eta \lessdot \sigma$ if $j \in [\![i+1,\, q-1]\!]$. Intuitively, $\sigma \lessdot \eta \lessdot \zeta$ (resp. $\zeta \lessdot \eta \lessdot \sigma$) if one meets η during the series of i updates $\sigma \to \zeta$ (resp. $q - i$ updates $\zeta \to \sigma$).

(4) For a subset $\mathcal{P} \subseteq \mathcal{X}$, we define

$$\mathfrak{O}(\mathcal{P}) := \bigcup_{\sigma,\,\zeta\in\mathcal{P}:\,r_\beta^{\mathrm{MH}}(\sigma,\,\zeta)>0} \mathfrak{O}(\sigma,\,\zeta). \tag{3.98}$$

The notion of orbits is necessary since all spin updates in an orbit $\mathfrak{O}_x(\sigma)$ attain the same level of height. More precisely, noting that

$$\mathfrak{O}_x(\sigma) = \{\sigma,\,\tau_x\sigma,\,\dots,\,\tau_x^{q-1}\sigma\},$$

we have for all $i \in [\![0,\,q-1]\!]$ that (cf. (3.7))

$$H(\tau_x^i\sigma,\,\tau_x^{i+1}\sigma) = \max_{j\in[\![0,\,q-1]\!]} H(\tau_x^j\sigma) = \max_{\mathfrak{O}_x(\sigma)} H. \tag{3.99}$$

Now, we introduce typical configurations subjected to the cyclic dynamics.

Definition 3.6.11 (Typical configurations of cyclic dynamics)**.** Recall the sets $\mathcal{R}_v^{a,\,b}$ and $\mathcal{Q}_v^{a,\,b}$ defined in Definition 3.4.10.

(1) For each regular configuration $\sigma \in \mathcal{R}_v^{a,\,b}$, we write

$$\overline{\sigma} := \bigcup_{x\in\Lambda} \mathfrak{O}_x(\sigma). \tag{3.100}$$

Then for $v \in [\![2,\,L-2]\!]$, we define

$$\overline{\mathcal{R}}_v^{a,\,b} := \bigcup_{\sigma\in\mathcal{R}_v^{a,\,b}} \overline{\sigma} \quad \text{and} \quad \overline{\mathcal{R}}_v := \bigcup_{a,\,b\in\Omega} \overline{\mathcal{R}}_v^{a,\,b}.$$

(2) For $v \in [\![2,\,L-3]\!]$, we define

$$\overline{\mathcal{Q}}_v^{a,\,b} := \mathfrak{O}(\mathcal{Q}_v^{a,\,b}) \quad \text{and} \quad \overline{\mathcal{Q}}_v := \bigcup_{a,\,b\in\Omega} \overline{\mathcal{Q}}_v^{a,\,b}.$$

(3) The set of (cyclic) *bulk typical configurations* between two ground states

$\boldsymbol{a}$ and $\boldsymbol{b}$ is defined by

$$\overline{\mathcal{B}}^{a,\,b} := \bigcup_{v\in[\![2,\,L-3]\!]} \overline{\mathcal{Q}}_v^{a,\,b} \cup \bigcup_{v\in[\![2,\,L-2]\!]} \overline{\mathcal{R}}_v^{a,\,b}.$$

We write

$$\overline{\mathcal{B}}_\Gamma^{a,\,b} := \Big[\bigcup_{v\in[\![2,\,L-3]\!]} \overline{\mathcal{Q}}_v^{a,\,b} \Big] \setminus \Big[\bigcup_{v\in[\![2,\,L-2]\!]} \overline{\mathcal{R}}_v^{a,\,b} \Big].$$

Then, we naturally define $\overline{\mathcal{B}} := \bigcup_{a,\,b\in\Omega} \overline{\mathcal{B}}^{a,\,b}$ and $\overline{\mathcal{B}}_\Gamma := \bigcup_{a,\,b\in\Omega} \overline{\mathcal{B}}_\Gamma^{a,\,b}$.

(4) For $a \in \Omega$, we define the set of (cyclic) *edge typical configurations* associated with spin a as $\overline{\mathcal{E}}^a := \widehat{\mathcal{N}}(\boldsymbol{a};\, \overline{\mathcal{B}}_\Gamma)$. Then, we set $\overline{\mathcal{E}} := \bigcup_{a\in\Omega} \overline{\mathcal{E}}^a$.

Notation. For each regular configuration $\xi_{\ell,\,v}^{a,\,b} \in \mathcal{R}_v^{a,\,b}$, we simply denote by $\overline{\xi}_{\ell,\,v}^{a,\,b}$ the collection $\overline{\xi_{\ell,\,v}^{a,\,b}}$ (cf. (3.100)).

With this new definition of the typical configurations, we can construct the saddle structure for the cyclic dynamics as we did in Proposition 3.4.17 for the MH dynamics.

Proposition 3.6.12. *The following properties hold.*

(1) For spins $a,\, b \in \Omega$, we have $\overline{\mathcal{E}}^a \cap \overline{\mathcal{E}}^b = \emptyset$.

(2) For spins $a,\, b \in \Omega$, we have $\overline{\mathcal{E}}^a \cap \overline{\mathcal{B}}^{a,\,b} = \overline{\mathcal{R}}_2^{a,\,b}$.

(3) For three spins $a,\, b,\, c \in \Omega$, we have $\overline{\mathcal{E}}^a \cap \overline{\mathcal{B}}^{b,\,c} = \emptyset$.

(4) It holds that $\overline{\mathcal{E}} \cup \overline{\mathcal{B}} = \widehat{\mathcal{N}}(\mathcal{S})$.

A detailed proof of this proposition is given in Section 3.11.2.

3.6.4 Graph structure of edge typical configurations

Recall that in the investigation of the edge typical configurations of the MH dynamics, the graph structure (cf. Section 3.4.5) played a significant role. In this subsection, we explain the corresponding results for the cyclic dynamics.

Recall the sets $\mathcal{Z}^{a,\,b}$ and $\mathcal{Z}_\ell^{a,\,b}$ from (3.51) and Definition 3.4.19, respectively, and define

$$\overline{\mathcal{Z}}^{a,\,b} := \mathfrak{O}(\mathcal{Z}^{a,\,b}) \quad \text{and} \quad \overline{\mathcal{Z}}_\ell^{a,\,b} := \mathfrak{O}(\mathcal{Z}_\ell^{a,\,b})$$

so that, by the characterization of the set $\mathcal{Z}^{a,\,b}$ in Proposition 3.4.18, we can decompose the set $\overline{\mathcal{Z}}^{a,\,b}$ into (similarly with (3.54))

$$\overline{\mathcal{Z}}^{a,\,b} = \begin{cases} \bigcup_{\ell\in\mathbb{T}_L} \overline{\mathcal{Z}}_\ell^{a,\,b} & \text{if } K < L, \\ \bigcup_{\ell\in\mathbb{T}_L} \overline{\mathcal{Z}}_\ell^{a,\,b} \cup \bigcup_{\ell\in\mathbb{T}_L} \Theta(\overline{\mathcal{Z}}_\ell^{a,\,b}) & \text{if } K = L. \end{cases} \tag{3.101}$$

Now, we define

$$\overline{\mathcal{Z}}^{a} := \bigcup_{b\in\Omega\setminus\{a\}} \overline{\mathcal{Z}}^{a,\,b}, \quad \overline{\mathcal{R}}^{a} := \bigcup_{b\in\Omega\setminus\{a\}} \overline{\mathcal{R}}_2^{a,\,b}, \quad \text{and} \quad \overline{\mathcal{D}}^{a} := \widehat{\mathcal{N}}(\boldsymbol{a};\, \overline{\mathcal{Z}}^{a}), \tag{3.102}$$

so that we have the following representations of $\overline{\mathcal{E}}^{a}$:

$$\begin{aligned} \overline{\mathcal{E}}^{a} &= \overline{\mathcal{D}}^{a} \cup \overline{\mathcal{Z}}^{a} \cup \overline{\mathcal{R}}^{a} \\ &= \begin{cases} \overline{\mathcal{D}}^{a} \cup \bigcup_{b\neq a} \bigcup_{\ell\in\mathbb{T}_L} [\overline{\mathcal{Z}}_\ell^{a,\,b} \cup \overline{\xi}_{\ell,\,2}^{a,\,b}] & \text{if } K < L, \\ \overline{\mathcal{D}}^{a} \cup \bigcup_{b\neq a} \bigcup_{\ell\in\mathbb{T}_L} [\overline{\mathcal{Z}}_\ell^{a,\,b} \cup \overline{\xi}_{\ell,\,2}^{a,\,b}] \cup \bigcup_{b\neq a} \bigcup_{\ell\in\mathbb{T}_L} [\Theta(\overline{\mathcal{Z}}_\ell^{a,\,b}) \cup \Theta(\overline{\xi}_{\ell,\,2}^{a,\,b})] & \text{if } K = L. \end{cases} \end{aligned}$$

A crucial difference here with the structure explained in Section 3.4 is that $\overline{\mathcal{Z}}^{a,\,b}$ ***is no longer disjoint with both*** $\overline{\mathcal{D}}^{a}$ ***and*** $\overline{\mathcal{R}}^{a}$***.*** In turn, here we should define the graph structure on the $\overline{\mathcal{Z}}^{a,\,b}$ itself and may exclude the sets $\overline{\mathcal{D}}^{a}$ and

$\overline{\mathcal{R}}^a$.

Definition 3.6.13. We fix $a,\, b \in \Omega$ and $\ell \in \mathbb{T}_L$. Then, we introduce a graph structure and a Markov chain on $\overline{\mathcal{Z}}_\ell^{a,\,b}$.

- **(Graph)** We first assign a graph structure (cf. (3.72))

$$\overline{\mathscr{G}}_\ell^{a,\,b} = (\overline{\mathscr{V}}_\ell^{a,\,b},\, \overline{\mathscr{E}}_\ell^{a,\,b}) := (\overline{\mathcal{Z}}_\ell^{a,\,b},\, E(\overline{\mathcal{Z}}_\ell^{a,\,b})).$$

  By symmetry, the graph structure $\overline{\mathscr{G}}_\ell^{a,\,b}$ does not depend on $\ell \in \mathbb{T}_L$ (or the transpose operator Θ if $K = L$), while ***it indeed depends on*** $a,\, b \in \Omega$ (actually on the value of $b - a$ modulo q) unlike in Definition 3.4.21. Thus, we omit the subscript ℓ and simply write $\overline{\mathscr{G}}^{a,\,b} = (\overline{\mathscr{V}}^{a,\,b},\, \overline{\mathscr{E}}^{a,\,b})$ when no risk of confusion arises.

- **(Target sets)** We define two disjoint subsets of $\overline{\mathscr{V}}^{a,\,b} = \overline{\mathcal{Z}}_\ell^{a,\,b}$ as

$$\overline{\mathscr{A}}^{a,\,b} = \overline{\mathscr{A}}_\ell^{a,\,b} := \overline{\mathcal{Z}}_\ell^{a,\,b} \cap \mathcal{N}(\boldsymbol{a}) \quad \text{and} \quad \overline{\mathscr{B}}^{a,\,b} = \overline{\mathscr{B}}_\ell^{a,\,b} := \overline{\mathcal{Z}}_\ell^{a,\,b} \cap \xi_{\ell,\,2}^{a,\,b}.$$

- **(Markov chain)** We define a symmetric rate function $\bar{\mathfrak{r}}^{a,\,b} : \overline{\mathscr{V}}^{a,\,b} \times \overline{\mathscr{V}}^{a,\,b} \to [0,\, \infty)$ in such a way that

$$\bar{\mathfrak{r}}^{a,\,b}(\sigma,\, \sigma') = \begin{cases} 1 & \text{if } \{\sigma,\, \sigma'\} \in \overline{\mathscr{E}}^{a,\,b} \text{ and } r_\beta(\sigma,\, \sigma') > 0, \\ 0 & \text{otherwise.} \end{cases}$$

  Then, define $\{\overline{\mathfrak{Z}}^{a,\,b}(t)\}_{t \ge 0}$ as the continuous-time Markov chain on $\overline{\mathscr{V}}^{a,\,b}$ with rate $\bar{\mathfrak{r}}^{a,\,b}(\cdot,\, \cdot)$. The Markov chain $\overline{\mathfrak{Z}}^{a,\,b}(\cdot)$ is invariant under the uniform distribution on $\overline{\mathscr{V}}^{a,\,b}$, but it is not reversible with respect to it. We denote by $\overline{\mathfrak{Z}}^{*,\,a,\,b}(\cdot)$ the adjoint Markov process of $\overline{\mathfrak{Z}}^{a,\,b}(\cdot)$. Denote by $\bar{\mathfrak{f}}_{\cdot,\,\cdot}^{a,\,b}(\cdot)$, $\overline{\mathfrak{cap}}^{a,\,b}(\cdot,\, \cdot)$ and $\overline{\mathfrak{D}}^{a,\,b}$ the equilibrium potential, capacity and Dirichlet form with respect to the Markov chain $\overline{\mathfrak{Z}}^{a,\,b}(\cdot)$, respectively. In addition, we denote by $\bar{\mathfrak{f}}_{\cdot,\,\cdot}^{*,\,a,\,b}(\cdot)$ the equilibrium potential with respect to the adjoint process $\overline{\mathfrak{Z}}^{*,\,a,\,b}(\cdot)$. Finally, we abbreviate

$$\overline{\mathfrak{f}}^{a,\,b} := \overline{\mathfrak{f}}^{a,\,b}_{\overline{\mathscr{A}}^{a,\,b},\,\overline{\mathscr{B}}^{a,\,b}} \quad \text{and} \quad \overline{\mathfrak{f}}^{*,\,a,\,b} = \overline{\mathfrak{f}}^{*,\,a,\,b}_{\overline{\mathscr{A}}^{a,\,b},\,\overline{\mathscr{B}}^{a,\,b}}.$$

Edge constant

We are now ready to define the edge constant $\mathfrak{e}_0$ that appears in (3.30) for the cyclic dynamics. We first define

$$\overline{\mathfrak{e}}_0^{a,\,b} := \frac{1}{|\overline{\mathscr{V}}^{a,\,b}| \cdot \overline{\mathfrak{cap}}^{a,\,b}(\overline{\mathscr{A}}^{a,\,b},\,\overline{\mathscr{B}}^{a,\,b})}. \tag{3.103}$$

The next proposition not only provides the bound on this constant, but also proves that this constant, somewhat surprisingly, does not depend on the choices of a and b.

Proposition 3.6.14. *The value of $\overline{\mathfrak{e}}_0^{a,\,b}$ does not depend on $a,\,b \in \Omega$, and moreover we have $\overline{\mathfrak{e}}_0^{a,\,b} < 2$.*

A proof of this proposition is given in Section 3.11.2. Thanks to this proposition, we can finally define the constant $\mathfrak{e}_0$ that appears in (3.30) for the cyclic dynamics:

$$\mathfrak{e}_0 := \overline{\mathfrak{e}}_0^{a,\,b} \quad \text{for any } a,\,b \in \Omega. \tag{3.104}$$

3.7 Test functions: cyclic dynamics

Fix two non-empty, disjoint $\mathcal{P}$ and $\mathcal{Q}$ of $\mathcal{S}$. The purpose of this section is to construct two test functions $\widetilde{h},\,\widetilde{h}^* : \mathcal{X} \to \mathbb{R}$ that appear in Proposition 3.2.9, and then to prove that these two test functions satisfy three conditions (3.38), (3.39) and (3.40). We again use Notation 3.5.1 throughout this section.

Remark 3.7.1. Of course, the test functions of the cyclic dynamics are different to (in fact, slightly more complex than) those of the MH dynamics.

However, most parts of the proofs of three conditions (3.38), (3.39) and (3.40) are quite similar or identical, and thus we omit the details for such cases. *This reveals that the proof of the non-reversible model based on our strategy does not possess additional difficulty compared to the proof of the reversible model.*

3.7.1 Test functions

In this subsection, we construct test functions $\widetilde{h}$ and $\widetilde{h}^*$ which are approximations of the equilibrium potentials $h_{\mathcal{P},\,\mathcal{Q}}$ and $h^*_{\mathcal{P},\,\mathcal{Q}}$, respectively. The following definition is an analogue of Definition 3.5.2.

Definition 3.7.2 (Test functions)**.** We construct $\widetilde{h},\, \widetilde{h}^* : \mathcal{X} \to \mathbb{R}$. Notation 3.5.1 is valid throughout. We first assume that $K < L$.

(1) **Construction on $\overline{\mathcal{E}}$.** We first define the function $\widetilde{h}$.

- For $\sigma \in \overline{\mathcal{E}}^a$, we define $\widetilde{h}(\sigma)$ as

$$\begin{cases} 1 & \text{if } \sigma \in \overline{\mathcal{D}}^a \cup \overline{\mathcal{Z}}^{a,\,a'} \cup \overline{\mathcal{R}}_2^{a,\,a'},\ a' \neq a, \\ 1 - \dfrac{\mathfrak{e}}{\kappa}(1 - \bar{\mathfrak{f}}^{a,\,b}(\sigma)) & \text{if } \sigma \in \overline{\mathcal{Z}}^{a,\,b}, \\ 1 - \dfrac{|\mathcal{Q}|}{|\mathcal{P}| + |\mathcal{Q}|}\dfrac{\mathfrak{e}}{\kappa}(1 - \bar{\mathfrak{f}}^{a,\,c}(\sigma)) & \text{if } \sigma \in \overline{\mathcal{Z}}^{a,\,c}. \end{cases} \tag{3.105}$$

- For $\sigma \in \overline{\mathcal{E}}^b$, we define $\widetilde{h}(\sigma)$ as

$$\begin{cases} 0 & \text{if } \sigma \in \overline{\mathcal{D}}^b \cup \overline{\mathcal{Z}}^{b,\,b'} \cup \overline{\mathcal{R}}_2^{b,\,b'},\ b' \neq b, \\ \dfrac{\mathfrak{e}}{\kappa}(1 - \bar{\mathfrak{f}}^{b,\,a}(\sigma)) & \text{if } \sigma \in \overline{\mathcal{Z}}^{b,\,a}, \\ \dfrac{|\mathcal{P}|}{|\mathcal{P}| + |\mathcal{Q}|}\dfrac{\mathfrak{e}}{\kappa}(1 - \bar{\mathfrak{f}}^{b,\,c}(\sigma)) & \text{if } \sigma \in \overline{\mathcal{Z}}^{b,\,c}. \end{cases}$$

- For $\sigma \in \overline{\mathcal{E}}^{c}$, we define $\widetilde{h}(\sigma)$ as

$$\begin{cases} \dfrac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|} & \text{in } \overline{\mathcal{D}}^{c} \cup \overline{\mathcal{Z}}^{c,\,c'} \cup \overline{\mathcal{R}}_2^{c,\,c'}, \\ \dfrac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|} + \dfrac{|\mathcal{Q}|}{|\mathcal{P}|+|\mathcal{Q}|}\dfrac{\mathfrak{e}}{\kappa}(1-\overline{\mathfrak{f}}^{c,\,a}(\sigma)) & \text{in } \overline{\mathcal{Z}}^{c,\,a}, \\ \dfrac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|} - \dfrac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|}\dfrac{\mathfrak{e}}{\kappa}(1-\overline{\mathfrak{f}}^{c,\,b}(\sigma)) & \text{in } \overline{\mathcal{Z}}^{c,\,b}. \end{cases}$$

The function $\widetilde{h}^*$ is defined in the same way, except that we substitute $\overline{\mathfrak{f}}^{*,\,s,\,s'}$ in place of $\overline{\mathfrak{f}}^{s,\,s'}$ for all $s,\, s' \in S$ above.

(2) **Construction on $\overline{\mathcal{B}}$.** We first set

$$\widetilde{h} \equiv \widetilde{h}^* \equiv \begin{cases} 1 & \text{on } \overline{\mathcal{B}}^{a,\,a'}, \\ 0 & \text{on } \overline{\mathcal{B}}^{b,\,b'}, \\ \dfrac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|} & \text{on } \overline{\mathcal{B}}^{c,\,c'}. \end{cases}$$

Next, we consider the construction on $\overline{\mathcal{B}}^{a,\,b}$ which is carried out by ***interpolating the value from*** $\dfrac{\mathfrak{b}+\mathfrak{e}}{\kappa}$ ***at*** $\overline{\mathcal{R}}_2^{a,\,b}$ ***to*** $\dfrac{\mathfrak{e}}{\kappa}$ ***at*** $\overline{\mathcal{R}}_{L-2}^{a,\,b}$ in the following way.

- For $\sigma \in \overline{\mathcal{R}}_v^{a,\,b}$ with $v \in [\![2,\, L-2]\!]$, we set

$$\widetilde{h}(\sigma) = \widetilde{h}^*(\sigma) = \frac{1}{\kappa}\Big[\frac{L-2-v}{L-4}\mathfrak{b} + \mathfrak{e}\Big].$$

- For $\sigma \in \mathcal{Q}_v^{a,\,b}$ with $v \in [\![2,\, L-3]\!]$, where $\sigma = \xi_{\ell,\,v;\,k,\,h}^{a,\,b,\,\pm}$ for some $\ell \in \mathbb{T}_L$, $k \in \mathbb{T}_K$ and $h \in [\![1,\, K-1]\!]$, we set

$$\widetilde{h}(\sigma) = \widetilde{h}^*(\sigma) = \frac{1}{\kappa}\Big[\frac{(K-2)(L-2-v)-(h-1)}{(K-2)(L-4)}\mathfrak{b} + \mathfrak{e}\Big].$$

- For $\sigma \in \overline{\mathcal{Q}}_v^{a,\,b} \setminus \mathcal{Q}_v^{a,\,b}$ with $v \in [\![2,\, L{-}3]\!]$, we have $\sigma \in \mathfrak{O}(\xi_{\ell,\,v;\,k,\,h}^{a,\,b,\,\pm},\, \xi_{\ell,\,v;\,k,\,h+1}^{a,\,b,\,\pm})$

or $\sigma \in \mathfrak{O}(\xi^{a,\,b,\,\pm}_{\ell,\,v;\,k,\,h},\ \xi^{a,\,b,\,\pm}_{\ell,\,v;\,k-1,\,h+1})$ for some $\ell \in \mathbb{T}_L$, $k \in \mathbb{T}_K$ and $h \in [\![1,\ K-2]\!]$. For the former case, we set

$$\widetilde{h}(\sigma) := \begin{cases} \widetilde{h}(\xi^{a,\,b,\,\pm}_{\ell,\,v;\,k,\,h+1}) & \text{if } \xi^{a,\,b,\,\pm}_{\ell,\,v;\,k,\,h} \lessdot \sigma \lessdot \xi^{a,\,b,\,\pm}_{\ell,\,v;\,k,\,h+1}, \\ \widetilde{h}(\xi^{a,\,b,\,\pm}_{\ell,\,v;\,k,\,h}) & \text{if } \xi^{a,\,b,\,\pm}_{\ell,\,v;\,k,\,h+1} \lessdot \sigma \lessdot \xi^{a,\,b,\,\pm}_{\ell,\,v;\,k,\,h}. \end{cases} \tag{3.106}$$

The value $\widetilde{h}^*(\sigma)$ is defined in the reversed way. For the latter case, i.e., the case of $\sigma \in \mathfrak{O}(\xi^{a,\,b,\,\pm}_{\ell,\,v;\,k,\,h},\ \xi^{a,\,b,\,\pm}_{\ell,\,v;\,k-1,\,h+1})$, the functions are constructed in the same manner.

Similarly, constructions on $\overline{\mathcal{B}}^{a,\,c}$ and $\overline{\mathcal{B}}^{c,\,b}$ can be done by interpolating from $\frac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|} + \frac{|\mathcal{Q}|}{|\mathcal{P}|+|\mathcal{Q}|}\frac{\mathfrak{b}+\mathfrak{e}}{\kappa}$ to $\frac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|} + \frac{|\mathcal{Q}|}{|\mathcal{P}|+|\mathcal{Q}|}\frac{\mathfrak{e}}{\kappa}$, and from $\frac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|}\frac{\mathfrak{b}+\mathfrak{e}}{\kappa}$ to $\frac{|\mathcal{P}|}{|\mathcal{P}|+|\mathcal{Q}|}\frac{\mathfrak{e}}{\kappa}$, respectively.

(3) **Construction on $\mathcal{X} \setminus (\overline{\mathcal{E}} \cup \overline{\mathcal{B}})$.** We set $\widetilde{h} \equiv \widetilde{h}^* \equiv 1$ thereon.

For the case of $K = L$, for all $\sigma \in \overline{\mathcal{E}} \cup \overline{\mathcal{B}}$ considered in parts (1) and (2) above, we additionally set $\widetilde{h}(\Theta(\sigma)) := \widetilde{h}(\sigma)$ and $\widetilde{h}^*(\Theta(\sigma)) := \widetilde{h}^*(\sigma)$.

Remark 3.7.3. It is immediate from the definition that (3.40) holds for the test functions $\widetilde{h}$ and $\widetilde{h}^*$.

It remains to prove conditions (3.38) and (3.39). We only verify these two conditions for $\widetilde{h}$, since the verification for $\widetilde{h}^*$ is essentially identical (done by reversing the order of orbits). Let us first check (3.39) for $\widetilde{h}$.

Proposition 3.7.4. *The function* $\widetilde{h}$ *satisfies* (3.39)*, i.e.,*

$$D_\beta(\widetilde{h}) = (1 + o(1)) \cdot \frac{|\mathcal{P}||\mathcal{Q}|}{\kappa(|\mathcal{P}| + |\mathcal{Q}|)} e^{-\Gamma\beta}.$$

Proof. We decompose $D_\beta(\widetilde{h})$ as

$$\frac{1}{2}\Big[\sum_{\sigma,\,\zeta\in\mathcal{X}\setminus(\overline{\mathcal{E}}\cup\overline{\mathcal{B}})}+\sum_{\substack{\sigma\in\overline{\mathcal{E}}\cup\overline{\mathcal{B}},\,\zeta\in\mathcal{X}\setminus(\overline{\mathcal{E}}\cup\overline{\mathcal{B}})\text{ or}\\ \zeta\in\overline{\mathcal{E}}\cup\overline{\mathcal{B}},\,\sigma\in\mathcal{X}\setminus(\overline{\mathcal{E}}\cup\overline{\mathcal{B}})}}+\sum_{\sigma,\,\zeta\in\overline{\mathcal{E}}\cup\overline{\mathcal{B}}}\Big]\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)[\widetilde{h}(\zeta)-\widetilde{h}(\sigma)]^2,$$

where all summations are carried over pairs $\sigma,\,\zeta$ such that $\sigma\sim\zeta$. Since $\widetilde{h}$ is defined as constant on $\mathcal{X}\setminus(\overline{\mathcal{E}}\cup\overline{\mathcal{B}})$, the first summation is 0. For the second summation, by (3.6), Lemma 3.6.7 and Proposition 3.6.12-(4), we have $\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)=O(e^{-(\Gamma+1)\beta})=o(e^{-\Gamma\beta})$ and thus this summation is negligible. It only remains to prove

$$\frac{1}{2}\sum_{\sigma,\,\zeta\in\overline{\mathcal{E}}\cup\overline{\mathcal{B}}}\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)[\widetilde{h}(\zeta)-\widetilde{h}(\sigma)]^2=(1+o(1))\cdot\frac{|\mathcal{P}||\mathcal{Q}|}{\kappa(|\mathcal{P}|+|\mathcal{Q}|)}e^{-\Gamma\beta}.$$

The proof of this estimate is essentially the same with the corresponding part in the proof of Proposition 3.5.6, and we omit the detail. □

3.7.2 Proof of H^1-approximation

In this section, we prove (3.38) for $\widetilde{h}$ and thus complete the proof of Proposition 3.2.9. The storyline is identical to the one given in Section 3.5.3. Note that the computation carried out in (3.82) is valid without reversibility and thus we have

$$D_\beta(h_{\mathcal{P},\,\mathcal{Q}}-\widetilde{h})=D_\beta(\widetilde{h})-\sum_{\sigma\in\mathcal{X}}h_{\mathcal{P},\,\mathcal{Q}}(\sigma)(-\mathcal{L}_\beta\widetilde{h})(\sigma)\mu_\beta(\sigma).$$

Hence, as in (3.83), it suffices to prove that

$$\sum_{\sigma\in\mathcal{X}}h_{\mathcal{P},\,\mathcal{Q}}(\sigma)\sum_{\zeta\in\mathcal{X}}\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)[\widetilde{h}(\sigma)-\widetilde{h}(\zeta)]=(1+o(1))\cdot\frac{|\mathcal{P}||\mathcal{Q}|}{\kappa(|\mathcal{P}|+|\mathcal{Q}|)}e^{-\Gamma\beta}. \tag{3.107}$$

To this end, we first demonstrate that the equilibrium potential $h_{\mathcal{P},\,\mathcal{Q}}$ is nearly constant on each neighborhood $\mathcal{N}(\sigma)$ for any $\sigma \in \mathcal{X}$, which is an analogue of Lemma 3.5.8.

Lemma 3.7.5. *For all $\sigma \in \mathcal{X}$, it holds that* $\max_{\zeta\in\mathcal{N}(\sigma)} \big|h_{\mathcal{P},\,\mathcal{Q}}(\zeta) - h_{\mathcal{P},\,\mathcal{Q}}(\sigma)\big| = o(1)$.

Note that the argument given in Lemma 3.5.8 relies on the reversibility only because of the cited result [70, Theorem 3.2-(iii)]. Thus, in this lemma, it suffices to replace this reference with [27, Propositions 3.10 and 3.18-(3)] which is a non-reversible generalization of [70, Theorem 3.2-(iii)]. In addition, we emphasize that the proof outlined in Remark 3.5.9 can also be applied to this lemma as well.

We now start to estimate the left-hand side of (3.107). As done in Section 3.5.3, write

$$\phi(\sigma) := \sum_{\zeta\in\mathcal{X}} \mu_\beta(\sigma) r_\beta(\sigma,\,\zeta)[\widetilde{h}(\sigma) - \widetilde{h}(\zeta)], \tag{3.108}$$

so that we can rewrite (3.107) as

$$\sum_{\sigma\in\mathcal{X}} h_{\mathcal{P},\,\mathcal{Q}}(\sigma)\phi(\sigma) = (1+o(1)) \cdot \frac{|\mathcal{P}||\mathcal{Q}|}{\kappa(|\mathcal{P}|+|\mathcal{Q}|)} e^{-\Gamma\beta}. \tag{3.109}$$

The following lemma can be proved in the same manner with Lemma 3.5.10; it suffices to use Lemma 3.6.7 instead of Lemma 3.4.6.

Lemma 3.7.6. *For all $\sigma \in \mathcal{X} \setminus \widehat{\mathcal{N}}(\mathcal{S})$, we have $\phi(\sigma) = o(e^{-\Gamma\beta})$.*

Next, we decompose $\phi = \phi_1 + \phi_2$ where for $\sigma \in \widehat{\mathcal{N}}(\mathcal{S})$,

$$\phi_1(\sigma) := \sum_{\zeta\in\widehat{\mathcal{N}}(\mathcal{S})} \mu_\beta(\sigma) r_\beta(\sigma,\,\zeta)[\widetilde{h}(\sigma) - \widetilde{h}(\zeta)],$$
$$\phi_2(\sigma) := \sum_{\zeta\notin\widehat{\mathcal{N}}(\mathcal{S})} \mu_\beta(\sigma) r_\beta(\sigma,\,\zeta)[\widetilde{h}(\sigma) - \widetilde{h}(\zeta)].$$

Next, we can show that ϕ_2 is negligible as in Lemma 3.5.11.

Lemma 3.7.7. *For all $\sigma \in \widehat{\mathcal{N}}(\mathcal{S})$, we have $\phi_2(\sigma) = o(e^{-\Gamma\beta})$.*

This can be proved in the same manner with Lemma 3.5.11. In addition to the replacement of Lemma 3.4.6 with Lemma 3.6.7, we need to replace Proposition 3.4.17-(4) with Proposition 3.6.12-(4). Summing up, instead of (3.109), it suffices to show that

$$\sum_{\sigma \in \widehat{\mathcal{N}}(\mathcal{S})} h_{\mathcal{P},\,\mathcal{Q}}(\sigma)\phi_1(\sigma) = (1+o(1)) \cdot \frac{|\mathcal{P}||\mathcal{Q}|}{\kappa(|\mathcal{P}|+|\mathcal{Q}|)} e^{-\Gamma\beta}. \tag{3.110}$$

Next, we investigate ϕ_1 in several lemmas. Let us first consider ϕ_1 on the bulk typical configurations.

Lemma 3.7.8. *For each $v \in [\![2,\, L-3]\!]$ and $a,\, b \in \Omega$, it holds that $\phi_1 \equiv 0$ on $\overline{\mathcal{Q}}_v^{a,\,b} \setminus (\overline{\mathcal{R}}_v^{a,\,b} \cup \overline{\mathcal{R}}_{v+1}^{a,\,b})$.*

Proof. We only prove that $\phi_1(\sigma) = 0$ for all $\sigma \in \mathfrak{O}(\xi_{\ell,\,v;\,k,\,h}^{a,\,b,\,+},\, \xi_{\ell,\,v;\,k,\,h+1}^{a,\,b,\,+})$ with $v \in [\![2,\, L-3]\!]$ and $h \in [\![1,\, K-2]\!]$, since the other orbits can be handled in the same way. Write $\xi_{\ell,\,v;\,k,\,h+1}^{a,\,b,\,+} = \tau_x^m \xi_{\ell,\,v;\,k,\,h}^{a,\,b,\,+}$ for some $x \in \Lambda$ and $m \in [\![1,\, q-1]\!]$[3], so that we can write

$$\sigma = \tau_x^i \xi_{\ell,\,v;\,k,\,h}^{a,\,b,\,+} \quad \text{for some } i \in [\![0,\, q-1]\!].$$

(Case 1: $i \neq 0,\, m$) We immediately have $\widetilde{h}(\tau_x\sigma) = \widetilde{h}(\sigma)$ by definition and thus

$$\phi_1(\sigma) = \mu_\beta(\sigma) r_\beta(\sigma,\, \tau_x\sigma)[\widetilde{h}(\sigma) - \widetilde{h}(\tau_x\sigma)] = 0,$$

where $\phi_1(\sigma)$ consists of only one term since we have $\tau_y\sigma \notin \widehat{\mathcal{N}}(\mathcal{S})$ for all $y \in \Lambda \setminus \{x\}$.

(Case 2: $\sigma = \xi_{\ell,\,v;\,k,\,h}^{a,\,b,\,+}$, so that $h \neq 1$ since $\sigma \notin \overline{\mathcal{R}}_v^{a,\,b}$) In this case, there are four updates (that does not exceed the energy level Γ) from σ along the orbits $\mathfrak{O}(\xi_{\ell,\,v;\,k,\,h}^{a,\,b,\,+},\, \xi_{\ell,\,v;\,k,\,h+1}^{a,\,b,\,+})$, $\mathfrak{O}(\xi_{\ell,\,v;\,k,\,h}^{a,\,b,\,+},\, \xi_{\ell,\,v;\,k-1,\,h+1}^{a,\,b,\,+})$, $\mathfrak{O}(\xi_{\ell,\,v;\,k,\,h-1}^{a,\,b,\,+},\, \xi_{\ell,\,v;\,k,\,h}^{a,\,b,\,+})$ and

[3] Actually, $m = b - a$ or $m = q + b - a$.

$\mathfrak{O}(\xi^{a,\,b,\,+}_{\ell,\,v;\,k+1,\,h-1},\,\xi^{a,\,b,\,+}_{\ell,\,v;\,k,\,h})$. By a direct computation with the definition of $\widetilde{h}$, we can check that for all these updates, which we denote as $\tau_{x_1},\,\tau_{x_2},\,\tau_{x_3},\,\tau_{x_4}$ respectively, we have

$$\mu_\beta(\sigma)r_\beta(\sigma,\,\tau_{x_i}\sigma)[\widetilde{h}(\sigma)-\widetilde{h}(\tau_{x_i}\sigma)] = \pm\frac{e^{-\Gamma\beta}}{Z_\beta}\cdot\frac{\mathfrak{b}}{\kappa(K-2)(L-4)} \quad \text{for } i \in [\![1,\,4]\!], \tag{3.111}$$

where the sign is plus for $i \in \{1,\,2\}$ and minus for $i \in \{3,\,4\}$. Therefore,

$$\begin{aligned}\phi_1(\sigma) &= \sum_{i=1}^{4}\mu_\beta(\sigma)r_\beta(\sigma,\,\tau_{x_i}\sigma)[\widetilde{h}(\sigma)-\widetilde{h}(\tau_{x_i}\sigma)]\\ &= \frac{e^{-\Gamma\beta}}{Z_\beta}\cdot\frac{\mathfrak{b}}{\kappa(K-2)(L-4)}\cdot(1+1-1-1)=0.\end{aligned}$$

(Case 3: $\sigma = \xi^{a,\,b,\,+}_{\ell,\,v;\,k,\,h+1}$, so that $h \neq K-2$ since $\sigma \notin \overline{\mathcal{R}}^{a,\,b}_{v+1}$) This case can be handled in the same manner with **(Case 2)**. □

Next, we handle $\overline{\mathcal{R}}^{a,\,b}_{v}$ for $a,\,b \in \Omega$ and $v \in [\![2,\,L-2]\!]$.

Lemma 3.7.9. *For each $v \in [\![2,\,L-2]\!]$ and $a,\,b \in \Omega$, it holds that*

$$\sum_{\sigma \in \overline{\mathcal{R}}^{a,\,b}_{v}} \phi_1(\sigma) = 0. \tag{3.112}$$

Moreover, there exists a constant $C > 0$ such that $|\phi_1(\sigma)| \le Ce^{-\Gamma\beta}$ for all $\sigma \in \overline{\mathcal{R}}^{a,\,b}_{v}$.

Proof. Let us first assume that $v \neq 2,\,L-2$. Recall that $\overline{\mathcal{R}}^{a,\,b}_{v} = \bigcup_{\sigma\in\mathcal{R}^{a,\,b}_{v}}\overline{\sigma}$. By the definition of $\widetilde{h}$, it holds that the function ϕ_1 vanishes outside

$$\bigcup_{\ell\in\mathbb{T}_L}\bigcup_{k\in\mathbb{T}_K}\{\xi^{a,\,b,\,+}_{\ell,\,v;\,k,\,1},\,\xi^{a,\,b,\,-}_{\ell,\,v;\,k,\,1},\,\xi^{a,\,b,\,+}_{\ell,\,v-1;\,k,\,K-1},\,\xi^{a,\,b,\,-}_{\ell+1,\,v-1;\,k,\,K-1}\}.$$

Thus, to prove (3.112), it suffices to verify that for all $\ell \in \mathbb{T}_L$ and $k \in \mathbb{T}_K$,

$$\phi_1(\xi^{a,\,b,\,+}_{\ell,\,v;\,k,\,1}) + \phi_1(\xi^{a,\,b,\,-}_{\ell,\,v;\,k,\,1}) + \phi_1(\xi^{a,\,b,\,+}_{\ell,\,v-1;\,k,\,K-1}) + \phi_1(\xi^{a,\,b,\,-}_{\ell+1,\,v-1;\,k,\,K-1}) = 0. \quad (3.113)$$

By definition of $\widetilde{h}$ on the bulk typical configurations, we have

$$\phi_1(\xi^{a,\,b,\,+}_{\ell,\,v;\,k,\,1}) = \phi_1(\xi^{a,\,b,\,-}_{\ell,\,v;\,k,\,1}) = \frac{e^{-\Gamma\beta}}{Z_\beta} \cdot \frac{\mathfrak{b}}{\kappa(K-2)(L-4)},$$
$$\phi_1(\xi^{a,\,b,\,+}_{\ell,\,v-1;\,k,\,K-1}) = \phi_1(\xi^{a,\,b,\,-}_{\ell+1,\,v-1;\,k,\,K-1}) = -\frac{e^{-\Gamma\beta}}{Z_\beta} \cdot \frac{\mathfrak{b}}{\kappa(K-2)(L-4)}.$$

Thus, (3.113) is a direct consequence of this computation. Moreover, we can also verify the second statement from this computation as well via Theorem 3.0.1 and (3.29).

The proof of cases $v = 2,\, L-2$ is a notational modification of that of Lemma 3.5.13, and thus we omit the details. □

Now, we consider the function ϕ_1 at the edge typical configurations.

Lemma 3.7.10. *We have $\phi_1(\sigma) = 0$ for*

(1) $\sigma \in (\overline{\mathcal{Z}}^{a,\,b} \cup \overline{\mathcal{Z}}^{a,\,c} \cup \overline{\mathcal{Z}}^{c,\,b}) \setminus \mathcal{N}(\mathcal{S})$ (cf. Notation 3.5.1) and

(2) $\sigma \in \overline{\mathcal{D}}^{s} \setminus \mathcal{N}(\boldsymbol{s})$ with $s \in S$.

Proof. Part (1) can be proved in the same way as we proved Lemma 3.5.14. On the other hand, part (2) directly follows from the fact that $\widetilde{h}$ is defined as constant on $\overline{\mathcal{D}}^{s}$ (cf. Definition 3.7.2-(1)). □

It remains to investigate ϕ_1 on the sets $\mathcal{N}(\boldsymbol{s})$, $\boldsymbol{s} \in \mathcal{S}$.

Lemma 3.7.11. *For* $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}$ *chosen according to Notation 3.5.1, we have*

$$\sum_{\sigma\in\mathcal{N}(\boldsymbol{a})}\phi_1(\sigma) = (1+o(1))\cdot\frac{|\mathcal{Q}|}{\kappa(|\mathcal{P}|+|\mathcal{Q}|)}e^{-\Gamma\beta}, \tag{3.114}$$

$$\sum_{\sigma\in\mathcal{N}(\boldsymbol{b})}\phi_1(\sigma) = -(1+o(1))\cdot\frac{|\mathcal{P}|}{\kappa(|\mathcal{P}|+|\mathcal{Q}|)}e^{-\Gamma\beta}, \tag{3.115}$$

$$\sum_{\sigma\in\mathcal{N}(\boldsymbol{c})}\phi_1(\sigma) = o(e^{-\Gamma\beta}). \tag{3.116}$$

Moreover, there exists a positive constant C *so that for all* $\sigma\in\mathcal{N}(\mathcal{S})$, $|\phi_1(\sigma)|\le Ce^{-\Gamma\beta}$.

Proof. The proof of this lemma is identical to that of Lemma 3.5.16 and we omit the detail. □

Finally, we are ready to prove Proposition 3.2.9 for the cyclic dynamics.

Proof of Proposition 3.2.9 for the cyclic dynamics. By Remark 3.7.3 and Proposition 3.7.4, if suffices to verify (3.38). We explained above that (3.38) follows if we can prove (3.110). By Lemmas 3.7.8 and 3.7.10, we have

$$\begin{aligned}\sum_{\sigma\in\widehat{\mathcal{N}}(\mathcal{S})}h_{\mathcal{P},\,\mathcal{Q}}(\sigma)\phi_1(\sigma) &= o(e^{-\Gamma\beta})+\sum_{s\in S}\sum_{\sigma\in\mathcal{N}(\boldsymbol{s})}h_{\mathcal{P},\,\mathcal{Q}}(\sigma)\phi_1(\sigma)\\ &= o(e^{-\Gamma\beta})+\sum_{s\in S}\Big[h_{\mathcal{P},\,\mathcal{Q}}(\boldsymbol{s})\sum_{\sigma\in\mathcal{N}(\boldsymbol{s})}\phi_1(\sigma)\Big],\end{aligned}$$

where the first identity follows from Lemma 3.7.5 and the last part of Lemma 3.7.9, and where the second identity follows from Lemma 3.7.5 and the last part of Lemma 3.7.11. Now, inserting (3.114), (3.115) and (3.116) completes the proof. □

3.8 Decomposition lemma

Before proceeding to the proofs of results stated in Sections 3.4 and 3.6, we provide a decomposition of neighborhoods which is crucially used in later discussions. Let $\mathcal{P}_1$, $\mathcal{P}_2$, and $\mathcal{Q}$ be pairwise disjoint subsets of $\mathcal{X}$. Then, by the definition of neighborhoods, we immediately have

$$\widehat{\mathcal{N}}(\mathcal{P}_1 \cup \mathcal{P}_2;\ \mathcal{Q}) = \widehat{\mathcal{N}}(\mathcal{P}_1;\ \mathcal{Q}) \cup \widehat{\mathcal{N}}(\mathcal{P}_2;\ \mathcal{Q}). \tag{3.117}$$

The following lemma is a refinement of this decomposition. Note that the proof works for both the MH and cyclic dynamics.

Lemma 3.8.1. *Suppose that $\mathcal{P}_1$, $\mathcal{P}_2$ and $\mathcal{Q}$ are pairwise disjoint subsets of $\mathcal{X}$. Then, it holds that*

$$\widehat{\mathcal{N}}(\mathcal{P}_1 \cup \mathcal{P}_2;\ \mathcal{Q}) = \widehat{\mathcal{N}}(\mathcal{P}_1;\ \mathcal{P}_2 \cup \mathcal{Q}) \cup \widehat{\mathcal{N}}(\mathcal{P}_2;\ \mathcal{P}_1 \cup \mathcal{Q}).$$

In particular, if $\mathcal{Q} = \emptyset$ then we have

$$\widehat{\mathcal{N}}(\mathcal{P}_1 \cup \mathcal{P}_2) = \widehat{\mathcal{N}}(\mathcal{P}_1;\ \mathcal{P}_2) \cup \widehat{\mathcal{N}}(\mathcal{P}_2;\ \mathcal{P}_1).$$

Proof. First, we consider the first identity. By (3.117) and the definition of restricted neighborhoods, we immediately have that

$$\widehat{\mathcal{N}}(\mathcal{P}_1 \cup \mathcal{P}_2;\ \mathcal{Q}) \supseteq \widehat{\mathcal{N}}(\mathcal{P}_1;\ \mathcal{P}_2 \cup \mathcal{Q}) \cup \widehat{\mathcal{N}}(\mathcal{P}_2;\ \mathcal{P}_1 \cup \mathcal{Q}). \tag{3.118}$$

To prove the reversed inclusion, we assume to the contrary that there exists $\sigma \in \mathcal{X}$ such that

$$\sigma \in \widehat{\mathcal{N}}(\mathcal{P}_1 \cup \mathcal{P}_2;\ \mathcal{Q}) \setminus \big[\widehat{\mathcal{N}}(\mathcal{P}_1;\ \mathcal{P}_2 \cup \mathcal{Q}) \cup \widehat{\mathcal{N}}(\mathcal{P}_2;\ \mathcal{P}_1 \cup \mathcal{Q})\big]. \tag{3.119}$$

By (3.117), we may assume without loss of generality that

$$\sigma \in \widehat{\mathcal{N}}(\mathcal{P}_1;\ \mathcal{Q}) \setminus \big[\widehat{\mathcal{N}}(\mathcal{P}_1;\ \mathcal{P}_2 \cup \mathcal{Q}) \cup \widehat{\mathcal{N}}(\mathcal{P}_2;\ \mathcal{P}_1 \cup \mathcal{Q})\big]. \tag{3.120}$$

Note that $\sigma \in \widehat{\mathcal{N}}(\mathcal{P}_1;\,\mathcal{Q})$ implies automatically that $H(\sigma) \le \Gamma$. Then, the fact that $\sigma \notin \widehat{\mathcal{N}}(\mathcal{P}_1;\,\mathcal{P}_2 \cup \mathcal{Q}) \cup \widehat{\mathcal{N}}(\mathcal{P}_2;\,\mathcal{P}_1 \cup \mathcal{Q})$ implies that we readily have $\sigma \notin \mathcal{P}_1 \cup \mathcal{P}_2$.

Now since $\sigma \in \widehat{\mathcal{N}}(\mathcal{P}_1;\,\mathcal{Q})$, we can find $(\omega_n)_{n=0}^N$ in $\mathcal{X} \setminus \mathcal{Q}$ with $N \ge 1$ such that $\omega_0 \in \mathcal{P}_1$, $\omega_N = \sigma$, $\omega_n \sim \omega_{n+1}$ and $H(\omega_n,\,\omega_{n+1}) \le \Gamma$. Let us assume that N is the smallest of all such sequences. If $\omega_n \notin \mathcal{P}_2$ for all $n \in [\![1,\,N-1]\!]$, then $(\omega_n)_{n=0}^N \subseteq \mathcal{X} \setminus (\mathcal{P}_2 \cup \mathcal{Q})$ so that we get a contradiction since we must have $\sigma \notin \widehat{\mathcal{N}}(\mathcal{P}_1;\,\mathcal{P}_2 \cup \mathcal{Q})$. Therefore, we can find $n_0 \in [\![1,\,N-1]\!]$ such that $\omega_{n_0} \in \mathcal{P}_2$. Since we have $\omega_n \notin \mathcal{P}_1$ for all $n \in [\![1,\,N]\!]$ by the minimality of the length N, we can notice that $(\omega_n)_{n=n_0}^N \subseteq (\mathcal{P}_1 \cup \mathcal{Q})^c$ and thus $\sigma \in \widehat{\mathcal{N}}(\mathcal{P}_2;\,\mathcal{P}_1 \cup \mathcal{Q})$. Thus, we get a contradiction to (3.120). Hence, we have proved the reversed inclusion of (3.118) and the proof of the first identity is completed.

Finally, the second identity of the lemma is immediate from Lemmas 3.4.6 and 3.6.7. □

3.9 Proof of results in Section 3.4

3.9.1 Preliminaries

First, we give in Proposition 3.9.3 a characterization of configurations which have energy less than Γ. For $a \in \Omega$, we write

$$\|\eta\|_a = \sum_{x \in \Lambda} \mathbb{1}\{\eta(x) = a\}, \tag{3.121}$$

which denotes the number of sites in η with spin a. We recall some notation from [69, Section 2.1].

Notation 3.9.1. We refer to Figure 3.7 for an illustration of the notions introduced below.

- For a configuration $\eta \in \mathcal{X}$, a *bridge*, which is a *horizontal* or *vertical bridge*, is a row or column, respectively, in which all spins are the same.

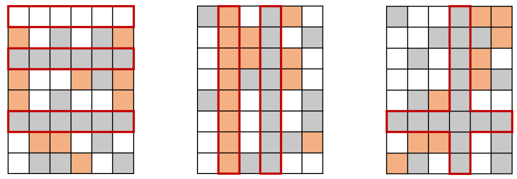


Figure 3.7: Figures for Notation 3.9.1. Configurations η_1, η_2 and η_3 have horizontal bridges, vertical bridges and a cross, respectively. Let $S = \{1, 2, 3\}$ and let white, gray and orange boxes denote sites with spin 1, 2 and 3, respectively. Then e.g., for configuration η_1, it holds that $B_1(\eta_1) = 1$, $B_2(\eta_1) = 2$, $B_3(\eta_1) = 0$, $\Delta H_{r_1}(\eta_1) = 5$ and $\Delta H_{c_2}(\eta_1) = 6$. Note that one should be careful about the periodic boundary condition when computing $\Delta H_{r_1}(\eta_1)$ and $\Delta H_{c_2}(\eta_1)$.

If a bridge consists of spin $a \in \Omega$, we call this bridge an a-bridge. Then, we denote by $B_a(\eta)$ the number of a-bridges with respect to η.

- In a configuration η, a *cross* is the union of a horizontal bridge and a vertical bridge. A cross consisting of spin $a \in \Omega$ is called an a-cross. Moreover, η is called *cross-free* if it does not have a cross.

- We denote by $r_1, \dots, r_L$ the rows and $c_1, \dots, c_K$ the columns of $\Lambda = \mathbb{T}_K \times \mathbb{T}_L$, starting from the lowest and the leftmost one, respectively. For $v \in [\![1, L]\!]$, $h \in [\![1, K]\!]$ and $\eta \in \mathcal{X}$, we define

$$\Delta H_{r_v}(\eta) = \sum_{\{x, y\} \subset r_v : x \sim y} \mathbb{1}\{\eta(x) \neq \eta(y)\}$$

and

$$\Delta H_{c_h}(\eta) = \sum_{\{x, y\} \subset c_h : x \sim y} \mathbb{1}\{\eta(x) \neq \eta(y)\},$$

so that

$$H(\eta) = \sum_{v \in [\![1, L]\!]} \Delta H_{r_v}(\eta) + \sum_{h \in [\![1, K]\!]} \Delta H_{c_h}(\eta). \tag{3.122}$$

An edge belonging to a row (resp. column) is called a horizontal (resp. vertical) edge.

The following lower bound for the Hamiltonian is useful.

Lemma 3.9.2. *It holds that*

$$H(\eta) \geq 2\Big[K + L - \sum_{a \in \Omega} B_a(\eta)\Big].$$

Proof. It follows directly from (3.122) since $\Delta H_{r_v}(\eta) \geq 2$ (resp. $\Delta H_{c_h}(\eta) \geq 2$) if r_v (resp. c_h) is not a bridge. □

Now, we classify the configurations with low energy.

Proposition 3.9.3. *Suppose that $\eta \in \mathcal{X}$ satisfies $H(\eta) < \Gamma$. Then, η satisfies exactly one of the following types.*

- **(L1)** *There exist $a,\, b \in \Omega$ and $v \in [\![2,\, L-2]\!]$ such that $\eta \in \mathcal{R}_v^{a,\,b}$. Here, $\mathcal{N}(\eta)$ is a singleton, i.e., $\mathcal{N}(\eta) = \{\eta\}$.*
- **(L2)** *There exist $a,\, b \in \Omega$ such that $\eta \in \mathcal{R}_1^{a,\,b}$. In this case, $\mathcal{N}(\eta) = \mathcal{N}(\boldsymbol{a})$.*
- **(L3)** *For some $a \in \Omega$, η has an a-cross. Then, $\mathcal{N}(\eta) = \mathcal{N}(\boldsymbol{a})$ and*

$$\sum_{b \neq a} \|\eta\|_b \leq \frac{H(\eta)^2}{16} \leq \frac{(2K+1)^2}{16}. \tag{3.123}$$

Proof. Fix $\eta \in \mathcal{X}$ with $H(\eta) < \Gamma = 2K+2$. It is obvious that no configuration can be of more than one type. Thus, we first show that η falls into exactly one among three categories, and then we will prove that configurations of each category satisfy each succeeding statement in the list.

By Lemma 3.9.2, η has at least L bridges. We take one of them and let this be an a-bridge for some $a \in \Omega$. Now, we consider three cases separately.

(Case 1: η has a horizontal a-bridge without a vertical a-bridge) Since $\Delta H_{c_h}(\eta) \geq 2$ for all $h \in [\![1,\, K]\!]$ and since $H(\eta) \leq \Gamma - 1 = 2K + 1$, we get from (3.122) that

$$\sum_{v \in [\![1,\, L]\!]} \Delta H_{r_v}(\eta) \leq 1.$$

Since we cannot have $\Delta H_{r_v}(\eta) = 1$, we must have $\Delta H_{r_v}(\eta) = 0$ for all $v \in [\![1,\, L]\!]$. This implies that $\eta \in \mathcal{R}_v^{a,\,b}$ for some $b \neq a$ and $v \in [\![0,\, L-1]\!]$ ($v = L$ is excluded because η must have an a-bridge). We consider three sub-cases separately.

- If $v \in [\![2,\, L-2]\!]$, then η satisfies **(L1)**.
- If $v = 0$, then $\eta = \boldsymbol{a}$ and thus η clearly has an a-cross, so that η satisfies **(L3)**.
- If $v = 1$ or $v = L - 1$, then η satisfies **(L2)** (if $v = L - 1$ then $\eta \in \mathcal{R}_{L-1}^{a,\,b} = \mathcal{R}_1^{b,\,a}$).

(Case 2: η has a vertical a-bridge without a horizontal a-bridge) Since $\Delta H_{r_v}(\eta) \geq 2$ for all $v \in [\![1,\, L]\!]$, we get from (3.122) that $2K + 2 > 2L$ and hence we must have $K = L$. The rest of the proof is now identical to **(Case 1)**; it suffices to switch the role of columns and rows.

(Case 3: η has an a-cross) Here, η readily satisfies **(L3)**.

Now, we verify the conditions of each category. If η satisfies **(L1)**, then it is clear that $\mathcal{N}(\eta)$ is a singleton since any configuration obtained from η by flipping a spin has energy greater than or equal to Γ. If η satisfies **(L2)**, then a part of a canonical path connecting $\boldsymbol{a}$ and η is a $(\Gamma - 2)$-path, and thus $\eta \in \mathcal{N}(\boldsymbol{a})$.

Finally, suppose that η satisfies **(L3)**. For this case, without loss of generality we may assume that $\mathbb{T}_K \times \{1\}$ and $\{1\} \times \mathbb{T}_L$ form the a-cross. Then, we update each spin to a in $[\![2,\, K]\!] \times [\![2,\, L]\!]$ in the ascending lexicographic order. The presence of a-bridges assures us that the Hamiltonian does not increase during the entire procedure. In the end we reach $\boldsymbol{a}$, and the maximal energy along the path is attained at the initial configuration, which is $H(\eta) < \Gamma$. Hence, we can conclude that $\eta \in \mathcal{N}(\boldsymbol{a})$.

Next, we verify the inequality (3.123). Define $\widetilde{\eta} \in \mathcal{X}$ as the configuration obtained from η by replacing all non-a spins by some fixed $b_0 \in S \setminus \{a\}$, i.e., for $x \in \Lambda$,

$$\widetilde{\eta}(x) = \begin{cases} a & \text{if } \eta(x) = a, \\ b_0 & \text{if } \eta(x) \neq a. \end{cases}$$

Then, it is straightforward from (3.122) that $H(\widetilde{\eta}) \le H(\eta)$. Moreover, as $\widetilde{\eta}$ also has an a-cross, we may regard clusters of spins b_0 in $\widetilde{\eta}$ as an object in $[\![2,\, K]\!] \times [\![2,\, L]\!] \subseteq \mathbb{Z}^2$. Thus, we can apply the well-known isoperimetric lemma [1, Corollary 2.5] to deduce

$$\|\widetilde{\eta}\|_{b_0} \le \frac{H(\widetilde{\eta})^2}{16} \le \frac{H(\eta)^2}{16} \le \frac{(2K+1)^2}{16},$$

where the last inequality follows from the assumption that $H(\eta) \le \Gamma - 1 = 2K + 1$. We also remark that the equality of the first inequality holds when the only cluster of spin b_0 in $\widetilde{\eta}$ forms a square. Since $\sum_{b \neq a} \|\eta\|_b = \|\widetilde{\eta}\|_{b_0}$, (3.123) is now proved and we conclude the proof. □

To conclude this subsection, we record a lemma regarding depths of valleys other than the metastable ones, which it is essential in the characterization of the three-dimensional metastable valleys in Chapter 4.

Lemma 3.9.4. *Let $\eta \in \mathcal{X}$ and $a \in \Omega$. For any standard sequence $(A_m)_{m=0}^{KL}$ of sets connecting $\emptyset$ and Λ and for $m \in [\![0,\, KL]\!]$, we define $\omega_m \in \mathcal{X}$ in such a manner that*

$$\omega_m(x) = \begin{cases} a & \text{if } x \in A_m, \\ \eta(x) & \text{if } x \in \Lambda \setminus A_m. \end{cases}$$

Then, we have that $H(\omega_m) \le H(\eta) + \Gamma$ for all $m \in [\![0,\, KL]\!]$.

Proof. As $\omega_{KL} = \boldsymbol{a}$, the lemma is immediate for $m = KL$. Thus, we prove this for $m \in [\![0,\, KL-1]\!]$.

Suppose that $m \in [\![K\ell,\, K(\ell+1)-1]\!]$ for some $\ell \in [\![0,\, L-1]\!]$ and write $\xi = \omega_m$. Suppose that $A_{K\ell} = \mathbb{T}_K \times P_\ell$, $A_{K(\ell+1)} = \mathbb{T}_K \times P_{\ell+1}$ and $P_{\ell+1} \setminus P_\ell = \{\ell_0\}$. By (3.122), we can write

$$H(\xi) - H(\eta) = \sum_{v \in [\![1,\, L]\!]} [\Delta H_{r_v}(\xi) - \Delta H_{r_v}(\eta)] + \sum_{h \in [\![1,\, K]\!]} [\Delta H_{c_h}(\xi) - \Delta H_{c_h}(\eta)]. \tag{3.124}$$

We start by considering the first summation at the right-hand side. For $v \in P_\ell$, we have $\Delta H_{r_v}(\xi) = 0$ and thus the summand is non-positive. For $v \in \mathcal{X} \setminus P_{\ell+1}$, the configurations η and ξ have the same v-th row and thus the summand is 0. Finally, for $v = \ell_0$, observe that ξ is obtained from η by changing spins at consecutive sites to b, and thus we can readily conclude that the energy has been increased by at most 2. Summing up, we obtain

$$\sum_{v \in [\![1,\, L]\!]} [\Delta H_{r_v}(\xi) - \Delta H_{r_v}(\eta)] \le 2. \tag{3.125}$$

By the same reasoning with the case of $v = \ell_0$ above, we can also observe that each summand of the second summation of (3.124) is at most 2 and hence

$$\sum_{h \in [\![1,\, K]\!]} [\Delta H_{c_h}(\xi) - \Delta H_{c_h}(\eta)] \le 2K. \tag{3.126}$$

By (3.124), (3.125) and (3.126), we get $H(\xi) - H(\eta) \le 2K + 2 = \Gamma$, and we have proved the lemma. □

3.9.2 Typical configurations

In this subsection, we prove Proposition 3.4.17. We first give two lemmas.

Lemma 3.9.5. *For $a, b \in \Omega$, suppose that $\eta_1 \in \mathcal{B}^{a,b}$ and $\eta_2 \in \mathcal{X}$ satisfy $\eta_1 \sim \eta_2$ and $H(\eta_2) \le \Gamma$. Then, the following statements hold.*

(1) If $\eta_1 \in \mathcal{R}_v^{a,b}$ *for* $v \in [\![2,\, L-2]\!]$*, then* $\eta_2 \in \mathcal{Q}_{v-1}^{a,b} \cup \mathcal{Q}_v^{a,b}$*. In particular, if* $v \in [\![3,\, L-3]\!]$ *then* $\eta_2 \in \mathcal{B}_\Gamma^{a,b}$*.*

(2) If $\eta_1 \in \mathcal{B}_\Gamma^{a,b}$*, then* $\eta_2 \in \mathcal{B}^{a,b}$*.*

In particular, it necessarily holds that $\eta_2 \in \mathcal{C}^{a,b}$*.*

Proof. We first assume that $K < L$ and consider two cases separately.

(Case 1: $\eta_1 = \xi_{\ell,v}^{a,b}$ **for some** $\ell \in \mathbb{T}_L$ **and** $v \in [\![2,\, L-2]\!]$**)** We can observe from the illustration given in Figure 3.1 that the only way of flipping a spin of η_1 in such a way that the resulting configuration has energy at most Γ is either to attach a protuberance of spin b to the cluster of spin b of η_1 or to attach a protuberance of spin a to the cluster of spin a of η_1. This implies that η_2 must be one of the following forms:

$$\xi_{\ell,v;k,1}^{a,b,\pm},\ \xi_{\ell,v-1;k,K-1}^{a,b,+},\ \xi_{\ell+1,v-1;k,K-1}^{a,b,-} \quad \text{for } k \in \mathbb{T}_K.$$

Hence, $\eta_2 \in \mathcal{Q}_{v-1}^{a,b} \cup \mathcal{Q}_v^{a,b}$. This proves the first assertion of part (1). The second assertion is straightforward.

(Case 2: $\eta_1 = \xi_{\ell,v;k,h}^{a,b,\pm}$ **for some** $\ell \in \mathbb{T}_L$**,** $v \in [\![2,\, L-3]\!]$**,** $k \in \mathbb{T}_K$**, and** $h \in [\![1,\, K-1]\!]$**)** In this case, we can also observe from the illustration given in Figure 3.1 that the only way of flipping a spin of η_1 without increasing the energy is to expand or shrink the protuberance of spin b attached at $\xi_{\ell,v}^{a,b}$, and therefore $\eta_2 = \xi_{\ell,v;k,h-1}^{a,b,\pm}$, $\xi_{\ell,v;k,h+1}^{a,b,\pm}$, $\xi_{\ell,v;k+1,h-1}^{a,b,\pm}$ or $\xi_{\ell,v;k-1,h+1}^{a,b,\pm}$. This proves that $\eta_2 \in \mathcal{B}^{a,b}$ and hence part (2) is now verified. Thus, we conclude the case of $K < L$.

The case of $K = L$ can be treated in the same manner. We just have to consider also the configurations transposed by the operator Θ. □

The previous lemma implies the following result.

Lemma 3.9.6. *It holds that* $\widehat{\mathcal{N}}(\mathcal{B};\, \mathcal{C} \setminus \mathcal{B}) = \mathcal{B}$*.*

Proof. Since the Hamiltonian of configurations belonging to $\mathcal{B}$ does not exceed Γ, it is immediate that

$$\widehat{\mathcal{N}}(\mathcal{B};\, \mathcal{C} \setminus \mathcal{B}) \supseteq \mathcal{B}.$$

Thus, it suffices to show the opposite inclusion. Since

$$\widehat{\mathcal{N}}(\mathcal{B};\, \mathcal{C} \setminus \mathcal{B}) = \bigcup_{a,\, b \in \Omega} \widehat{\mathcal{N}}(\mathcal{B}^{a,\, b};\, \mathcal{C} \setminus \mathcal{B}) \subseteq \bigcup_{a,\, b \in \Omega} \widehat{\mathcal{N}}(\mathcal{B}^{a,\, b};\, \mathcal{C}^{a,\, b} \setminus \mathcal{B}^{a,\, b}),$$

it suffices to show that for $a,\, b \in \Omega$,

$$\widehat{\mathcal{N}}(\mathcal{B}^{a,\, b};\, \mathcal{C}^{a,\, b} \setminus \mathcal{B}^{a,\, b}) \subseteq \mathcal{B}^{a,\, b}. \tag{3.127}$$

Take $\eta \in \widehat{\mathcal{N}}(\mathcal{B}^{a,\, b};\, \mathcal{C}^{a,\, b} \setminus \mathcal{B}^{a,\, b})$. Then, we have a Γ-path $(\omega_n)_{n=0}^{N}$ in $\mathcal{X} \setminus (\mathcal{C}^{a,\, b} \setminus \mathcal{B}^{a,\, b}) = (\mathcal{X} \setminus \mathcal{C}^{a,\, b}) \cup \mathcal{B}^{a,\, b}$ from $\mathcal{B}^{a,\, b}$ to η. Suppose the contrary that $\eta \notin \mathcal{B}^{a,\, b}$. Then, as $\omega_0 \in \mathcal{B}^{a,\, b}$, there exists $n_0 \in [\![0,\, N-1]\!]$ such that $\omega_{n_0} \in \mathcal{B}^{a,\, b}$ and $\omega_{n_0+1} \in \mathcal{X} \setminus \mathcal{B}^{a,\, b}$. Since $(\omega_n)_{n=0}^{N}$ is a path in $(\mathcal{X} \setminus \mathcal{C}^{a,\, b}) \cup \mathcal{B}^{a,\, b}$, we get

$$\omega_{n_0+1} \in (\mathcal{X} \setminus \mathcal{B}^{a,\, b}) \cap \big[(\mathcal{X} \setminus \mathcal{C}^{a,\, b}) \cup \mathcal{B}^{a,\, b}\big] = \mathcal{X} \setminus \mathcal{C}^{a,\, b}.$$

On the other hand, since $\omega_{n_0} \in \mathcal{B}^{a,\, b}$ we must have $\omega_{n_0+1} \in \mathcal{C}^{a,\, b}$ by Lemma 3.9.5 and thus we get a contradiction. Therefore, we must have $\eta \in \mathcal{B}^{a,\, b}$ and thus we get (3.127). $\square$

Now, we are ready to present a proof of Proposition 3.4.17.

Proof of Proposition 3.4.17. We first prove that

$$\{\boldsymbol{b}\} \cap \widehat{\mathcal{N}}(\boldsymbol{a};\, \mathcal{B}_\Gamma) = \emptyset. \tag{3.128}$$

Let us suppose the contrary that $(\omega_n)_{n=0}^{N}$ is a Γ-path from $\boldsymbol{a}$ to $\boldsymbol{b}$ in $\mathcal{X} \setminus \mathcal{B}_\Gamma$.

We now follow the idea of [69, Proposition 2.6]. Define $u : [\![0,\, N]\!] \to \mathbb{R}$ as

$$u(n) = B_b(\omega_n) \quad \text{for all } n \in [\![0,\, N]\!],$$

where $B_b(\cdot)$ is defined in Notation 3.9.1. Then, we have that

$$u(0) = 0,\ u(N) = K + L,\ \text{and } |u(n+1) - u(n)| \le 2 \text{ for all } n \in [\![0,\, N-1]\!]. \tag{3.129}$$

Thus, the following instant n^* is well defined:

$$n^* = \min\{n \in [\![0,\, N-1]\!] : u(n),\, u(n+1) \ge 2\}. \tag{3.130}$$

Note that, since we need to change at least $2K - 1$ spins from $\boldsymbol{a}$ to get $u(t) \ge 2$, we clearly have $n^* \ge 2K - 1$. By (3.129), we have $B_b(\omega_{n^*}) = 2$ or 3. We divide the proof into three cases as in Proposition 3.9.3.

(Case 1: ω_{n^*} has a horizontal b-bridge without a vertical b-bridge) For this case, if $B_b(\omega_{n^*}) = 3$, we have $B_b(\omega_{n^*-1}) \ge 2$ and thus we get a contradiction to the minimality of n^*. Thus, we must have $B_b(\omega_{n^*}) = 2$.

Since ω_{n^*} cannot have any vertical bridges, we get $\Delta H_{c_h}(\omega_{n^*}) \ge 2$ for all $h \in [\![1,\, K]\!]$. In view of (3.122) and the fact that $H(\omega_{n^*}) \le \Gamma = 2K + 2$, we can readily conclude that the only possibility is $\omega_{n^*} \in \mathcal{R}_2^{a_0,\, b}$ or $\mathcal{Q}_2^{a_0,\, b}$ for some $a_0 \ne b$. The latter case yields an immediate contradiction since $\mathcal{Q}_2^{a_0,\, b} \subseteq \mathcal{B}_\Gamma^{a_0,\, b} \subseteq \mathcal{B}_\Gamma$. Summing up, we must have $\omega_{n^*} \in \mathcal{R}_2^{a_0,\, b}$ for some $a_0 \ne b$. Since $H(\omega_{n^*+1}) \le \Gamma$, the only possibility to get ω_{n^*+1} from ω_{n^*} is either to change a spin a_0 neighboring the cluster of spin b to b, or to change a spin b neighboring the cluster of spin a_0 to a_0. Both cases yield a contradiction, since in the former we get $\omega_{n^*+1} \in \mathcal{B}_\Gamma^{a,\, b} \subseteq \mathcal{B}_\Gamma$ while in the latter $u(n^*+1) = 1$.

(Case 2: ω_{n^*} has a vertical b-bridge without a horizontal b-bridge) This case is similar to **(Case 1)** and we omit the detail.

(Case 3: ω_{n^*} has a b-cross) In this case, ω_{n^*} does not have a bridge whose spin is not b and thus, by (3.129), the configuration ω_{n^*} has at most 3 bridges.

Therefore, by Lemma 3.9.2, it holds that

$$H(\omega_{n^*}) \geq 2(K+L-3) > \Gamma.$$

This contradicts the assumption that $(\omega_n)_{n=0}^{N}$ is a Γ-path. Therefore, we conclude the proof of (3.128).

(1) This is direct from (3.128), since otherwise we can construct a Γ-path from $\boldsymbol{a}$ to $\boldsymbol{b}$ avoiding $\mathcal{B}_\Gamma$ by reversing and concatenating.

(2) First, we have $\mathcal{B}^{a,\,b} \supseteq \mathcal{R}_2^{a,\,b}$ from the definition of the set $\mathcal{B}^{a,\,b}$. Moreover, since a canonical path connecting $\mathcal{R}_2^{a,\,b}$ and $\boldsymbol{a}$ is a Γ-path in $\mathcal{X} \setminus \mathcal{B}_\Gamma$, we also have $\mathcal{E}^a \supseteq \mathcal{R}_2^{a,\,b}$. This concludes that

$$\mathcal{E}^a \cap \mathcal{B}^{a,\,b} \supseteq \mathcal{R}_2^{a,\,b}. \tag{3.131}$$

Now, we claim that the reversed inclusion also holds. To this end, we start by observing that, since $\mathcal{B}_\Gamma^{a,\,b}$ and $\mathcal{E}^a$ are disjoint from the definition (3.50),

$$\mathcal{E}^a \cap \mathcal{B}^{a,\,b} \subseteq \mathcal{B}^{a,\,b} \setminus \mathcal{B}_\Gamma^{a,\,b} = \bigcup_{v \in [\![2,\,L-2]\!]} \mathcal{R}_v^{a,\,b}.$$

For $\eta \in \mathcal{R}_v^{a,\,b}$ with $v \in [\![3,\,L-3]\!]$, we cannot have a Γ-path in $\mathcal{X} \setminus \mathcal{B}_\Gamma$ from $\boldsymbol{a}$ to η by part (1) of Lemma 3.9.5. Thus, such an η cannot belong to $\mathcal{E}^a$ and we deduce that

$$\mathcal{E}^a \cap \mathcal{B}^{a,\,b} \subseteq \mathcal{R}_2^{a,\,b} \cup \mathcal{R}_{L-2}^{a,\,b}. \tag{3.132}$$

Note that we have $\mathcal{E}^b \supseteq \mathcal{R}_{L-2}^{a,\,b}$ by the same reason with $\mathcal{E}^a \supseteq \mathcal{R}_2^{a,\,b}$ that we proved before; hence, any configuration $\eta \in \mathcal{R}_{L-2}^{a,\,b}$ cannot belong to $\mathcal{E}^a$ by part (1). This observation and (3.132) implies that $\mathcal{E}^a \cap \mathcal{B}^{a,\,b} \subseteq \mathcal{R}_2^{a,\,b}$. This along with (3.131) completes the proof of part (2).

(3) We can deduce $\mathcal{E}^a \cap \mathcal{B}^{b,\,c} \subseteq \mathcal{R}_2^{b,\,c} \cup \mathcal{R}_{L-2}^{b,\,c}$ by the the same logic as we obtained (3.132). Then, since $\mathcal{R}_2^{b,\,c} \subseteq \mathcal{E}^b$ and $\mathcal{R}_{L-2}^{b,\,c} \subseteq \mathcal{E}^c$, part (1) implies that $\mathcal{E}^a \cap \mathcal{B}^{b,\,c} = \emptyset$.

(4) The inclusion $\mathcal{E} \subseteq \widehat{\mathcal{N}}(\mathcal{S})$ is immediate from the definition of $\mathcal{E}$, and the inclusion $\mathcal{B} \subseteq \widehat{\mathcal{N}}(\mathcal{S})$ is direct from the fact that any configuration in $\mathcal{B}^{a,\,b}$ is obtained starting from $\boldsymbol{a}$ via a canonical path which is a Γ-path (cf. Lemma 3.4.13-(3)). Thus, we get

$$\mathcal{E} \cup \mathcal{B} \subseteq \widehat{\mathcal{N}}(\mathcal{S}). \tag{3.133}$$

On the other hand, by Lemma 3.8.1 with $\mathcal{P}_1 = \mathcal{C} \setminus \mathcal{B}$, $\mathcal{P}_2 = \mathcal{B}$ and $\mathcal{Q} = \emptyset$ and Lemma 3.4.8, we can write

$$\widehat{\mathcal{N}}(\mathcal{C}) = \widehat{\mathcal{N}}(\mathcal{B};\, \mathcal{C} \setminus \mathcal{B}) \cup \widehat{\mathcal{N}}(\mathcal{C} \setminus \mathcal{B};\, \mathcal{B}). \tag{3.134}$$

First, by Lemma 3.9.6,

$$\widehat{\mathcal{N}}(\mathcal{B};\, \mathcal{C} \setminus \mathcal{B}) = \mathcal{B}. \tag{3.135}$$

On the other hand, since any configuration in $\mathcal{C} \setminus \mathcal{B}$ is obtained starting from a ground state by a part of a canonical path which is a Γ-path in $\mathcal{X} \setminus \mathcal{B}_\Gamma$, we get

$$\widehat{\mathcal{N}}(\mathcal{C} \setminus \mathcal{B};\, \mathcal{B}) \subseteq \widehat{\mathcal{N}}(\mathcal{C} \setminus \mathcal{B};\, \mathcal{B}_\Gamma) = \widehat{\mathcal{N}}(\mathcal{S};\, \mathcal{B}_\Gamma) = \mathcal{E}. \tag{3.136}$$

By combining (3.134), (3.135) and (3.136), we get $\widehat{\mathcal{N}}(\mathcal{C}) \subseteq \mathcal{B} \cup \mathcal{E}$. Since $\mathcal{S} \subseteq \mathcal{C}$, the opposite inclusion of (3.133) holds, and the proof is completed. □

3.9.3 Edge typical configurations

Here, we prove Propositions 3.4.18 and 3.4.20.

Proof of Proposition 3.4.18. To begin with, we consider the case of $K < L$. First, we prove the only if part. Fix $\eta \in \mathcal{Z}^{a,\,b}$ and take a path $(\omega_n)_{n=0}^N$ in $\mathcal{X} \setminus \mathcal{B}_\Gamma$ such that $\omega_0 = \xi_{\ell,\,2}^{a,\,b}$ for some $\ell \in \mathbb{T}_L$, $\omega_N = \eta$ and $H(\omega_n) = \Gamma$ for all $n \in [\![1,\, N]\!]$. It suffices to prove that ω_n satisfies all requirements **[Z1]**, **[Z2]** and **[Z3]** for all $n \in [\![1,\, N]\!]$. We prove this by induction on n. First, consider the case $n = 1$. Then, since $\omega_0 = \xi_{\ell,\,2}^{a,\,b}$ and $\omega_1 \notin \mathcal{B}_\Gamma$, the proof of Lemma 3.9.5

implies that

$$\omega_1 \in \bigcup_{k\in\mathbb{T}_K} \{\xi^{a,\,b,\,+}_{\ell,\,1;\,k,\,K-1},\, \xi^{a,\,b,\,-}_{\ell+1,\,1;\,k,\,K-1}\}.$$

In any case [**Z1**] and [**Z2**] are obvious, and since $G_a(\eta)$ is a singleton subset of $\mathbb{T}_K \times \{\ell,\, \ell+1\}$, [**Z3**] also holds. These observations conclude the first step of $n = 1$.

Now, suppose that the three conditions hold for ω_n, and then we consider ω_{n+1}. Note that $H(\omega_n) = H(\omega_{n+1}) = \Gamma$. We denote by $z \in \Lambda$ the site where the spin update happens from ω_n to ω_{n+1}, which does not change the energy. By simple inspection, any spin update outside $\mathbb{T}_K \times \{\ell,\, \ell+1\}$ strictly increases the energy, and thus $z \in \mathbb{T}_K \times \{\ell,\, \ell+1\}$. Moreover, any spin update to a third spin (other than a and b) strictly increases the energy, since the fact that $G_a(\omega_n)$ is a sub-tree in $\mathbb{T}_K \times \{\ell,\, \ell+1\}$ implies that there is no isolated spin. Therefore, the spin update at site z must be $b \to a$ or $a \to b$ inside $\mathbb{T}_K \times \{\ell,\, \ell+1\}$. This observation verifies both [**Z1**] and [**Z2**] for the new configuration ω_{n+1}.

To check [**Z3**] for ω_{n+1}, we divide into two cases.

- If the update at z is $b \to a$, then $z \notin G_a(\omega_n)$ and $G_a(\omega_{n+1}) = G_a(\omega_n) \cup \{z\}$. Since $H(\omega_n) = H(\omega_{n+1})$, z must have exactly two neighboring sites with spin a and two neighboring sites with spin b. Since z has exactly one neighbor outside $\mathbb{T}_K \times \{\ell,\, \ell+1\}$ which has spin a by condition [**Z1**], z must have exactly one neighbor with spin a inside $\mathbb{T}_K \times \{\ell,\, \ell+1\}$. This implies that $G_a(\omega_{n+1}) = G_a(\omega_n) \cup \{z\}$ is still a tree.

- If the update at z is $a \to b$, then $z \in G_a(\omega_n)$ and $G_a(\omega_{n+1}) = G_a(\omega_n) \setminus \{z\}$. The same logic as above indicates that z has exactly one neighbor with spin a inside $\mathbb{T}_K \times \{\ell,\, \ell+1\}$. This is equivalent to saying that z is an external vertex of the tree $G_a(\omega_n)$ and that $\{z\} \subseteq G_a(\omega_n)$ with proper inclusion. Therefore, $G_a(\omega_{n+1}) = G_a(\omega_n) \setminus \{z\}$ is also a tree. This concludes the proof of the only if part.

Now, we prove the if part. Suppose that [**Z1**], [**Z2**] and [**Z3**] hold for a configuration $\eta \in \mathcal{X}$. Then, since $G_a(\eta)$ is a tree in $\mathbb{T}_K \times \{\ell,\, \ell+1\}$, we may enumerate

$$G_a(\eta) = \{x_1,\, x_2,\, \dots,\, x_m\}$$

in a way that $\{x_i,\, \dots,\, x_m\}$ is still a tree for all $i \in [\![1,\, m]\!]$. Indeed, we can just inductively choose an external vertex x_i in each $G_a(\eta) \setminus \{x_1,\, \dots,\, x_{i-1}\}$. Then, starting from η, we define a path $(\omega_n)_{n=0}^m$ such that for each $n \in [\![1,\, m]\!]$, ω_n is obtained from ω_{n-1} by flipping the spin a on x_n to spin b (i.e., $\omega_n = \omega_{n-1}^{x_n,\, b}$). Then, by the same logic used in the two cases above, we have $H(\omega_n) = H(\omega_{n-1})$ for $n \in [\![1,\, m-1]\!]$. On the other hand, the final update from ω_{m-1} to ω_m decreases the energy by 2 since in ω_{m-1}, x_m has three neighboring sites with spin b and one neighboring site with spin a. Moreover, $G_a(\omega_m) = \emptyset$ which implies that $\omega_m = \xi_{\ell,\,2}^{a,\,b} \in \mathcal{R}_2^{a,\,b}$. Therefore, the reversed path $(\omega_{m-n})_{n=0}^m$ guarantees by definition that $\omega_0 = \eta \in \mathcal{Z}^{a,\,b}$. This concludes the proof of the case of $K < L$.

Finally, the case of $K = L$ can be dealt with in an identical manner; the only difference is that we may also have $\omega_0 = \Theta(\xi_{\ell,\,2}^{a,\,b})$ for some $\ell \in \mathbb{T}_L$, so that in [**Z2**] we may have $P_b(\eta) \subseteq \{\ell,\, \ell+1\} \times \mathbb{T}_K$. Everything else works in the same way. □

Before proceeding to the proof of Proposition 3.4.20, we give an additional property of the set $\mathcal{Z}^{a,\,b}$.

Lemma 3.9.7. *Let $a,\, b \in \Omega$ and $\eta \in \mathcal{Z}^{a,\,b}$. Then, the followings hold.*

(1) There exists a Γ-path from $\boldsymbol{a}$ to η in $\mathcal{X} \setminus \mathcal{B}_\Gamma$.

(2) If another $\xi \in \mathcal{X}$ satisfies $\eta \sim \xi$ and $H(\xi) \le \Gamma$, then we have $\xi \in \mathcal{Z}^{a,\,b} \cup \mathcal{N}(\boldsymbol{a}) \cup \mathcal{R}_2^{a,\,b}$.

Proof. (1) Without loss of generality, we assume that $K < L$. According to the notation and statements from Proposition 3.4.18, $G_a(\eta)$, the collection of sites in $\mathbb{T}_K \times \{\ell,\, \ell+1\}$ with spin a, is a tree. Then, we may enumerate

$$\big[\mathbb{T}_K \times \{\ell,\, \ell+1\}\big] \setminus G_a(\eta) = \{y_1,\, \dots,\, y_M\}$$

in a way that $G_a(\eta) \cup \{y_1,\, \dots,\, y_i\}$ is connected for all $i \in [\![1,\, M]\!]$. Indeed, we can just inductively choose a neighboring site to $G_a(\eta) \cup \{y_1,\, \dots,\, y_i\}$. Then, we define a path $(\omega_n)_{n=0}^M$ such that for each $n \in [\![1,\, M]\!]$, ω_n is obtained from ω_{n-1} by flipping the spin b on y_n to spin a (i.e., $\omega_n = \omega_{n-1}^{y_n,\, a}$). By our construction, on each step n, the site y_n has at least two neighboring sites with spin a (one in $G_a(\eta) \cup \{y_1,\, \dots,\, y_{n-1}\}$ and another outside $\mathbb{T}_K \times \{\ell,\, \ell+1\}$), which implies that $H(\omega_n) \le H(\omega_{n-1})$. Moreover, it is clear that $H(\omega_M) = \boldsymbol{a}$. Therefore, $(\omega_n)_{n=0}^M$ is a $H(\eta)$-path from η to $\boldsymbol{a}$. Since $H(\eta) = \Gamma$ and it is clear by construction that $\omega_n \notin \mathcal{B}_\Gamma$, we conclude that $(\omega_n)_{n=0}^M$ satisfies the requirements of part (1).

(2) Let $(\omega_n)_{n=0}^N$ be a path in $\mathcal{X} \setminus \mathcal{B}_\Gamma$ from $\mathcal{R}_2^{a,\, b}$ to η such that $H(\omega_n) = \Gamma$ for $n \in [\![1,\, N]\!]$ (cf. (3.51)). Suppose first that $H(\xi) = \Gamma$. Then by part (3) of Lemma 3.9.5, it follows that $\xi \notin \mathcal{B}_\Gamma$. Hence, by letting $\omega_{N+1} = \xi$, the path $(\omega_n)_{n=0}^{N+1}$ in $\mathcal{X} \setminus \mathcal{B}_\Gamma$ is from $\mathcal{R}_2^{a,\, b}$ to ξ and satisfies $H(\omega_n) = \Gamma$ for $n \in [\![1,\, N+1]\!]$. Thus, by (3.51), we get $\xi \in \mathcal{Z}^{a,\, b}$.

Next, we consider the case $H(\xi) < \Gamma$. Using Proposition 3.9.3 and considering the conditions [**Z1**], [**Z2**] and [**Z3**] in Proposition 3.4.18 that η must satisfy, we can easily deduce that $\xi \in \mathcal{R}_2^{a,\, b}$ or ξ has an a-cross. In the latter case, again by Proposition 3.9.3 it holds that $\xi \in \mathcal{N}(\boldsymbol{a})$. Thus, we conclude the proof. □

Now, we prove Proposition 3.4.20.

Proof of Proposition 3.4.20. First, we demonstrate that

$$\mathcal{E}^a = \widehat{\mathcal{N}}(\boldsymbol{a};\, \mathcal{Z}^a \cup \mathcal{R}^a \cup \mathcal{B}_\Gamma) \cup \mathcal{Z}^a \cup \mathcal{R}^a. \tag{3.137}$$

Recall that $\mathcal{E}^a = \widehat{\mathcal{N}}(\boldsymbol{a};\, \mathcal{B}_\Gamma) = \widehat{\mathcal{N}}(\mathcal{N}(\boldsymbol{a});\, \mathcal{B}_\Gamma)$. Since $\mathcal{Z}^a$ is connected to

$\mathcal{N}(\boldsymbol{a})$ by a Γ-path outside $\mathcal{B}_\Gamma$ by Lemma 3.9.7-(1), we have $\widehat{\mathcal{N}}(\mathcal{Z}^a;\, \mathcal{B}_\Gamma) = \widehat{\mathcal{N}}(\mathcal{N}(\boldsymbol{a});\, \mathcal{B}_\Gamma)$. Moreover, $\mathcal{R}^a$ is connected to $\boldsymbol{a}$ by a part of a canonical path outside $\mathcal{B}_\Gamma$, so that $\widehat{\mathcal{N}}(\mathcal{R}^a;\, \mathcal{B}_\Gamma) = \widehat{\mathcal{N}}(\mathcal{N}(\boldsymbol{a});\, \mathcal{B}_\Gamma)$. Thus, we obtain

$$\mathcal{E}^a = \widehat{\mathcal{N}}\big(\mathcal{N}(\boldsymbol{a}) \cup \mathcal{Z}^a \cup \mathcal{R}^a;\, \mathcal{B}_\Gamma\big).$$

Then, by Lemma 3.8.1 with $\mathcal{P}_1 = \mathcal{N}(\boldsymbol{a})$, $\mathcal{P}_2 = \mathcal{Z}^a \cup \mathcal{R}^a$ and $\mathcal{Q} = \mathcal{B}_\Gamma$, we obtain

$$\mathcal{E}^a = \widehat{\mathcal{N}}(\mathcal{N}(\boldsymbol{a});\, \mathcal{Z}^a \cup \mathcal{R}^a \cup \mathcal{B}_\Gamma) \cup \widehat{\mathcal{N}}(\mathcal{Z}^a \cup \mathcal{R}^a;\, \mathcal{N}(\boldsymbol{a}) \cup \mathcal{B}_\Gamma).$$

Since it is clear that $\widehat{\mathcal{N}}(\mathcal{N}(\boldsymbol{a});\, \mathcal{Z}^a \cup \mathcal{R}^a \cup \mathcal{B}_\Gamma) = \widehat{\mathcal{N}}(\boldsymbol{a};\, \mathcal{Z}^a \cup \mathcal{R}^a \cup \mathcal{B}_\Gamma)$, it suffices to prove that

$$\widehat{\mathcal{N}}(\mathcal{Z}^a \cup \mathcal{R}^a;\, \mathcal{N}(\boldsymbol{a}) \cup \mathcal{B}_\Gamma) = \mathcal{Z}^a \cup \mathcal{R}^a. \tag{3.138}$$

Subjected to the energy barrier Γ, the first exit from $\mathcal{Z}^a$ is to $\mathcal{N}(\boldsymbol{a}) \cup \mathcal{R}^a$ by Lemma 3.9.7-(2), and the first exit from $\mathcal{R}^a$ is to $\mathcal{Z}^a \cup \mathcal{B}^\Gamma$ by Lemma 3.9.5-(1) and (3.51). Thus, we can deduce (3.138) by the same logic that we used to prove (3.127). Thus, we have proved (3.137).

Now, to conclude the proof of Proposition 3.4.20 it remains to prove that $\widehat{\mathcal{N}}(\boldsymbol{a};\, \mathcal{Z}^a \cup \mathcal{R}^a \cup \mathcal{B}_\Gamma) = \mathcal{D}^a$. Note that $\mathcal{D}^a = \widehat{\mathcal{N}}(\boldsymbol{a};\, \mathcal{Z}^a)$. It is clear that $\widehat{\mathcal{N}}(\boldsymbol{a};\, \mathcal{Z}^a \cup \mathcal{R}^a \cup \mathcal{B}_\Gamma) \subseteq \widehat{\mathcal{N}}(\boldsymbol{a};\, \mathcal{Z}^a)$. Suppose that there exists $\eta \in \widehat{\mathcal{N}}(\boldsymbol{a};\, \mathcal{Z}^a) \setminus \widehat{\mathcal{N}}(\boldsymbol{a};\, \mathcal{Z}^a \cup \mathcal{R}^a \cup \mathcal{B}_\Gamma)$. This implies that not only there exists a Γ-path ω from $\boldsymbol{a}$ to η in $\mathcal{X} \setminus \mathcal{Z}^a$, but also all such paths must visit $\mathcal{R}^a \cup \mathcal{B}_\Gamma$. Thus, we may define

$$n_1 := \min\{n \geq 0 : \omega_n \in \mathcal{R}^a \cup \mathcal{B}_\Gamma\}.$$

By Lemma 3.9.5 and (3.51), we readily have three possibilities:

$$\omega_{n_1-1} \in \mathcal{Z}^a \cup \bigcup_{b\in\Omega\setminus\{a\}} \bigcup_{v\in[\![3,\, L-3]\!]} \mathcal{R}_v^{a,\,b} \cup \bigcup_{b\in\Omega\setminus\{a\}} \mathcal{R}_{L-2}^{a,\,b}.$$

The first possibility, $\omega_{n_1-1} \in \mathcal{Z}^a$, is clearly impossible by the definition of ω. The second possibility, $\omega_{n_1-1} \in \mathcal{R}_v^{a,b}$ for some $b \neq a$ and $v \in [\![3, L-3]\!]$, is also impossible since then by Lemma 3.9.5-(1), $\omega_{n_1-2} \in \mathcal{B}_\Gamma$ which contradicts the minimality of n_1. Finally, the third possibility, $\omega_{n_1-1} \in \mathcal{R}_{L-2}^{a,b}$ for some $b \neq a$, implies that $\omega_{n_1-1} \in \mathcal{E}^b$ and this is again impossible since $\mathcal{E}^a \cap \mathcal{E}^b = \emptyset$ by Proposition 3.4.17-(1). Therefore, all cases reject the possibility that such η exists, and we conclude the proof. □

3.9.4 Graph structure

In this subsection, we prove Propositions 3.4.22 and 3.4.23.

Proof of Proposition 3.4.22. By symmetry, it suffices to prove only for the projection $\Pi_\ell^{a,b} : \mathcal{N}(\boldsymbol{a}) \cup \mathcal{Z}_\ell^{a,b} \cup \{\xi_{\ell,2}^{a,b}\} \to \mathscr{V}$. We first consider part (1). Suppose that $\eta_1, \eta_2 \neq \boldsymbol{a}$. If $\eta_1 \nsim \eta_2$, then both sides of (3.61) are clearly 0 and there is nothing to prove. If $\eta_1 \sim \eta_2$ so that $\{\eta_1, \eta_2\} \in \mathscr{E}$, then by (2.2) and (3.60), we can write

$$\frac{1}{q}e^{-\Gamma\beta}\mathfrak{r}(\Pi_\ell^{a,b}(\eta_1), \Pi_\ell^{a,b}(\eta_2)) = \frac{1}{q}e^{-\Gamma\beta} = \frac{Z_\beta}{q} \cdot \mu_\beta(\eta_1) r_\beta(\eta_1, \eta_2),$$

since $\min\{\mu_\beta(\eta_1), \mu_\beta(\eta_2)\} = \frac{1}{Z_\beta}e^{-\Gamma\beta}$. By Theorem 3.0.1, the right-hand side of the last display becomes $(1+o(1)) \cdot \mu_\beta(\eta_1) r_\beta(\eta_1, \eta_2)$.

We next consider part (2) so that $\eta_1 \neq \boldsymbol{a}$. Similarly, we may assume $\{\eta_1, \boldsymbol{a}\} \in \mathscr{E}$ since otherwise both sides of (3.62) become 0. Then by (3.60), we can write

$$\begin{aligned}\frac{1}{q}e^{-\Gamma\beta}\mathfrak{r}(\Pi_\ell^{a,b}(\eta_1), \boldsymbol{a}) &= \frac{1}{q}e^{-\Gamma\beta}|\{\xi \in \mathcal{N}(\boldsymbol{a}) : \xi \sim \eta_1\}| \\ &= |\{\xi \in \mathcal{N}(\boldsymbol{a}) : \xi \sim \eta_1\}| \cdot \frac{Z_\beta}{q} \cdot \mu_\beta(\eta_1).\end{aligned}$$

Since $\min\{\mu_\beta(\eta_1), \mu_\beta(\xi)\} = \mu_\beta(\eta_1) = \frac{1}{Z_\beta}e^{-\Gamma\beta}$ for all $\xi \in \mathcal{N}(\boldsymbol{a})$, by (2.2) and

Theorem 3.0.1, the right-hand side equals

$$(1+o(1)) \cdot \sum_{\xi \in \mathcal{N}(\boldsymbol{a})} \mu_\beta(\eta_1) r_\beta(\eta_1,\, \xi).$$

This concludes the proof. □

Proof of Proposition 3.4.23. We fix $a,\, b \in \Omega$ and $\ell \in \mathbb{T}_L$. Recall (3.65). Note that

$$\mathfrak{cap}(\boldsymbol{a},\, \xi_{\ell,\,2}^{a,\,b}) = \mathfrak{D}(\mathfrak{f}) = \sum_{\{x,\,y\} \subseteq \mathscr{V}} \frac{1}{|\mathscr{V}|} \mathfrak{r}(x,\, y)[\mathfrak{f}(y) - \mathfrak{f}(x)]^2.$$

For each $k \in \mathbb{T}_K$, consider a path $\omega^k = (\omega_n^k)_{n=0}^K$ such that

$$\omega_0^k = \boldsymbol{a} \quad \text{and} \quad \omega_n^k = \xi_{\ell,\,1;\,k,\,n}^{a,\,b,\,+} \quad \text{for } n \in [\![1,\, K]\!].$$

This is indeed a path from $\boldsymbol{a}$ to $\xi_{\ell,\,2}^{a,\,b}$ subjected to the process $\mathfrak{Z}(\cdot)$ since $\omega_0^k = \xi_{\ell,\,1}^{a,\,b} \in \mathcal{N}(\boldsymbol{a})$ and $\omega_K^k = \xi_{\ell,\,1;\,k,\,K}^{a,\,b,\,+} = \xi_{\ell,\,2}^{a,\,b}$. Therefore, we may calculate along only these K paths:

$$\begin{aligned}
\mathfrak{cap}(\boldsymbol{a},\, \xi_{\ell,\,2}^{a,\,b}) &\geq \sum_{k \in \mathbb{T}_K} \sum_{n=0}^{K-1} \frac{1}{|\mathscr{V}|} \mathfrak{r}(\omega_n^k,\, \omega_{n+1}^k)[\mathfrak{f}(\omega_{n+1}^k) - \mathfrak{f}(\omega_n^k)]^2 \\
&= \frac{1}{|\mathscr{V}|} \sum_{k \in \mathbb{T}_K} \sum_{n=0}^{K-1} [\mathfrak{f}(\omega_{n+1}^k) - \mathfrak{f}(\omega_n^k)]^2.
\end{aligned}$$

By the Cauchy–Schwarz inequality, we obtain

$$\begin{aligned}
\mathfrak{cap}(\boldsymbol{a},\, \xi_{\ell,\,2}^{a,\,b}) &\geq \frac{1}{|\mathscr{V}|} \sum_{k \in \mathbb{T}_K} \frac{1}{K} \Big[\sum_{n=0}^{K-1} [\mathfrak{f}(\omega_{n+1}^k) - \mathfrak{f}(\omega_n^k)] \Big]^2 \\
&= \frac{1}{|\mathscr{V}|} \sum_{k \in \mathbb{T}_K} \frac{1}{K} [\mathfrak{f}(\boldsymbol{a}) - \mathfrak{f}(\xi_{\ell,\,2}^{a,\,b})]^2.
\end{aligned}$$

Since $\mathfrak{f}(\boldsymbol{a}) = 1$ and $\mathfrak{f}(\xi_{\ell,\,2}^{a,\,b}) = 0$, we deduce that $\mathfrak{cap}(\boldsymbol{a},\, \xi_{\ell,\,2}^{a,\,b}) \geq |\mathscr{V}|^{-1}$ which concludes the proof. □

3.9.5 Gateway configurations

In this subsection, we define the notion of *gateway configurations.* which is essential in the 3D Ising/Potts models in Chapter 4.

Definition 3.9.8 (Gateway configurations)**.** Recall the collection $\mathcal{Z}^{a,\,b}$ defined in (3.51). Define the gateway $\mathcal{G}^{a,\,b}$ between $\boldsymbol{a}$ and $\boldsymbol{b}$ as

$$\mathcal{G}^{a,\,b} = \mathcal{Z}^{a,\,b} \cup \mathcal{B}^{a,\,b} \cup \mathcal{Z}^{b,\,a}, \tag{3.139}$$

where this expression gives a decomposition of $\mathcal{G}^{a,\,b}$. Since $\mathcal{B}^{a,\,b} = \mathcal{B}^{b,\,a}$, we have $\mathcal{G}^{a,\,b} = \mathcal{G}^{b,\,a}$. A configuration belonging to $\mathcal{G}^{a,\,b}$ is called a *gateway configuration* between $\boldsymbol{a}$ and $\boldsymbol{b}$.

Remark 3.9.9. In the terminology which was first suggested in [67] and widely used since then, *gate* configurations are the ones which serve as effective checkpoints of the transition, along with the property that their energy equals the exact energy barrier (i.e., Γ in our case). On the other hand, in our sense (cf. Definition 3.9.8), *gateway* configurations may have energy less than Γ; indeed, we have $\mathcal{R}_v^{a,\,b} \subseteq \mathcal{G}^{a,\,b}$ for $v \in [\![2,\, L-2]\!]$ where each configuration in $\mathcal{R}_v^{a,\,b}$, $v \in [\![2,\, L-2]\!]$ has energy $\Gamma - 2 < \Gamma$. Nevertheless, our definition of gateway configurations still works properly since the gateway configurations with energy less than Γ must immediately visit the ones with energy Γ before preceding further. This fact is interpreted in part (1) of Lemma 3.9.5.

Lemma 3.9.10. *For $a,\, b \in \Omega$, suppose that two configurations η and ξ satisfy*

$$\eta \in \mathcal{G}^{a,\,b},\ \ \xi \notin \mathcal{G}^{a,\,b},\ \ \eta \sim \xi,\ \ \text{and}\ H(\xi) \le \Gamma.$$

Then, we have either $\xi \in \mathcal{N}(\boldsymbol{a})$ and $\eta \in \mathcal{Z}^{a,\,b}$ or $\xi \in \mathcal{N}(\boldsymbol{b})$ and $\eta \in \mathcal{Z}^{b,\,a}$. In particular, we cannot have $\eta \in \mathcal{B}^{a,\,b}$.

Proof. The proof is straightforward from Lemmas 3.9.5 and 3.9.7. □

3.10 Dirichlet form on gateway configurations

In this short section, we record a result which is needed in Chapter 4. *In this subsection, we assume that $q=2$.*

Proposition 3.10.1. *Recall the test function $\widetilde{h}:\mathcal{X}=\{1,\,2\}^\Lambda\to\mathbb{R}$ from Definition 3.5.2. Then, it holds that*

$$\sum_{\{\eta,\xi\}\subseteq\mathcal{X}:\,\{\eta,\xi\}\cap\mathcal{G}^{1,\,2}\neq\emptyset}\mu_\beta(\eta)r_\beta(\eta,\,\xi)\{\widetilde{h}(\xi)-\widetilde{h}(\eta)\}^2=\frac{1+o(1)}{2\kappa}e^{-\Gamma\beta}.$$

Proof. It has already been verified in the proof of Proposition 3.5.6 that

$$\sum_{\{\eta,\xi\}\subseteq\mathcal{E}\cup\mathcal{B}}\mu_\beta(\eta)r_\beta(\eta,\,\xi)\{\widetilde{h}(\xi)-\widetilde{h}(\eta)\}^2=\frac{1+o(1)}{2\kappa}e^{-\Gamma\beta}. \tag{3.140}$$

Then, by the definition of $\widetilde{h}$ given in Definition 3.5.2, $\widetilde{h}\equiv 1$ on $\mathcal{D}^1$ and $\widetilde{h}\equiv 0$ on $\mathcal{D}^2$. Thus, the summation in the left-hand side vanishes if

$$\{\eta,\,\xi\}\subseteq\mathcal{D}^1\quad\text{or}\quad\{\eta,\,\xi\}\subseteq\mathcal{D}^2. \tag{3.141}$$

Proposition 3.4.20 and Definition 3.9.8 imply the following decomposition:

$$\mathcal{E}\cup\mathcal{B}=\mathcal{D}^1\cup\mathcal{G}^{1,\,2}\cup\mathcal{D}^2.$$

Therefore, by (3.141), the left-hand side of (3.140) equals

$$\sum_{\{\eta,\xi\}\subseteq\mathcal{X}:\,\{\eta,\xi\}\cap\mathcal{G}^{1,\,2}\neq\emptyset}\mu_\beta(\eta)r_\beta(\eta,\,\xi)\{\widetilde{h}(\xi)-\widetilde{h}(\eta)\}^2,$$

which concludes the proof of the proposition. □

3.11 Proof of results in Section 3.6

3.11.1 Energy barrier

Proof of Proposition 3.6.5. We fix such a path ω, so that $\omega_0 = \boldsymbol{a}$ and $\omega_N = \boldsymbol{b}$ for some $\boldsymbol{b} \in \breve{\boldsymbol{a}}$, and suppose the contrary that $\Phi_\omega \le 2K+3$. By the formula (3.95), we note that

$$\max_{m\in[\![0,\,KL]\!]} H(\omega_m) \le \max_{m\in[\![0,\,KL-1]\!]} \max_{a\in\Omega} H(\omega_m^{x_m,\,a}) = \Phi_\omega \le 2K+3, \tag{3.142}$$

where x_m is the location of the spin update from ω_m to ω_{m+1}. Therefore, each configuration ω_m has energy at most $2K+3$.

We claim that there exists $m \in [\![0,\, KL]\!]$ such that $\omega_m \in \mathcal{Q}_v^{a_0,\,b}$ for some $a_0 \neq b$ and $v \in [\![2,\, L-3]\!]$, and that the size of protuberance of spin b belongs to $[\![2,\, K-2]\!]$. First, we assume that the claim holds and then prove the theorem. If the claim holds, then we can easily check that $H(\omega_m) = 2K+2$ and for every $x \in \Lambda$,

$$\max_{a\in\Omega} H(\omega_m^{x,\,a}) \in \{2K+4,\, 2K+5,\, 2K+6\}.$$

Here, it is used that $q \ge 3$; this no longer holds if $q = 2$. This implies that

$$\Phi_\omega \ge \max_{a\in\Omega} H(\omega_m^{x_m,\,a}) \ge 2K+4,$$

which contradicts the assumption and thus concludes the proof.

It remains to verify the claim. To this end, we take maximal $m \in [\![0,\, KL]\!]$ such that $\|\omega_m\|_b = \lfloor KL/2 \rfloor + 3$ (cf. (3.121)). We divide the proof into three cases.

(Case 1: ω_m has a horizontal b-bridge without a vertical b-bridge) For this case, since $\Delta H_{c_h}(\omega_m) \ge 2$ for all $h \in [\![1,\, K]\!]$, by (3.122), the fact that $H(\omega_m) \le 2K+3$, and the fact that $\Delta H_{r_v}(\omega_m) \ge 2$ if $\Delta H_{r_v}(\omega_m) > 0$, we deduce that the possibilities lie among:

- **(C1)** $\sum_{v\in\mathbb{T}_L} \Delta H_{r_v}(\omega_m) = 0$ and $\sum_{h\in\mathbb{T}_K} \Delta H_{c_h}(\omega_m) = 2K$,
- **(C2)** $\sum_{v} \Delta H_{r_v}(\omega_m) = 0$ and $\sum_{h} \Delta H_{c_h}(\omega_m) = 2K+1$,
- **(C3)** $\sum_{v} \Delta H_{r_v}(\omega_m) = 0$ and $\sum_{h} \Delta H_{c_h}(\omega_m) = 2K+2$,
- **(C4)** $\sum_{v} \Delta H_{r_v}(\omega_m) = 0$ and $\sum_{h} \Delta H_{c_h}(\omega_m) = 2K+3$,
- **(C5)** $\sum_{v} \Delta H_{r_v}(\omega_m) = 2$ and $\sum_{h} \Delta H_{c_h}(\omega_m) = 2K$,
- **(C6)** $\sum_{v} \Delta H_{r_v}(\omega_m) = 2$ and $\sum_{h} \Delta H_{c_h}(\omega_m) = 2K+1$,
- **(C7)** $\sum_{v} \Delta H_{r_v}(\omega_m) = 3$ and $\sum_{h} \Delta H_{c_h}(\omega_m) = 2K$.

In sub-cases **(C1)**, **(C2)**, **(C3)** and **(C4)**, all rows must be bridges so that all columns are the same. This is impossible since $\|\omega_m\|_b = \lfloor KL/2\rfloor + 3$ cannot be a multiple of $K \geq 11$. In sub-case **(C5)**, it necessarily holds that $\Delta H_{c_h}(\omega_m) = 2$ for all $h \in [\![1, K]\!]$. Then, it is easy to deduce that $\omega_m \in \mathcal{Q}_v^{a_0,b}$ for some $a_0 \neq b$. Moreover, the size of protuberance of b cannot be 1 or $K-1$ since $\lfloor KL/2\rfloor + 3$ cannot be equivalent to ± 1 modulo K. Thus, the claim is proved in this case. In sub-case **(C6)**, the only possible configuration is the one which is obtained from a regular configuration by attaching a protuberance of a third spin. This is impossible by the same logic that $\lfloor KL/2\rfloor + 3$ cannot be equivalent to 0 or ± 1 modulo K. Finally, in sub-case **(C7)**, there exists $v_0 \in \mathbb{T}_L$ such that $\Delta H_{r_{v_0}}(\omega_m) = 3$ and $\Delta H_{r_v}(\omega_m) = 0$ for all $v \neq v_0$. This implies that there are three types of spins in the row r_{v_0} and all the other rows are bridges, but this contradicts the fact that $\Delta H_{c_h}(\omega_m)$ must be 2 for all $h \in \mathbb{T}_K$. Thus, this sub-case is impossible.

Therefore, we conclude the proof of the claim in this case.

(Case 2: ω_m has a vertical b-bridge without a horizontal b-bridge) This case can be handled by the identical manner to **(Case 1)** and we omit the details.

(Case 3: ω_m has a b-cross) In this case, as in the proof of Proposition 3.9.3, define $\widetilde{\sigma} \in \mathcal{X}$ as the configuration obtained from ω_m by replacing all non-b spins with some fixed $a_0 \in S \setminus \{b\}$, i.e., for $x \in \Lambda$,

$$\widetilde{\sigma}(x) = \begin{cases} b & \text{if } \omega_m(x) = b, \\ a_0 & \text{if } \omega_m(x) \neq b, \end{cases}$$

so that $H(\widetilde{\sigma}) \le H(\omega_m)$. Then, we can apply the well-known isoperimetric inequality (e.g. [1, Corollary 2.5]) to the a_0-clusters of $\widetilde{\sigma}$ to deduce

$$H(\widetilde{\sigma}) \ge 4\sqrt{\|\widetilde{\sigma}\|_{a_0}} = 4\sqrt{KL - \left\lfloor \frac{KL}{2} \right\rfloor - 3} > 2K + 4,$$

where we used $L \ge K \ge 11$ at the last inequality. Thus, we obtain $H(\omega_m) > 2K + 3$ which contradicts (3.142). This completes the proof. $\square$

3.11.2 Typical configurations

From now on, we provide proofs of the characterization of typical configurations subjected to the cyclic dynamics, which are formulated in Section 3.6.3. Since the structure is highly similar to the typical configurations with respect to the MH dynamics, we will omit the details if there are no specific novel ideas involved compared to the corresponding previous versions in Sections 3.4 and 3.9.

First, we prove Proposition 3.6.12. We need two lemmas.

Lemma 3.11.1. *For $a, b \in \Omega$, suppose that $\sigma_1 \in \overline{\mathcal{B}}^{a,b}$ and $\sigma_2 \in \mathcal{X}$ satisfy $\sigma_1 \sim \sigma_2$ and $H(\sigma_1, \sigma_2) \le \Gamma$. Then, the following statements hold.*

(1) If $\sigma_1 \in \overline{\mathcal{R}}_v^{a,b}$ for $v \in [\![2, L-2]\!]$, then $\sigma_2 \in \overline{\mathcal{R}}_v^{a,b} \cup \overline{\mathcal{Q}}_{v-1}^{a,b} \cup \overline{\mathcal{Q}}_v^{a,b}$.

(2) If $\sigma_1 \in \overline{\mathcal{B}}_\Gamma^{a,\,b}$*, then* $\sigma_2 \in \overline{\mathcal{B}}^{a,\,b}$*.*

Proof. This lemma can be proved in the exact same way as Lemma 3.9.5, and thus we omit the proof. □

We employ the previous lemma to prove the following crucial lemma.

Lemma 3.11.2. *It holds that* $\widehat{\mathcal{N}}(\overline{\mathcal{B}};\, \overline{\mathcal{E}} \setminus \overline{\mathcal{B}}) = \overline{\mathcal{B}}$*.*

Proof. It suffices to show $\widehat{\mathcal{N}}(\overline{\mathcal{B}};\, \overline{\mathcal{E}} \setminus \overline{\mathcal{B}}) \subseteq \overline{\mathcal{B}}$. If we suppose the contrary, then there must be a first exit from the set $\overline{\mathcal{B}}$ outside $\overline{\mathcal{E}} \setminus \overline{\mathcal{B}}$. This is impossible, since Lemma 3.11.1 implies that we first exit from $\overline{\mathcal{B}}$ via a configuration in $\overline{\mathcal{R}}_2 \subseteq \overline{\mathcal{E}}$. This concludes the proof. □

Proof of Proposition 3.6.12. (1) It suffices to prove that $\{\boldsymbol{b}\} \cap \widehat{\mathcal{N}}(\boldsymbol{a};\, \overline{\mathcal{B}}_\Gamma) = \emptyset$. Suppose the contrary that $(\omega_n)_{n=0}^N$ is a sequence from $\boldsymbol{a}$ to $\boldsymbol{b}$ in $\mathcal{X} \setminus \overline{\mathcal{B}}_\Gamma$ so that $\omega_n \sim \omega_{n+1}$ and $H(\omega_n,\, \omega_{n+1}) \le \Gamma$. Following the proof of Proposition 3.6.5, we again claim that there exists $m \in [\![0,\, KL]\!]$ such that $\omega_m \in \mathcal{Q}_v^{a_0,\,b}$ for some $a_0 \ne b$ and $v \in [\![2,\, L-3]\!]$ and that the size of protuberance of spin b belongs to $[\![2,\, K-2]\!]$. Such configuration belongs to $\overline{\mathcal{B}}_\Gamma$, and thus we are able to conclude the proof by contradiction.

As before, we take maximal $m \in [\![0,\, KL]\!]$ such that $\|\omega_m\|_b = \lfloor KL/2 \rfloor + 3$ (cf. (3.121)). The only difference here with the proof of Proposition 3.6.5 is that we also allow ω_m to have energy $2K + 4$. In turn, we have four additional sub-cases added to the seven sub-cases in **(Case 1)** in the proof of Proposition 3.6.5, namely,

- **(C8)** $\sum_v \Delta H_{r_v}(\omega_m) = 0$ and $\sum_h \Delta H_{c_h}(\omega_m) = 2K + 4$,
- **(C9)** $\sum_v \Delta H_{r_v}(\omega_m) = 2$ and $\sum_h \Delta H_{c_h}(\omega_m) = 2K + 2$,
- **(C10)** $\sum_v \Delta H_{r_v}(\omega_m) = 3$ and $\sum_h \Delta H_{c_h}(\omega_m) = 2K + 1$,

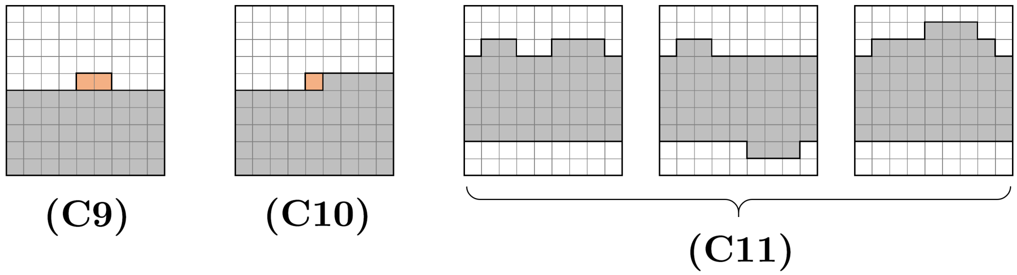


Figure 3.8: Illustration for the proof of Proposition 3.6.12. The figures represent configurations belonging to sub-cases **(C9)**, **(C10)**, and **(C11)**, respectively.

- **(C11)** $\sum_v \Delta H_{r_v}(\omega_m) = 4$ and $\sum_h \Delta H_{c_h}(\omega_m) = 2K$.

Sub-case **(C8)** is impossible since $\|\omega_m\|_b$ cannot be a multiple of K. For sub-case **(C9)**, the only possible type is illustrated in Figure 3.8-left and thus in this case we must have $\|\omega_m\|_b = \lfloor KL/2 \rfloor + 3 \equiv 0$ or ± 2 modulo K. This is impossible for $K \geq 11$.

For **(C10)**, the only possible type of configuration is given in Figure 3.8-middle. Then, to obtain the next configuration ω_{m+1} without exceeding the energy barrier $\Gamma = 2K + 4$, it is mandatory that the spin flip $\omega_m \to \omega_{m+1}$ happens on the single protuberance spin. Since m is maximal, the resulting spin must be b, so that we obtain $\omega_{m+1} \in \overline{\mathcal{B}}_\Gamma$ which contradicts our assumption (here we employed the fact that $\|\omega_m\|_b = \lfloor KL/2 \rfloor + 3$ cannot be equivalent to -2 modulo K). Finally, for sub-case **(C11)**, the possible types of configurations are given in Figure 3.8-right. Note that any update from a configuration of one of these types attains energy barrier at least $2K + 6$, and thus we obtain a contradiction. This completes the proof of part (1).

(2) By definition, we have $\overline{\mathcal{R}}_2^{a,b} \subseteq \overline{\mathcal{B}}^{a,b}$. Moreover, it is verified in Definition 3.6.1 and Lemma 3.6.3 that a part of a canonical path from $\boldsymbol{a}$ to $\boldsymbol{b}$ becomes a Γ-path from $\boldsymbol{a}$ to $\mathcal{R}_2^{a,b}$ in $\mathcal{X} \setminus \overline{\mathcal{B}}_\Gamma$, so that $\mathcal{R}_2^{a,b} \subseteq \overline{\mathcal{E}}^a$. This automatically

implies that $\overline{\mathcal{R}}_2^{a,\,b} \subseteq \overline{\mathcal{E}}^a$. Hence, we have proved

$$\overline{\mathcal{E}}^a \cap \overline{\mathcal{B}}^{a,\,b} \supseteq \overline{\mathcal{R}}_2^{a,\,b}. \tag{3.143}$$

To prove the other direction, observe that

$$\overline{\mathcal{E}}^a \cap \overline{\mathcal{B}}^{a,\,b} \subseteq \overline{\mathcal{B}}^{a,\,b} \setminus \overline{\mathcal{B}}_\Gamma^{a,\,b} = \bigcup_{v \in [\![2,\,L-2]\!]} \overline{\mathcal{R}}_v^{a,\,b}.$$

For $\sigma \in \overline{\mathcal{R}}_v^{a,\,b}$ with $v \in [\![3,\,L-3]\!]$, we cannot have a Γ-path in $\mathcal{X} \setminus \overline{\mathcal{B}}_\Gamma$ from $\boldsymbol{a}$ to σ by part (1) of Lemma 3.11.1. Thus, such σ cannot belong to $\overline{\mathcal{E}}^a$ and we deduce that

$$\overline{\mathcal{E}}^a \cap \overline{\mathcal{B}}^{a,\,b} \subseteq \overline{\mathcal{R}}_2^{a,\,b} \cup \overline{\mathcal{R}}_{L-2}^{a,\,b}. \tag{3.144}$$

Since $\overline{\mathcal{R}}_{L-2}^{a,\,b} \subseteq \overline{\mathcal{E}}^b$ and $\overline{\mathcal{E}}^a \cap \overline{\mathcal{E}}^b = \emptyset$ by part (1), we conclude that

$$\overline{\mathcal{E}}^a \cap \overline{\mathcal{B}}^{a,\,b} \subseteq \overline{\mathcal{R}}_2^{a,\,b}. \tag{3.145}$$

The proof is completed by (3.143) and (3.145).

(3) By the same logic as we obtained (3.144), we deduce that $\overline{\mathcal{E}}^a \cap \overline{\mathcal{B}}^{b,\,c} \subseteq \overline{\mathcal{R}}_2^{b,\,c} \cup \overline{\mathcal{R}}_{L-2}^{b,\,c}$. Since $\overline{\mathcal{R}}_2^{b,\,c} \subseteq \overline{\mathcal{E}}^b$ and $\overline{\mathcal{R}}_{L-2}^{b,\,c} \subseteq \overline{\mathcal{E}}^c$, part (1) implies that $\overline{\mathcal{E}}^a \cap \overline{\mathcal{B}}^{b,\,c} = \emptyset$.

(4) It suffices to prove that

$$\widehat{\mathcal{N}}(\overline{\mathcal{E}} \cup \overline{\mathcal{B}}) \subseteq \overline{\mathcal{E}} \cup \overline{\mathcal{B}}, \tag{3.146}$$

since it is clear that $\overline{\mathcal{E}} \cup \overline{\mathcal{B}} \subseteq \widehat{\mathcal{N}}(\overline{\mathcal{E}} \cup \overline{\mathcal{B}}) = \widehat{\mathcal{N}}(\mathcal{S})$. Indeed, the canonical paths defined in Definition 3.6.1 assure us that $\widehat{\mathcal{N}}(\overline{\mathcal{B}}) = \widehat{\mathcal{N}}(\mathcal{S})$ and by definition and Lemma 3.6.9, $\widehat{\mathcal{N}}(\overline{\mathcal{E}}) \subseteq \widehat{\mathcal{N}}(\mathcal{S})$. To prove (3.146), by Lemma 3.8.1 with $\mathcal{P}_1 = \overline{\mathcal{B}}$, $\mathcal{P}_2 = \overline{\mathcal{E}} \setminus \overline{\mathcal{B}}$, and $\mathcal{Q} = \emptyset$ and Lemma 3.6.9,

$$\widehat{\mathcal{N}}(\overline{\mathcal{E}} \cup \overline{\mathcal{B}}) = \widehat{\mathcal{N}}(\overline{\mathcal{B}};\, \overline{\mathcal{E}} \setminus \overline{\mathcal{B}}) \cup \widehat{\mathcal{N}}(\overline{\mathcal{E}} \setminus \overline{\mathcal{B}};\, \overline{\mathcal{B}}).$$

This completes the proof of (3.146) by Lemma 3.11.2, since we have $\widehat{\mathcal{N}}(\overline{\mathcal{E}} \setminus \overline{\mathcal{B}};\, \overline{\mathcal{B}}) \subseteq \widehat{\mathcal{N}}(\overline{\mathcal{E}};\, \overline{\mathcal{B}}_\Gamma) = \overline{\mathcal{E}}$. $\square$

Finally, we proceed to prove Proposition 3.6.14. First, we state a few lemmas. For $a \in \Omega$, we denote by $\mathcal{N}^{\mathrm{MH}}(\boldsymbol{a})$ the neighborhood of $\boldsymbol{a}$ in the sense of the MH dynamics (cf. Definition 3.4.2).

Lemma 3.11.3. *For every $a \in \Omega$, it holds that $\mathcal{N}^{\mathrm{MH}}(\boldsymbol{a}) \subseteq \mathcal{N}(\boldsymbol{a})$.*

Proof. We take $\sigma \in \mathcal{N}^{\mathrm{MH}}(\boldsymbol{a})$ and prove that $\sigma \in \mathcal{N}(\boldsymbol{a})$. There exists a path $\widetilde{\omega} : \boldsymbol{a} \to \sigma$ subject to the MH dynamics such that $\Phi_{\widetilde{\omega}} \le 2K + 1$. Now, we define a path $\omega : \boldsymbol{a} \to \sigma$ by enlarging each MH-spin update in $\widetilde{\omega}$ by iterating spin rotations on the corresponding site. Then, to prove that $\sigma \in \mathcal{N}(\boldsymbol{a})$, it suffices to demonstrate that $\Phi_\omega \le 2K + 3$.

Consider each pair $(\widetilde{\omega}_m,\, \widetilde{\omega}_{m+1})$ with $\widetilde{\omega}_{m+1} = \widetilde{\omega}_m^{x_m,\, b}$ for some $x_m \in \Lambda$ and $b \in \Omega$, from which the enlarged path becomes $(\omega_n,\, \omega_{n+1},\, \dots,\, \omega_{n+r})$ (so that $\omega_n = \widetilde{\omega}_m$ and $\omega_{n+r} = \widetilde{\omega}_{m+1}$). Then, by (3.5),

$$H(\omega_{n+i},\, \omega_{n+i+1}) = \max_{c \in \Omega} H(\widetilde{\omega}_m^{x_m,\, c}) \quad \text{for all } i \in [\![0,\, r-1]\!].$$

Since $\widetilde{\omega}_m(x_m) \ne \widetilde{\omega}_{m+1}(x_m)$ and $\widetilde{\omega}_m(x) = \widetilde{\omega}_{m+1}(x)$ for all $x \ne x_m$, it holds that

$$\min\Big\{ \sum_{x:\, x \sim x_m} \mathbb{1}\{\widetilde{\omega}_m(x) = \widetilde{\omega}_m(x_m)\},\, \sum_{x:\, x \sim x_m} \mathbb{1}\{\widetilde{\omega}_{m+1}(x) = \widetilde{\omega}_{m+1}(x_m)\} \Big\} \le 2.$$

Indeed, if the minimum is bigger than 2, then x_m must have at least three neighboring sites with spin $\widetilde{\omega}_m(x_m)$ and also at least three neighboring sites with spin $\widetilde{\omega}_{m+1}(x_m)$, which is absurd since x_m has exactly four neighboring sites in Λ. Thus, we deduce that

$$\max_{c \in \Omega} H(\widetilde{\omega}_m^{x_m,\, c}) \le \max\{H(\widetilde{\omega}_m),\, H(\widetilde{\omega}_{m+1})\} + 2.$$

This concludes the proof since Φ_ω equals

$$\max_{n\geq 0} H(\omega_n,\, \omega_{n+1}) \leq \max_{m\geq 0} \big[\max\{H(\widetilde{\omega}_m),\, H(\widetilde{\omega}_{m+1})\} + 2\big] = \Phi_{\widetilde{\omega}} + 2 \leq 2K + 3.$$

□

Lemma 3.11.4. *Fix $a,\, b \in \Omega$ and $\ell \in \mathbb{T}_L$. The following statements hold.*

(1) The sets $\overline{\mathscr{A}}_\ell^{a,\,b}$ and $\overline{\mathscr{B}}_\ell^{a,\,b}$ belong to $\mathcal{Z}_\ell^{a,\,b}$.

(2) It holds that

$$\overline{\mathscr{A}}_\ell^{a,\,b} = \big\{\sigma \in \mathcal{Z}_\ell^{a,\,b} : \exists \zeta \in \mathcal{N}^{\mathrm{MH}}(\boldsymbol{a}) \text{ such that } r_\beta^{\mathrm{MH}}(\sigma,\, \zeta) > 0\big\}, \quad (3.147)$$

(3) It holds that

$$\overline{\mathscr{B}}_\ell^{a,\,b} = \big\{\sigma \in \mathcal{Z}_\ell^{a,\,b} : r_\beta^{\mathrm{MH}}(\sigma,\, \xi_{\ell,\,2}^{a,\,b}) > 0\big\}. \quad (3.148)$$

Proof. (1) Recall from Definition 3.6.13 that

$$\overline{\mathscr{A}}_\ell^{a,\,b} = \overline{\mathcal{Z}}_\ell^{a,\,b} \cap \mathcal{N}(\boldsymbol{a}) \quad \text{and} \quad \overline{\mathscr{B}}_\ell^{a,\,b} = \overline{\mathcal{Z}}_\ell^{a,\,b} \cap \overline{\xi}_{\ell,\,2}^{a,\,b}.$$

It suffices to prove that a configuration $\sigma \in \overline{\mathcal{Z}}_\ell^{a,\,b} \setminus \mathcal{Z}_\ell^{a,\,b}$ cannot belong to $\mathcal{N}(\boldsymbol{a}) \cup \overline{\xi}_{\ell,\,2}^{a,\,b}$. Indeed, such σ has a single spin $c \in \Omega \setminus \{a,\, b\}$ which is obtained by a spin update from a configuration in $\mathcal{Z}_\ell^{a,\,b}$, and thus we can verify that this update increases the energy by 2 and thus $H(\sigma) = 2K + 4$. This clearly implies that $\sigma \notin \mathcal{N}(\boldsymbol{a})$, since every configuration in $\mathcal{N}(\boldsymbol{a})$ has energy at most $2K + 3$. Moreover, suppose the contrary that $\sigma \in \overline{\xi}_{\ell,\,2}^{a,\,b}$. Then, since σ has a single spin c and $H(\xi_{\ell,\,2}^{a,\,b}) = 2K$, σ must be obtained from $\xi_{\ell,\,2}^{a,\,b}$ by an update from a spin (a or b) to c which increases the energy by 4. This contradicts the previous observation, and thus we conclude that $\sigma \notin \overline{\xi}_{\ell,\,2}^{a,\,b}$.

(2) First, we prove the $\supseteq$-part of (3.147). To this end, suppose that $\sigma \in \mathcal{Z}_\ell^{a,\,b}$ and $\zeta \in \mathcal{N}^{\mathrm{MH}}(\boldsymbol{a})$ satisfy $r_\beta^{\mathrm{MH}}(\sigma,\, \zeta) > 0$. By property **[Z1]** of Proposition

3.4.18, σ consists of spins a and b only. Moreover, the fact that $r_\beta^{\mathrm{MH}}(\sigma, \zeta) > 0$ and $H(\zeta) < H(\sigma)$ implies that the MH-spin flip $\sigma \to \zeta$ occurs on some $x_0 \in \Lambda$ in either way:

- $a \to b$ where a has three neighboring spins b and one neighboring spin a,
- $b \to a$ where b has three neighboring spins a and one neighboring spin b.

In any cases, we may obtain σ by iterating the spin rotation τ_{x_0} to ζ. Then, by (3.5) and the presence of three same spins on the nearest neighbors of x_0, the height along that path $\zeta \to \sigma$ equals (cf. (3.99))

$$\max_{\mathfrak{O}(\zeta,\sigma)} H = 2K + 3.$$

Next, by Lemma 3.11.3, we have $\zeta \in \mathcal{N}(\boldsymbol{a})$ and thus there exists a $(2K+3)$-path from $\boldsymbol{a}$ to ζ. Therefore, concatenating this path before the previously-defined path $\zeta \to \sigma$, we obtain a $(2K+3)$-path from $\boldsymbol{a}$ to σ. This deduces that $\sigma \in \mathcal{N}(\boldsymbol{a})$, and thus we have proved the $\supseteq$-part.

To prove the $\subseteq$-part of (3.147), fix $\sigma \in \overline{\mathscr{A}}_\ell^{a,b} = \overline{\mathcal{Z}}_\ell^{a,b} \cap \mathcal{N}(\boldsymbol{a})$. By part (1), we know that $\sigma \in \mathcal{Z}_\ell^{a,b} \cap \mathcal{N}(\boldsymbol{a})$, so that we may apply Proposition 3.4.18. Since $\sigma \in \mathcal{N}(\boldsymbol{a})$, there exists $\sigma_0 \in \mathcal{X}$ such that $r_\beta(\sigma_0, \sigma) > 0$ and $H(\sigma_0, \sigma) \le 2K+3$. Then, it is immediate that $r_\beta^{\mathrm{MH}}(\sigma, \sigma_0) > 0$. According to properties **[Z1]** and **[Z2]** in Proposition 3.4.18, this can only happen when the MH-spin flip $\sigma \to \sigma_0$ occurs on $x_0 \in \Lambda$ in either way:

- $a \to c$ for some $c \neq a$, where a has three neighboring spins b and one neighboring spin a,
- $b \to c$ for some $c \neq b$, where b has three neighboring spins a and one neighboring spin b.

According to Proposition 3.4.18, the former case implies that x_0 is the only site with spin a on the strip $\mathbb{T}_K \times \{\ell,\, \ell+1\}$ (or $\{\ell,\, \ell+1\} \times \mathbb{T}_K$ if $K = L$), and thus $\sigma \in \overline{\mathcal{R}}_2^{a,\,b}$, which is clearly impossible. Therefore, the second case must hold.

Now, we define a new configuration σ_1 as

$$\sigma_1(x) = \begin{cases} \sigma(x) & \text{if } x \neq x_0, \\ a & \text{if } x = x_0. \end{cases}$$

Then, $r_\beta^{\mathrm{MH}}(\sigma,\, \sigma_1) > 0$. Moreover, since x_0 has three neighboring spins a, $H(\sigma_1) = 2K$. Thus, by Proposition 3.9.3, we readily deduce that $\sigma_1 \in \mathcal{N}^{\mathrm{MH}}(\boldsymbol{a})$. This concludes the proof of part (2).

(3) This can be proved in a nearly same manner to part (2), and thus we omit the proof. □

Finally, we present a proof of Proposition 3.6.14.

Proof of Proposition 3.6.14. To prove that the constant $\overline{\mathfrak{e}}_0^{a,\,b}$ is independent of $a,\, b \in \Omega$, we first denote by $\widetilde{\mathfrak{Z}}_\ell^{a,\,b}(\cdot)$ the trace of the process $\overline{\mathfrak{Z}}_\ell^{a,\,b}(\cdot)$ to the subset $\mathcal{Z}_\ell^{a,\,b} \subseteq \overline{\mathcal{Z}}_\ell^{a,\,b}$ (cf. Section 3.1.2). Then, by [5, Corollary 6.2], the jump rate $\widetilde{\mathfrak{r}}_\ell^{a,\,b}(\cdot,\, \cdot)$ of the process $\widetilde{\mathfrak{Z}}_\ell^{a,\,b}(\cdot)$ can be written as

$$\widetilde{\mathfrak{r}}_\ell^{a,\,b}(\sigma_1,\, \sigma_2) = \overline{\mathfrak{r}}_\ell^{a,\,b}(\sigma_1,\, \sigma_2) + \sum_{\zeta \in \overline{\mathcal{Z}}_\ell^{a,\,b} \setminus \mathcal{Z}_\ell^{a,\,b}} \overline{\mathfrak{r}}_\ell^{a,\,b}(\sigma_1,\, \zeta) \cdot \mathbf{P}_\zeta[\tau_{\mathcal{Z}_\ell^{a,\,b}} = \tau_{\sigma_2}]$$

for all $\sigma_1,\, \sigma_2 \in \mathcal{Z}_\ell^{a,\,b}$, where $\mathbf{P}_\zeta$ denotes the law of the process $\overline{\mathfrak{Z}}_\ell^{a,\,b}(\cdot)$ starting from ζ. Thus, by the cyclic structure of the set $\overline{\mathcal{Z}}_\ell^{a,\,b}$, we can observe that

$$\widetilde{\mathfrak{r}}_\ell^{a,\,b}(\sigma_1,\, \sigma_2) = \mathbb{1}\big\{r_\beta^{\mathrm{MH}}(\sigma_1,\, \sigma_2) > 0\big\},$$

and hence the trace process $\widetilde{\mathfrak{Z}}_\ell^{a,\,b}(\cdot)$ is equivalent to the Markov chain defined in Definition 3.4.21 restricted to $\mathcal{Z}_\ell^{a,\,b}$. In particular, it does not depend on

$a,\, b \in \Omega$.

Denote by $\widetilde{\mathfrak{cap}}^{a,\,b}(\cdot,\,\cdot)$ the capacity with respect to the process $\widetilde{\mathfrak{Z}}_\ell^{a,\,b}(\cdot)$ on $\mathscr{Z}_\ell^{a,\,b}$. Then, by [7, (A.10)], we can write (recall that $\overline{\mathscr{A}}_\ell^{a,\,b}$ and $\overline{\mathscr{B}}_\ell^{a,\,b}$ are subsets of $\mathscr{Z}_\ell^{a,\,b}$ by Lemma 3.11.4-(1)),

$$\frac{1}{\bar{\mathfrak{e}}_0^{a,\,b}} = |\overline{\mathscr{V}}_\ell^{a,\,b}| \cdot \overline{\mathfrak{cap}}^{a,\,b}(\overline{\mathscr{A}}_\ell^{a,\,b},\, \overline{\mathscr{B}}_\ell^{a,\,b}) = \big(|\overline{\mathscr{A}}_\ell^{a,\,b}| + |\overline{\mathscr{B}}_\ell^{a,\,b}|\big) \cdot \widetilde{\mathfrak{cap}}^{a,\,b}(\overline{\mathscr{A}}_\ell^{a,\,b},\, \overline{\mathscr{B}}_\ell^{a,\,b}). \tag{3.149}$$

By Proposition 3.4.18, Definition 3.4.19, and Lemma 3.11.4, we notice that the Markov chain $\widetilde{\mathfrak{Z}}_\ell^{a,\,b}(\cdot)$ and the sets $\overline{\mathscr{A}}_\ell^{a,\,b}$ and $\overline{\mathscr{B}}_\ell^{a,\,b}$ have the same structure for all $a,\, b \in \Omega$. Therefore, we conclude from the expression (3.149) that the constant $\bar{\mathfrak{e}}_0^{a,\,b}$ does not depend on $a,\, b \in \Omega$, and we have proved the first statement of the proposition.

Next, we estimate $\bar{\mathfrak{e}}_0^{a,\,b}$. Since it does not depend on $a,\, b \in \Omega$ by the first statement, we may assume that $a = 1$ and $b = 2$. By the same logic with the proof of Proposition 3.4.23 (given in Section 3.9.4), we write

$$\overline{\mathfrak{cap}}_\ell^{1,\,2}(\overline{\mathscr{A}}_\ell^{1,\,2},\, \overline{\mathscr{B}}_\ell^{1,\,2}) = \overline{\mathfrak{D}}^{1,\,2}(\bar{\mathfrak{f}}^{1,\,2}) = \frac{1}{2} \sum_{x,\, y \in \overline{\mathscr{V}}^{1,\,2}} \frac{1}{|\overline{\mathscr{V}}^{1,\,2}|} \bar{\mathfrak{r}}^{1,\,2}(x,\, y)[\bar{\mathfrak{f}}^{1,\,2}(y) - \bar{\mathfrak{f}}^{1,\,2}(x)]^2.$$

For each $k \in \mathbb{T}_K$, we consider a path $\omega^{(k)} = (\omega_n^{(k)})_{n=0}^{K-2}$ where $\omega_n^{(k)} = \xi_{\ell,\,1;\,k,\,n+1}^{1,\,2,\,+}$ for $n \in [\![0,\, K-2]\!]$. Note that $\xi_{\ell,\,1;\,k,\,1}^{1,\,2,\,+} \in \overline{\mathscr{A}}_\ell^{1,\,2}$ and $\xi_{\ell,\,1;\,k,\,K-1}^{1,\,2,\,+} \in \overline{\mathscr{B}}_\ell^{1,\,2}$. Thus, we have

$$\overline{\mathfrak{cap}}_\ell^{1,\,2}(\overline{\mathscr{A}}_\ell^{1,\,2},\, \overline{\mathscr{B}}_\ell^{1,\,2}) \geq \frac{1}{2} \sum_{k \in \mathbb{T}_K} \sum_{n=0}^{K-3} \frac{1}{|\overline{\mathscr{V}}^{1,\,2}|} [\bar{\mathfrak{f}}^{1,\,2}(\omega_{n+1}^{(k)}) - \bar{\mathfrak{f}}^{1,\,2}(\omega_n^{(k)})]^2.$$

By the Cauchy–Schwarz inequality,

$$\begin{aligned}\overline{\mathfrak{cap}}_\ell^{1,2}(\overline{\mathscr{A}}_\ell^{1,2},\,\overline{\mathscr{B}}_\ell^{1,2}) &\ge \frac{1}{2|\overline{\mathscr{V}}^{1,2}|}\sum_{k\in\mathbb{T}_K}\frac{1}{K-2}\Big[\sum_{n=0}^{K-3}[\bar{\mathfrak{f}}^{1,2}(\omega_{n+1}^{(k)})-\bar{\mathfrak{f}}^{1,2}(\omega_n^{(k)})]\Big]^2\\ &=\frac{K}{2(K-2)|\overline{\mathscr{V}}^{1,2}|},\end{aligned}$$

where the last equality follows from

$$\bar{\mathfrak{f}}^{1,2}(\omega_0^{(k)})=\bar{\mathfrak{f}}^{1,2}(\xi_{\ell,\,1;\,k,\,1}^{1,\,2,\,+})=1\quad\text{and}\quad\bar{\mathfrak{f}}^{1,2}(\omega_{K-2}^{(k)})=\bar{\mathfrak{f}}^{1,2}(\xi_{\ell,\,1;\,k,\,K-1}^{1,\,2,\,+})=0.$$

This proves that $\overline{\mathfrak{cap}}_\ell^{1,2}(\overline{\mathscr{A}}_\ell^{1,2},\,\overline{\mathscr{B}}_\ell^{1,2})\cdot|\overline{\mathscr{V}}^{1,2}|>\frac{1}{2}$, and the proof is completed. □

Chapter 4

Three-dimensional model

In this chapter, we deal with the Ising/Potts models with zero external fields on the 3D lattice. We fix three positive integers $K \le L \le M$. Then, we denote by

$$\Lambda = [\![1,\, K]\!] \times [\![1,\, L]\!] \times [\![1,\, M]\!]$$

the 3D lattice box. Again, we impose either open or periodic boundary conditions upon the lattice box Λ. For the latter boundary condition, we can write

$$\Lambda = \mathbb{T}_K \times \mathbb{T}_L \times \mathbb{T}_M. \tag{4.1}$$

The Hamiltonian and the Gibbs distribution are given as in (3.2) and Definition 2.0.2. Moreover, the ground states are collected, as done in the previous chapter, as

$$\mathcal{S} = \{\mathbf{1},\, \mathbf{2},\, \dots,\, \boldsymbol{q}\}. \tag{4.2}$$

The following theorem is an analogue of Theorem 3.0.1.

Theorem 4.0.1. *We have*

$$Z_\beta = q + O(e^{-6\beta}). \tag{4.3}$$

Thus, we obtain

$$\lim_{\beta\to\infty} \mu_\beta(\boldsymbol{s}) = \frac{1}{q} \textit{ for all } \boldsymbol{s} \in \mathcal{S} \quad \textit{and} \quad \lim_{\beta\to\infty} \mu_\beta(\mathcal{S}) = 1.$$

On this model, we impose the MH dynamics $\sigma_\beta(t) = \sigma_\beta^{\mathrm{MH}}(t)$, $t \geq 0$ as defined in Definition (2.0.1). For $\sigma, \zeta \in \mathcal{X}$, we write $\sigma \sim \zeta$ if $r_\beta(\sigma, \zeta) > 0$. Again, the detailed balance condition holds:

$$\mu_\beta(\sigma) r_\beta(\sigma, \zeta) = \mu_\beta(\zeta) r_\beta(\zeta, \sigma) = \begin{cases} \min\{\mu_\beta(\sigma), \mu_\beta(\zeta)\} & \text{if } \sigma \sim \zeta, \\ 0 & \text{otherwise.} \end{cases} \tag{4.4}$$

Remark 4.0.2. We employ the continuous-time dynamics (as applied in numerous previous studies) because it offers a simpler presentation than the corresponding discrete dynamics (as demonstrated in [9, 22, 69]), for which the jump probability is given by

$$p_\beta(\sigma, \zeta) = \begin{cases} \dfrac{1}{q|\Lambda|} \cdot e^{-\beta \max\{H(\zeta) - H(\sigma), 0\}} & \text{if } \zeta = \sigma^{x, a} \neq \sigma, \ x \in \Lambda, \ a \in \Omega, \\ 1 - \displaystyle\sum_{x \in \Lambda, a \in \Omega: \sigma^{x, a} \neq \sigma} p_\beta(\sigma, \sigma^{x, a}) & \text{if } \zeta = \sigma, \\ 0 & \text{otherwise.} \end{cases} \tag{4.5}$$

However, our computations can be applied to this model as well. See also Remark 4.1.11.

4.1 Main results

4.1.1 Large deviation-type results

Here, we explain the large deviation-type results obtained for the metastable behavior.

Energy barrier between ground states

Recall the energy barrier and communication height defined in Section 3.1. We define

$$\Gamma = \Gamma^{3D} = \Gamma^{3D}(K,\, L,\, M) = \Phi(\boldsymbol{s},\, \boldsymbol{s'}) \quad \text{for all } \boldsymbol{s},\, \boldsymbol{s'} \in \mathcal{S}.$$

Note that $\Phi(\boldsymbol{s},\, \boldsymbol{s'})$ does not depend on the selections of $\boldsymbol{s},\, \boldsymbol{s'} \in \mathcal{S}$, owing to the model symmetry. Additionally, note that Γ represents the *energy barrier* between ground states, because the dynamics must overcome this energy level to make a transition from one ground state to another.

To characterize the energy barrier, we must check the maximum energy of all paths connecting the ground states. Thus, the energy barrier is a global feature of the energy landscape, and characterizing it is a non-trivial task. For the current model, we can identify the exact value of the energy barrier. Recall that we assumed $K \le L \le M$.

Theorem 4.1.1. *For all sufficiently large K, it holds that*

$$\Gamma = \begin{cases} 2KL + 2K + 2 & \textit{under periodic boundary conditions,} \\ KL + K + 1 & \textit{under open boundary conditions.} \end{cases} \tag{4.6}$$

Remark 4.1.2. Our arguments state that this theorem holds for $K \ge 2829$, where the threshold 2829 may be sub-optimal (cf. Remark 4.5.4). However, the optimality of this threshold is a minor issue, because our main concern is the spin system on large boxes. *Henceforth, we assume that K satisfies this condition, i.e., $K \ge 2829$.*

Theorem 4.1.1 is proved in Section 4.5.

Remark 4.1.3. Several remarks regarding the previous theorem are in order.

(1) Note that Theorem 4.1.1 does not depend on the value of q, because in the transition from $\boldsymbol{a}$ to $\boldsymbol{b}$ for $a,\, b \in \Omega$, no spins besides a and b play a significant role.

(2) Suppose temporarily that Γ_d is the energy barrier, defined in the same way as above, subjected to Ising/Potts models defined on a d-dimensional lattice box of size $K_1 \times \cdots \times K_d$ with $K_1 \leq \cdots \leq K_d$. Then, we expect that $\Gamma_d = 2 + 2\sum_{n=1}^{d-1}\prod_{i=1}^{n} K_i$ under periodic boundary conditions and $\Gamma_d = 1 + \sum_{n=1}^{d-1}\prod_{i=1}^{n} K_i$ under open boundary conditions for all $d \geq 2$. Notice that the case of $d = 2$ is handled in [69, Theorem 1.1] and the case of $d = 3$ is handled in Theorem 4.1.1. We leave the verification of this conjecture for the case of $d \geq 4$ as a future research problem.

Large deviation-type results based on pathwise approach

Here, we explain the large deviation-type analysis of the metastable behavior of the Metropolis–Hastings dynamics. These results can be obtained via the pathwise approach developed in [24], provided that we can analyze the model energy landscape to a certain degree of precision. We refer to the monograph [75] for an extensive summary of the pathwise approach. This approach allows us to analyze the metastability from three different perspectives: transition time, spectral gap, and mixing time. All these quantities are crucial for quantifying the metastable behavior. First, we explicitly define them as follows:

- For $\boldsymbol{s} \in \mathcal{S}$, we write $\breve{\boldsymbol{s}} = \mathcal{S} \setminus \{\boldsymbol{s}\}$. Then, our primary concern is the hitting time $\tau_{\breve{\boldsymbol{s}}}$ or $\tau_{\boldsymbol{s}'}$ for $\boldsymbol{s}' \in \breve{\boldsymbol{s}}$ when the dynamics starts from $\boldsymbol{s} \in \mathcal{S}$.
- The *mixing time* corresponding to the level $\epsilon \in (0, 1)$ is defined as

$$t_\beta^{\mathrm{mix}}(\epsilon) = \min\left\{t \geq 0 : \max_{\sigma \in \mathcal{X}} \|\mathbb{P}_\sigma[\sigma_\beta(t) \in \cdot] - \mu_\beta(\cdot)\|_{\mathrm{TV}} \leq \epsilon\right\},$$

where $\|\cdot\|_{\mathrm{TV}}$ represents the total variation distance between measures (cf. [66, Chapter 4]).

- We denote by λ_β the *spectral gap* of the MH dynamics.

The 2D version of the following theorem was established in [69] using the refined pathwise approach developed in [27, 67, 70]. We extend their results to the 3D model.

Theorem 4.1.4. *The following statements hold.*

(1) ***(Transition time)*** *For all* $\boldsymbol{s}$, $\boldsymbol{s'} \in \mathcal{S}$ *and* $\epsilon > 0$*, we have*

$$\lim_{\beta\to\infty} \mathbb{P}_{\boldsymbol{s}}[e^{\beta(\Gamma-\epsilon)} < \tau_{\breve{\boldsymbol{s}}} \le \tau_{\boldsymbol{s'}} < e^{\beta(\Gamma+\epsilon)}] = 1, \tag{4.7}$$

$$\lim_{\beta\to\infty} \frac{1}{\beta} \log \mathbb{E}_{\boldsymbol{s}}[\tau_{\breve{\boldsymbol{s}}}] = \lim_{\beta\to\infty} \frac{1}{\beta} \log \mathbb{E}_{\boldsymbol{s}}[\tau_{\boldsymbol{s'}}] = \Gamma. \tag{4.8}$$

Moreover, under $\mathbb{P}_{\boldsymbol{s}}$*, as* $\beta \to \infty$*,*

$$\frac{\tau_{\breve{\boldsymbol{s}}}}{\mathbb{E}_{\boldsymbol{s}}[\tau_{\breve{\boldsymbol{s}}}]},\ \frac{\tau_{\boldsymbol{s'}}}{\mathbb{E}_{\boldsymbol{s}}[\tau_{\boldsymbol{s'}}]} \rightharpoonup \mathrm{Exp}(1), \tag{4.9}$$

where Exp(1) *is the exponential random variable with a mean value of* 1*.*

(2) ***(Mixing time)*** *For all* $\epsilon \in (0,\, 1/2)$*, the mixing time satisfies*

$$\lim_{\beta\to\infty} \frac{1}{\beta} \log t_\beta^{\mathrm{mix}}(\epsilon) = \Gamma.$$

(3) ***(Spectral gap)*** *There exist two constants* $0 < c_1 \le c_2$ *such that*

$$c_1 e^{-\beta\Gamma} \le \lambda_\beta \le c_2 e^{-\beta\Gamma}.$$

Remark 4.1.5. The above theorem holds under both open and periodic boundary conditions.

Theorem 4.1.4 states that the metastable transition time, mixing time, and inverse spectral gap become exponentially large as $\beta \to \infty$, and their exponential growth rates are determined by the energy barrier Γ.

The robust methodology developed in [27, 67, 70] implies that characterizing the energy barrier between ground states and identifying all the deepest valleys suffice (up to several technical issues) to confirm the results presented in Theorem 4.1.4. In [69], the authors performed corresponding analyses of the energy landscape; then, they used this robust methodology to prove Theorem 4.1.4 for two dimensions. We perform the corresponding analysis of the energy landscape for the 3D model as well in Sections 4.3, 4.4, and 4.5. The proof of Theorem 4.1.4 is given in Section 4.5.3. Analysis of the energy landscape is far more difficult than that of the 2D one considered in Chapter 3 for several reasons. Details are presented at the beginning of Section 4.3.

Characterization of transition path

Our analysis of the energy landscape is sufficiently precise to characterize all the possible transition paths between ground states in a high level of detail. The *transition paths* are rigorously defined in Definition 4.6.13; we do not present explicit definitions here, because we would have to define a large amount of notation. The following theorem asserts that, with dominating probability, the MH dynamics evolves along one of the transition paths when a transition occurs from one ground state to another.

Theorem 4.1.6. *For all $\boldsymbol{s} \in \mathcal{S}$, we have*

$$\mathbb{P}_{\boldsymbol{s}}\big[\exists 0 < t_1 < \cdots < t_N < \tau_{\breve{\boldsymbol{s}}} \textit{ s.t. } (\sigma_\beta(t_n))_{n=1}^N \textit{ is a transition path } \boldsymbol{s} \leftrightarrow \breve{\boldsymbol{s}}\big]$$
$$= 1 - o(1).$$

The characterization of the transition paths and the proof of this theorem are given in Section 4.6.4.

4.1.2 Eyring–Kramers formula and model reduction

The following results constitute more quantitative analyses of the metastable behavior obtained using potential-theoretic methods. In particular, we obtain the Eyring–Kramers formula (which is a considerable refinement of (4.8)) and the Markov chain model reduction of metastable behavior.

For these results, we require an accurate understanding of the energy landscape and the behavior of the MH dynamics on a large set of saddle configurations between ground states. We conduct these analyses in Sections 4.6 and 4.7.

We further remark that the quantitative results given below depend on the selection of boundary condition, in contrast to Theorems 4.1.4 and 4.1.6 (cf. Remark 4.1.5). For brevity, we assume periodic boundary conditions throughout this subsection. We can treat the open boundary case in a similar manner; the results and a sketch of the proof are presented in Section 4.8.

Eyring–Kramers formula

The following result constitutes a refinement of (4.8) (and hence of (4.9)) that allows us to pin down the sub-exponential prefactor associated with the large deviation-type exponential estimates of the mean transition time between ground states.

Theorem 4.1.7. *There exists a constant* $\kappa = \kappa(K,\, L,\, M) > 0$ *such that for all* $\boldsymbol{s},\, \boldsymbol{s'} \in \mathcal{S}$*,*

$$\mathbb{E}_{\boldsymbol{s}}^{\beta}[\tau_{\breve{\boldsymbol{s}}}] = (1 + o(1)) \cdot \frac{\kappa}{q-1} e^{\Gamma\beta} \quad \textit{and} \quad \mathbb{E}_{\boldsymbol{s}}^{\beta}[\tau_{\boldsymbol{s'}}] = (1 + o(1)) \cdot \kappa e^{\Gamma\beta}. \tag{4.10}$$

Moreover, the constant κ *satisfies*

$$\lim_{K\to\infty} \kappa(K,\, L,\, M) = \begin{cases} 1/8 & \textit{if } K < L < M, \\ 1/16 & \textit{if } K = L < M \textit{ or } K < L = M, \\ 1/48 & \textit{if } K = L = M. \end{cases} \tag{4.11}$$

Remark 4.1.8. Here, we make several comments regarding Theorem 4.8.1.

(1) Although we do not present the exact formula for the constant κ in

the theorem, they can be explicitly expressed in terms of potential-theoretic notions relevant to a random walk defined in a complicated space (cf. (4.15) and (4.16) for the formulas). This random walk is vague (cf. Proposition 4.6.9) compared with the corresponding random walk identified in Proposition 3.4.23 for the 2D model, which reflects the complexity of the energy landscape of the 3D model compared with that of the 2D one.

(2) The constant κ is model-dependent. For different Glauber dynamics (even with identical boundary conditions), this constant may differ.

(3) If $K < L < M$, the transition between ground states must occur in a specific direction; meanwhile, if $K = L < M$ or $K < L = M$, there are two possible directions for the transition. If $K = L = M$, there are six possible directions. This explains the dependence of the asymptotics of κ on the relationships among K, L, and M.

We require precise analyses of the energy landscape and the behavior of the underlying metastable processes on a certain neighborhood of saddle configurations between metastable sets. In most other models for which the Eyring–Kramers formula can be obtained via such robust strategies, the energy landscape is relatively simple; hence, the landscape only marginally presents serious mathematical issues. However, in the current model, the saddle consists of a very large collection of saddle configurations, which form a complex structure. Analyzing this structure is a highly complicated task; moreover, it is difficult to assess the behavior of the dynamics in the neighborhood of this large set with adequate precision. The achievement of these tasks is one of the main contributions presented in this chapter. We emphasize here that the H^1-approximation technique, which is used in the proof of the main results in a critical manner, is particularly handy for models with complicated landscapes, such as the one considered here.

Markov chain model reduction of metastable behavior

Recall the accelerated process $\widehat{\sigma}_\beta(t)$, $t \ge 0$ and the accelerated trace process $Y_\beta(t)$, $t \ge 0$ introduced in Section 3.1.2, here subjected to the 3D model. Moreover, in view of the second estimate of (4.10), we define the limiting Markov chain $\{Y(t)\}_{t\ge 0}$ on $\mathcal{S}$, which expresses the asymptotic behavior of the accelerated process $\widehat{\sigma}_\beta(\cdot)$ between the ground states as a continuous-time Markov chain with jump rate

$$r_Y(\boldsymbol{s},\, \boldsymbol{s'}) = \kappa^{-1} \quad \text{for all } \boldsymbol{s},\, \boldsymbol{s'} \in \mathcal{S}. \tag{4.12}$$

Theorem 4.1.9. *The following statements hold.*

(1) The law of the Markov chain $Y_\beta(\cdot)$ converges to that of the limiting Markov chain $Y(\cdot)$ as $\beta \to \infty$, in the usual Skorokhod topology.

(2) It holds that

$$\lim_{\beta\to\infty} \max_{\boldsymbol{s}\in\mathcal{S}} \mathbb{E}_{\boldsymbol{s}}\Big[\int_0^t \mathbb{1}\{\widehat{\sigma}_\beta(u) \notin \mathcal{S}\} du\Big] = 0.$$

Remark 4.1.10. Temporarily, we denote by $\mathbf{E}_{\boldsymbol{s}}$ the law of the limiting Markov chain $Y(\cdot)$ starting from $\boldsymbol{s} \in \mathcal{S}$. Theorem 4.1.9 is consistent with Theorem 4.1.7, in that for any $\boldsymbol{s'} \in \breve{\boldsymbol{s}}$, we have $\mathbf{E}_{\boldsymbol{s}}[\tau_{\boldsymbol{s'}}] = \kappa$.

Remark 4.1.11 (Discrete Metropolis–Hastings dynamics). The only difference in the discrete dynamics defined by (4.5) is that it is $q|\Lambda|$ times slower than the continuous dynamics (in the average sense). Therefore, Theorems 4.1.1, 4.1.4, and 4.1.6 are valid for this dynamics without any modification. Theorems 4.8.1 and 4.1.9 hold provided that we replace the constant κ with $\kappa' = q|\Lambda| \cdot \kappa$. The rigorous verification of the result proceeds in a similar way; thus, we do not repeat it here.

Outlook of proofs of main results

To prove Theorems 4.1.1 and 4.1.4, which fall into the category of pathwise-type metastability results, we investigate the energy landscape of the Ising/Potts models on the 3D lattice Λ, as described in Sections 4.3, 4.4, and 4.5. Along the investigation, we present proofs of Theorems 4.1.1 and 4.1.4 in Section 4.5. Then, we proceed to the proofs of Theorems 4.8.1 and 4.1.9, which require more accurate analyses of the energy landscape than the previous theorems. These detailed analyses are presented in Section 4.6, and as a byproduct we present the proof of Theorem 4.1.6 in Section 4.6.4. Then, we present the proofs of Theorems 4.8.1 and 4.1.9 in Section 4.7.

Non-reversible models

The stochastic system considered in this chapter is the continuous-time MH dynamics, which is reversible with respect to the Gibbs distribution μ_β. In fact, as done in Chapter 3, we can consider various dynamics with invariant distribution μ_β but are non-reversible with respect to this measure. Since the approximation method and the pathwise approach used in the proof of the main results presented above are robust and can be used in the non-reversible setting as well, we can analyze the 3D version of the non-reversible models and obtain similar results.

4.2 Outline of the proof

Recall the strategy explained in Section 3.2. We define the constant $\kappa = \kappa(K,\, L,\, M)$ that appears in Theorems 4.8.1 and 4.1.9.

- Let $\mathfrak{m}_K = \lfloor K^{2/3} \rfloor$, and let $\kappa^{2\text{D}} = \kappa^{2\text{D}}(K,\, L)$ be the constant $\kappa(K,\, L)$ that appears in Theorem (3.1.2). Then, for $n \in [\![1,\, q-1]\!]$, the bulk constant $\mathfrak{b}(n)$ is defined explicitly as

$$\mathfrak{b}(n)=\begin{cases}\dfrac{1}{n(q-n)}\cdot\dfrac{M-2\mathfrak{m}_K}{2M}\cdot\kappa^{2\mathrm{D}}(K,\,L) & \text{if } K<L<M,\\ \dfrac{1}{n(q-n)}\cdot\dfrac{M-2\mathfrak{m}_K}{2M}\cdot\kappa^{2\mathrm{D}}(K,\,L) & \text{if } K=L<M,\\ \dfrac{1}{n(q-n)}\cdot\dfrac{M-2\mathfrak{m}_K}{4M}\cdot\kappa^{2\mathrm{D}}(K,\,L) & \text{if } K<L=M,\\ \dfrac{1}{n(q-n)}\cdot\dfrac{M-2\mathfrak{m}_K}{6M}\cdot\kappa^{2\mathrm{D}}(K,\,L) & \text{if } K=L=M.\end{cases} \tag{4.13}$$

- The edge constant $\mathfrak{e}(n)$, $n\in[\![1,\,q-1]\!]$, is defined in (4.116). Furthermore, it is verified in Proposition 4.6.9 that

$$0<\mathfrak{e}(n)\le\frac{1}{K^{1/3}}\quad\text{for all } n\in[\![1,\,q-1]\!]. \tag{4.14}$$

- Then, for $n\in[\![1,\,q-1]\!]$, we define the constant

$$\mathfrak{c}(n)=\mathfrak{b}(n)+\mathfrak{e}(n)+\mathfrak{e}(q-n). \tag{4.15}$$

We remark that by definition, $\mathfrak{b}(n)=\mathfrak{b}(q-n)$ for $n\in[\![1,\,q-1]\!]$; therefore, we have $\mathfrak{c}(n)=\mathfrak{c}(q-n)$. Finally, we define the constant κ that appears in Theorem 4.1.7 as

$$\kappa=(q-1)\mathfrak{c}(1). \tag{4.16}$$

For $A\subseteq\Omega$, we define (cf. (4.2))

$$\mathcal{S}(A)=\{\boldsymbol{a}:a\in A\}.$$

A pair $(A,\,B)$ of two subsets A and B of Ω is referred to as a *proper partition* of Ω if A and B are non-empty subsets of Ω satisfying $A\cup B=\Omega$ and $A\cap B=\emptyset$. Our aim is to estimate the capacity between $\mathcal{S}(A)$ and $\mathcal{S}(B)$

for proper partitions $(A,\, B)$ of Ω. The following theorem expresses the key capacity estimate:

Theorem 4.2.1. *It holds for any proper partition* $(A,\, B)$ *of* Ω *that*

$$\mathrm{Cap}_\beta(\mathcal{S}(A),\, \mathcal{S}(B)) = \frac{1+o(1)}{q\mathfrak{c}(|A|)} e^{-\Gamma\beta}, \tag{4.17}$$

where $\mathfrak{c}(|A|)$ *is the constant defined in* (4.15).

We conclude the proofs of Theorems 4.8.1 and 4.1.9 by assuming Theorem 4.2.1.

Proof of Theorem 4.1.7. Recall the magic formula (3.24):

$$\mathbb{E}_{\boldsymbol{s}}[\tau_{\breve{\boldsymbol{s}}}] = \frac{1}{\mathrm{Cap}_\beta(\boldsymbol{s},\, \breve{\boldsymbol{s}})} \sum_{\sigma\in\mathcal{X}} \mu_\beta(\sigma) h_{\boldsymbol{s},\,\breve{\boldsymbol{s}}}(\sigma).$$

Using Theorem 4.0.1 and the fact that $h_{\boldsymbol{s},\,\breve{\boldsymbol{s}}}(\boldsymbol{s}) = 1$ and $h_{\boldsymbol{s},\,\breve{\boldsymbol{s}}} \equiv 0$ on $\breve{\boldsymbol{s}}$, we can rewrite the last summation as

$$\frac{1}{q} + o(1) + \sum_{\sigma\in\mathcal{X}\setminus\mathcal{S}} \mu_\beta(\sigma) h_{\boldsymbol{s},\,\breve{\boldsymbol{s}}}(\sigma) = \frac{1}{q} + o(1),$$

where the identity follows from the trivial bound $|h_{\boldsymbol{s},\,\breve{\boldsymbol{s}}}| \le 1$ (cf. (3.18)). Summing up the computations above and applying Theorem 4.2.1, we obtain

$$\mathbb{E}_{\boldsymbol{s}}[\tau_{\breve{\boldsymbol{s}}}] = \frac{1}{\mathrm{Cap}_\beta(\boldsymbol{s},\, \breve{\boldsymbol{s}})} \Big[\frac{1}{q} + o(1)\Big] = (1+o(1)) \cdot \frac{\kappa}{q-1} e^{\Gamma\beta}. \tag{4.18}$$

We next address the second estimate of (4.10). Assume that the process $\sigma_\beta(\cdot)$ starts from $\boldsymbol{s}$ and that $\boldsymbol{s} \neq \boldsymbol{s'}$. We define a sequence of stopping times $(J_n)_{n=0}^\infty$ by $J_0 = 0$ and

$$J_{n+1} = \inf\{t \ge J_n : \sigma_\beta(t) \in \mathcal{S} \setminus \sigma_\beta(J_n)\} \quad \text{for } n \ge 0.$$

In other words, $(J_n)_{n=0}^{\infty}$ is the sequence of random times at which the process $\sigma_\beta(\cdot)$ visits a new ground state. By (4.18) and the strong Markov property, we have for all $n \geq 0$ that

$$\mathbb{E}_{\boldsymbol{s}}[J_{n+1} - J_n] = (1 + o(1)) \cdot \frac{\kappa}{q-1} e^{\Gamma\beta}. \tag{4.19}$$

Then, we define

$$n(\boldsymbol{s'}) = \inf\{n \geq 0 : \sigma_\beta(J_n) = \boldsymbol{s'}\}$$

such that $\tau_{\boldsymbol{s'}} = J_{n(\boldsymbol{s'})}$; thus, we can write

$$\tau_{\boldsymbol{s'}} = \sum_{i=0}^{n(\boldsymbol{s'})-1} (J_{i+1} - J_i). \tag{4.20}$$

Note that because we have assumed $\boldsymbol{s} \neq \boldsymbol{s'}$, it holds that $n(\boldsymbol{s'}) \geq 1$. By symmetry, we observe that $n(\boldsymbol{s'})$ is a geometric random variable with success probability $1/(q-1)$ that is independent of the sequence $(J_n)_{n=0}^{\infty}$. Thus, we get from (4.19) and (4.20) that

$$\mathbb{E}_{\boldsymbol{s}}[\tau_{\boldsymbol{s'}}] = (1 + o(1)) \cdot \frac{\kappa}{q-1} e^{\Gamma\beta} \cdot (q-1) = (1 + o(1)) \cdot \kappa e^{\Gamma\beta}.$$

Finally, from (3.14), (4.13), (4.14), and (4.15), we can easily see that κ satisfies the asymptotics (4.11). This completes the proof. □

Next, we consider Theorem 4.1.9. Before stating the proof, we remark that two alternative approaches are available for the Markov chain model reduction in the context of metastability: an approach based on the Poisson equation [58, 61, 76, 77], and one based on the resolvent equation [57, 65].

Proof of Theorem 4.1.9. We first consider part (1). We denote by $r_{Y_\beta} : \mathcal{S} \times \mathcal{S} \to [0, \infty)$ the transition rate of the trace process $Y_\beta(\cdot)$. In view of the rate (4.12) of the limiting Markov chain, it suffices to prove that $r_{Y_\beta}(\boldsymbol{s}, \boldsymbol{s'}) = (1+o(1))/\kappa$ for all $\boldsymbol{s}, \boldsymbol{s'} \in \mathcal{S}$. Since $r_\beta(\boldsymbol{s}, \boldsymbol{s'})$ does not depend on the selections of $\boldsymbol{s}$, $\boldsymbol{s'} \in \mathcal{S}$ by the symmetry of the model, it remains to prove that

$$r_{Y_\beta}(\boldsymbol{s},\, \breve{\boldsymbol{s}}) = (1+o(1)) \cdot \frac{q-1}{\kappa} \quad \text{for all } \boldsymbol{s} \in \mathcal{S}. \tag{4.21}$$

We temporarily denote by $\mathbf{E}_{\boldsymbol{s}}$ the law of the trace process $Y_\beta(\cdot)$ starting from $\boldsymbol{s}$. Then,

$$\frac{1}{r_{Y_\beta}(\boldsymbol{s},\, \breve{\boldsymbol{s}})} = \mathbf{E}_{\boldsymbol{s}}[\tau_{\breve{\boldsymbol{s}}}] = e^{-\Gamma\beta} \cdot \mathbb{E}_{\boldsymbol{s}}\Big[\int_0^{\tau_{\breve{\boldsymbol{s}}}} \mathbb{1}\{\sigma_\beta(t) \in \mathcal{S}\}dt\Big], \tag{4.22}$$

where the factor $e^{-\Gamma\beta}$ is included because we accelerated the process by the factor $e^{\Gamma\beta}$; the integrand $\mathbb{1}\{\sigma_\beta(t) \in \mathcal{S}\}$ arises because the trace process is obtained from the accelerated process by turning off the clock when the process resides outside $\mathcal{S}$. Then, by [5, Proposition 6.10], we can write

$$\begin{aligned}&\mathbb{E}_{\boldsymbol{s}}\Big[\int_0^{\tau_{\breve{\boldsymbol{s}}}} \mathbb{1}\{\sigma_\beta(t) \in \mathcal{S}\}dt\Big] \\ &= \frac{1}{\mathrm{Cap}_\beta(\boldsymbol{s},\, \breve{\boldsymbol{s}})} \sum_{\sigma\in\mathcal{X}} \mu_\beta(\sigma)\mathbb{1}\{\sigma \in \mathcal{S}\} h_{\boldsymbol{s},\,\breve{\boldsymbol{s}}}(\sigma) = \frac{\mu_\beta(\boldsymbol{s})}{\mathrm{Cap}_\beta(\boldsymbol{s},\, \breve{\boldsymbol{s}})},\end{aligned}$$

where the second identity follows from the fact that $h_{\boldsymbol{s},\,\breve{\boldsymbol{s}}}(\boldsymbol{s}) = 1$ and $h_{\boldsymbol{s},\,\breve{\boldsymbol{s}}} \equiv 0$ on $\breve{\boldsymbol{s}}$. Therefore, by Theorems 4.0.1 and 4.2.1, we obtain

$$\mathbb{E}_{\boldsymbol{s}}\Big[\int_0^{\tau_{\breve{\boldsymbol{s}}}} \mathbb{1}\{\sigma_\beta(t) \in \mathcal{S}\}dt\Big] = (1+o(1)) \cdot \frac{\kappa}{q-1} e^{\Gamma\beta}.$$

Inserting this into (4.22) yields (4.21).

Part (2) can be proved in the exact same way as Theorem 3.1.4. □

Finally, to prove Theorem 4.2.1, we apply the H^1-approximation method given in Proposition 3.2.9. This is done by constructing the explicit test function in Section 4.7.

4.3 Canonical configurations and paths

Analyzing the energy landscape of the 3D model is far more complex than that of the 2D model; below, we briefly list the main differences between them that serve to complexify the problem. Below, for the 2D objects, we added the superscripts 2D.

(1) In the 2D model, the energy of the gateway configuration is either Γ^{2D} or $\Gamma^{2D} - 2$. Thus, a Γ^{2D}-path on the gateway configurations does not have the freedom to move. On the other hand, in the 3D model, the energy of the gateway configuration ranges from $\Gamma - 2K - 2$ to Γ. This implies that the behavior of a Γ-path around a gateway configuration of energy $\Gamma - 2K - 2$ (which is a regular configuration) cannot be characterized precisely.

(2) In the 2D model, a Γ^{2D}-path from $\boldsymbol{a}^{2D}$ to $\boldsymbol{b}^{2D}$ must visit a configuration in $\mathcal{R}_2^{a,\,b,\,2D}$. Then, it successively visits $\mathcal{R}_3^{a,\,b,\,2D}$, ..., $\mathcal{R}_{L-2}^{a,\,b,\,2D}$ and finally arrives at $\boldsymbol{b}^{2D}$. Remarkably, this path does not need to visit a configuration in $\mathcal{R}_1^{a,\,b,\,2D}$ and in $\mathcal{R}_{L-1}^{a,\,b,\,2D}$; this fact essentially arises from the features of the 2D geometry. In the 3D model, we observe a similar phenomenon. To explain this, let us temporarily denote by $\mathcal{R}_v^{a,\,b}$, $v \in [\![1,\, L-1]\!]$ the collection of 3D configurations such that there are v consecutive $K \times L$ slabs of spins b and such that the spins at the remaining sites are a. Then, there exists an integer $n = n_{K,\,L,\,M}$ such that any Γ-path connecting $\boldsymbol{a}$ and $\boldsymbol{b}$ must successively visit configurations in $\mathcal{R}_n^{a,\,b}$, $\mathcal{R}_{n+1}^{a,\,b}$, $\ldots$, $\mathcal{R}_{M-n}^{a,\,b}$ but need not visit $\mathcal{R}_i^{a,\,b}$ for $i \in [\![1,\, n-1]\!]$ and $i \in [\![M-n+1,\, M-1]\!]$. In the 2D model, the number corresponding to this $n = n_{K,\,L,\,M}$ is 2. We guess that in the 3D model, $n \sim K^{1/2}$; however, we cannot determine the exact value of n. This fact reveals the complex structure of the energy landscape in the 3D model. Instead,

we prove below (cf. Propositions 4.3.14 and 4.5.1) that

$$\lfloor K^{1/2} \rfloor \le n \le \lfloor K^{2/3} \rfloor.$$

Fortunately, this bound suffices to complete our analysis without identifying the exact value of n.

(3) In the 2D model, the $\mathcal{N}^{\mathrm{2D}}$-neighborhoods are fully characterized in Proposition 3.9.3; meanwhile, in the 3D case, we cannot obtain such a specific and simple result. We overcome the absence of this result by using the 2D result obtained in Proposition 3.9.3, through suitably applying it to the analysis of the 3D model. *Indeed, this absence is a crucial difficulty in extending the analysis to the four- or higher-dimensional models.*

(4) Because of the aforementioned complexity of the energy landscape, the transition may encounter a dead-end with energy Γ, even in the bulk part of the transition; this is not the case in the 2D model. Therefore, another technical challenge is that of carefully characterizing these dead-ends and appropriately excluding them from the computation.

As explained above, the energy landscape of the 3D model is more complex than that of the 2D one, and we are unable to present a complete description of the energy landscape for the former. Nevertheless, we analyze the landscape with the precision required to prove our main results.

In Section 4.3, we introduce canonical configurations and paths. Their definitions are direct generalizations of those in the 2D model. Then, we explain several applications of these canonical objects.

We first collect several notation which will be frequently used throughout the remainder of the article.

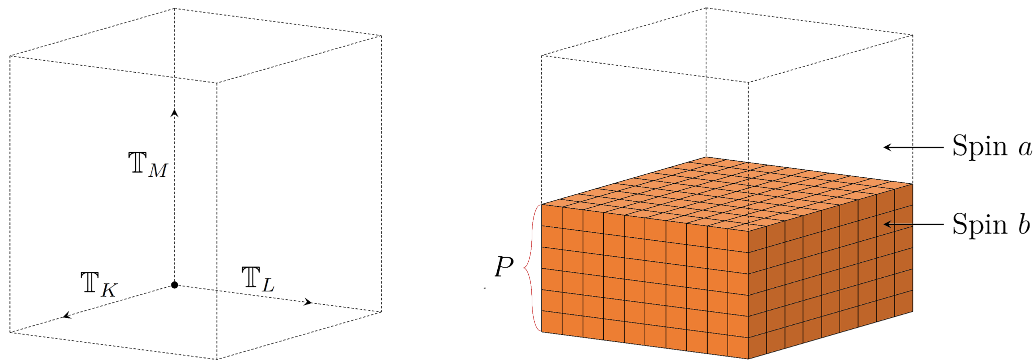


Figure 4.1: Figures on Notation 4.3.1. This form of figure is used throughout the remainder of the article to illustrate a 3D configuration consisting of two types of spins only. The large dotted box denotes $\Lambda = \mathbb{T}_K \times \mathbb{T}_L \times \mathbb{T}_M$. The orange unit boxes denote the sites with spin b, and the empty part denotes the cluster of spin a. For some cases when we only concern the shape of the cluster of spin b (e.g. in Figure 4.2), we omit the dotted box representing Λ.

Notation 4.3.1. We refer to Figure 4.1[1] for an illustration of the notation below.

- For $m \in \mathbb{T}_M$, the slab $\mathbb{T}_K \times \mathbb{T}_L \times \{m\} \subseteq \Lambda$ is called an *m-th floor*. For each configuration $\sigma \in \mathcal{X}$, we denote by $\sigma^{(m)}$ the configuration of σ at the m-th floor, i.e.,

$$\sigma^{(m)}(k,\,\ell) = \sigma(k,\,\ell,\,m);\;k \in \mathbb{T}_K,\;\ell \in \mathbb{T}_L. \tag{4.23}$$

  Thus, $\sigma^{(m)} \in \mathcal{X}^{\text{2D}}$ is a spin configuration in $\Lambda^{\text{2D}} = \mathbb{T}_K \times \mathbb{T}_L$.

- For $a,\,b \in \Omega$ and $P \subseteq \mathbb{T}_M$, we denote by $\sigma_P^{a,\,b} \in \mathcal{X}$ the configuration satisfying

$$\sigma_P^{a,\,b}(k,\,\ell,\,m) = b \cdot \mathbb{1}\{m \in P\} + a \cdot \mathbb{1}\{m \notin P\}. \tag{4.24}$$

[1]In fact, this figure and all the 3D figures below contradict our assumption that $K \geq 2829$. However, we believe that there will be absolutely no confusion with these figures which only provide simple illustrations of complicated notions.

Also, recall the definition of neighborhoods given in Definition 3.4.2, but now subjected to the 3D energy barrier $\Gamma = \Gamma^{3D}$.

4.3.1 Canonical configurations

The following notation is used frequently.

Notation 4.3.2. We first introduce several maps on $\mathcal{X}$. If $K = L$, we define a bijection $\Theta^{(12)} : \mathcal{X} \to \mathcal{X}$ as the map switching the first and second coordinates, i.e., for all $\sigma \in \mathcal{X}$ and $(k, \ell, m) \in \Lambda$,

$$(\Theta^{(12)}(\sigma))(k, \ell, m) = \sigma(\ell, k, m).$$

If $L = M$, we can similarly define a bijection $\Theta^{(23)}$ on $\mathcal{X}$ switching the second and third coordinates. Finally, for the case of $K = L = M$, we can even define the bijection $\Theta^{(13)}$ on $\mathcal{X}$ switching the first and third coordinates.

Then, for $\mathcal{A} \subseteq \mathcal{X}$, we define $\Upsilon(\mathcal{A})$ as

$$\Upsilon(\mathcal{A}) = \begin{cases} \mathcal{A} & \text{if } K < L < M, \\ \mathcal{A} \cup \Theta^{(12)}(\mathcal{A}) & \text{if } K = L < M, \\ \mathcal{A} \cup \Theta^{(23)}(\mathcal{A}) & \text{if } K < L = M, \\ \mathcal{A} \cup \Theta^{(12)}(\mathcal{A}) \cup \Theta^{(23)}(\mathcal{A}) \cup \Theta^{(13)}(\mathcal{A}) & \\ \quad \cup (\Theta^{(12)} \circ \Theta^{(23)})(\mathcal{A}) \cup (\Theta^{(23)} \circ \Theta^{(12)})(\mathcal{A}) & \text{if } K = L = M. \end{cases}$$

Note that the set $\Upsilon(\mathcal{A})$ for the case of $K = L = M$ denotes the set of all configurations obtained by permuting the coordinates of the configurations in $\mathcal{A}$.

Now, we define canonical configurations of our 3D model.

Definition 4.3.3 (Canonical configurations)**.** We refer to Figure 4.2 for a visualization of the objects introduced below. Recall Notation 3.4.11. We first introduce some building blocks in the definition of canonical and gateway

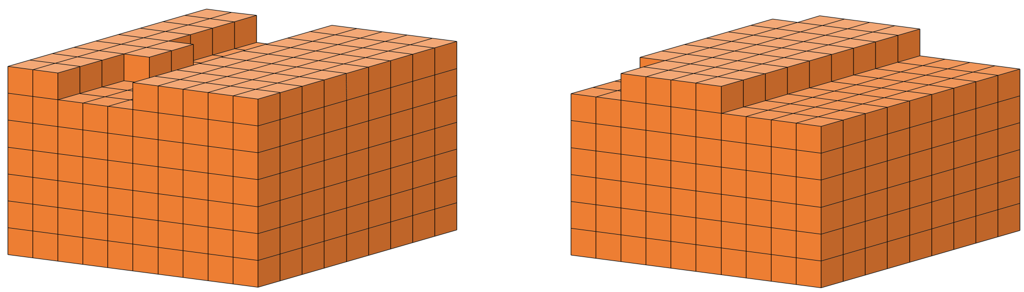


Figure 4.2: Canonical configurations. These two configurations belong to $\mathcal{C}_6^{a,\,b}$ (if the orange boxes represent the sites with spin b as in Figure 4.1), since the 2D configurations at the 7-th floor are 2D canonical configurations $\xi_{6,\,7;\,5,\,2}^{a,\,b,\,+}$ and $\xi_{3,\,4;\,2,\,6}^{a,\,b,\,-}$, respectively.

configurations. For $a,\,b\in\Omega$ and $P,\,Q\in\mathfrak{S}_M$ with $P\prec Q$, we define $\widetilde{\mathcal{C}}_{P,\,Q}^{a,\,b}\subseteq\mathcal{X}$ as

$$\sigma\in\widetilde{\mathcal{C}}_{P,\,Q}^{a,\,b}\quad\Leftrightarrow\quad\begin{cases}\sigma^{(m)}=\boldsymbol{b}^{\mathrm{2D}} & \text{if } m\in P,\\ \sigma^{(m)}=\boldsymbol{a}^{\mathrm{2D}} & \text{if } m\in Q^c,\\ \sigma^{(m)}\in\mathcal{C}^{a,\,b,\,\mathrm{2D}} & \text{if } m\in Q\setminus P,\end{cases}$$

where the 2D objects are defined in Chapter 3. Then, we set

$$\mathcal{C}_{P,\,Q}^{a,\,b}=\Upsilon(\widetilde{\mathcal{C}}_{P,\,Q}^{a,\,b}).\tag{4.25}$$

We then define, for $i\in[\![0,\,M-1]\!]$,

$$\mathcal{C}_i^{a,\,b}=\bigcup_{P,\,Q\in\mathfrak{S}_M:\,|P|=i\text{ and }P\prec Q}\mathcal{C}_{P,\,Q}^{a,\,b}\quad\text{and}\quad\mathcal{C}^{a,\,b}=\bigcup_{i=0}^{M-1}\mathcal{C}_i^{a,\,b}.\tag{4.26}$$

Finally, for a proper partition $(A,\,B)$ of Ω, we write

$$\mathcal{C}_i^{A,\,B}=\bigcup_{a\in A}\bigcup_{b\in B}\mathcal{C}_i^{a,\,b}\quad\text{and}\quad\mathcal{C}^{A,\,B}=\bigcup_{a\in A}\bigcup_{b\in B}\mathcal{C}^{a,\,b}.$$

A configuration belonging to $\mathcal{C}^{a,\,b}$ for some $a,\,b\in\Omega$ is called a *canonical* *configuration* between $\boldsymbol{a}$ and $\boldsymbol{b}$.

In view of the definition above, the role of the map Υ is clear. When $K < L < M$ there is only one direction of transition, if $K = L < M$ or $K < L = M$ there are $2 = 2!$ possible directions, while if $K = L = M$ there are $6 = 3!$ possible directions. The map Υ reflects this observation into the definition. Next, let us define regular configurations which are the special ones among the canonical configurations.

Definition 4.3.4 (Regular configurations)**.** For $a,\, b \in \Omega$ and $P \in \mathfrak{S}_M$, recall the configuration $\sigma_P^{a,\,b}$ from (4.24) and define

$$\widetilde{\mathcal{R}}_i^{a,\,b} = \{\sigma_P^{a,\,b} : P \in \mathfrak{S}_M,\ |P| = i\}; \quad i \in [\![0,\, M]\!]. \tag{4.27}$$

Note that $\widetilde{\mathcal{R}}_i^{a,\,b}$ is a collection of configurations consisting of spins a and b only, where spins a and b are located at slabs $\mathbb{T}_K \times \mathbb{T}_L \times (\mathbb{T}_M \setminus P)$ and $\mathbb{T}_K \times \mathbb{T}_L \times P$, respectively, for $P \in \mathfrak{S}_M$ with $|P| = i$. Then, define (cf. Notation 4.3.2)

$$\mathcal{R}_i^{a,\,b} = \Upsilon(\widetilde{\mathcal{R}}_i^{a,\,b}). \tag{4.28}$$

A configuration belonging to $\mathcal{R}_i^{a,\,b}$ for some $i \in [\![0,\, M]\!]$ is called a *regular configuration*. Clearly, we have $\mathcal{R}_0^{a,\,b} = \{\boldsymbol{a}\}$ and $\mathcal{R}_M^{a,\,b} = \{\boldsymbol{b}\}$. For a proper partition $(A,\, B)$ of Ω, we write

$$\mathcal{R}_i^{A,\,B} = \bigcup_{a\in A} \bigcup_{b\in B} \mathcal{R}_i^{a,\,b}. \tag{4.29}$$

4.3.2 Energy of canonical configurations

One can compute the energy of canonical configurations readily by elementary computations, but we provide a more systematic approach which will be frequently used in later computations. To this end, we first introduce a notation.

Notation 4.3.5. For $(k,\, \ell) \in \mathbb{T}_K \times \mathbb{T}_L$, we denote by $\sigma^{\langle k,\, \ell \rangle} \in S^{\mathbb{T}_M}$ the configuration of σ on the $(k,\, \ell)$-th pillar $\{k\} \times \{\ell\} \times \mathbb{T}_M$, i.e.,

$$\sigma^{\langle k,\, \ell \rangle}(m) = \sigma(k,\, \ell,\, m); \quad m \in \mathbb{T}_M. \tag{4.30}$$

The energy of the 1D configuration $\sigma^{\langle k,\, \ell \rangle}$ is denoted by

$$H^{\mathrm{1D}}(\sigma^{\langle k,\, \ell \rangle}) = \sum_{m \in \mathbb{T}_M} \mathbb{1}\{\sigma(k,\, \ell,\, m) \neq \sigma(k,\, \ell,\, m+1)\}. \tag{4.31}$$

In the following lemma, we decompose the 3D energy into lower-dimensional ones. Here, H^{2D} is the Hamiltonian of the 2D Ising/Potts configurations.

Lemma 4.3.6. *For each $\sigma \in \mathcal{X}$, it holds that*

$$H(\sigma) = \sum_{m \in \mathbb{T}_M} H^{\mathrm{2D}}(\sigma^{(m)}) + \sum_{(k,\, \ell) \in \mathbb{T}_K \times \mathbb{T}_L} H^{\mathrm{1D}}(\sigma^{\langle k,\, \ell \rangle}). \tag{4.32}$$

Proof. We can write $H(\sigma)$ as

$$\begin{aligned} &\sum_{m \in \mathbb{T}_M} \Big[\sum_{k \in \mathbb{T}_K} \sum_{\ell \in \mathbb{T}_L} \mathbb{1}_{\{\sigma(k+1,\, \ell,\, m) \neq \sigma(k,\, \ell,\, m)\}} + \mathbb{1}_{\{\sigma(k,\, \ell+1,\, m) \neq \sigma(k,\, \ell,\, m)\}} \Big] \\ &+ \sum_{k \in \mathbb{T}_K} \sum_{\ell \in \mathbb{T}_L} \Big[\sum_{m \in \mathbb{T}_M} \mathbb{1}_{\{\sigma(k,\, \ell,\, m) \neq \sigma(k,\, \ell,\, m+1)\}} \Big]. \end{aligned}$$

The first and second lines correspond to the first and second terms at the right-hand side of (4.32), respectively. □

Based on the previous expression, we deduce the following proposition.

Proposition 4.3.7 (Energy of canonical configurations)**.** *The following properties hold.*

(1) For each canonical configuration σ, we have $H(\sigma) \leq \Gamma$.

(2) *For each configuration* $\sigma \in \mathcal{C}_i^{a,\,b}$ *for some* $a,\, b \in \Omega$ *and* $i \in [\![1,\, M-2]\!]$, *we have*

$$H(\sigma) \in [\![\Gamma - 2K - 2,\, \Gamma]\!].$$

Proof. Observe that for a canonical configuration σ, we have $H^{1\mathrm{D}}(\sigma^{\langle k,\,\ell\rangle}) \le 2$ for all $(k,\, \ell) \in \mathbb{T}_K \times \mathbb{T}_L$, and $H^{2\mathrm{D}}(\sigma^{(m)}) = 0$ for all $m \in \mathbb{T}_M \setminus \{m_0\}$ for some $m_0 \in \mathbb{T}_M$, at which it holds that $H^{2\mathrm{D}}(\sigma^{(m_0)}) \le 2K+2$ (cf. (3.48)). Thus, by Lemma 4.3.6,

$$H(\sigma) \le (2K+2) + 2KL = \Gamma.$$

For part (2), it suffices to additionally observe that $H^{1\mathrm{D}}(\sigma^{\langle k,\,\ell\rangle}) = 2$ for all $(k,\, \ell) \in \mathbb{T}_K \times \mathbb{T}_L$ if $i \in [\![1,\, M-2]\!]$ and thus

$$H(\sigma) \ge 2KL = \Gamma - 2K - 2.$$

□

Remark 4.3.8. In particular, we have $H(\sigma) = \Gamma - 2K - 2 = 2KL$ for any $\sigma \in \mathcal{R}_i^{A,\,B}$, $i \in [\![1,\, M-1]\!]$. Hence, a Γ-path at a regular configuration can evolve in a non-canonical way, since we still have a spare of $2K+2$ to reach the energy barrier Γ. Incorporating all these behaviors in the metastability analysis is a demanding part of the 3D model. For this reason, the regular configuration plays a crucial role. We remark that for the 2D case, any optimal path at a regular configuration does not have freedom, and that helped a lot simplifying the arguments.

4.3.3 Canonical paths

In this subsection, we define 3D canonical paths between ground states. They generalize the 2D paths recalled in Definition 3.4.12. Refer to Figure 4.3 for an illustration.

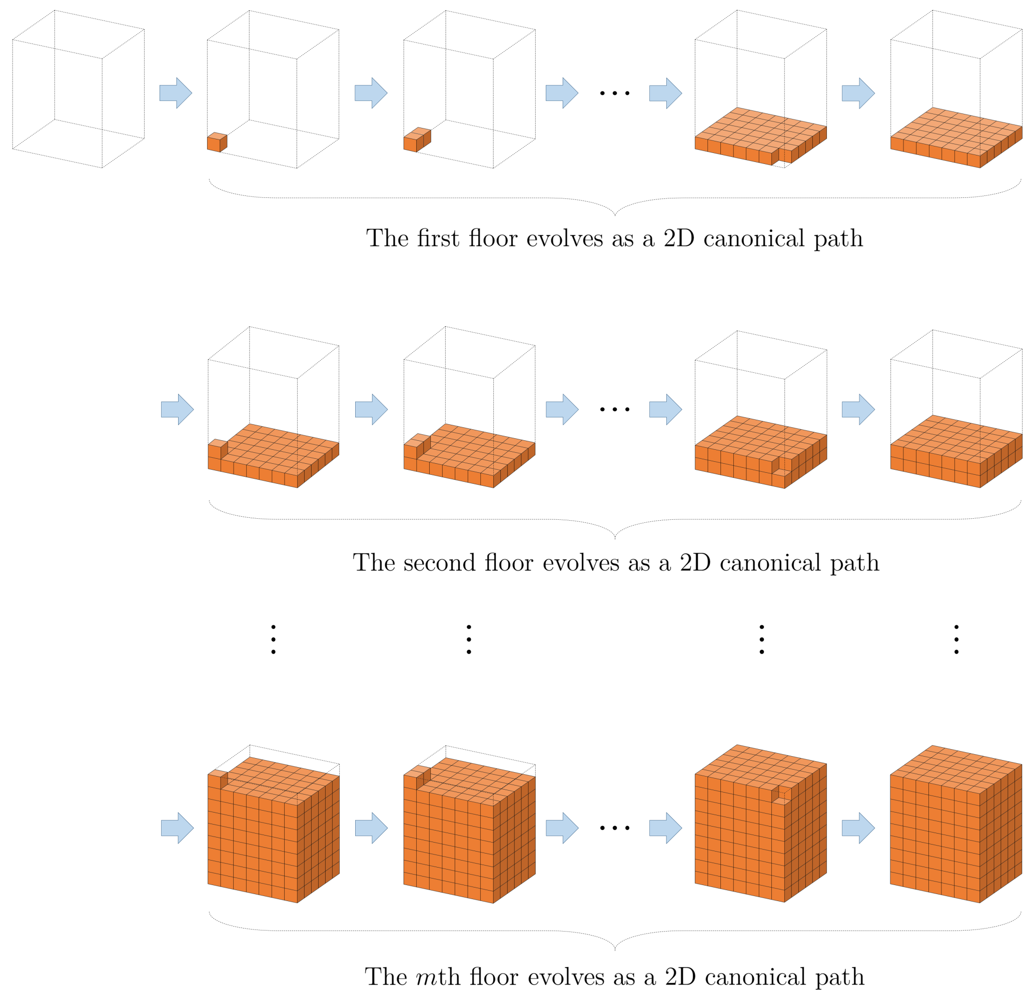


Figure 4.3: Canonical path connecting $\boldsymbol{a}$ and $\boldsymbol{b}$.

Definition 4.3.9 (Canonical paths)**.** We recall Notation 3.4.11. Let us fix $a,\, b \in \Omega$. A path $(\omega_t)_{t=0}^{KLM}$ is called a *pre-canonical path* connecting $\boldsymbol{a}$ and $\boldsymbol{b}$ if there exists an increasing sequence $(P_i)_{i=0}^{M}$ in $\mathfrak{S}_M$ such that

- for each $i \in [\![0,\, M]\!]$, we have that $\omega_{KLi} = \sigma_{P_i}^{a,\, b}$ (cf. (4.24)), and
- for each $i \in [\![0,\, M-1]\!]$, there exists a 2D canonical path $(\gamma_t^i)_{t=0}^{KL}$ from $\boldsymbol{a}^{\mathrm{2D}}$ to $\boldsymbol{b}^{\mathrm{2D}}$ defined in Definition 3.4.12 such that

$$\omega_t^{(m)} = \begin{cases} \boldsymbol{b}^{\mathrm{2D}} & \text{if } m \in P_i, \\ \boldsymbol{a}^{\mathrm{2D}} & \text{if } m \in \mathbb{T}_M \setminus P_{i+1}, \\ \gamma_{t-KLi}^i & \text{if } m \in P_{i+1} \setminus P_i, \end{cases} \quad \text{for all } t \in [\![KLi,\, KL(i+1)]\!].$$

If $K < L < M$, a path is called a *canonical path* if it is a pre-canonical path. If $K = L < M$, a path is called a *canonical path* if it is either a pre-canonical one or the image of a pre-canonical one with respect to the map $\Theta^{(12)}$. We can define canonical paths for the cases of $K < L = M$ and $K = L = M$ in a similar manner.

Remark 4.3.10*.* We emphasize that for a canonical path $(\omega_t)_{t=0}^{KLM}$, all configurations ω_t, $t \in [\![0,\, KLM]\!]$, are canonical configurations, and hence any canonical path is a Γ-path by part (1) of Proposition 4.3.7.

Canonical paths provide optimal paths between two ground states, and hence we can confirm the following upper bound for the energy barrier.

Proposition 4.3.11. *For* $\boldsymbol{s},\, \boldsymbol{s'} \in \mathcal{S}$*, we have that* $\Phi(\boldsymbol{s},\, \boldsymbol{s'}) \le \Gamma$.

Proof. By Remark 4.3.10, it suffices to take a canonical path connecting $\boldsymbol{s}$ and $\boldsymbol{s'}$. □

We prove $\Phi(\boldsymbol{s},\, \boldsymbol{s'}) \ge \Gamma$ in Section 4.5 to verify $\Phi(\boldsymbol{s},\, \boldsymbol{s'}) = \Gamma$. This reversed inequality requires a much more complicated proof.

4.3.4 Characterization of the deepest valleys

We show in this subsection that using the canonical paths, the valleys in the energy landscape, except for the ones associated to the ground states, have depths less than Γ. Note that Theorem 4.1.1, although not yet proved, indicates that the valleys associated to the ground states have depth Γ. This characterization of the depths of other valleys is essentially required since we have to reject the possibility of being trapped in a deeper valley in the course of transition. This fact is crucially used in the application of the pathwise approach to metastability.

Notation 4.3.12. For the convenience of notation, we call $(\omega_t)_{t=0}^{T}$ a pseudo-path if either $\omega_t \sim \omega_{t+1}$ or $\omega_t = \omega_{t+1}$ for all $t \in [\![0,\, T-1]\!]$.

Proposition 4.3.13. *For $\sigma \in \mathcal{X} \setminus \mathcal{S}$, we have*

$$\Phi(\sigma,\, \mathcal{S}) - H(\sigma) \leq \Gamma - 2 < \Gamma.$$

Proof. Main idea of the proof is inherited from the proof of [69, Theorem 2.1]. Let us find two spins $a,\, b \in \Omega$ so that σ has spins a and b at some sites, which is clearly possible since $\sigma \notin \mathcal{S}$. Let us fix a canonical path $(\omega_t)_{t=0}^{KLM}$ connecting $\boldsymbol{a}$ and $\boldsymbol{b}$. Then, we write

$$A_t = \{x \in \Lambda : \omega_t(x) = b\}; \quad t \in [\![0,\, KLM]\!],$$

so that we have $\emptyset = A_0 \subseteq A_1 \subseteq \cdots \subseteq A_{KLM} = \Lambda$ and $|A_t| = t$ for all $t \in [\![0,\, KLM]\!]$. We can take the path $(\omega_t)_{t=0}^{KLM}$ in a way that

$$A_1 = \{x_0\} \quad \text{and} \quad \sigma(x_0) = b. \tag{4.33}$$

Now, we define a pseudo-path (cf. Notation 4.3.12) $(\widetilde{\omega}_t)_{t=0}^{KLM}$ connecting σ

and $\boldsymbol{b}$ as

$$\widetilde{\omega}_t(x) = \begin{cases} \sigma(x) & \text{if } x \notin A_t, \\ b & \text{if } x \in A_t. \end{cases}$$

In other words, we update the spins in an exactly same manner with the canonical path $(\omega_t)_{t=0}^{KLM}$. We claim that

$$H(\widetilde{\omega}_t) - H(\sigma) \le 2KL + 2K = \Gamma - 2 \quad \text{for all } t \in [\![0,\, KLM]\!]. \tag{4.34}$$

It is immediate that this claim concludes the proof. To prove this claim, we recall the decomposition obtained in Lemma 4.3.6 and write $\widetilde{\omega}_t = \zeta$. Then, we can write $H(\zeta) - H(\sigma)$ as

$$\sum_{m\in\mathbb{T}_M} [H^{\rm 2D}(\zeta^{(m)}) - H^{\rm 2D}(\sigma^{(m)})] + \sum_{(k,\,\ell)\in\mathbb{T}_K\times\mathbb{T}_L} [H^{\rm 1D}(\zeta^{\langle k,\,\ell\rangle}) - H^{\rm 1D}(\sigma^{\langle k,\,\ell\rangle})]. \tag{4.35}$$

Let us first consider the first summation of (4.35). We suppose that $t \in [\![KLi,\, KL(i+1)]\!]$ and write $\omega_{KLi} = \sigma_P^{a,\,b}$ and $\omega_{KL(i+1)} = \sigma_Q^{a,\,b}$ where $P \prec Q$. Write $Q \setminus P = \{m'\}$. Then, we have that

$$H^{\rm 2D}(\zeta^{(m)}) - H^{\rm 2D}(\sigma^{(m)}) = \begin{cases} -H^{\rm 2D}(\sigma^{(m)}) \le 0 & \text{if } m \in P, \\ 0 & \text{if } m \in Q^c, \end{cases} \tag{4.36}$$

since $\zeta^{(m)} = \boldsymbol{b}^{\rm 2D}$ for $m \in P$ and $\zeta^{(m)} = \sigma^{(m)}$ for $m \in Q^c$. On the other hand, by Lemma 3.9.4, we have that

$$H^{\rm 2D}(\zeta^{(m')}) - H^{\rm 2D}(\sigma^{(m')}) \le 2K + 2. \tag{4.37}$$

By (4.36) and (4.37), we conclude that

$$\sum_{m\in\mathbb{T}_M} [H^{\rm 2D}(\zeta^{(m)}) - H^{\rm 2D}(\sigma^{(m)})] \le 2K + 2. \tag{4.38}$$

Now, we turn to the second summation of (4.35). Note that $\zeta^{\langle k,\,\ell\rangle}$ is obtained from $\sigma^{\langle k,\,\ell\rangle}$ by flipping the spins in consecutive sites in Q to b. From this, we can readily deduce that

$$H^{\rm 1D}(\zeta^{\langle k,\,\ell\rangle}) - H^{\rm 1D}(\sigma^{\langle k,\,\ell\rangle}) \le 2 \quad \text{for all } k \in \mathbb{T}_K \text{ and } \ell \in \mathbb{T}_L. \tag{4.39}$$

Moreover, if $x_0 = (k_0,\, \ell_0,\, m_0)$, we can check that

$$H^{\rm 1D}(\zeta^{\langle k_0,\,\ell_0\rangle}) - H^{\rm 1D}(\sigma^{\langle k_0,\,\ell_0\rangle}) \le 0. \tag{4.40}$$

By (4.39) and (4.40), we get

$$\sum_{(k,\,\ell)\in\mathbb{T}_K\times\mathbb{T}_L} [H^{\rm 1D}(\zeta^{\langle k,\,\ell\rangle}) - H^{\rm 1D}(\sigma^{\langle k,\,\ell\rangle})] \le 2(KL-1). \tag{4.41}$$

Now, the claim (4.34) follows from (4.35), (4.38), and (4.41). □

4.3.5 Auxiliary result on saddle configurations

In the 2D case, in the analysis of the energy landscape, the collection $\mathcal{R}_2^{\rm 2D}$ plays a significant role since to make an optimal transition (not exceeding the energy barrier $2K+2$), we may skip the collection $\mathcal{R}_1^{\rm 2D}$ but must pass through $\mathcal{R}_2^{\rm 2D}$. Thus, the integer 2 worked as some kind of a threshold for metastable transitions. We expect a similar pattern in the 3D case, and we briefly explain this phenomenon in this subsection.

Let us define

$$\mathfrak{m}_K = \lfloor K^{2/3} \rfloor. \tag{4.42}$$

Then, we shall prove in Corollary 4.5.5 below that

$$\Phi(\boldsymbol{a},\, \sigma^{a,\,b}_{[\![1,\,n]\!]}) = \Gamma \quad \text{for all } n \in [\![\mathfrak{m}_K,\, M-\mathfrak{m}_K]\!]. \tag{4.43}$$

Thus, we can define (cf. Figure 4.5 below)

$$n_{K,\,L,\,M} = \min\{n \in [\![1,\, M-1]\!] : \Phi(\boldsymbol{a},\, \sigma^{a,\,b}_{[\![1,\,n]\!]}) = \Gamma\}. \tag{4.44}$$

We strongly believe that this quantity does not depend on M, but we do not have a proof for it at the moment. Note that this number was just 2 in the 2D case. In the 3D model, we do not know this number exactly, since non-canonical movements at the early stage of transitions are hard to characterize. However, the upper bound $n_{K,\,L,\,M} \le \mathfrak{m}_K = \lfloor K^{2/3} \rfloor$ obtained from (4.43) is enough for our purpose, as we shall see later.

The main result of this subsection is the corresponding lower bound. This result will not be used in the proofs later, but emphasizes the complexity of the energy landscape near ground states.

Proposition 4.3.14. *We have* $n_{K,\,L,\,M} \ge \lfloor K^{1/2} \rfloor$.

Proof. It suffices to prove that

$$\Phi(\mathbf{1},\, \sigma^{1,\,2}_{[\![1,\,n]\!]}) \le \Gamma - 2 \quad \text{for all } n \in [\![1,\, \lfloor K^{1/2} \rfloor - 1]\!].$$

We fix such an n and write $\sigma = \sigma^{1,\,2}_{[\![1,\,n]\!]}$. We now construct an explicit path from σ to $\mathbf{1}$ without exceeding the energy $\Gamma - 2$. Note that $\sigma^{1,\,2}_{[\![1,\,n]\!]}$ has spins 2 at $\mathbb{T}_K \times \mathbb{T}_L \times [\![1,\, n]\!]$ and spins 1 at all the other sites. In this proof, we regard $\mathbb{T}_K = [\![1,\, K]\!]$ and $\mathbb{T}_L = [\![1,\, L]\!]$ in order to simplify the explanation of the order of spin flips in a lexicographic manner.

- First, starting from σ, we change spins 2 to 1 in $[\![1,\, K]\!] \times [\![1,\, n]\!] \times [\![1,\, n]\!]$ in ascending lexicographic order. Denote by $\zeta \in \mathcal{X}$ the obtained spin configuration, which has spins 2 only on $[\![1,\, K]\!] \times [\![n+1,\, L]\!] \times [\![1,\, n]\!]$. Then, the variation of the Hamiltonian from σ to ζ can be expressed by the following $n \times n$ matrices:

$$\begin{bmatrix} +2 & +0 & \cdots & +0 \\ +4 & +2 & \cdots & +2 \\ & & \vdots & \\ +4 & +2 & \cdots & +2 \end{bmatrix}, \quad \begin{bmatrix} +0 & -2 & \cdots & -2 \\ \mathbf{+2} & +0 & \cdots & +0 \\ & & \vdots & \\ +2 & +0 & \cdots & +0 \end{bmatrix} \times (K-2), \quad \begin{bmatrix} -2 & -4 & \cdots & -4 \\ +0 & -2 & \cdots & -2 \\ & & \vdots & \\ +0 & -2 & \cdots & -2 \end{bmatrix}.$$

Here, each $n \times n$ matrix represents $\{i\} \times [\![1,\, n]\!] \times [\![1,\, n]\!]$ for $1 \le i \le K$, in which the numbers represent the variation of the energy which should be read in ascending lexicographic order. From this path, we obtain

$$\Phi(\sigma,\, \zeta) \le 2KL + 2n^2 + 2n - 2, \tag{4.45}$$

where the maximum of the energy is obtained right after flipping the spin at $(2,\, 1,\, n-1)$, which is denoted by bold font at the matrices above.

- Next, starting from ζ, we change spins 2 to 1 in $[\![1,\, K]\!] \times \{i\} \times [\![1,\, n]\!]$ in the ascending lexicographic order for $i \in [\![n+1,\, L-1]\!]$, from $i = n+1$ to $i = L-1$. Denote by $\zeta' \in \mathcal{X}$ the obtained spin configuration, which has spins 2 only on $[\![1,\, K]\!] \times \{L\} \times [\![1,\, n]\!]$. In each step, the variation of the Hamiltonian is represented by the $n \times K$ matrix

$$\begin{bmatrix} +0 & -2 & \cdots & -2 & -4 \\ +2 & +0 & \cdots & +0 & -2 \\ & & \vdots & & \\ \mathbf{+2} & +0 & \cdots & +0 & -2 \end{bmatrix}.$$

Since $H(\zeta) = 2KL$, we can verify that

$$\Phi(\zeta,\, \zeta') \le 2KL + 2, \tag{4.46}$$

where the maximum is obtained right after flipping the spin at $(1,\, n+1,\, 1)$ (cf. bold font $\mathbf{+2}$).

- Finally, starting from ζ', we change spins 2 to 1 in the ascending lexicographic order. The variation of the Hamiltonian is represented by

$$\begin{bmatrix} -2 & -4 & \cdots & -4 & -6 \\ +0 & -2 & \cdots & -2 & -4 \\ & & \vdots & & \\ +0 & -2 & \cdots & -2 & -4 \end{bmatrix}.$$

Hence, the Hamiltonian monotonically decreases from $H(\zeta') = 2K(n+1)$ to arrive at $H(\mathbf{1}) = 0$. Hence, we have

$$\Phi(\zeta',\, \mathbf{1}) \le 2K(n+1). \tag{4.47}$$

Therefore, by (4.45), (4.46), and (4.47), we have

$$\Phi(\sigma,\, \mathbf{1}) \le 2KL + 2n^2 + 2n - 2.$$

Since $n \in [\![1,\, \lfloor K^{1/2} \rfloor - 1]\!]$, it holds that $2n^2 + 2n - 2 \le 2K$. This concludes the proof. □

4.4 Gateway configurations

In the analysis of the 3D model, a crucial notion is the concept of gateway configurations. The gateway configurations of the 3D model play a far more significant role than those of the 2D model.

We fix a proper partition $(A,\, B)$ of Ω throughout this section.

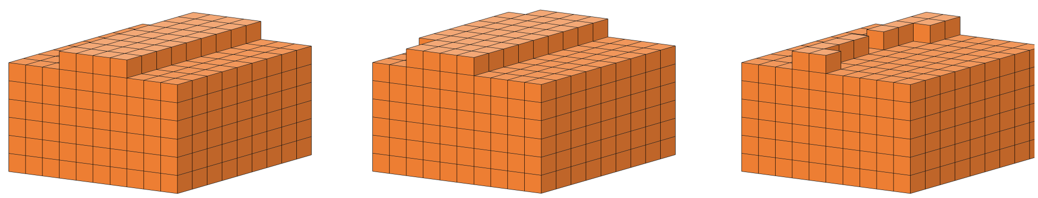


Figure 4.4: Examples of gateway configurations. Each configuration above represents a gateway configuration of type 1 (left), type 2 (middle), or type 3 (right), respectively.

4.4.1 Gateway configurations

We refer to Figure 4.4 for an illustration of gateway configurations defined below.

Definition 4.4.1 (Gateway configurations)**.** For $a,\, b \in \Omega$ and $P,\, Q \in \mathfrak{S}_M$ with $P \prec Q$, we define $\widetilde{\mathcal{G}}_{P,\,Q}^{a,\,b} \subseteq \widetilde{\mathcal{C}}_{P,\,Q}^{a,\,b}$ as

$$\sigma \in \widetilde{\mathcal{G}}_{P,\,Q}^{a,\,b} \quad \Leftrightarrow \quad \begin{cases} \sigma^{(m)} = \boldsymbol{b}^{2\mathrm{D}} & \text{if } m \in P, \\ \sigma^{(m)} = \boldsymbol{a}^{2\mathrm{D}} & \text{if } m \in Q^c, \\ \sigma^{(m)} \in \mathcal{G}^{a,\,b,\,2\mathrm{D}} & \text{if } m \in Q \setminus P, \end{cases}$$

where $\mathcal{G}^{a,\,b,\,2\mathrm{D}}$ is defined in Definition 3.9.8. Then, we define (cf. Notation 4.3.2)

$$\mathcal{G}_{P,\,Q}^{a,\,b} = \Upsilon(\widetilde{\mathcal{G}}_{P,\,Q}^{a,\,b}).$$

Then, recall $\mathfrak{m}_K$ from (4.42) and define, for $i \in [\![0,\, M-1]\!]$,

$$\mathcal{G}_i^{a,\,b} = \bigcup_{P,\,Q \in \mathfrak{S}_M :\, |P|=i \text{ and } P \prec Q} \mathcal{G}_{P,\,Q}^{a,\,b} \quad \text{and} \quad \mathcal{G}^{a,\,b} = \bigcup_{i=\mathfrak{m}_K-1}^{M-\mathfrak{m}_K} \mathcal{G}_i^{a,\,b}. \tag{4.48}$$

Notice that the crucial difference between (4.48) and (4.26) is the fact that the second union in (4.48) is taken only over $i \in [\![\mathfrak{m}_K - 1,\, M - \mathfrak{m}_K]\!]$. This is related to (4.43), and we give a more detailed reasoning in Section 4.4.2.

A configuration belonging to $\mathcal{G}^{a,\,b}$ for some $a,\, b \in \Omega$ is called a *gateway configuration*.

Finally, for a proper partition $(A,\, B)$ of Ω, we write for $i \in [\![0,\, M-1]\!]$,

$$\mathcal{G}_i^{A,\,B} = \bigcup_{a\in A}\bigcup_{b\in B}\mathcal{G}_i^{a,\,b} \quad \text{and} \quad \mathcal{G}^{A,\,B} = \bigcup_{a\in A}\bigcup_{b\in B}\mathcal{G}^{a,\,b}. \tag{4.49}$$

Notation 4.4.2. For $a,\, b \in \Omega$ and $P,\, Q \in \mathfrak{S}_M$ with $P \prec Q$, $Q \setminus P = \{m_0\}$, and $|P| \in [\![\mathfrak{m}_K - 1,\, M - \mathfrak{m}_K]\!]$, we decompose

$$\widetilde{\mathcal{G}}_{P,\,Q}^{a,\,b} = \widetilde{\mathcal{G}}_{P,\,Q}^{a,\,b,\,[1]} \cup \widetilde{\mathcal{G}}_{P,\,Q}^{a,\,b,\,[2]} \cup \widetilde{\mathcal{G}}_{P,\,Q}^{a,\,b,\,[3]},$$

where (cf. Definition 3.4.14)

$$\begin{aligned}
\widetilde{\mathcal{G}}_{P,\,Q}^{a,\,b,\,[1]} &= \{\sigma \in \widetilde{\mathcal{G}}_{P,\,Q}^{a,\,b} : \sigma^{(m_0)} \in \mathcal{B}^{a,\,b,\,2\mathrm{D}} \setminus \mathcal{B}_{\Gamma}^{a,\,b,\,2\mathrm{D}}\},\\
\widetilde{\mathcal{G}}_{P,\,Q}^{a,\,b,\,[2]} &= \{\sigma \in \widetilde{\mathcal{G}}_{P,\,Q}^{a,\,b} : \sigma^{(m_0)} \in \mathcal{B}_{\Gamma}^{a,\,b,\,2\mathrm{D}}\},\\
\widetilde{\mathcal{G}}_{P,\,Q}^{a,\,b,\,[3]} &= \{\sigma \in \widetilde{\mathcal{G}}_{P,\,Q}^{a,\,b} : \sigma^{(m_0)} \in \mathcal{Z}^{a,\,b,\,2\mathrm{D}} \cup \mathcal{Z}^{b,\,a,\,2\mathrm{D}}\}.
\end{aligned}$$

Then, write $\mathcal{G}_{P,\,Q}^{a,\,b,\,[n]} = \Upsilon(\widetilde{\mathcal{G}}_{P,\,Q}^{a,\,b,\,[n]})$, $n \in \{1,\, 2,\, 3\}$. A configuration $\sigma \in \mathcal{G}^{A,\,B}$ is called a *gateway configuration of type* n, $n \in \{1,\, 2,\, 3\}$, if $\sigma \in \mathcal{G}_{P,\,Q}^{a,\,b,\,[n]}$ for some $a \in A$, $b \in B$ and $P,\, Q \in \mathfrak{S}_M$ with $P \prec Q$.

The following proposition is direct from the definition of gateway configurations.

Proposition 4.4.3. *For $\sigma \in \mathcal{G}^{A,\,B}$, we have $H(\sigma) \in \{\Gamma - 2,\, \Gamma\}$. Moreover, we have $H(\sigma) = \Gamma - 2$ if and only if σ is a gateway configuration of type 1 and $H(\sigma) = \Gamma$ if and only if σ is a gateway configuration of type 2 or 3.*

Proof. Let $\sigma \in \widetilde{\mathcal{G}}_{P,\,Q}^{a,\,b}$ for some $a \in A$, $b \in B$ and $P,\, Q \in \mathfrak{S}_M$ with $P \prec Q$, $Q \setminus P = \{m_0\}$, and $|P| \in [\![\mathfrak{m}_K - 1,\, M - \mathfrak{m}_K]\!]$. Then, by Lemma 4.3.6, we can write

$$H(\sigma) = H^{2\mathrm{D}}(\sigma^{(m_0)}) + 2KL$$

since $H^{2\mathrm{D}}(\sigma^{(m)}) = 0$ for all $m \neq m_0$ and $H^{1\mathrm{D}}(\sigma^{\langle k,\,\ell\rangle}) = 2$ for all $k \in \mathbb{T}_K$ and $\ell \in \mathbb{T}_L$. Hence, by definition, we have

$$H(\sigma) = \begin{cases} 2KL + 2K = \Gamma - 2 & \text{if } \sigma \in \widetilde{\mathcal{G}}_{P,\,Q}^{a,\,b,\,[1]}, \\ 2KL + 2K + 2 = \Gamma & \text{if } \sigma \in \widetilde{\mathcal{G}}_{P,\,Q}^{a,\,b,\,[2]} \cup \widetilde{\mathcal{G}}_{P,\,Q}^{a,\,b,\,[3]}. \end{cases}$$

Since the Hamiltonian is invariant under Υ, the proof is completed. □

4.4.2 Properties of gateway configurations

Next, we investigate several crucial properties of the gateway configurations which will be used frequently in the following discussions. The following notation will be useful in the remaining parts of the article.

Notation 4.4.4. For any integers u, v such that $0 \leq u < v \leq M$, we write

$$\mathcal{K}_{[u,\,v]}^{a,\,b} = \bigcup_{i=u}^{v} \mathcal{K}_i^{a,\,b} \quad \text{and} \quad \mathcal{K}_{[u,\,v]}^{A,\,B} = \bigcup_{i=u}^{v} \mathcal{K}_i^{A,\,B},$$

where $\mathcal{K} \in \{\mathcal{C},\, \mathcal{G},\, \mathcal{R}\}$. In particular, by (4.48) and (4.49), we can write

$$\mathcal{G}^{A,\,B} = \mathcal{G}_{[\mathfrak{m}_K - 1,\, M - \mathfrak{m}_K]}^{A,\,B}. \tag{4.50}$$

In this section, we focus on the relation between gateway configurations and neighborhoods of regular configurations. We refer to Figure 4.5 for an illustration of the relations obtained in the current subsection.

The first one below states that we have to escape from a gateway configuration via a neighborhood of regular configurations, unless we touch a configuration with energy higher than Γ.

Lemma 4.4.5. *For a proper partition $(A,\, B)$ of Ω, the following statements hold.*

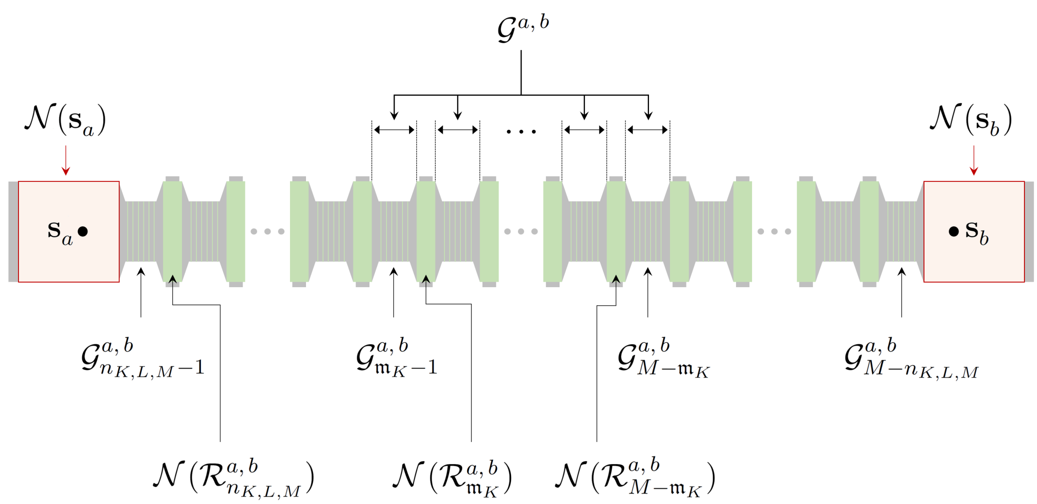


Figure 4.5: Structure of gateway configurations between $\boldsymbol{a}$ and $\boldsymbol{b}$. The grey regions consist of configurations of energy Γ. The green boxes denote the sets of the form $\mathcal{N}(\mathcal{R}_i^{a,b})$ for $i \in [\![n_{K,L,M},\, M-n_{K,L,M}]\!]$ (cf. (4.44)), while the green lines denote the gateway configurations of type 1 whose energy is $\Gamma - 2$ (cf. Proposition 4.4.3). Later in Proposition 4.5.1, we shall show that $\mathfrak{m}_K \geq n_{K,L,M}$. The structure given in this figure (especially between $\mathcal{G}^{a,b}_{\mathfrak{m}_K-1}$ and $\mathcal{G}^{a,b}_{M-\mathfrak{m}_K}$) is confirmed in Lemma 4.4.5. We remark that the dead-ends are attached to $\mathcal{N}(\boldsymbol{a})$, $\mathcal{N}(\boldsymbol{b})$, and $\mathcal{N}(\mathcal{R}_i^{a,b})$, $i \in [\![n_{K,L,M},\, M-n_{K,L,M}]\!]$. In particular, the configurations in $\mathcal{G}_i^{a,b}$ with $i < n_{K,L,M} - 1$ belong to the dead-ends attached to the set $\mathcal{N}(\boldsymbol{a})$.

(1) For $a \in A$, $b \in B$, and $i \in [\![\mathfrak{m}_K - 1,\, M - \mathfrak{m}_K]\!]$, we suppose that $\sigma \in \mathcal{G}_i^{a,\,b}$ and $\zeta \in \mathcal{X} \setminus \mathcal{G}_i^{a,\,b}$ satisfy $\sigma \sim \zeta$ and $H(\zeta) \le \Gamma$. Then, we have $\zeta \in \mathcal{N}(\mathcal{R}_{[i,\,i+1]}^{a,\,b})$, and moreover σ is a gateway configuration of type 3.

(2) Suppose that $\sigma \in \mathcal{G}^{A,\,B}$ and $\zeta \in \mathcal{X} \setminus \mathcal{G}^{A,\,B}$ satisfy $\sigma \sim \zeta$ and $H(\zeta) \le \Gamma$. Then, we have $\zeta \in \mathcal{N}(\mathcal{R}_{[\mathfrak{m}_K-1,\, M-\mathfrak{m}_K+1]}^{A,\,B})$, and moreover σ is a gateway configuration of type 3.

Proof. We first suppose that $\sigma \in \widetilde{\mathcal{G}}_{P,Q}^{a,\,b}$ and $\zeta \in \mathcal{X} \setminus \widetilde{\mathcal{G}}_{P,Q}^{a,\,b}$ for some $a \in A$, $b \in B$ and $P,\, Q \in \mathfrak{S}_M$ with $P \prec Q$ and $|P| \in [\![\mathfrak{m}_K - 1,\, M - \mathfrak{m}_K]\!]$. We write $Q \setminus P = \{m_0\}$. Then, we claim that $\zeta \in \mathcal{N}(\{\sigma_P^{a,\,b},\, \sigma_Q^{a,\,b}\})$, and σ is of type 3.

Let us first show that σ is a gateway configuration of type 3. If σ is of type 1, then we have $H(\sigma) = \Gamma - 2$, $H^{\mathrm{2D}}(\sigma^{(m_0)}) = 2K$, and $\sigma^{(m_0)} \in \mathcal{B}^{a,\,b,\,\mathrm{2D}}$. To update a spin in σ without increasing the energy by 3 or more, it can be readily observed that we have to update a spin of σ at the m_0-th floor to get ζ with $H^{\mathrm{2D}}(\zeta^{(m_0)}) \le 2K + 2$. In such a situation, Lemma 3.9.10 asserts that $\sigma^{(m_0)} \notin \mathcal{B}^{a,\,b,\,\mathrm{2D}}$ and we get a contradiction. A similar argument can be applied if σ is of type 2, and hence we can conclude that σ is of type 3.

Now, since σ is of type 3, we have $H(\sigma) = \Gamma$, $H^{\mathrm{2D}}(\sigma^{(m_0)}) = 2K + 2$, and $\sigma^{(m_0)} \in \mathcal{Z}^{a,\,b,\,\mathrm{2D}} \cup \mathcal{Z}^{b,\,a,\,\mathrm{2D}}$ (cf. (3.51)). In order not to increase the energy by flipping a site of σ, it is clear that we have to flip a spin at the m_0-th floor (cf. Figure 4.4). This means that, by Lemma 3.9.10, we have $\zeta^{(m_0)} \in \mathcal{N}^{\mathrm{2D}}(\boldsymbol{a}^{\mathrm{2D}}) \cup \mathcal{N}^{\mathrm{2D}}(\boldsymbol{b}^{\mathrm{2D}})$. Now, we suppose first that $\zeta^{(m_0)} \in \mathcal{N}^{\mathrm{2D}}(\boldsymbol{a}^{\mathrm{2D}})$. Then, there exists a 2D $(2K+1)$-path $(\omega_t)_{t=0}^T$ in $\mathcal{X}^{\mathrm{2D}} = S^{\Lambda^{\mathrm{2D}}}$ such that $\omega_0 = \boldsymbol{a}^{\mathrm{2D}}$ and $\omega_T = \zeta^{(m_0)}$. Define a 3D path $(\widetilde{\omega}_t)_{t=0}^T$ as

$$\widetilde{\omega}_t^{(m)} = \begin{cases} \omega_t^{(m)} & \text{if } m = m_0, \\ \zeta^{(m)} = \sigma^{(m)} & \text{if } m \ne m_0. \end{cases}$$

Then, $(\widetilde{\omega}_t)_{t=0}^T$ is a $(\Gamma - 1)$-path connecting $\sigma_P^{a,\,b}$ and ζ, and thus we get $\zeta \in \mathcal{N}(\sigma_P^{a,\,b})$. Similarly, we can deduce that $\zeta^{(m_0)} \in \mathcal{N}^{\mathrm{2D}}(\boldsymbol{b}^{\mathrm{2D}})$ implies $\zeta \in \mathcal{N}(\sigma_Q^{a,\,b})$. This concludes the proof of the claim.

Now, we return to the lemma. For part (1), suppose that $\sigma \in \mathcal{G}_{P,Q}^{a,b}$ for some $a \in A$, $b \in B$ and $P, Q \in \mathfrak{S}_M$ with $|P| = i \in [\![\mathfrak{m}_K - 1, M - \mathfrak{m}_K]\!]$ and $P \prec Q$. If $\sigma \in \widetilde{\mathcal{G}}_{P,Q}^{a,b}$, then by the claim above, we get

$$\zeta \in \mathcal{N}(\{\sigma_P^{a,b}, \sigma_Q^{a,b}\}) \subseteq \mathcal{N}(\mathcal{R}_{[i,i+1]}^{a,b}),$$

and moreover σ is a gateway configuration of type 3. On the other hand, if $\sigma \in \Theta(\widetilde{\mathcal{G}}_{P,Q}^{a,b})$ for some permutation operator Θ that appears in Notation 4.3.2, then by the same logic as above, we obtain that

$$\zeta \in \mathcal{N}(\{\Theta(\sigma_P^{a,b}), \Theta(\sigma_Q^{a,b})\}) \subseteq \mathcal{N}(\Theta(\widetilde{\mathcal{R}}_{[i,i+1]}^{a,b})) \subseteq \mathcal{N}(\mathcal{R}_{[i,i+1]}^{a,b}),$$

and that σ is a gateway configuration of type 3. This completes the proof of part (1). Part (2) is direct from part (1). $\square$

Next, we establish a relation between $\mathcal{G}^{A,B}$ and $\mathcal{N}(\mathcal{R}_{[0,M]}^{A,B})$ for proper partitions (A, B) of S.

Lemma 4.4.6. *For a proper partition (A, B) of Ω, the two sets $\mathcal{G}^{A,B}$ and $\mathcal{N}(\mathcal{R}_{[0,M]}^{A,B})$ are disjoint and moreover, it holds that*

$$\widehat{\mathcal{N}}\big(\mathcal{G}^{A,B}; \mathcal{N}(\mathcal{R}_{[0,M]}^{A,B})\big) = \mathcal{G}^{A,B}. \tag{4.51}$$

Proof. We first claim that, for any $a \in A$, $b \in B$, and $P, Q \in \mathfrak{S}_M$ with $P \prec Q$ and $|P| \in [\![\mathfrak{m}_K - 1, M - \mathfrak{m}_K]\!]$[2],

$$\widetilde{\mathcal{G}}_{P,Q}^{a,b} \cap \mathcal{N}(\mathcal{R}_{[0,M]}^{A,B}) = \emptyset. \tag{4.52}$$

Suppose the contrary that we can take a configuration $\sigma \in \widetilde{\mathcal{G}}_{P,Q}^{a,b} \cap \mathcal{N}(\mathcal{R}_{[0,M]}^{A,B})$. Then, since $\sigma \in \widetilde{\mathcal{G}}_{P,Q}^{a,b}$ and since $H(\sigma) < \Gamma$ as $\sigma \in \mathcal{N}(\mathcal{R}_{[0,M]}^{A,B})$, the configuration σ must be a gateway configuration of type 1 by Proposition 4.4.3. Since $\sigma \in \mathcal{N}(\mathcal{R}_{[0,M]}^{A,B})$, there exists a $(\Gamma - 1)$-path connecting σ and $\mathcal{R}_{[0,M]}^{A,B}$.

[2]In fact, it holds even if $|P| \in [\![0, M-1]\!]$.

However, it is clear that (cf. Figure 4.4) any configuration ζ such that $\zeta \sim \sigma$ has energy at least Γ. This yields a contradiction. By the same argument, we can show that $\Theta(\widetilde{\mathcal{G}}^{a,\,b}_{P,\,Q})$ is also disjoint with $\mathcal{N}(\mathcal{R}^{A,\,B}_{[0,\,M]})$ where Θ is one of the permutation operators introduced in Notation 4.3.2, and hence it holds that $\mathcal{G}^{a,\,b}_{P,\,Q}$ is disjoint with $\mathcal{N}(\mathcal{R}^{A,\,B}_{[0,\,M]})$. Hence, the two sets $\mathcal{G}^{A,\,B}$ and $\mathcal{N}(\mathcal{R}^{A,\,B}_{[0,\,M]})$ are disjoint.

Next, we turn to (4.51). Since $\mathcal{G}^{A,\,B} \subseteq \widehat{\mathcal{N}}(\mathcal{G}^{A,\,B};\, \mathcal{N}(\mathcal{R}^{A,\,B}_{[0,\,M]}))$ easily follows from (4.52), it suffices to show that

$$\widehat{\mathcal{N}}(\mathcal{G}^{A,\,B};\, \mathcal{N}(\mathcal{R}^{A,\,B}_{[0,\,M]})) \subseteq \mathcal{G}^{A,\,B}.$$

Suppose the contrary that we can take $\sigma \in \widehat{\mathcal{N}}(\mathcal{G}^{A,\,B};\, \mathcal{N}(\mathcal{R}^{A,\,B}_{[0,\,M]}))$ which does not belong to $\mathcal{G}^{A,\,B}$. Let $(\omega_t)_{t=0}^T$ be a Γ-path in $\mathcal{X} \setminus \mathcal{N}(\mathcal{R}^{A,\,B}_{[0,\,M]})$ connecting $\mathcal{G}^{A,\,B}$ and σ. Since we have assumed that $\sigma \notin \mathcal{G}^{A,\,B}$, we can take

$$t_0 = \min\{t : \omega_t \notin \mathcal{G}^{A,\,B}\}.$$

Since $\omega_{t_0-1} \in \mathcal{G}^{A,\,B}$, $\omega_{t_0} \notin \mathcal{G}^{A,\,B}$, and $\omega_{t_0-1} \sim \omega_{t_0}$, by Lemma 4.4.5, we have $\omega_{t_0-1} \in \mathcal{N}(\mathcal{R}^{A,\,B}_{[\mathfrak{m}_K-1,\, M-\mathfrak{m}_K+1]})$. This contradicts the fact that $(\omega_t)_{t=0}^T$ is a path in $\mathcal{X} \setminus \mathcal{N}(\mathcal{R}^{A,\,B}_{[0,\,M]})$. □

4.5 Energy barrier between ground states

The main objective of the current section is to analyze the energy barrier and optimal paths between ground states. In this section, we fix a proper partition $(A,\, B)$ of S. The main result of the current section is the following result regarding the energy barrier between the ground states.

Proposition 4.5.1. *The following statements hold.*

(1) For $\boldsymbol{s},\, \boldsymbol{s'} \in \mathcal{S}$, we have that $\Phi(\boldsymbol{s},\, \boldsymbol{s'}) \geq \Gamma$.

(2) Let $(\omega_t)_{t=0}^T$ be a path in $\mathcal{X} \setminus \mathcal{G}^{A,\,B}$ connecting $\mathcal{S}(A)$ and $\mathcal{S}(B)$. Then, there exists $t \in [\![0,\,T]\!]$ such that $H(\omega_t) \geq \Gamma + 1$.

Part (1) of the previous proposition gives an opposite bound of Proposition 4.3.11 and hence completes the proof of the characterization of the energy barrier. *Moreover, in part (2), it is verified that any optimal path connecting $\mathcal{S}(A)$ and $\mathcal{S}(B)$ must visit a gateway configuration between them.* Before proceeding further, we officially conclude the proof of Theorem 4.1.1 by assuming Proposition 4.5.1.

Proof of Theorem 4.1.1. The conclusion of the theorem holds by Proposition 4.3.11 and part (1) of Proposition 4.5.1. □

We provide the proof of Proposition 4.5.1 in Sections 4.5.1 and 4.5.2. Then, in Section 4.5.3, we prove the large deviation-type results, namely Theorem 4.1.4, based on the analysis of energy landscape that we carried out so far.

4.5.1 Preliminary analysis on energy landscape

The purpose of this subsection is to provide a lemma (cf. Lemma 4.5.3 below) regarding the communication height between two far away configurations, which will be the crucial tool in the proof of Proposition 4.5.1.

Before proceeding to this result, we first introduce a lower bound on the Hamiltonian H which will be used frequently in the remaining computations of the current section. For $\sigma \in \mathcal{X}$ and $a \in \Omega$, denote by $\mathcal{D}_a(\sigma) \subseteq \mathbb{T}_K \times \mathbb{T}_L$ the collection of monochromatic pillars in σ of spin a:

$$\mathcal{D}_a(\sigma) = \{(k,\,\ell) \in \mathbb{T}_K \times \mathbb{T}_L : \sigma^{\langle k,\,\ell\rangle}(m) = a \text{ for all } m \in \mathbb{T}_M\}.$$

Then, let $\mathcal{D}(\sigma) = \bigcup_{a\in\Omega} \mathcal{D}_a(\sigma)$ and write

$$d_a(\sigma) = |\mathcal{D}_a(\sigma)| \quad \text{and} \quad d(\sigma) = |\mathcal{D}(\sigma)| = \sum_{a\in\Omega} d_a(\sigma). \tag{4.53}$$

Now, we derive a lower bound on H.

Lemma 4.5.2. *For each $\sigma \in \mathcal{X}$, it holds that*

$$H(\sigma) \geq 2KL - 2d(\sigma) + \sum_{m\in\mathbb{T}_M} H^{2\mathrm{D}}(\sigma^{(m)}), \tag{4.54}$$

and the equality holds if and only if $H^{1\mathrm{D}}(\sigma^{\langle k,\,\ell\rangle}) = 2$ for all $(k,\,\ell) \in (\mathbb{T}_K \times \mathbb{T}_L) \setminus \mathcal{D}(\sigma)$.

Proof. Since $H^{1\mathrm{D}}(\sigma^{\langle k,\,\ell\rangle}) = 0$ if $(k,\,\ell) \in \mathcal{D}(\sigma)$ and $H^{1\mathrm{D}}(\sigma^{\langle k,\,\ell\rangle}) \geq 2$ otherwise, we have that

$$\sum_{(k,\,\ell)\in\mathbb{T}_K\times\mathbb{T}_L} H^{1\mathrm{D}}(\sigma^{\langle k,\,\ell\rangle}) \geq 2(KL - d(\sigma)). \tag{4.55}$$

Hence, we can deduce (4.54) from Lemma 4.3.6. The conclusion on the equality condition is immediate from the argument above. □

Now, we proceed to the main result of this subsection. For the simplicity of notation, we write, for $a \in \Omega$,

$$\mathcal{V}^a := \mathcal{N}^{2\mathrm{D}}(\boldsymbol{a}^{2\mathrm{D}}) \subseteq \mathcal{X}^{2\mathrm{D}} \quad \text{and} \quad \Delta^{2\mathrm{D}} := \mathcal{X}^{2\mathrm{D}} \setminus \bigcup_{a=1}^{q} \mathcal{V}^a \tag{4.56}$$

so that we have the following natural decomposition of the set $\mathcal{X}^{2\mathrm{D}}$:

$$\mathcal{X}^{2\mathrm{D}} = \Big(\bigcup_{a=1}^{q} \mathcal{V}^a\Big) \cup \Delta^{2\mathrm{D}}. \tag{4.57}$$

Note that the set $\Delta^{2\mathrm{D}}$ is non-empty by the definition of $\mathcal{N}^{2\mathrm{D}}$. Recall $\mathfrak{m}_K \in \mathbb{N}$ from (4.42). The following lemma, which is the main technical result in the analysis of the energy landscape, asserts that *we have to overcome an energy barrier of* Γ *in order to change a 2D configuration at a certain floor from a neighborhood of a ground state to a neighborhood of another ground state.*

Lemma 4.5.3. *Suppose that* $a,\, b \in \Omega$*. Moreover, let* U *and* V *be two disjoint subsets of* $\mathbb{T}_M$ *satisfying* $|U|,\, |V| \geq \mathfrak{m}_K$*, and let* $\sigma \in \mathcal{X}$ *be a configuration satisfying*

$$\sigma^{(m)} \in \mathcal{V}^a \text{ for all } m \in U \quad \text{and} \quad \sigma^{(m)} \in \mathcal{V}^b \text{ for all } m \in V.$$

Suppose that another configuration $\zeta \in \mathcal{X}$ *satisfies either* $\zeta^{(m)} \in \mathcal{V}^{a_1}$ *for some* $m \in U$ *and* $a_1 \neq a$ *or* $\zeta^{(m)} \in \mathcal{V}^{b_1}$ *for some* $m \in V$ *and* $b_1 \neq b$*. Finally, we assume that* σ *satisfies*

$$d(\sigma) < 200. \tag{4.58}$$

Then, both of the following statements hold.

(1) It holds that $\Phi(\sigma,\, \zeta) \geq \Gamma$*.*

(2) For any path $(\omega_t)_{t=0}^T$ *in* $\mathcal{X} \setminus \mathcal{G}^{a,b}$ *connecting* σ *and* ζ*, there exists* $t \in [\![0,\, T]\!]$ *such that* $H(\omega_t) \geq \Gamma + 1$*.*

Proof. We first consider part (1). Let $(\omega_t)_{t=0}^T$ be a path connecting σ and ζ. For convenience of notation, we define a collection $(c_m)_{m\in U\cup V}$ such that

$$c_m = \begin{cases} a & \text{if } m \in U, \\ b & \text{if } m \in V. \end{cases} \tag{4.59}$$

Then, we define

$$T_0 = \min\{t : H^{\text{2D}}(\omega_t^{(m)}) \notin \mathcal{V}^{c_m} \text{ for some } m \in U \cup V\},$$

where the existence of $t \in [\![1,\, T-1]\!]$ such that $H^{\text{2D}}(\omega_t^{(m)}) \notin \mathcal{V}^{c_m}$ for some $m \in U \cup V$ is guaranteed by the conditions on σ and ζ. Now, we find $m_0 \in$

$U \cup V$ such that

$$H^{2\mathrm{D}}(\omega_{T_0}^{(m_0)}) \notin \mathcal{V}^{c_{m_0}}. \tag{4.60}$$

By the definitions of $\mathcal{V}^a$ and T_0, we have that

$$H^{2\mathrm{D}}(\omega_{T_0}^{(m_0)}) \geq \Gamma^{2\mathrm{D}} = 2K + 2. \tag{4.61}$$

If $H(\omega_{T_0}) \geq \Gamma$, there is nothing to prove. Hence, let us assume from now on that

$$H(\omega_{T_0}) < \Gamma. \tag{4.62}$$

Then, by Lemma 4.5.2 with $\sigma = \omega_{T_0}$ and by recalling the definition (4.53) of $d(\sigma)$, we have

$$2\sum_{n\in\Omega} d_n(\omega_{T_0}) + 2K + 2 > \sum_{m\in\mathbb{T}_M} H^{2\mathrm{D}}(\omega_{T_0}^{(m)}). \tag{4.63}$$

Since we get a contradiction to (4.61) if $\mathcal{D}_n(\omega_{T_0}) = \emptyset$ for all $n \in \Omega$, there exists $n \in \Omega$ such that $\mathcal{D}_n(\omega_{T_0}) \neq \emptyset$. Suppose first that $n \in \Omega \setminus \{b\}$. For this case, we claim that

$$H^{2\mathrm{D}}(\omega_{T_0}^{(m)}) \geq 4 \text{ for all } m \in V. \tag{4.64}$$

Assume not, so that we have $\omega_{T_0}^{(m)} = \boldsymbol{n}^{2\mathrm{D}}$ for some $m \in V$. If $m = m_0$, this obviously cannot happen. On the other hand, if $m \in V \setminus \{m_0\}$, we have $\omega_{T_0}^{(m)} \in \mathcal{V}^b$ by the definition of T_0 and thus $\omega_{T_0}^{(m)}$ cannot be $\boldsymbol{n}^{2\mathrm{D}}$ as $b \neq n$. Therefore, we verified (4.64). Similarly, if $n \in \Omega \setminus \{a\}$, we obtain

$$H^{2\mathrm{D}}(\omega_{T_0}^{(m)}) \geq 4 \text{ for all } m \in U. \tag{4.65}$$

Since either (4.64) or (4.65) must happen, and since $|U|$, $|V| \geq \mathfrak{m}_K$, we get from (4.61) and (4.63) that

$$2\sum_{n\in\Omega} d_n(\omega_{T_0}) + 2K + 2 > (2K+2) + 4(\mathfrak{m}_K - 1), \tag{4.66}$$

and hence

$$\sum_{n\in\Omega} d_n(\omega_{T_0}) \geq 2\mathfrak{m}_K - 1. \tag{4.67}$$

Thus, we have either

$$\sum_{n\in\Omega\setminus\{a\}} d_n(\omega_{T_0}) \geq \mathfrak{m}_K \quad \text{or} \quad \sum_{n\in\Omega\setminus\{b\}} d_n(\omega_{T_0}) \geq \mathfrak{m}_K.$$

Then for K satisfying the condition in Theorem 4.1.1, we have $\mathfrak{m}_K \geq 200$ and thus by the condition (4.58), we can take $T_1 < T_0$ such that

$$T_1 = \min\Big\{t : \sum_{n\in\Omega\setminus\{a\}} d_n(\omega_t) = h_K^2 \quad \text{or} \quad \sum_{n\in\Omega\setminus\{b\}} d_n(\omega_t) = h_K^2\Big\} \tag{4.68}$$

where $h_K = \lfloor\sqrt{\mathfrak{m}_K - 1}\rfloor$. Since $T_1 < T_0$, by the definition of T_0, we have

$$\omega_{T_1}^{(m)} \in \mathcal{V}^a, \quad \forall m \in U \quad \text{and} \quad \omega_{T_1}^{(m)} \in \mathcal{V}^b, \quad \forall m \in V. \tag{4.69}$$

We first suppose that $\sum_{n\in\Omega\setminus\{a\}} d_n(\omega_{T_1}) = h_K^2$. Since (cf. (3.121))

$$\|\omega_{T_1}^{(m)}\|_n \geq d_n(\omega_{T_1}) \quad \text{for all } m \in \mathbb{T}_M,\ n \in \Omega,$$

we can assert from (4.69) and **(L2)**, **(L3)** of Proposition 3.9.3 that

$$H^{2\mathrm{D}}(\omega_{T_1}^{(m)}) \geq 4\Big(\sum_{n\in\Omega\setminus\{a\}} d_n(\omega_{T_1})\Big)^{1/2} = 4h_K \quad \text{for all } m \in U. \tag{4.70}$$

Therefore, by Lemma 4.5.2 with $\sigma = \omega_{T_1}$, the definition of T_1, and (4.70), we get

$$H(\omega_{T_1}) \geq 2KL - 4h_K^2 + 4h_K|U| \geq 2KL - 4h_K^2 + 4h_K\mathfrak{m}_K > 2KL + 2K + 2 = \Gamma,$$

where the last inequality holds for $K \geq 32$. Of course, we get the same conclusion for the case of $\sum_{n\in\Omega\setminus\{b\}} d_n(\omega_{T_1}) = h_K^2$ by an identical argument. Therefore, we can conclude that $H(\omega_{T_1}) > \Gamma$, and thus part (1) is verified.

Now, we turn to part (2). We now assume that, for some σ and ζ satisfying the assumptions of the lemma, there exists a path $(\omega_t)_{t=0}^T$ in $\mathcal{X} \setminus \mathcal{G}^{a,b}$ connecting σ and ζ with

$$H(\omega_t) \leq \Gamma \quad \text{for all } t \in [\![0, T]\!]. \tag{4.71}$$

Without loss of generality, we can assume that the triple $(\sigma, \zeta, (\omega_t)_{t=0}^T)$ that we selected has the smallest path length T among all such triples.

Recall T_0 from the proof of the first part. If $\mathcal{D}_n(\omega_{T_0}) \neq \emptyset$ for some $n \in \Omega$, we can repeat the same argument with part (1) to deduce $H(\omega_{T_1}) > \Gamma$, where T_1 is defined in (4.68). This contradicts (4.71).

Next, we consider the case when $\mathcal{D}_n(\omega_{T_0}) = \emptyset$ for all $n \in \Omega$. The contradiction for this case is more involved than that of the corresponding case of part (1). By Lemma 4.5.2, we have that

$$2K + 2 \geq \sum_{m\in\mathbb{T}_M} H^{2\mathrm{D}}(\omega_{T_0}^{(m)}). \tag{4.72}$$

Recall m_0 from (4.60). Since $H^{2\mathrm{D}}(\omega_{T_0}^{(m_0)}) = 2K + 2$ by (4.61), we not only have

$$H^{2\mathrm{D}}(\omega_{T_0}^{(m)}) = 0 \quad \text{for all } m \in \mathbb{T}_M \setminus \{m_0\}, \tag{4.73}$$

but also the equality in (4.72) holds, i.e.,

$$\sum_{m\in\mathbb{T}_M} H^{\mathrm{2D}}(\omega_{T_0}^{(m)}) = 2K+2. \tag{4.74}$$

Hence, by the last part of Lemma 4.5.2, we must have

$$H^{\mathrm{1D}}(\omega_{T_0}^{\langle k,\,\ell\rangle}) = 2 \quad \text{for all } (k,\,\ell)\in\mathbb{T}_K\times\mathbb{T}_L. \tag{4.75}$$

From these observations, we can deduce the following facts:

- By (4.74), (4.75), and Lemma 4.5.2, we have $H(\omega_{T_0}) = \Gamma$.
- By (4.73) and (4.75), we have $\omega_{T_0}^{(m)} \in \{\boldsymbol{a}^{\mathrm{2D}},\, \boldsymbol{b}^{\mathrm{2D}}\}$ for all $m\in\mathbb{T}_M\setminus\{m_0\}$.

Moreover, the spins must be aligned so that (4.75) holds. Without loss of generality, we assume that $m_0\in U$, since the case $m_0\in V$ can be handled in an identical manner. Starting from ω_{T_0}, suppose that we flip a spin at m-th floor, $m\neq m_0$, without decreasing the 2D energy of the m_0-th floor. Then, since each non-m_0-th floor is monochromatic and (4.75) holds, the 3D energy of σ increases by at least four and we obtain a contradiction to the fact that $(\omega_t)_{t=0}^T$ is a Γ-path. Thus, we must decrease the 2D energy of the m_0-th floor before modifying the other floors. Define

$$T_2 = \min\{t > T_0 : H^{\mathrm{2D}}(\omega_t^{(m_0)}) < 2K+2\}.$$

Then, by Proposition 3.9.3, it suffices to consider the following two cases:

- **(Case 1: $\omega_{T_2}^{(m_0)} \in \mathcal{V}^n$ for some $n\in\Omega$)** Since $\omega_{T_0}^{(m_0)}\in\mathcal{X}^{\mathrm{2D}}$ is the first escape from the valley $\mathcal{V}^a$, it holds from the minimality of T_2 that $\omega_{T_2}^{(m_0)}\notin\mathcal{V}^n$ for $n\in\Omega\setminus\{a\}$ (the 2D path must visit a number of regular configurations first; see part (1) of Proposition 3.4.17). On the other hand, if $\omega_{T_2}^{(m_0)}\in\mathcal{V}^a$, then we obtain a contradiction from the minimality of the length of $(\omega_t)_{t=0}^T$, as we have a shorter path from ω_{T_2} to ζ where ω_{T_2} clearly satisfies the conditions imposed to σ.

- **(Case 2: $\omega_{T_2}^{(m_0)}$ is a 2D regular configuration)** Since we have assumed that $m_0 \in U$, we have $\omega_{T_2}^{(m_0)} \in \mathcal{R}_2^{a,\,b'}$ for some $b' \in \Omega \setminus \{a\}$ (by the minimality of T_2 and part (1) of Proposition 3.4.17). Now, we claim that $b' = b$. To this end, let us suppose that $b' \neq b$. Then as $\omega_{T_2}^{(m)} \in \{\boldsymbol{a}^{\rm 2D},\, \boldsymbol{b}^{\rm 2D}\}$ for $m \neq m_0$, we have $H^{\rm 1D}(\omega_{T_2}^{\langle k,\,\ell\rangle}) \geq 3$ for $(k,\,\ell) \in \mathbb{T}_K \times \mathbb{T}_L$ satisfying $\omega_{T_2}^{(m_0)}(k,\,\ell) = b'$. Because there are exactly $2K$ such $(k,\,\ell)$, by Lemma 4.5.2, we have

$$H(\omega_{T_2}) = \sum_{(k,\,\ell)\in\mathbb{T}_K\times\mathbb{T}_L} H^{\rm 1D}(\omega_{T_2}^{\langle k,\,\ell\rangle}) + \sum_{m\in\mathbb{T}_M} H^{\rm 2D}(\omega_{T_2}^{(m)})$$
$$\geq 3\times 2K + 2\times(KL-2K) + 2K > \Gamma,$$

  where at the first inequality we used the fact that $H^{\rm 2D}(\omega_{T_2}^{(m_0)}) = 2K$. This contradicts the fact that $(\omega_t)_{t=0}^T$ is a Γ-path. Therefore, we must have $b' = b$, which implies along with (4.75) that $\omega_{T_2} \in \mathcal{G}^{a,\,b}$. Hence, we get a contradiction as we assumed that $(\omega_t)_{t=0}^T$ is a path in $\mathcal{X} \setminus \mathcal{G}^{a,\,b}$.

Since we get a contradiction for both cases, we completed the proof of part (2). □

Remark 4.5.4. We remark that (4.68) is exactly the place from which the lower bound 2829 of K in Theorem 4.1.1 originates.

The following is a direct consequence of the previous lemma which will be used later.

Corollary 4.5.5. *Suppose that $P,\, Q \in \mathfrak{S}_M$ and $|P| \in [\![\mathfrak{m}_K,\, M-\mathfrak{m}_K]\!]$. Then for $a,\, b \in \Omega$, we have $\Phi(\sigma_P^{a,\,b},\, \sigma_Q^{a,\,b}) = \Gamma$. In particular, we have $\Phi(\sigma_P^{a,\,b},\, \boldsymbol{a}) = \Gamma$.*

Proof. We can apply Lemma 4.5.3 with $\sigma = \sigma_P^{a,\,b}$ and $\zeta = \sigma_Q^{a,\,b}$ to get

$$\Phi(\sigma_P^{a,\,b},\, \sigma_Q^{a,\,b}) \geq \Gamma. \tag{4.76}$$

On the other hand, by taking a canonical path connecting $\boldsymbol{a}$ and $\sigma_P^{a,\,b}$, we get $\Phi(\boldsymbol{a},\,\sigma_P^{a,\,b}) \le \Gamma$. Similarly, we get $\Phi(\boldsymbol{a},\,\sigma_Q^{a,\,b}) \le \Gamma$. Hence, we obtain

$$\Phi(\sigma_P^{a,\,b},\,\sigma_Q^{a,\,b}) \le \max\{\Phi(\boldsymbol{a},\,\sigma_P^{a,\,b}),\,\Phi(\boldsymbol{a},\,\sigma_Q^{a,\,b})\} \le \Gamma. \tag{4.77}$$

Combining (4.76) and (4.77) proves $\Phi(\sigma_P^{a,\,b},\,\sigma_Q^{a,\,b}) = \Gamma$. By inserting $Q = \emptyset$, we get $\Phi(\sigma_P^{a,\,b},\,\boldsymbol{a}) = \Gamma$. $\square$

4.5.2 Proof of Proposition 4.5.1

Recall (3.121). Note that

$$\|\sigma\|_a = \sum_{m\in\mathbb{T}_M} \|\sigma^{(m)}\|_a. \tag{4.78}$$

We are now ready to prove Proposition 4.5.1. We first prove this proposition when $q = 2$. Then, the general case can be verified from this result via a projection-type argument.

Proof of Proposition 4.5.1: $q = 2$. Since $q = 2$, we only have two spins 1 and 2 and hence we let $\boldsymbol{s} = \mathbf{1}$ and $\boldsymbol{s'} = \mathbf{2}$. We fix an arbitrary path $(\omega_t)_{t=0}^T$ connecting $\boldsymbol{s}$ and $\boldsymbol{s'}$, and take $\sigma \in (\omega_t)_{t=0}^T$ such that

$$\|\sigma\|_1 = \lfloor KLM/2 \rfloor + 1. \tag{4.79}$$

Since there is nothing to prove if $H(\sigma) \ge \Gamma + 1$, we assume that

$$H(\sigma) \le \Gamma. \tag{4.80}$$

Then, we claim that there exists $t \in [\![0,\,T]\!]$ such that $H(\omega_t) = \Gamma$. Moreover, we claim that if $(\omega_t)_{t=0}^T$ is a path in $\mathcal{X} \setminus \mathcal{G}^{1,\,2}$, there exists $t \in [\![0,\,T]\!]$ such that $H(\omega_t) = \Gamma + 1$. It is clear that a verification of these claims immediately proves the case of $q = 2$.

We recall the decomposition (4.57) of $\mathcal{X}^{2\mathrm{D}}$ and write

$$\begin{aligned} P_n &= P_n(\sigma) = \{m \in \mathbb{T}_M : \sigma^{(m)} \in \mathcal{V}^n\}; \quad n \in \{1, 2\}, \\ R &= R(\sigma) = \{m \in \mathbb{T}_M : \sigma^{(m)} \in \Delta^{2\mathrm{D}}\}, \end{aligned}$$

so that $\mathbb{T}_M$ can be decomposed into $\mathbb{T}_M = P_1 \cup P_2 \cup R$. Write $p_1 = |P_1|$, $p_2 = |P_2|$, and $r = |R|$ so that the previous decomposition of $\mathbb{T}_M$ implies

$$p_1 + p_2 + r = M. \tag{4.81}$$

We also write $d_1 = d_1(\sigma)$, $d_2 = d_2(\sigma)$, and $d = d(\sigma)$ so that $d = d_1 + d_2$. The following facts are crucially used:

- By Lemma 4.5.2 and (4.80), it holds that

$$d_1 + d_2 + K + 1 \geq \frac{1}{2} \sum_{m \in \mathbb{T}_M} H^{2\mathrm{D}}(\sigma^{(m)}). \tag{4.82}$$

- We have

$$\begin{cases} H^{2\mathrm{D}}(\sigma^{(m)}) \geq 4\|\sigma^{(m)}\|_2^{1/2} \geq 4d_2^{1/2} & \text{if } m \in P_1, \\ H^{2\mathrm{D}}(\sigma^{(m)}) \geq 4\|\sigma^{(m)}\|_1^{1/2} \geq 4d_1^{1/2} & \text{if } m \in P_2, \\ H^{2\mathrm{D}}(\sigma^{(m)}) \geq 2K & \text{if } m \in R, \end{cases} \tag{4.83}$$

  where the first two bounds follow from **(L2)** and **(L3)** of Proposition 3.9.3, while the last one follows from **(L1)** of Proposition 3.9.3.

- By inserting (4.83) to (4.82), we get

$$d_1 + d_2 + K + 1 \geq 2p_1 d_2^{1/2} + 2p_2 d_1^{1/2} + Kr. \tag{4.84}$$

We consider four cases separately based on the conditions on p_1, p_2, and r. Recall that we assumed $K \geq 2829$; several arguments below require K to be large enough, and they indeed hold for K in this range.

(Case 1: $p_1, p_2 \geq 1$**)** Since both P_1 and P_2 are non-empty, the first two bounds in (4.83) activate and thus

$$d_1,\, d_2 \leq \frac{(2K+1)^2}{16}. \tag{4.85}$$

We note that, since the function $f(x) = x - 2ax^{1/2}$ is convex on $[0, \infty)$ for $a > 0$, by (4.85) we have

$$\begin{aligned} d_1 - 2p_2 d_1^{1/2} &\leq \max\left\{0,\, \frac{(2K+1)^2}{16} - \frac{2K+1}{2}p_2\right\}, \\ d_2 - 2p_1 d_2^{1/2} &\leq \max\left\{0,\, \frac{(2K+1)^2}{16} - \frac{2K+1}{2}p_1\right\}. \end{aligned} \tag{4.86}$$

Inserting (4.86) to (4.84), we get

$$Kr \leq K + 1 + \sum_{i=1}^{2} \max\left\{0,\, \frac{(2K+1)^2}{16} - \frac{2K+1}{2}p_i\right\}. \tag{4.87}$$

We now consider three sub-cases:

- $p_1, p_2 \leq (2K+1)/8$: For this case, we can rewrite (4.87) as

  $$Kr \leq K+1+\frac{(2K+1)^2}{8}-\frac{2K+1}{2}(p_1+p_2) < K+1+\frac{(2K+1)^2}{8}-K(p_1+p_2).$$

  Inserting (4.81) yields a contradiction since $K \leq M$.

- $p_1 \leq (2K+1)/8 < p_2$ or $p_2 \leq (2K+1)/8 < p_1$: By symmetry, it suffices to consider the former case, for which we can rewrite (4.87) as

  $$\begin{aligned} Kr &\leq K + 1 + \frac{(2K+1)^2}{16} - \frac{2K+1}{2}p_1 \\ &< 2K + \frac{(2K+1)^2}{16} - Kp_1. \end{aligned}$$

Thus, we get

$$p_1 + r \leq 2 + \frac{(2K+1)^2}{16K},$$

and thus by the second bound in (4.83),

$$\begin{aligned} \|\sigma\|_2 &\geq p_2\Big(KL - \frac{(2K+1)^2}{16}\Big) \\ &\geq \Big(M - 2 - \frac{(2K+1)^2}{16K}\Big)\Big(KL - \frac{(2K+1)^2}{16}\Big). \end{aligned}$$

We get a contradiction to (4.79) since the right-hand side is greater than $\lfloor KLM/2 \rfloor + 1$.

- p_1, $p_2 > (2K+1)/8$: By (4.87), we can notice that $r = 0$ or 1. By (4.79), the first bound in (4.83), and (4.78), we get

$$\Big\lfloor \frac{KLM}{2} \Big\rfloor + 1 = \|\sigma\|_1 \geq \sum_{m \in P_1} \|\sigma^{(m)}\|_1 \geq p_1\Big(KL - \frac{(2K+1)^2}{16}\Big),$$

and thus,

$$p_2 \geq M - 1 - p_1 \geq M - 1 - \frac{\lfloor KLM/2 \rfloor + 1}{KL - (2K+1)^2/16} \geq \frac{2K+1}{7}. \quad (4.88)$$

Similarly, we get

$$p_1 \geq \frac{2K+1}{7}. \quad (4.89)$$

Now, by (4.85), (4.88) and (4.89), it holds that

$$p_2 \geq \frac{4}{7} d_1^{1/2} \quad \text{and} \quad p_1 \geq \frac{4}{7} d_2^{1/2}.$$

Inserting this along with (4.88) and (4.89) to the right-hand side of

(4.84), we get

$$
\begin{aligned}
2p_1 d_2^{1/2} + 2p_2 d_1^{1/2} + Kr &\geq \Big(d_2 + \frac{1}{4} p_1 d_2^{1/2}\Big) + \Big(d_1 + \frac{1}{4} p_2 d_1^{1/2}\Big) \\
&\geq d + \frac{2K+1}{28} d^{1/2},
\end{aligned}
$$

where the last inequality follows from the inequality $x^{1/2} + y^{1/2} \geq (x + y)^{1/2}$. Applying this to (4.84), we conclude that

$$
d \leq \Big(\frac{28(K+1)}{2K+1}\Big)^2 < 200.
$$

This proves the condition (4.58) for σ. Moreover, since $p_1, p_2 > (2K + 1)/8 \geq \mathfrak{m}_K$, we can now apply part (1) of Lemma 4.5.3 to deduce $\Phi(\sigma, \boldsymbol{s'}) \geq \Gamma$, and this proves the first part of the claim. Moreover, if $(\omega_t)_{t=0}^T$ is a path in $\mathcal{X} \setminus \mathcal{G}^{1,2}$, then the sub-path from σ to $\omega_T = \boldsymbol{s'}$ is also in $\mathcal{X} \setminus \mathcal{G}^{1,2}$, and thus part (2) of Lemma 4.5.3 verifies the second assertion of the claim as well.

(Case 2: $p_1 \geq 1,\ p_2 = 0,\ r \geq 1$ or $p_1 \geq 1,\ p_2 = 0,\ r \geq 1$**)** By symmetry, it suffices to consider the former case. Similarly as in **(Case 1)**, we can apply the first bound in (4.83) to deduce

$$
d_2 \leq \frac{(2K+1)^2}{16}. \tag{4.90}
$$

Again by the first bound in (4.83), we have

$$
\|\sigma^{(m)}\|_1 \geq KL - \frac{(2K+1)^2}{16} \quad \text{for all } m \in P_1,
$$

and thus we get

$$
\sum_{m \in R} \|\sigma^{(m)}\|_1 = \|\sigma\|_1 - \sum_{m \in P_1} \|\sigma^{(m)}\|_1 \leq \frac{KLM}{2} + 1 - p_1\Big(KL - \frac{(2K+1)^2}{16}\Big).
$$

Therefore, there exists $m_0 \in R$ such that

$$\begin{aligned}
\|\sigma^{(m_0)}\|_1 &\le \frac{1}{r}\Big[\frac{KLM}{2} + 1 - p_1\Big(KL - \frac{(2K+1)^2}{16}\Big)\Big] \\
&= KL - \frac{(2K+1)^2}{16} + \frac{1}{r}\Big[-\frac{KLM}{2} + \frac{(2K+1)^2M}{16} + 1\Big] \\
&\le KL - \frac{(2K+1)^2}{16} - \frac{1}{r}\Big[\frac{KLM}{4} - \frac{K^2M}{20}\Big],
\end{aligned}$$

where at the second line we used $p_1 = M - r$. Thus, we have

$$d_1 \le \|\sigma^{(m_0)}\|_1 \le KL - \frac{(2K+1)^2}{16} - \frac{1}{r}\Big[\frac{KLM}{4} - \frac{K^2M}{20}\Big]. \tag{4.91}$$

Inserting this to (4.84), we get

$$2p_1 d_2^{1/2} + Kr \le d_2 + \Big[KL - \frac{(2K+1)^2}{16} - \frac{1}{r}\Big(\frac{KLM}{4} - \frac{K^2M}{20}\Big)\Big] + K + 1.$$

Reorganizing and applying a similar estimate as in (4.86), we get

$$\begin{aligned}
&Kr + \frac{1}{r}\Big[\frac{KLM}{4} - \frac{K^2M}{20}\Big] \le KL - \frac{(2K+1)^2}{16} + K + 1 + (d_2 - 2p_1 d_2^{1/2}) \\
&\le KL - \frac{(2K+1)^2}{16} + K + 1 + \max\Big\{0, \frac{(2K+1)^2}{16} - \frac{2K+1}{2}p_1\Big\} \\
&= KL + K + 1 - \min\Big\{\frac{(2K+1)^2}{16}, \frac{2K+1}{2}p_1\Big\}.
\end{aligned} \tag{4.92}$$

Now, we analyze two sub-cases separately.

- $p_1 \le (2K+1)/8$: Then, we can rewrite (4.92) as

$$Kr + \frac{1}{r}\Big[\frac{KLM}{4} - \frac{K^2M}{20}\Big] \le KL + K + 1 - \frac{2K+1}{2}p_1 \le KL + K.$$

  Multiplying r/K in both sides, we reorganize the previous inequality as

$$\Big(r - \frac{L+1}{2}\Big)^2 \le \frac{(L+1)^2}{4} - \frac{LM}{4} + \frac{KM}{20} \le \frac{L^2+10L+5}{20}. \qquad (4.93)$$

Since $p_1 \le (2K+1)/8$, we have

$$r \ge M - \frac{2K+1}{8} \ge \frac{3}{4}L - 1. \qquad (4.94)$$

Inserting (4.94) to (4.93) yields a contradiction for $L \ge K \ge 2829$.

- $p_1 > (2K+1)/8$: For this case, (4.92) becomes

$$Kr + \frac{1}{r}\Big[\frac{KLM}{4} - \frac{K^2M}{20}\Big] \le KL + K + 1 - \frac{(2K+1)^2}{16}$$
$$\le KL - \frac{K^2}{4} + K.$$

Multiplying both sides by r/K and reorganizing, we get

$$\Big(r - \frac{L}{2} + \frac{K}{8} - \frac{1}{2}\Big)^2 \le \frac{1}{64}(4L - K + 4)^2 - \frac{LM}{4} + \frac{KM}{20}.$$

Since the right-hand side is negative for $K \ge 9$, we get a contradiction.

(Case 3: $p_1 \ge 1$, $p_2 = 0$, $r = 0$ or $p_1 = 0$, $p_2 \ge 1$, $r = 0$**)** As before, we only consider the former case. In this case, indeed $P_1 = \mathbb{T}_M$. Thus, by the first bound in (4.83) we have

$$\|\sigma\|_1 = \sum_{m \in \mathbb{T}_M} \|\sigma^{(m)}\|_1 \ge M\Big(KL - \frac{(2K+1)^2}{16}\Big) > \frac{KLM}{2} + 2.$$

This contradicts (4.79).

(Case 4: $p_1 = p_2 = 0$**)** For this case, we have $\sigma^{(m)} \in \Delta^{2\mathrm{D}}$ for all $m \in \mathbb{T}_M$. Hence, $H^{2\mathrm{D}}(\sigma^{(m)}) \ge 2K$ for all $m \in \mathbb{T}_M$ by **(L1)** of Proposition 3.9.3, and thus by (4.82) we get

$$d_1 + d_2 \geq K(M-1) - 1. \tag{4.95}$$

Since $d_1 + d_2 = d \leq KL$, we get $M = L+1$ or L.

If $M = L+1$, we must have $d_1 + d_2 = KL$ or $KL-1$. If this is KL, then all floors should have the same configuration, which is impossible since $\|\sigma\|_1 = \lfloor KLM/2 \rfloor + 1$ cannot be a multiple of M. If this is $KL-1$, then the equality in (4.95) must hold and thus we have $H^{2D}(\sigma^{(m)}) = 2K$ for all $m \in \mathbb{T}_M$. Hence, by **(L1)** of Proposition 3.9.3, $\|\sigma^{(m)}\|_1$, $m \in \mathbb{T}_M$, is a multiple of K, and thus $\|\sigma\|_1 = \sum_{m\in\mathbb{T}_M} \|\sigma^{(m)}\|_1$ is also a multiple of K. This is impossible since $\|\sigma\|_1 = \lfloor KLM/2 \rfloor + 1$ is not a multiple of K.

It remains to consider the case of $M = L$. For this case, (4.95) becomes

$$d_1 + d_2 \geq K(L-1) - 1. \tag{4.96}$$

Define

$$\mathcal{E}(\sigma) = (\mathbb{T}_K \times \mathbb{T}_L) \setminus (\mathcal{D}_1(\sigma) \cup \mathcal{D}_2(\sigma)) \tag{4.97}$$

so that we have $|\mathcal{E}(\sigma)| \leq K+1$ by (4.96). We now have three sub-cases. We note that $H^{2D}(\sigma^{(m)})$ is an even integer for each $m \in \mathbb{T}_M$, as $q = 2$.

- First, we assume that $H^{2D}(\sigma^{(m)}) = 2K$ for all $m \in \mathbb{T}_M$. Then, as in the previous discussion on the case of $M = L+1$, we get a contradiction since $\|\sigma\|_1$ must be a multiple of K for this case.

- Next, we assume that $H^{2D}(\sigma^{(m)}) \geq 2K+2$ for all $m \in \mathbb{T}_M$. Then, by (4.82),

  $$d = d_1 + d_2 \geq (K+1)(L-1). \tag{4.98}$$

  If $d = KL$, then as in the case of $M = L+1$, we get a contradiction since $\|\sigma\|_1 = \lfloor KLM/2 \rfloor + 1$ cannot be a multiple of M. Hence, we have $d \leq KL-1$, and combining this with (4.98) implies that we must have

$K = L$ (and thus $K = L = M$), and moreover

$$d = KL - 1 \quad \text{and} \quad H^{2D}(\sigma^{(m)}) = 2K + 2 \quad \text{for all } m \in \mathbb{T}_M.$$

Hence, we have $|\mathcal{E}(\sigma)| = KL - d = 1$. Write $\mathcal{E}(\sigma) = \{(k_0, \ell_0)\}$. By Lemma 3.9.2, we can deduce that the configuration $\sigma^{(m)}$ has at least $L - 1 \geq 3$ monochromatic bridges, and thus we have at least one monochromatic bridge of the form $\mathbb{T}_K \times \{\ell\}$ or $\{k\} \times \mathbb{T}_L$ that does not touch $\mathcal{E}(\sigma)$, so that it is a subset of either $\mathcal{D}_1(\sigma)$ or $\mathcal{D}_2(\sigma)$. Suppose first that this bridge is $\mathbb{T}_K \times \{\ell\}$ for some $\ell \in \mathbb{T}_L$. Then, the slab $\mathbb{T}_K \times \{\ell\} \times \mathbb{T}_M$ is monochromatic. Therefore, by replacing the role of the second and third coordinates, which is possible since $K = L = M$, the proof is reduced to one of **(Case 1)**, **(Case 2)**, and **(Case 3)** as there is a monochromatic floor so that either p_1 or p_2 is positive. This completes the proof. Similarly, if the monochromatic bridge is $\{k\} \times \mathbb{T}_L$, then we replace the role of the first and third coordinates to complete the proof.

- Now, we lastly assume that $H^{2D}(\sigma^{(i_0)}) = 2K$ for some $i_0 \in \mathbb{T}_M$ and $H^{2D}(\sigma^{(j_0)}) \geq 2K + 2$ for some $j_0 \in \mathbb{T}_M$. By (4.82), we get

$$d \geq KL - K, \tag{4.99}$$

and hence, we have $|\mathcal{E}(\sigma)| \leq K$ (cf. (4.97)). Now, we consider two sub-sub-cases separately.

  - $|\mathcal{E}(\sigma)| \leq K - 1$: First, suppose that $K < L$. By **(L1)** of Proposition 3.9.3, we have $\sigma^{(i_0)} \in \mathcal{R}_v^{1,2}$ for some $v \in [\![2, L-2]\!]$. Since $|\mathcal{E}(\sigma)| \leq K - 1 \leq L - 1$, there exists $\ell_1 \in \mathbb{T}_L$ such that

$$(\mathbb{T}_K \times \{\ell_1\}) \cap \mathcal{E}(\sigma) = \emptyset.$$

We further have $\mathbb{T}_K \times \{\ell_1\} \subseteq \mathcal{D}_1(\sigma)$ or $\mathbb{T}_K \times \{\ell_1\} \subseteq \mathcal{D}_2(\sigma)$ since $\sigma^{(i_0)} \in \mathcal{R}_v^{1,2}$. This implies that all sites in the slab $\mathbb{T}_K \times \{\ell_1\} \times \mathbb{T}_M$ have the same spin n under σ. Since $L = M$, we can replace the role of the second and third coordinates to reduce the proof to one of **(Case 1)**, **(Case 2)** and **(Case 3)**. This completes the proof. Next, if $K = L$, then since there further exists $k_1 \in \mathbb{T}_K$ such that $(\{k_1\} \times \mathbb{T}_L) \cap \mathcal{E}(\sigma) = \emptyset$, we can use the same argument as above to handle this case as well.

– $|\mathcal{E}(\sigma)| = K$: The equality in (4.99) must hold, and thus we get $H^{2\mathrm{D}}(\sigma^{(j_0)}) = 2K + 2$ and $H^{2\mathrm{D}}(\sigma^{(m)}) = 2K$ for all $m \in \mathbb{T}_M \setminus \{j_0\}$. We first suppose that $K < L$. By **(L1)** of Proposition 3.9.3, we get $\sigma^{(m)} = \xi_{\ell_m, v_m}^{1,2}$ for some $\ell_m \in \mathbb{T}_L$ and $v_m \in [\![2, L-2]\!]$ for all $m \in \mathbb{T}_M \setminus \{j_0\}$. Then, since L is strictly bigger than $K = |\mathcal{E}(\sigma)|$, we can always find a row in $\mathbb{T}_K \times \mathbb{T}_L$ which is either a subset of $\mathcal{D}_1(\sigma)$ or $\mathcal{D}_2(\sigma)$. Thus, by changing the role of the second and third coordinates, which is possible since $L = M$, we find a monochromatic floor and the proof is reduced to one of **(Case 1)**, **(Case 2)** and **(Case 3)**. Next, we handle the case $K = L$, so that for all $m \in \mathbb{T}_M \setminus \{j_0\}$, $\sigma^{(m)} = \xi_{\ell_m, v_m}^{1,2}$ or $\Theta(\xi_{\ell_m, v_m}^{1,2})$ (cf. Definition 3.4.10) for some $\ell_m \in \mathbb{T}_L$ and $v_m \in [\![2, L-2]\!]$. First of all, assume that all of them are of the same direction. Without loss of generality, assume that $\sigma^{(m)} = \xi_{\ell_m, v_m}^{1,2}$ for all $m \in \mathbb{T}_M \setminus \{j_0\}$. If $\sigma^{(m_1)} \neq \sigma^{(m_2)}$ for some $m_1, m_2 \in \mathbb{T}_M \setminus \{j_0\}$, then $\mathcal{E}(\sigma)$ must be exactly the line where they differ and hence we can write $\mathcal{E}(\sigma) = \mathbb{T}_K \times \{\ell_0\}$ for some $\ell_0 \in \mathbb{T}_L$. Then, by taking any $\ell \in \mathbb{T}_L \setminus \{\ell_0\}$, we notice that $\mathbb{T}_K \times \{\ell\}$ is not only monochromatic in $\sigma^{(m)}$ with $m \in \mathbb{T}_M \setminus \{j_0\}$, but also a subset of either $\mathcal{D}_1(\sigma)$ or $\mathcal{D}_2(\sigma)$; hence, $\mathbb{T}_K \times \{\ell\} \times \mathbb{T}_M$ is a monochromatic slab. By replacing the role of the second and third coordinates, which is possible since $L = M$, we find a monochromatic floor and the proof is reduced to one of **(Case 1)**, **(Case 2)** and **(Case 3)**. On the contrary, suppose that $\sigma^{(m_1)} = \sigma^{(m_2)}$ for all $m_1,\, m_2 \in \mathbb{T}_M \setminus \{j_0\}$. If there exists a row or column which is disjoint with $\mathcal{E}(\sigma)$, then we can argue as above. If not, then we can easily deduce that for the j_0-th floor,

$$H^{\rm 2D}(\sigma^{(j_0)}) \ge 4(K-4) > 2K+2,$$

which contradicts the assumption that $H^{\rm 2D}(\sigma^{(j_0)}) = 2K+2$. Finally, we consider the case when $\sigma^{(m)} = \xi^{1,\,2}_{\ell,\,v}$ and $\sigma^{(m')} = \Theta(\xi^{1,\,2}_{\ell',\,v'})$ for some $m,\, m' \in \mathbb{T}_M \setminus \{j_0\}$ simultaneously. In this case, we have

$$d_1 \le (K-v)(K-v') \quad \text{and} \quad d_2 \le vv'.$$

Thus, we get a contradiction since

$$\begin{aligned} |\mathcal{E}(\sigma)| &\ge K^2 - (K-v)(K-v') - vv' \\ &= \frac{1}{2}K^2 - \frac{1}{2}(K-2v)(K-2v') \\ &\ge \frac{1}{2}K^2 - \frac{1}{2}(K-4)^2 = 4K-8 > K, \end{aligned}$$

where the second inequality holds since $v,\, v' \in [\![2,\, K-2]\!]$.

□

Now, we consider the general case of Proposition 4.5.1.

Proof of Proposition 4.5.1: general case. We fix a proper partition $(A,\, B)$ of S and then fix $a \in A$ and $b \in B$. Let $(\omega_t)_{t=0}^T$ be a path connecting $\boldsymbol{a}$ and $\boldsymbol{b}$. For each $\sigma \in \mathcal{X}$, we denote by $\widetilde{\sigma}$ the configuration obtained from σ by changing all spins in A to 1 and spins in B to 2. Thus, $\widetilde{\sigma}$ becomes an Ising configuration, i.e. a spin configuration for $q = 2$. Note that

$$
\begin{aligned}
H(\widetilde{\sigma}) &= \sum_{\{x,\,y\}\subseteq\Lambda:\,x\sim y} \mathbb{1}\{\widetilde{\sigma}(x) \neq \widetilde{\sigma}(y)\} \\
&= \sum_{\{x,\,y\}\subseteq\Lambda:\,x\sim y} \mathbb{1}\{\sigma(x) \in A,\, \sigma(y) \in B \text{ or } \sigma(x) \in B,\, \sigma(y) \in A\} \\
&\le \sum_{\{x,\,y\}\subseteq\Lambda:\,x\sim y} \mathbb{1}\{\sigma(x) \neq \sigma(y)\} = H(\sigma).
\end{aligned}
\tag{4.100}
$$

Now, we consider the induced pseudo-path $(\widetilde{\omega}_t)_{t=0}^T$ of $(\omega_t)_{t=0}^T$ (cf. Notation 4.3.12). Thus, by the proof above for $q = 2$, there exists $t_1 \in [\![0,\, T]\!]$ such that $H(\widetilde{\omega}_{t_1}) \ge \Gamma$. Thus, we get from (4.100) that

$$
\Gamma \le H(\widetilde{\omega}_{t_1}) \le H(\omega_{t_1}),
$$

and we complete the proof for part (1).

For part (2), suppose that $(\omega_t)_{t=0}^T$ is a path such that

$$
H(\omega_t) \le \Gamma \quad \text{for all } t \in [\![0,\, T]\!]. \tag{4.101}
$$

Then, by (4.100), we have $H(\widetilde{\omega}_t) \le \Gamma$ for all $t \in [\![0,\, T]\!]$. Thus, by the proof above for $q = 2$, there exists $s \in [\![0,\, T]\!]$ such that $\widetilde{\omega}_s \in \mathcal{G}^{1,\,2}$. We now claim that $\omega_s \in \mathcal{G}^{A,\,B}$. It is immediate that this claim finishes the proof.

To prove this claim, we write

$$
\mathcal{U}_n = \{x \in \Lambda : \widetilde{\omega}_s(x) = n\}; \quad n = 1,\, 2.
$$

Then, we have

$$
\omega_s(x) \in A \text{ for } x \in \mathcal{U}_1 \quad \text{and} \quad \omega_s(x) \in B \text{ for } x \in \mathcal{U}_2. \tag{4.102}
$$

Now, we assume that

$$\omega_s(x) \neq \omega_s(y) \text{ for some } x,\, y \in \mathcal{U}_1 \text{ or } x,\, y \in \mathcal{U}_2 \text{ with } x \sim y. \tag{4.103}$$

We now express the energy $H(\omega_s)$ as

$$H(\omega_s) = \Big[\sum_{\{x,\,y\}\subseteq\mathcal{U}_1 \text{ or } \{x,\,y\}\subseteq\mathcal{U}_2} + \sum_{x\in\mathcal{U}_1,\, y\in\mathcal{U}_2} \Big] \mathbb{1}\{\omega_s(x) \neq \omega_s(y)\}, \tag{4.104}$$

where the summation is carried over x, y satisfying $x \sim y$. Note that the second summation is equal to $H(\widetilde{\omega}_s)$ by (4.102). On the other hand, we can readily deduce from Figure 4.4 that the first summation of (4.104) is at least 4 if $\widetilde{\omega}_s$ is a gateway configuration of type 1, and at least 2 if $\widetilde{\omega}_s$ is a gateway configuration of type 2 or 3 (cf. Notation 4.4.2). Thus, by Proposition 4.4.3, we can conclude that the right-hand side of (4.104) is at least $\Gamma + 2$; i.e., we get $H(\omega_s) \geq \Gamma + 2$. This contradicts (4.101) and hence, we cannot have (4.103). This finally implies that there exist $a_0 \in A$ and $b_0 \in B$ such that

$$\omega_s(x) = \begin{cases} a_0 & \text{if } x \in \mathcal{U}_1, \\ b_0 & \text{if } x \in \mathcal{U}_2, \end{cases}$$

and thus we have $\omega_s \in \mathcal{G}^{a_0,\, b_0} \subseteq \mathcal{G}^{A,\, B}$ as claimed. □

4.5.3 Proof of Theorem 4.1.4

Theorem 4.1.4 is now a consequence of our analysis on the energy landscape and the general theory developed in [69, 70].

Proof of Theorem 4.1.4. We have two results on the energy barrier; Theorem 4.1.1 and Proposition 4.3.13. The theory developed in [70] implies that these two are sufficient to conclude Theorem 4.1.4[3]. This implication has been

[3] We remark that the second convergence of (4.9) is not a consequence of an analysis of the energy barrier, but of the first convergence of (4.9) and the symmetry of the model.

rigorously verified in [69] for the case of $d = 2$, and this argument extends to the case of $d = 3$ without a modification. Hence, we do not repeat the argument here, and refer the readers to [69, Section 3] for a detailed proof. □

4.6 Typical configurations and optimal paths

In the previous sections, we proved large deviation-type results regarding the metastable behavior by analyzing the energy barrier in terms of canonical and gateway configurations. In order to get precise quantitative results such as Theorems 4.8.1 and 4.1.9 or to get a characterization of optimal paths, we need a more refined analysis of the energy landscape based on the typical configurations which will be introduced and analyzed in the current section.

We fix a proper partition $(A,\, B)$ of Ω throughout the section.

4.6.1 Typical configurations

Let us start by defining the typical configurations. We consistently refer to Figure 4.6 for an illustration of our construction.

For $a,\, b \in \Omega$ and $i \in [\![0,\, M]\!]$, we define

$$\widehat{\mathcal{R}}_i^{a,\,b} = \widehat{\mathcal{N}}(\mathcal{R}_i^{a,\,b};\, \mathcal{G}^{a,\,b}). \tag{4.105}$$

We also define

$$\widehat{\mathcal{R}}_i^{A,\,B} = \widehat{\mathcal{N}}(\mathcal{R}_i^{A,\,B};\, \mathcal{G}^{A,\,B});\quad i \in [\![0,\, M]\!].$$

Remark 4.6.1. For $i \in [\![\mathfrak{m}_K,\, M - \mathfrak{m}_K]\!]$, we have that

$$\widehat{\mathcal{R}}_i^{A,\,B} = \bigcup_{a\in A,\, b\in B} \widehat{\mathcal{R}}_i^{a,\,b}.$$

This argument is also given in [69, Section 3] for $d = 2$, and an identical one works for $d = 3$.

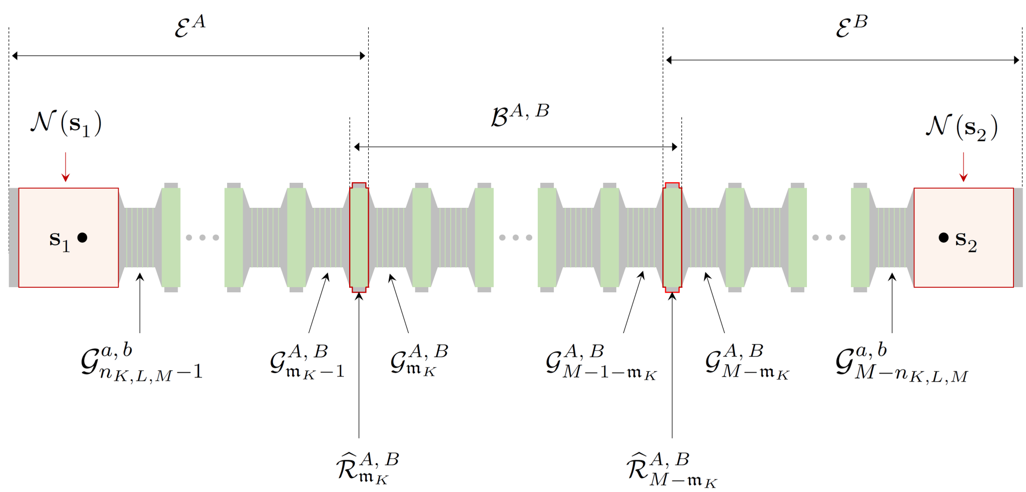


Figure 4.6: 3D typical configurations for the Ising model. Suppose that $q = 2$, $A = \{1\}$, and $B = \{2\}$ (one can compare this figure with Figure 4.5). The given figure provides an illustration of the complete structure of the set $\widehat{\mathcal{N}}(\mathcal{S})$. This characterization is verified in Proposition 4.6.6. We take bulk ones only from $\mathfrak{m}_K$ to $M - \mathfrak{m}_K$ instead of $n_{K,L,M}$ (cf. (4.44)) to $M - n_{K,L,M}$ since we do not know the exact value of $n_{K,L,M}$. Because of this, the structure of the edge typical configurations is a little bit more complicated than in the 2D case.

To check this, it suffices to check $\widehat{\mathcal{N}}(\mathcal{R}_i^{a,\,b};\,\mathcal{G}^{a,\,b}) = \widehat{\mathcal{N}}(\mathcal{R}_i^{a,\,b};\,\mathcal{G}^{A,\,B})$ provided that $a \in A$ and $b \in B$. This follows from Lemma 4.5.3 since $\mathcal{R}_i^{a,\,b}$ cannot be connected to a configuration in $\mathcal{G}^{A,\,B} \setminus \mathcal{G}^{a,\,b}$ via a Γ-path in $\mathcal{X} \setminus \mathcal{G}^{a,\,b}$ by part (2) of Lemma 4.5.3.

Remark 4.6.2. By Lemma 4.5.3, two sets $\widehat{\mathcal{R}}_i^{A,\,B}$ and $\widehat{\mathcal{R}}_j^{A,\,B}$ for different $i,\,j$ are disjoint if either $i \in [\![\mathfrak{m}_K,\,M-\mathfrak{m}_K]\!]$ or $j \in [\![\mathfrak{m}_K,\,M-\mathfrak{m}_K]\!]$. Moreover by Proposition 4.5.1, they are disjoint if $i \in [\![0,\,\mathfrak{m}_K-1]\!]$ and $j \in [\![M-\mathfrak{m}_K+1,\,M]\!]$ or vice versa. On the other hand, they might be the same set if $i,\,j \in [\![0,\,\mathfrak{m}_K-1]\!]$ or $i,\,j \in [\![M-\mathfrak{m}_K+1,\,M]\!]$. In particular, we have

$$\widehat{\mathcal{R}}_0^{A,\,B} = \widehat{\mathcal{R}}_1^{A,\,B} = \cdots = \widehat{\mathcal{R}}_{n_{K,L,M}-1}^{A,\,B},$$

where $n_{K,\,L,\,M}$ is defined in (4.44). The same result holds for $\widehat{\mathcal{R}}_i^{a,\,b}$ instead of $\widehat{\mathcal{R}}_i^{A,\,B}$.

Now, we define the typical configurations. We recall Notation 4.4.4.

Definition 4.6.3 (Typical configurations)**.** For a proper partition $(A,\,B)$ of Ω, we define the typical configurations as follows.

- **Bulk typical configurations:** We define, for $a,\,b \in \Omega$,

$$\mathcal{B}^{a,\,b} = \mathcal{G}^{a,\,b}_{[\mathfrak{m}_K,\,M-\mathfrak{m}_K-1]} \cup \widehat{\mathcal{R}}^{a,\,b}_{[\mathfrak{m}_K,\,M-\mathfrak{m}_K]},$$

  and then define

$$\mathcal{B}^{A,\,B} = \bigcup_{a\in A}\bigcup_{b\in B} \mathcal{B}^{a,\,b} = \mathcal{G}^{A,\,B}_{[\mathfrak{m}_K,\,M-\mathfrak{m}_K-1]} \cup \widehat{\mathcal{R}}^{A,\,B}_{[\mathfrak{m}_K,\,M-\mathfrak{m}_K]}, \tag{4.106}$$

  where the second identity holds because of Remark 4.6.1. A configuration belonging to $\mathcal{B}^{A,\,B}$ is called a *bulk typical configuration* between $\mathcal{S}(A)$ and $\mathcal{S}(B)$.

- **Edge typical configurations:** We define

$$\mathcal{E}^A = \mathcal{G}^{A,B}_{\mathfrak{m}_K-1} \cup \widehat{\mathcal{R}}^{A,B}_{[0,\mathfrak{m}_K]} \quad \text{and} \quad \mathcal{E}^B = \mathcal{G}^{A,B}_{M-\mathfrak{m}_K} \cup \widehat{\mathcal{R}}^{A,B}_{[M-\mathfrak{m}_K,M]}. \tag{4.107}$$

  Finally, we define $\mathcal{E}^{A,B} = \mathcal{E}^A \cup \mathcal{E}^B$. A configuration belonging to $\mathcal{E}^{A,B}$ is called an *edge typical configuration* between $\mathcal{S}(A)$ and $\mathcal{S}(B)$.

Later in Proposition 4.6.6, we shall show that $\mathcal{B}^{A,B} \cup \mathcal{E}^{A,B} = \widehat{\mathcal{N}}(\mathcal{S})$ and hence all relevant configurations in the analysis of metastable behavior between $\mathcal{S}(A)$ and $\mathcal{S}(B)$ belong to either $\mathcal{B}^{A,B}$ or $\mathcal{E}^{A,B}$.

Remark 4.6.4. Since $\mathcal{R}^{A,B}_0 = \mathcal{S}(A)$ and $\mathcal{R}^{A,B}_M = \mathcal{S}(B)$ (cf. (4.29)), we can readily observe that $\mathcal{S}(A) \subseteq \mathcal{E}^A$ and $\mathcal{S}(B) \subseteq \mathcal{E}^B$.

4.6.2 Properties of typical configurations

In this subsection, we analyze some properties of the edge and bulk typical configurations. In fact, we have to take K large enough (i.e., $K \geq 2829$) in order to get the structural properties of edge and bulk typical configurations given in the current section.

The first property asserts that $\mathcal{E}^A$ and $\mathcal{E}^B$ are disjoint.

Proposition 4.6.5. *The two sets $\mathcal{E}^A$ and $\mathcal{E}^B$ are disjoint.*

Proof. By part (2) of Lemma 4.5.3 (cf. Remark 4.6.2), the set $\widehat{\mathcal{R}}^{A,B}_{\mathfrak{m}_K}$ is disjoint with $\mathcal{E}^B$; similarly, the set $\widehat{\mathcal{R}}^{A,B}_{M-\mathfrak{m}_K}$ is disjoint with $\mathcal{E}^A$. It is direct from the definition that $\mathcal{G}^{A,B}_{\mathfrak{m}_K-1}$ and $\mathcal{G}^{A,B}_{M-\mathfrak{m}_K}$ are disjoint. By definition, $\mathcal{G}^{A,B}_{\mathfrak{m}_K-1}, \mathcal{G}^{A,B}_{M-\mathfrak{m}_K} \subseteq \mathcal{G}^{A,B}$ are mutually disjoint with $\widehat{\mathcal{R}}^{A,B}_{[0,\mathfrak{m}_K]}$ and $\widehat{\mathcal{R}}^{A,B}_{[M-\mathfrak{m}_K,M]}$. Hence, it suffices to prove that $\widehat{\mathcal{R}}^{A,B}_{[0,\mathfrak{m}_K-1]}$ and $\widehat{\mathcal{R}}^{A,B}_{[M-\mathfrak{m}_K+1,M]}$ are disjoint. Otherwise, we can take a configuration σ such that

$$\sigma \in \widehat{\mathcal{R}}^{A,B}_{[0,\mathfrak{m}_K-1]} \cap \widehat{\mathcal{R}}^{A,B}_{[M-\mathfrak{m}_K+1,M]}.$$

Since $\sigma \in \widehat{\mathcal{R}}^{A,B}_{[0,\mathfrak{m}_K-1]}$, there exists a Γ-path in $\mathcal{X}\setminus\mathcal{G}^{A,B}$ (which is indeed a part of a canonical path) connecting σ and $\mathcal{S}(A)$. Similarly, there exists a Γ-path in $\mathcal{X}\setminus\mathcal{G}^{A,B}$ connecting σ and $\mathcal{S}(B)$. By concatenating them, we can find a Γ-path $(\omega_t)_{t=0}^T$ in $\mathcal{X}\setminus\mathcal{G}^{A,B}$ connecting $\mathcal{S}(A)$ and $\mathcal{S}(B)$. This contradicts part (2) of Proposition 4.5.1. □

Now, we analyze the crucial features of the typical configurations. Note that this is a 3D version of Proposition 3.4.17.

Proposition 4.6.6. *For a proper partition $(A,\,B)$ of S, the following properties hold for the typical configurations.*

(1) It holds that $\mathcal{E}^A\cap\mathcal{B}^{A,B}=\widehat{\mathcal{R}}^{A,B}_{\mathfrak{m}_K}$ and $\mathcal{E}^B\cap\mathcal{B}^{A,B}=\widehat{\mathcal{R}}^{A,B}_{M-\mathfrak{m}_K}$.

(2) We have $\mathcal{E}^{A,B}\cup\mathcal{B}^{A,B}=\widehat{\mathcal{N}}(\mathcal{S})$.

Proof. (1) It suffices to prove the first identity, as the second one follows similarly. One can observe that the set $\mathcal{G}^{A,B}_{\mathfrak{m}_K-1}\subseteq\mathcal{G}^{A,B}$ is disjoint with $\mathcal{B}^{A,B}$ from (4.106), and the set $\mathcal{G}^{A,B}_{[\mathfrak{m}_K,\,M-\mathfrak{m}_K-1]}\subseteq\mathcal{G}^{A,B}$ is disjoint with $\mathcal{E}^A$ in view of the expression (4.107). Therefore, by (4.106) and (4.107), we get

$$\mathcal{E}^A\cap\mathcal{B}^{A,B}=\widehat{\mathcal{R}}^{A,B}_{[0,\mathfrak{m}_K]}\cap\widehat{\mathcal{R}}^{A,B}_{[\mathfrak{m}_K,\,M-\mathfrak{m}_K]}. \tag{4.108}$$

By Lemma 4.5.3, the two sets $\mathcal{R}^{A,B}_{[0,\mathfrak{m}_K-1]}$ and $\mathcal{R}^{A,B}_{[\mathfrak{m}_K,\,M-\mathfrak{m}_K]}$ cannot be connected by a Γ-path in $\mathcal{X}\setminus\mathcal{G}^{A,B}$, and hence $\widehat{\mathcal{R}}^{A,B}_{[0,\mathfrak{m}_K-1]}$ and $\widehat{\mathcal{R}}^{A,B}_{[\mathfrak{m}_K,\,M-\mathfrak{m}_K]}$ are disjoint. Therefore, we have

$$\widehat{\mathcal{R}}^{A,B}_{[0,\mathfrak{m}_K]}\cap\widehat{\mathcal{R}}^{A,B}_{[\mathfrak{m}_K,\,M-\mathfrak{m}_K]}=\widehat{\mathcal{R}}^{A,B}_{\mathfrak{m}_K}\cap\widehat{\mathcal{R}}^{A,B}_{[\mathfrak{m}_K,\,M-\mathfrak{m}_K]}=\widehat{\mathcal{R}}^{A,B}_{\mathfrak{m}_K}. \tag{4.109}$$

The proof is completed by (4.108) and (4.109).

(2) We will first prove that

$$\widehat{\mathcal{N}}(\mathcal{S})=\widehat{\mathcal{N}}(\mathcal{N}(\mathcal{R}^{A,B}_{[0,\,M]})\cup\mathcal{G}^{A,B}). \tag{4.110}$$

Since it is immediate that $\mathcal{S}$ is a subset of the right-hand side, we have $\widehat{\mathcal{N}}(\mathcal{S}) \subseteq \widehat{\mathcal{N}}(\mathcal{N}(\mathcal{R}_{[0,\,M]}^{A,\,B}) \cup \mathcal{G}^{A,\,B})$. On the other hand, since $\mathcal{N}(\mathcal{R}_{[0,\,M]}^{A,\,B}) \cup \mathcal{G}^{A,\,B} \subseteq \widehat{\mathcal{N}}(\mathcal{S})$ clearly holds, we also have $\widehat{\mathcal{N}}(\mathcal{N}(\mathcal{R}_{[0,\,M]}^{A,\,B}) \cup \mathcal{G}^{A,\,B}) \subseteq \widehat{\mathcal{N}}(\mathcal{S})$. This proves (4.110). Since the sets $\mathcal{N}(\mathcal{R}_{[0,\,M]}^{A,\,B})$ and $\mathcal{G}^{A,\,B}$ are disjoint by Lemma 4.4.6, we can apply Lemmas 3.8.1 and 4.4.6 to deduce

$$\begin{aligned}\widehat{\mathcal{N}}(\mathcal{S}) &= \widehat{\mathcal{N}}(\mathcal{N}(\mathcal{R}_{[0,\,M]}^{A,\,B});\, \mathcal{G}^{A,\,B}) \cup \widehat{\mathcal{N}}(\mathcal{G}^{A,\,B};\, \mathcal{N}(\mathcal{R}_{[0,\,M]}^{A,\,B})).\\ &= \widehat{\mathcal{N}}(\mathcal{R}_{[0,\,M]}^{A,\,B};\, \mathcal{G}^{A,\,B}) \cup \mathcal{G}^{A,\,B} = \widehat{\mathcal{R}}_{[0,\,M]}^{A,\,B} \cup \mathcal{G}^{A,\,B}.\end{aligned}$$

This completes the proof since by (4.50), (4.106) and (4.107), we have $\mathcal{E}^{A,\,B} \cup \mathcal{B}^{A,\,B} = \mathcal{G}^{A,\,B} \cup \widehat{\mathcal{R}}_{[0,\,M]}^{A,\,B}$. □

4.6.3 Structure of edge typical configurations

As in the 2D case, Sections 3.4.4 and 3.4.5, we analyze the structure of edge typical configurations.

We remark that we fixed a proper partition $(A,\, B)$ of S. Decompose

$$\mathcal{E}^A = \mathcal{O}^A \cup \mathcal{I}^A \tag{4.111}$$

where

$$\mathcal{O}^A = \{\sigma \in \mathcal{E}^A : H(\sigma) = \Gamma\} \quad \text{and} \quad \mathcal{I}^A = \{\sigma \in \mathcal{E}^A : H(\sigma) < \Gamma\}.$$

We now take a subset $\overline{\mathcal{I}}^A$ of $\mathcal{I}^A$ so that we can decompose $\mathcal{I}^A$ into the following disjoint union:

$$\mathcal{I}^A = \bigcup_{\sigma \in \overline{\mathcal{I}}^A} \mathcal{N}(\sigma).$$

Consequently, we get the following decomposition of $\mathcal{E}^A$:

$$\mathcal{E}^A = \mathcal{O}^A \cup \Big(\bigcup_{\sigma \in \overline{\mathcal{I}}^A} \mathcal{N}(\sigma) \Big). \tag{4.112}$$

Notation 4.6.7. For $\sigma \in \mathcal{I}^A$, we denote by $\overline{\sigma} \in \overline{\mathcal{I}}^A$ the unique configuration satisfying $\sigma \in \mathcal{N}(\overline{\sigma})$.

By part (1) of Lemma 4.5.3, for $\sigma,\, \sigma' \in \mathcal{R}_{\mathfrak{m}_K}^{A,\, B}$, the two sets $\mathcal{N}(\sigma)$ and $\mathcal{N}(\sigma')$ are disjoint. By a similar reasoning, we know that for any $\sigma \in \mathcal{R}_{\mathfrak{m}_K}^{A,\, B}$ and $a \in A$, the sets $\mathcal{N}(\sigma)$ and $\mathcal{N}(\boldsymbol{a})$ are disjoint. Thus, we can assume that

$$\mathcal{R}_{\mathfrak{m}_K}^{A,\, B} \cup \mathcal{S}(A) \subseteq \overline{\mathcal{I}}^A. \tag{4.113}$$

The following construction of an auxiliary Markov chain is an analogue of Definition 3.4.21.

Definition 4.6.8. For a proper partition $(A,\, B)$ of Ω, we define a Markov chain $Z^A(\cdot)$ on $\overline{\mathcal{I}}^A \cup \mathcal{O}^A$.

- **(Graph)** We define the graph structure $\mathscr{G}^A = (\mathscr{V}^A,\, \mathscr{E}^A)$ for $\mathscr{V}^A = \mathcal{O}^A \cup \overline{\mathcal{I}}^A$. The edge set $\mathscr{E}^A$ is defined by declaring that $\{\sigma,\, \sigma'\} \in \mathscr{E}^A$ for $\sigma,\, \sigma' \in \mathscr{V}^A$ if

$$\begin{cases} \sigma,\, \sigma' \in \mathcal{O}^A \text{ and } \sigma \sim \sigma' \text{ or} \\ \sigma \in \mathcal{O}^A,\; \sigma' \in \overline{\mathcal{I}}^A, \;\text{ and } \sigma \sim \zeta \text{ for some } \zeta \in \mathcal{N}(\sigma'). \end{cases}$$

- **(Markov chain)** We first define a rate $r^A : \mathscr{V}^A \times \mathscr{V}^A \to [0,\, \infty)$. If $\{\sigma,\, \sigma'\} \notin \mathscr{E}^A$, we set $r^A(\sigma,\, \sigma') = 0$, and if $\{\sigma,\, \sigma'\} \in \mathscr{E}^A$, we set

$$r^A(\sigma,\, \sigma') = \begin{cases} 1 & \text{if } \sigma,\, \sigma' \in \mathcal{O}^A, \\ |\{\zeta \in \mathcal{N}(\sigma) : \zeta \sim \sigma'\}| & \text{if } \sigma \in \overline{\mathcal{I}}^A \text{ and } \sigma' \in \mathcal{O}^A, \\ |\{\zeta \in \mathcal{N}(\sigma') : \zeta \sim \sigma\}| & \text{if } \sigma \in \mathcal{O}^A \text{ and } \sigma' \in \overline{\mathcal{I}}^A. \end{cases} \tag{4.114}$$

  We now let $\{Z^A(t)\}_{t \ge 0}$ be the continuous-time Markov chain on $\mathscr{V}^A$ with rate $r^A(\cdot,\, \cdot)$. Note that the uniform distribution on $\mathscr{V}^A$ is the invariant measure for the chain $Z^A(\cdot)$, and indeed this chain is reversible with respect to this measure.

- **(Potential-theoretic objects)** Denote by L^A, $h^A_{\cdot,\cdot}(\cdot)$, and $\mathrm{cap}^A(\cdot,\,\cdot)$ the generator, equilibrium potential, and capacity with respect to the Markov chain $Z^A(\cdot)$, respectively.

We now give three important propositions regarding the objects constructed above. These propositions play fundamental roles in the construction of the test function on the edge typical configurations.

We remark from (4.113) that $\mathcal{S}(A),\, \mathcal{R}^{A,\,B}_{\mathfrak{m}_K} \subseteq \overline{\mathcal{I}}^A \subseteq \mathscr{V}^A$. Potential-theoretic objects between these two sets are crucially used in our discussion. We define

$$\mathfrak{e}(A) = \frac{1}{|\mathscr{V}^A|\mathrm{cap}^A(\mathcal{S}(A),\, \mathcal{R}^{A,\,B}_{\mathfrak{m}_K})}. \tag{4.115}$$

For $n \in [\![1,\, q-1]\!]$ (with a slight abuse of notation) we can write

$$\mathfrak{e}(n) = \frac{1}{|\mathscr{V}^{A_n}|\mathrm{cap}^{A_n}(\mathcal{S}(A_n),\, \mathcal{R}^{A_n,\,B_n}_{\mathfrak{m}_K})}, \tag{4.116}$$

where $A_n = [\![1,\, n]\!]$ and $B_n = [\![n+1,\, q]\!]$. Since $\mathfrak{e}(A)$ depends on A only through $|A|$, it holds that $\mathfrak{e}(A) = \mathfrak{e}(|A|)$. We next derive a rough bound of $\mathfrak{e}(n)$ via the Thomson principle (cf. Theorem 3.2.7).

Proposition 4.6.9. *For all $n \in [\![1,\, q-1]\!]$, we have that $\mathfrak{e}(n) \le \dfrac{1}{K^{1/3}}$.*

Proof. We shall construct below a *unit flow* ψ from $\mathcal{S}(A)$ to $\mathcal{R}^{A,\,B}_{\mathfrak{m}_K}$ that satisfies

$$\|\psi\|^2 < \frac{\mathfrak{m}_K|\mathscr{V}^A|}{2M}. \tag{4.117}$$

Then, by Theorem 3.2.7, we have

$$\mathrm{cap}^A(\mathcal{S}(A),\, \mathcal{R}^{A,\,B}_{\mathfrak{m}_K}) \ge \frac{1}{\|\psi\|^2} > \frac{2M}{|\mathscr{V}^A|\mathfrak{m}_K} \ge \frac{K^{1/3}}{|\mathscr{V}^A|}.$$

Recalling the definition (4.115), this completes the proof.

Now, it remains to construct a *unit flow* ψ from $\mathcal{S}(A)$ to $\mathcal{R}^{A,\,B}_{\mathfrak{m}_K}$ satisfying bound (4.117). To this end, let us first fix $a \in A$ and $b \in B$. Define

$$i_{K,L,M} = \max\{m \geq 1 : \Phi(\mathcal{S}(A), \mathcal{R}_m^{A,B}) < \Gamma\}. \tag{4.118}$$

By Corollary 4.5.5, we know that $i_{K,L,M} < \mathfrak{m}_K$.

Let us start by fixing $P, Q \in \mathfrak{S}_M$ such that $P \prec Q$, $Q \setminus P = \{m\}$, $i_{K,L,M} \leq |P| < |Q| \leq \mathfrak{m}_K$, $a \in A$, and $b \in B$. Then, we first define a flow $\psi_{P,Q}$ connecting $\overline{\sigma}_P^{a,b} = \overline{\sigma_P^{a,b}}$ and $\overline{\sigma}_Q^{a,b} = \overline{\sigma_Q^{a,b}}$ (cf. Notation 4.6.7). First, we set

$$\psi_{P,Q}(\sigma, \zeta) = -\psi_{P,Q}(\zeta, \sigma) = \frac{1}{2KLM} \tag{4.119}$$

if $\sigma, \zeta \in \mathcal{C}_{P,Q}^{a,b}$ satisfy, for some $\ell \in \mathbb{T}_L$, $k \in \mathbb{T}_K$, $v \in [\![1, L-2]\!]$, and $h \in [\![1, K-2]\!]$,

$$\begin{cases} \sigma^{(m)} = \xi_{\ell,v}^{a,b} \text{ and } \zeta^{(m)} = \xi_{\ell,v;k,1}^{a,b,+}, \\ \sigma^{(m)} = \xi_{\ell,v;k,h}^{a,b,+} \text{ and } \zeta^{(m)} = \xi_{\ell,v;k,h+1}^{a,b,+}, \\ \sigma^{(m)} = \xi_{\ell,v;k,K-1}^{a,b,+} \text{ and } \zeta^{(m)} = \xi_{\ell,v+1}^{a,b}. \end{cases} \tag{4.120}$$

Now, we claim that all configurations that appear in (4.120) except for the ones corresponding to $\xi_{\ell,1}^{a,b}$ and $\xi_{\ell,L-1}^{a,b}$ belong to $\mathscr{V}^A$. To check this, observe first that if the m-th floor of $\sigma \in \mathcal{C}_{P,Q}^{a,b}$ is of the form $\sigma^{(m)} = \xi_{\ell,v;k,h}^{a,b,+}$, we have $H(\sigma) = \Gamma$ and hence $\sigma \in \mathcal{O}^A$. On the other hand, if the m-th floor of $\sigma \in \mathcal{C}_{P,Q}^{a,b}$ is of the form $\sigma^{(m)} = \xi_{\ell,v}^{a,b}$ for $v \in [\![2, L-2]\!]$, we have $H(\sigma) = \Gamma - 2$ and moreover $\mathcal{N}(\sigma) = \{\sigma\}$. This implies that $\sigma \in \overline{\mathcal{I}}^A$. This proves the claim. On the other hand, since if $\sigma^{(m)} = \xi_{\ell,1}^{a,b}$ then $\sigma \in \mathcal{N}(\sigma_P^{a,b})$, and if $\sigma^{(m)} = \xi_{\ell,L-1}^{a,b}$ then $\sigma \in \mathcal{N}(\sigma_Q^{a,b})$ (cf. the canonical paths provide $(\Gamma-1)$-paths), we can replace the configurations corresponding to $\xi_{\ell,1}^{a,b}$ and $\xi_{\ell,L-1}^{a,b}$ that appear in (4.120) with $\overline{\sigma}_P^{a,b}$ and $\overline{\sigma}_Q^{a,b}$, respectively, to get a flow connecting $\overline{\sigma}_P^{a,b}$ and $\overline{\sigma}_Q^{a,b}$. We remark that we may have $\overline{\sigma}_P^{a,b} = \overline{\sigma}_Q^{a,b}$.

We deduce from the definition of the flow norm that

$$\|\psi_{P,Q}\|^2 = \frac{|\mathscr{V}^A|}{(2KLM)^2} \times K^2 L(L-2) < \frac{|\mathscr{V}^A|}{4M^2}, \tag{4.121}$$

where $K^2L(L-2)$ is the number of edges that appear in (4.120). Next, we define

$$\psi = \sum_{r=i_{K,\,L,\,M}}^{\mathfrak{m}_K-1} \sum_{P,\,Q\in\mathfrak{S}_M:\,|P|=r,\,P\prec Q} \psi_{P,\,Q}.$$

Notice from (4.118) that a configuration of the form $\overline{\sigma}_{P,\,Q}^{a,\,b}$ with $|P| = i_{K,\,L,\,M}$ is indeed an element of $\mathcal{S}(A)$. Then, from the definition (4.119), we can readily check that $\psi(x) = 0$ for all $x \notin \mathcal{S}(A) \cup \mathcal{R}_{\mathfrak{m}_K}^{A,\,B}$ (by using the fact that the flow on each edge has a constant magnitude $\dfrac{1}{2KLM}$), and moreover it holds that (cf. (4.113))

$$\sum_{x\in\mathcal{S}(A)} \sum_{y\in\mathscr{V}^A} \psi(x,\,y) = 1. \tag{4.122}$$

Indeed, to prove the last assertion, it suffices to observe that

$$\begin{aligned}\sum_{x\in\mathcal{S}(A)} \sum_{y\in\mathscr{V}^A} \psi(x,\,y) &= \sum_{P,\,Q\in\mathfrak{S}_M:\,|P|=i_{K,\,L,\,M},\,P\prec Q} \; \sum_{\zeta\in\mathscr{V}^A:\,\overline{\sigma}_P^{a,\,b}\sim\zeta} \psi_{P,\,Q}(\overline{\sigma}_P^{a,\,b},\,\zeta) \\ &= \frac{1}{2KLM} \times KL \times 2M = 1,\end{aligned}$$

where KL is the number of configurations in $\mathcal{C}_{P,\,Q}^{a,\,b}$ connected to $\overline{\sigma}_P^{a,\,b}$, and $2M$ is the number of possible choices of P and Q. Consequently, the flow ψ is a unit flow from $\mathcal{S}(A)$ to $\mathcal{R}_{\mathfrak{m}_K}^{A,\,B}$.

Thus, it suffices to verify (4.117). Since the support of $\psi_{P,\,Q}$ (which is the collection of edges on which $\psi_{P,\,Q}$ is non-zero) for different pairs $(P,\,Q)$ are disjoint, we deduce from (4.121) that

$$\|\psi\|^2 = \sum_{r=i_{K,\,L,\,M}}^{\mathfrak{m}_K-1} \sum_{P,\,Q\in\mathfrak{S}_M:\,|P|=r,\,P\prec Q} \|\psi_{P,\,Q}\|^2 < \mathfrak{m}_K \times 2M \times \frac{|\mathscr{V}^A|}{4M^2} = \frac{\mathfrak{m}_K|\mathscr{V}^A|}{2M},$$

and therefore ψ satisfies (4.117). $\square$

For simplicity, we write (cf. (4.113))

$$\mathfrak{h}^A(\cdot) = h^A_{\mathcal{S}(A),\, \mathcal{R}^{a,\,b}_{\mathfrak{m}_K}}(\cdot) \tag{4.123}$$

where h^A is the equilibrium potential defined in Definition 4.6.8. This function is a fundamental object in the construction of the test function in Section 4.7.

Proposition 4.6.10. *For $\sigma \in \widehat{\mathcal{R}}^{A,\,B}_{\mathfrak{m}_K} \cap \mathcal{O}^A \subseteq \mathscr{V}^A$, we have $\mathfrak{h}^A(\sigma) = 0$.*

Proof. We fix $\sigma \in \widehat{\mathcal{R}}^{A,\,B}_{\mathfrak{m}_K} \cap \mathcal{O}^A$. It suffices to prove that any Γ-path $(\omega_t)_{t=0}^T$ from σ to $\mathcal{S}(A)$ must visit $\mathcal{N}(\mathcal{R}^{A,\,B}_{\mathfrak{m}_K})$. Suppose first that the path $(\omega_t)_{t=0}^T$ does not visit $\mathcal{G}^{A,\,B}$. Since $\sigma \in \widehat{\mathcal{R}}^{A,\,B}_{\mathfrak{m}_K}$, there exists a Γ-path in $\mathcal{X} \setminus \mathcal{G}^{A,\,B}$ connecting $\mathcal{R}^{A,\,B}_{\mathfrak{m}_K}$ and σ, and therefore by concatenating this path with $(\omega_t)_{t=0}^T$, we get a Γ-path in $\mathcal{X} \setminus \mathcal{G}^{A,\,B}$ connecting $\mathcal{R}^{A,\,B}_{\mathfrak{m}_K}$ and $\mathcal{S}(A)$. This contradicts part (2) of Lemma 4.5.3. Thus, the path $(\omega_t)_{t=0}^T$ must visit $\mathcal{G}^{A,\,B}$ and we let

$$t_0 = \min\{t : \omega_t \in \mathcal{G}^{A,\,B}\}.$$

By part (2) of Lemma 4.4.5, we have $\omega_{t_0-1} \in \mathcal{N}(\mathcal{R}^{A,\,B}_{[\mathfrak{m}_K-1,\, M-\mathfrak{m}_K+1]})$. If $\omega_{t_0-1} \in \mathcal{N}(\mathcal{R}^{A,\,B}_i)$ for some $i \in [\![\mathfrak{m}_K - 1,\, M - \mathfrak{m}_K + 1]\!] \setminus \{\mathfrak{m}_K\}$, then $(\omega_t)_{t=0}^{t_0-1}$ induces a Γ-path from $\mathcal{R}^{A,\,B}_{\mathfrak{m}_K}$ from $\mathcal{R}^{A,\,B}_i$ avoiding $\mathcal{G}^{A,\,B}$, which contradicts part (2) of Lemma 4.5.3. Hence, we can conclude that $\omega_{t_0-1} \in \mathcal{N}(\mathcal{R}^{A,\,B}_{\mathfrak{m}_K})$, as desired. □

Remark 4.6.11. The previous proposition implies that configurations σ that belong to $\widehat{\mathcal{R}}^{A,\,B}_{\mathfrak{m}_K} \cap \mathcal{O}^A$ are dead-ends attached to $\mathcal{N}(\mathcal{R}^{A,\,B}_{\mathfrak{m}_K})$ (cf. grey protuberances attached to green boxes in Figures 4.5 and 4.6).

The next proposition highlights the fact that the auxiliary process $Z^A(\cdot)$ defined in Definition 4.6.8 approximates the behavior of the Metropolis–Hastings dynamics at the edge typical configurations.

Proposition 4.6.12. *Define a projection map* $\Pi^A : \mathcal{E}^A \to \mathscr{V}^A$ *by (cf. Notation 4.6.7)*

$$\Pi^A(\sigma) = \begin{cases} \overline{\sigma} & \text{if } \sigma \in \mathcal{I}^A, \\ \sigma & \text{if } \sigma \in \mathcal{O}^A. \end{cases}$$

Then, there exists $C = C(K,\, L,\, M) > 0$ *such that*

(1) for $\sigma_1,\, \sigma_2 \in \mathcal{O}^A$*, we have*

$$\Big| \frac{1}{q} e^{-\Gamma\beta} r^A(\Pi^A(\sigma_1),\, \Pi^A(\sigma_2)) - \mu_\beta(\sigma_1) r_\beta(\sigma_1,\, \sigma_2) \Big| \le C e^{-(\Gamma+1)\beta}, \quad (4.124)$$

(2) for $\sigma_1 \in \mathcal{O}^A$ *and* $\sigma_2 \in \overline{\mathcal{I}}^A$*, we have*

$$\Big| \frac{1}{q} e^{-\Gamma\beta} r^A(\Pi^A(\sigma_1),\, \Pi^A(\sigma_2)) - \sum_{\zeta \in \mathcal{N}(\sigma_2)} \mu_\beta(\sigma_1) r_\beta(\sigma_1,\, \zeta) \Big| \le C e^{-(\Gamma+1)\beta}. \quad (4.125)$$

Proof. As the proof is identical to that of Proposition 3.4.22, we omit the details. □

4.6.4 Analysis of 3D transition paths

In this section, we finally define the collection of transition paths between ground states that appear in Theorem 4.1.6.

Definition 4.6.13 (Transition paths)**.** Write

$$\mathcal{H}^{A,\,B} = \mathcal{G}^{A,\,B} \cup \widehat{\mathcal{R}}^{A,\,B}_{[\mathfrak{m}_K,\, M-\mathfrak{m}_K]}. \quad (4.126)$$

A path $(\omega_t)_{t=0}^T$ is called a *transition path between* $\mathcal{S}(A)$ *and* $\mathcal{S}(B)$ if

$$\omega_0 \in \widehat{\mathcal{N}}(\mathcal{S}(A);\, \mathcal{G}^{A,\,B}),\ \omega_T \in \widehat{\mathcal{N}}(\mathcal{S}(B);\, \mathcal{G}^{A,\,B}),\ \text{and}$$
$$\omega_t \in \mathcal{H}^{A,\,B} \text{ for all } t \in [\![1,\, T-1]\!].$$

In particular, we have $\omega_0 \in \mathcal{N}(\mathcal{R}^{A,\,B}_{\mathfrak{m}_K-1})$, $\omega_1 \in \mathcal{G}^{A,\,B}_{\mathfrak{m}_K-1}$, $\omega_{T-1} \in \mathcal{G}^{A,\,B}_{M-\mathfrak{m}_K}$, and $\omega_T \in \mathcal{N}(\mathcal{R}^{A,\,B}_{M-\mathfrak{m}_K+1})$ by part (1) of Lemma 4.4.5.

Remark 4.6.14. The two sets $\widehat{\mathcal{N}}(\mathcal{S}(A);\,\mathcal{G}^{A,\,B})$ and $\widehat{\mathcal{N}}(\mathcal{S}(B);\,\mathcal{G}^{A,\,B})$ are disjoint thanks to part (2) of Proposition 4.5.1.

Now, we characterize all the optimal paths between ground states in terms of the transition paths.

Theorem 4.6.15. *Let $(\omega_t)_{t=0}^T$ be a Γ-path connecting $\mathcal{S}(A)$ and $\mathcal{S}(B)$. Then, $(\omega_t)_{t=0}^T$ has a transition path between $\mathcal{S}(A)$ and $\mathcal{S}(B)$ as a sub-path.*

Proof. Let $(\omega_t)_{t=0}^T$ be a Γ-path connecting $\mathcal{S}(A)$ and $\mathcal{S}(B)$, and define

$$T' = \min\{t : \omega_t \in \widehat{\mathcal{N}}(\mathcal{S}(B);\,\mathcal{G}^{A,\,B})\}.$$

Then, define

$$t' = \max\{t < T' : \omega_t \in \widehat{\mathcal{N}}(\mathcal{S}(A);\,\mathcal{G}^{A,\,B})\}.$$

We claim that the sub-path $(\omega_t)_{t=t'}^{T'}$ is a transition path between $\mathcal{S}(A)$ and $\mathcal{S}(B)$. By part (1) of Lemma 4.4.5, we have

$$\omega_{t'} \in \mathcal{N}(\mathcal{R}^{A,\,B}_{\mathfrak{m}_K-1}),\ \omega_{t'+1} \in \mathcal{G}^{A,\,B}_{\mathfrak{m}_K-1},\ \omega_{T'-1} \in \mathcal{G}^{A,\,B}_{M-\mathfrak{m}_K},\ \text{and } \omega_{T'} \in \mathcal{N}(\mathcal{R}^{A,\,B}_{M-\mathfrak{m}_K+1}).$$

In particular, we get $\omega_{t'+1}, \omega_{T'-1} \in \mathcal{H}^{A,\,B}$. To complete the proof of the claim, it suffices to check that, if $\sigma \in \mathcal{H}^{A,\,B}$ and $\zeta \notin \mathcal{H}^{A,\,B}$ satisfy $\sigma \sim \zeta$ and $H(\zeta) \le \Gamma$, then $\zeta \in \mathcal{N}(\mathcal{R}^{A,\,B}_{\mathfrak{m}_K-1}) \cup \mathcal{N}(\mathcal{R}^{A,\,B}_{M-\mathfrak{m}_K+1})$. To prove this, let us first assume that $\sigma \in \widehat{\mathcal{R}}^{a,\,b}_i$ for some $a \in A$, $b \in B$, and $i \in [\![\mathfrak{m}_K,\, M-\mathfrak{m}_K]\!]$ (cf. (4.126)). Then, since $\zeta \notin \widehat{\mathcal{R}}^{a,\,b}_i$ and $H(\zeta) \le \Gamma$, by the definition of $\widehat{\mathcal{R}}^{a,\,b}_i$ we must have $\zeta \in \mathcal{G}^{A,\,B}$, and hence we get a contradiction to the fact that $\zeta \notin \mathcal{H}^{A,\,B}$. Next, we assume that $\sigma \in \mathcal{G}^{A,\,B}_i$ for some $i \in [\![\mathfrak{m}_K-1,\, M-\mathfrak{m}_K]\!]$. Since $\zeta \in \mathcal{X}\setminus\mathcal{H}^{A,\,B}$, by Lemma 4.4.5, we have $\zeta \in \mathcal{N}(\mathcal{R}^{A,\,B}_{\mathfrak{m}_K-1}) \cup \mathcal{N}(\mathcal{R}^{A,\,B}_{M-\mathfrak{m}_K+1})$. This completes the proof. $\square$

Therefore, we can now say that the set $\mathcal{G}^{A,\,B} \cup \widehat{\mathcal{R}}^{A,\,B}_{[\mathfrak{m}_K,\,M-\mathfrak{m}_K]}$ consists of a saddle plateau between $\mathcal{S}(A)$ and $\mathcal{S}(B)$, which is a huge set of saddle configurations.

Now, we can prove Theorem 4.1.6.

Proof of Theorem 4.1.6. Denote by $\widehat{\tau}$ the hitting time of the set $\{\sigma \in \mathcal{X} : H(\sigma) \geq \Gamma + 1\}$. Then, by the large deviation principle (e.g. [70, Theorem 3.2]), we have that

$$\mathbb{P}_{\boldsymbol{s}}[\widehat{\tau} < e^{\beta(\Gamma+1/2)}] = o(1).$$

Hence, by part (1) of Theorem 4.1.4, we have that $\mathbb{P}_{\boldsymbol{s}}[\tau_{\breve{\boldsymbol{s}}} < \widehat{\tau}] = 1 - o(1)$. Thus, the conclusion of the theorem follows immediately from Theorem 4.6.15. $\square$

4.7 Construction of test function

We fix in this section a proper partition $(A,\,B)$ of Ω. The main purpose of the current section is to construct a test function $\widetilde{h} = \widetilde{h}_{\mathcal{S}(A),\,\mathcal{S}(B)} : \mathcal{X} \to \mathbb{R}$ that satisfies the requirements of Proposition 3.2.9. We remark that, since the process is reversible, we only need to construct one test object $\widetilde{h}$ which approximates both $h_{\mathcal{S}(A),\,\mathcal{S}(B)} = h^*_{\mathcal{S}(A),\,\mathcal{S}(B)}$.

Notation 4.7.1. Since the partition $(A,\,B)$ is fixed, we simply write $\mathfrak{b} = \mathfrak{b}(|A|)$, $\mathfrak{e}_A = \mathfrak{e}(|A|)$, $\mathfrak{e}_B = \mathfrak{e}(|B|)$, and $\mathfrak{c} = \mathfrak{c}(|A|)$ so that $\mathfrak{c} = \mathfrak{b} + \mathfrak{e}_A + \mathfrak{e}_B$ throughout the current section.

4.7.1 Construction of test function

We now define a function $\widetilde{h} : \mathcal{X} \to \mathbb{R}$ which indeed fulfills all requirements in Proposition 3.2.9, as we shall verify later.

Definition 4.7.2 (Test function)**.** We construct the test function $\widetilde{h}$ on $\mathcal{E}^{A,\,B}$, $\mathcal{B}^{A,\,B}$, and $(\mathcal{E}^{A,\,B} \cup \mathcal{B}^{A,\,B})^c$ separately. Recall Notation 4.6.7.

(1) **Construction of $\widetilde{h}$ on edge typical configurations $\mathcal{E}^{A,\,B} = \mathcal{E}^A \cup \mathcal{E}^B$.**

- For $\sigma \in \mathcal{E}^A$, we recall the decomposition (4.112) of $\mathcal{E}^A$ and define

$$\widetilde{h}(\sigma) = \begin{cases} 1 - \dfrac{\mathfrak{e}_A}{\mathfrak{c}}(1 - \mathfrak{h}^A(\sigma)) & \text{if } \sigma \in \mathcal{O}^A, \\ 1 - \dfrac{\mathfrak{e}_A}{\mathfrak{c}}(1 - \mathfrak{h}^A(\overline{\sigma})) & \text{if } \sigma \in \mathcal{I}^A. \end{cases} \tag{4.127}$$

- For $\sigma \in \mathcal{E}^B$, we similarly define

$$\widetilde{h}(\sigma) = \begin{cases} \dfrac{\mathfrak{e}_B}{\mathfrak{c}}(1 - \mathfrak{h}^B(\sigma)) & \text{if } \sigma \in \mathcal{O}^B, \\ \dfrac{\mathfrak{e}_B}{\mathfrak{c}}(1 - \mathfrak{h}^B(\overline{\sigma})) & \text{if } \sigma \in \mathcal{I}^B. \end{cases} \tag{4.128}$$

(2) **Construction of $\widetilde{h}$ on bulk typical configurations $\mathcal{B}^{A,\,B}$.** Recall the 2D test function $\widetilde{h}^{\rm 2D}$ explained in Proposition 3.10.1. We define the test function on each component of the decomposition (4.106) of $\mathcal{B}^{A,\,B}$.

- Construction on $\mathcal{G}^{A,\,B}_{[\mathfrak{m}_K,\,M-\mathfrak{m}_K-1]}$: Let us first fix $P,\,Q \in \mathfrak{S}_M$ such that $P \prec Q$ and $|P| \in [\![\mathfrak{m}_K,\,M-\mathfrak{m}_K-1]\!]$. Write

$$\mathcal{G}^{A,\,B}_{P,\,Q} = \bigcup_{a\in A,\,b\in B} \mathcal{G}^{a,\,b}_{P,\,Q}.$$

The test function $\widetilde{h}$ is defined on $\mathcal{G}^{A,\,B}_{P,\,Q}$ by

$$\widetilde{h}(\sigma) = \frac{1}{\mathfrak{c}}\Big[\frac{M - \mathfrak{m}_K - |P| - (1 - \widetilde{h}^{\rm 2D}(\sigma^{(m)}))}{M - 2\mathfrak{m}_K}\mathfrak{b} + \mathfrak{e}_B\Big]; \quad \sigma \in \mathcal{G}^{A,\,B}_{P,\,Q}, \tag{4.129}$$

where $\{m\} = Q \setminus P$ so that $\sigma^{(m)}$ is a 2D gateway configuration between $\boldsymbol{a}^{\rm 2D}$ and $\boldsymbol{b}^{\rm 2D}$ for some $(a,\,b) \in A \times B$. Since $\mathcal{G}^{A,\,B}_{[\mathfrak{m}_K,\,M-\mathfrak{m}_K-1]}$

can be decomposed into

$$\mathcal{G}^{A,\,B}_{[\mathfrak{m}_K,\,M-\mathfrak{m}_K-1]} = \bigcup_{i=\mathfrak{m}_K}^{M-\mathfrak{m}_K-1} \bigcup_{P,\,Q\in\mathfrak{S}_M:\,P\prec Q \text{ and } |P|=i} \mathcal{G}^{A,\,B}_{P,\,Q},$$

we can combine the constructions (4.129) to define the test function on $\mathcal{G}^{A,\,B}_{[\mathfrak{m}_K,\,M-\mathfrak{m}_K-1]}$.

- Construction on $\widehat{\mathcal{R}}^{A,\,B}_i$ for $i \in [\![\mathfrak{m}_K,\, M-\mathfrak{m}_K]\!]$: We set

$$\widetilde{h}(\sigma) = \frac{1}{\mathfrak{c}}\Big[\frac{M-\mathfrak{m}_K-i}{M-2\mathfrak{m}_K}\mathfrak{b} + \mathfrak{e}_B\Big];\quad \sigma \in \widehat{\mathcal{R}}^{A,\,B}_i, \tag{4.130}$$

so that the function $\widetilde{h}$ is constant on each $\widehat{\mathcal{R}}^{A,\,B}_i$, $i \in [\![\mathfrak{m}_K,\, M-\mathfrak{m}_K]\!]$.

(3) Construction of $\widetilde{h}$ on the remainder set $\mathcal{X} \setminus (\mathcal{E}^{A,\,B} \cup \mathcal{B}^{A,\,B})$: We define $\widetilde{h}(\sigma) = 1$ for all $\sigma \in \mathcal{X} \setminus (\mathcal{E}^{A,\,B} \cup \mathcal{B}^{A,\,B})$.

Remark 4.7.3. From the definition above, we can readily observe the following properties of the test function $\widetilde{h}$.

(1) In view of part (1) of Proposition 4.6.6, we should check that the definitions of $\widetilde{h}$ on $\mathcal{E}^{A,\,B}$ and $\mathcal{B}^{A,\,B}$ agree on $\widehat{\mathcal{R}}^{A,\,B}_{\mathfrak{m}_K}$ and $\widehat{\mathcal{R}}^{A,\,B}_{M-\mathfrak{m}_K}$. This can be verified from (4.127), (4.128), (4.130), and Proposition 4.6.10. In particular, both definitions imply that the value of $\widetilde{h}$ on the former set is *constantly* $\dfrac{\mathfrak{b}+\mathfrak{e}_B}{\mathfrak{c}}$, while the value of $\widetilde{h}$ on the latter set is *constantly* $\dfrac{\mathfrak{e}_B}{\mathfrak{c}}$.

(2) It is obvious that $\widetilde{h} \equiv 1$ on $\mathcal{S}(A)$ and $\widetilde{h} \equiv 0$ on $\mathcal{S}(B)$, and moreover we can readily verify from the definition that $0 \le \widetilde{h} \le 1$.

The remainder of this section is devoted to proving parts (1) and (2) of Proposition 3.2.9. In the remainder of the current section, *we assume for* *simplicity that* $K < L < M$*.* The other cases, $K = L < M$, $K < L = M$, or $K = L = M$, can be handled in the exact same manner.

4.7.2 Dirichlet form of test function

We first prove that the test function $\widetilde{h}$ satisfies property (2) of Proposition 3.2.9.

Proof of part (2) of Proposition 3.2.9. We divide the Dirichlet form into three parts as

$$\Big[\sum_{\{\sigma,\zeta\}\subseteq\mathcal{E}^{A,B}\cup\mathcal{B}^{A,B}}+\sum_{\substack{\sigma\in\mathcal{E}^{A,B}\cup\mathcal{B}^{A,B}\\ \zeta\in(\mathcal{E}^{A,B}\cup\mathcal{B}^{A,B})^c}}+\sum_{\{\sigma,\zeta\}\subseteq(\mathcal{E}^{A,B}\cup\mathcal{B}^{A,B})^c}\Big]\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)\{\widetilde{h}(\zeta)-\widetilde{h}(\sigma)\}^2.$$

We first consider the second summation. Observe first that, by part (2) of Proposition 4.6.6, we have $\mathcal{E}^{A,B}\cup\mathcal{B}^{A,B}=\widehat{\mathcal{N}}(\mathcal{S})$ and thus we get $H(\zeta)\ge\Gamma+1$ if $\sigma\sim\zeta$. Hence, by (4.4) and Theorem 4.0.1, we get

$$\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)=\min\{\mu_\beta(\sigma),\,\mu_\beta(\zeta)\}=\mu_\beta(\zeta)\le Ce^{-(\Gamma+1)\beta}.$$

From the fact that $0\le\widetilde{h}\le 1$ (cf. part (2) of Remark 4.7.3), we can conclude that the second summation is $o(1)e^{-\Gamma\beta}$. The third summation is trivially 0 by the definition of the test function on $(\mathcal{E}^{A,B}\cup\mathcal{B}^{A,B})^c$. Therefore, it remains to show that

$$\sum_{\{\sigma,\zeta\}\subseteq\mathcal{E}^{A,B}\cup\mathcal{B}^{A,B}}\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)\{\widetilde{h}(\zeta)-\widetilde{h}(\sigma)\}^2=\frac{1+o(1)}{\mathfrak{c}q}e^{-\Gamma\beta}. \tag{4.131}$$

By part (1) of Proposition 4.6.6 and the fact that $\widetilde{h}$ is constant on each $\widehat{\mathcal{R}}_i^{A,B}$,

$i \in [\![\mathfrak{m}_K,\, M - \mathfrak{m}_K]\!]$ (cf. (4.130)), we can decompose the left-hand side into

$$\Big[\sum_{\{\sigma,\,\zeta\} \subseteq \mathcal{B}^{A,\,B}} + \sum_{\{\sigma,\,\zeta\} \subseteq \mathcal{E}^{A}} + \sum_{\{\sigma,\,\zeta\} \subseteq \mathcal{E}^{B}} \Big] \mu_\beta(\sigma) r_\beta(\sigma,\, \zeta) \{\widetilde{h}(\zeta) - \widetilde{h}(\sigma)\}^2. \tag{4.132}$$

Again by the fact that $\widetilde{h}$ is constant on each $\widehat{\mathcal{R}}_i^{A,\,B}$, we can express the first summation as

$$\sum_{i=\mathfrak{m}_K}^{M-\mathfrak{m}_K-1} \sum_{a\in A,\, b\in B} \sum_{\substack{P,\, Q \in \mathfrak{S}_M: \\ P \prec Q,\, |P|=i}} \sum_{\{\sigma,\,\zeta\} \subseteq \mathcal{B}^{a,\,b}:\, \{\sigma,\,\zeta\} \cap \mathcal{G}_{P,\,Q}^{a,\,b} \neq \emptyset} \mu_\beta(\sigma) r_\beta(\sigma,\, \zeta) \{\widetilde{h}(\zeta) - \widetilde{h}(\sigma)\}^2. \tag{4.133}$$

By (4.129) and (4.130), Theorem 4.0.1 and (4.3), we can write the last summation as $(1 + o(1))$ times

$$\frac{2\mathfrak{b}^2 e^{-2KL\beta}}{q\mathfrak{c}^2 (M - 2\mathfrak{m}_K)^2} \sum_{\{\sigma,\,\zeta\} \subseteq \mathcal{B}^{a,\,b}:\, \{\sigma,\,\zeta\} \cap \mathcal{G}_{P,\,Q}^{a,\,b} \neq \emptyset} \mu_\beta^{2\mathrm{D}}(\sigma^{(m)}) r_\beta^{2\mathrm{D}}(\sigma^{(m)},\, \zeta^{(m)}) \{\widetilde{h}^{2\mathrm{D}}(\zeta^{(m)}) - \widetilde{h}^{2\mathrm{D}}(\sigma^{(m)})\}^2, \tag{4.134}$$

where $\{m\} = Q \setminus P$ and $\sigma^{(m)}$ and $\zeta^{(m)}$ are regarded as 2D Ising configurations. By Proposition 3.10.1, the last summation is $\dfrac{1 + o(1)}{2\kappa^{2\mathrm{D}}} e^{-\Gamma^{2\mathrm{D}}\beta}$. Therefore, display (4.134) equals

$$\frac{\mathfrak{b}^2 e^{-2KL\beta}}{\mathfrak{c}^2 (M - 2\mathfrak{m}_K)^2} \times \frac{(1 + o(1)) e^{-\Gamma^{2\mathrm{D}}\beta}}{q\kappa^{2\mathrm{D}}}. \tag{4.135}$$

Inserting this to (4.133) (and recalling (4.13)), we get

$$\sum_{\{\sigma,\,\zeta\} \subseteq \mathcal{B}^{A,\,B}} \mu_\beta(\sigma) r_\beta(\sigma,\, \zeta) \{\widetilde{h}(\zeta) - \widetilde{h}(\sigma)\}^2 = \frac{\mathfrak{b} + o(1)}{\mathfrak{c}^2 q} e^{-\Gamma\beta}. \tag{4.136}$$

Next, we deal with the second and third summations of (4.132). By

(4.127) and Proposition 4.6.12, the second summation equals

$$\frac{e^{-\Gamma\beta}}{q}\sum_{\{\sigma,\,\zeta\}\subseteq\mathscr{V}^A}\frac{\mathfrak{e}_A^2 r^A(\sigma,\,\zeta)\{\mathfrak{h}^A(\zeta)-\mathfrak{h}^A(\sigma)\}^2}{\mathfrak{c}^2}+o(1)e^{-\Gamma\beta}=\frac{\mathfrak{e}_A+o(1)}{\mathfrak{c}^2 q}e^{-\Gamma\beta}. \tag{4.137}$$

Similarly, we get

$$\sum_{\{\sigma,\,\zeta\}\subseteq\mathcal{E}^B}\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)\{\widetilde{h}(\zeta)-\widetilde{h}(\sigma)\}^2=\frac{\mathfrak{e}_B+o(1)}{\mathfrak{c}^2 q}e^{-\Gamma\beta}. \tag{4.138}$$

Therefore, by (4.136), (4.137), and (4.138), we can conclude that the left-hand side of (4.131) is equal to

$$(1+o(1))\times\frac{\mathfrak{b}+\mathfrak{e}_A+\mathfrak{e}_B}{\mathfrak{c}^2 q}e^{-\Gamma\beta}=\frac{1+o(1)}{q\mathfrak{c}}e^{-\Gamma\beta}.$$

This concludes the proof. □

4.7.3 H^1-approximation

Now it remains to prove that the test function $\widetilde{h}$ satisfies part (1) of Proposition 3.2.9. We shall carry this out in the current section to conclude the proof of Proposition 3.2.9.

We abbreviate $h = h_{\mathcal{S}(A),\,\mathcal{S}(B)}$ in the remainder of the section. Then, the next lemma asserts that the equilibrium potential is nearly constant on each $\mathcal{N}$-neighborhood. Since this lemma can be proved in the exact same manner as Lemma 3.5.8, we omit the proof.

Lemma 4.7.4. *For any $\sigma\in\mathcal{X}$ such that $H(\sigma)<\Gamma$, it holds that*

$$\max_{\zeta\in\mathcal{N}(\sigma)}|h(\zeta)-h(\sigma)|=o(1).$$

Now we proceed to the proof of (3.38). By (3.20), we can write

$$\begin{aligned} D_\beta(h-\widetilde{h}) &= \langle h-\widetilde{h},\, -\mathcal{L}_\beta h + \mathcal{L}_\beta \widetilde{h}\rangle_{\mu_\beta} \\ &= D_\beta(h) + D_\beta(\widetilde{h}) - \langle h,\, -\mathcal{L}_\beta \widetilde{h}\rangle_{\mu_\beta} - \langle \widetilde{h},\, -\mathcal{L}_\beta h\rangle_{\mu_\beta}. \end{aligned}$$

Since $\widetilde{h} \equiv h \equiv 1$ on $\mathcal{S}(A)$, $\widetilde{h} \equiv h \equiv 0$ on $\mathcal{S}(B)$ (cf. Remark 4.7.3-(2)), and $\mathcal{L}_\beta h \equiv 0$ on $\mathcal{X} \setminus \mathcal{S}$ (cf. (3.19)), we have

$$\begin{aligned} \langle \widetilde{h},\, -\mathcal{L}_\beta h\rangle_{\mu_\beta} &= \sum_{\boldsymbol{s}\in\mathcal{S}(A)} \widetilde{h}(\boldsymbol{s})(-\mathcal{L}_\beta h)(\boldsymbol{s})\mu_\beta(\boldsymbol{s}) \\ &= \sum_{\boldsymbol{s}\in\mathcal{S}(A)} h(\boldsymbol{s})(-\mathcal{L}_\beta h)(\boldsymbol{s})\mu_\beta(\boldsymbol{s}) = D_\beta(h). \end{aligned}$$

By the last two displayed equations, we obtain that

$$D_\beta(h-\widetilde{h}) = D_\beta(\widetilde{h}) - \sum_{\sigma\in\mathcal{X}} h(\sigma)(-\mathcal{L}_\beta \widetilde{h})(\sigma)\mu_\beta(\sigma). \tag{4.139}$$

Therefore, by part (2) of Proposition 3.2.9 proved in the previous subsection and the definition of $\mathcal{L}_\beta$ (cf. (2.1)), we are left to prove that

$$\sum_{\sigma\in\mathcal{X}} h(\sigma) \sum_{\zeta\in\mathcal{X}} \mu_\beta(\sigma) r_\beta(\sigma,\, \zeta)[\widetilde{h}(\sigma) - \widetilde{h}(\zeta)] = \frac{1+o(1)}{q\mathfrak{c}} e^{-\Gamma\beta}. \tag{4.140}$$

For simplicity, we define

$$\psi(\sigma) = \sum_{\zeta\in\mathcal{X}} \mu_\beta(\sigma) r_\beta(\sigma,\, \zeta)[\widetilde{h}(\sigma) - \widetilde{h}(\zeta)], \tag{4.141}$$

so that we can rewrite our objective (4.140) as

$$\sum_{\sigma\in\mathcal{X}} h(\sigma)\psi(\sigma) = \frac{1+o(1)}{q\mathfrak{c}} e^{-\Gamma\beta}. \tag{4.142}$$

In summary, it suffices to prove (4.142) to prove that $\widetilde{h}$ satisfies part (1) of

Proposition 3.2.9. The proof of (4.142) is divided into several lemmas. First, we demonstrate that $\psi(\sigma)$ is negligible if σ is not a typical configuration.

Lemma 4.7.5. *For every $\sigma \in \mathcal{X} \setminus (\mathcal{E}^{A,\,B} \cup \mathcal{B}^{A,\,B})$ (i.e., $\sigma \notin \widehat{\mathcal{N}}(\mathcal{S})$ by Proposition 4.6.6), it holds that $\psi(\sigma) = o(e^{-\Gamma\beta})$.*

Proof. Since $\widetilde{h} \equiv 1$ on $\mathcal{X} \setminus (\mathcal{E}^{A,\,B} \cup \mathcal{B}^{A,\,B})$ by part (3) of Definition 4.7.2, it readily holds that

$$\psi(\sigma) = \sum_{\zeta \in \mathcal{E}^{A,\,B} \cup \mathcal{B}^{A,\,B}} \mu_\beta(\sigma) r_\beta(\sigma,\,\zeta)[\widetilde{h}(\sigma) - \widetilde{h}(\zeta)].$$

Then, by (4.4) and part (2) of Proposition 4.6.6, if $\zeta \in \mathcal{E}^{A,\,B} \cup \mathcal{B}^{A,\,B}$ with $\sigma \sim \zeta$ then $H(\sigma) \geq \Gamma + 1$, and thus

$$\mu_\beta(\sigma) r_\beta(\sigma,\,\zeta) = \mu_\beta(\sigma) = O(e^{-(\Gamma+1)\beta}).$$

Along with the fact that $0 \leq \widetilde{h} \leq 1$, we conclude that $\psi(\sigma) = O(e^{-(\Gamma+1)\beta}) = o(e^{-\Gamma\beta})$. $\square$

We are left to consider $\psi(\sigma)$ for $\sigma \in \mathcal{E}^{A,\,B} \cup \mathcal{B}^{A,\,B} = \widehat{\mathcal{N}}(\mathcal{S})$. To this end, we decompose as $\psi = \psi_1 + \psi_2$ where

$$\psi_1(\sigma) = \sum_{\zeta \in \mathcal{E}^{A,\,B} \cup \mathcal{B}^{A,\,B}} \mu_\beta(\sigma) r_\beta(\sigma,\,\zeta)[\widetilde{h}(\sigma) - \widetilde{h}(\zeta)], \tag{4.143}$$
$$\psi_2(\sigma) = \sum_{\zeta \notin \mathcal{E}^{A,\,B} \cup \mathcal{B}^{A,\,B}} \mu_\beta(\sigma) r_\beta(\sigma,\,\zeta)[\widetilde{h}(\sigma) - \widetilde{h}(\zeta)].$$

In fact, we can show that $\psi_2(\sigma)$ is negligible.

Lemma 4.7.6. *For $\sigma \in \mathcal{E}^{A,\,B} \cup \mathcal{B}^{A,\,B}$, we have $\psi_2(\sigma) = o(e^{-\Gamma\beta})$.*

Proof. This follows directly by the same argument presented in the proof of Lemma 4.7.5. $\square$

Now, to estimate $\psi_1(\sigma)$, let us first look at the bulk typical configurations that are not the edge typical configurations.

Lemma 4.7.7. *We have that* $\psi_1(\sigma) = o(e^{-\Gamma\beta})$ *for all* $\sigma \in \mathcal{G}^{A,\,B}_{[\mathfrak{m}_K,\, M-\mathfrak{m}_K-1]}$.

Proof. For $\sigma \in \mathcal{G}^{A,\,B}_{[\mathfrak{m}_K,\, M-\mathfrak{m}_K-1]}$, by definition we can write

$$\begin{aligned}\psi_1(\sigma) &= \sum_{\zeta\in\mathcal{E}^{A,\,B}\cup\mathcal{B}^{A,\,B}} \mu_\beta(\sigma) r_\beta(\sigma,\,\zeta)[\widetilde{h}(\sigma) - \widetilde{h}(\zeta)] \\ &= \frac{\mathfrak{b}}{\mathfrak{c}(M - 2\mathfrak{m}_K)} \sum_{\zeta\in\mathcal{E}^{A,\,B}\cup\mathcal{B}^{A,\,B}} \mu_\beta(\sigma) r_\beta(\sigma,\,\zeta)[\widetilde{h}^{\rm 2D}(\sigma^{(m)}) - \widetilde{h}^{\rm 2D}(\zeta^{(m)})]\end{aligned}$$

for some $m \in Q \setminus P$ with $P \prec Q$ (cf. Definition 4.7.2), where $\sigma^{(m)}$ and $\zeta^{(m)}$ are considered as 2D Ising configurations. Then, by Theorem 4.0.1 and (4.3), the last display equals

$$\frac{2\mathfrak{b}(1 + o(1))}{q\mathfrak{c}(M - 2\mathfrak{m}_K)} e^{-2KL\beta} \times \sum_{\zeta\in\mathcal{E}^{A,\,B}\cup\mathcal{B}^{A,\,B}} \mu^{\rm 2D}_\beta(\sigma) r^{\rm 2D}_\beta(\sigma,\,\zeta)[\widetilde{h}^{\rm 2D}(\sigma^{(m)}) - \widetilde{h}^{\rm 2D}(\zeta^{(m)})].$$

Since $\sigma^{(m)}$ is a 2D gateway configuration, by the results in Section 3.5.3, the last summation equals $o(e^{-\Gamma^{\rm 2D}\beta})$. Therefore, we conclude that

$$\psi_1(\sigma) = \frac{2\mathfrak{b}(1 + o(1))}{q\mathfrak{c}(M - 2\mathfrak{m}_K)} e^{-2KL\beta} \times o(e^{-\Gamma^{\rm 2D}\beta}) = o(e^{-\Gamma\beta}).$$

□

Lemma 4.7.8. *For all* $i \in [\![\mathfrak{m}_K + 1,\, M - \mathfrak{m}_K - 1]\!]$, *we have that*

$$\sum_{\sigma\in\widehat{\mathcal{R}}^{A,\,B}_i} \psi_1(\sigma) = 0.$$

Moreover, $|\psi_1(\sigma)| \le Ce^{-\beta\Gamma}$ *for all* $\sigma \in \widehat{\mathcal{R}}^{A,\,B}_i$, *for some fixed constant* $C > 0$.

Proof. Recall from the definition that $\widetilde{h}$ is defined as constant on each $\widehat{\mathcal{R}}^{A,\,B}_i$.

Thus, $\psi_1(\sigma) = 0$ for all $\sigma \in \widehat{\mathcal{R}}_i^{A,\,B} \setminus \mathcal{N}(\mathcal{R}_i^{A,\,B})$ and it suffices to show that

$$\sum_{\sigma \in \mathcal{N}(\mathcal{R}_i^{A,\,B})} \psi_1(\sigma) = o(e^{-\beta\Gamma}).$$

It remains to prove that for all $a \in A$, $b \in B$, and $P \in \mathfrak{S}_M$ such that $|P| \in [\![\mathfrak{m}_K + 1,\, M - \mathfrak{m}_K - 1]\!]$,

$$\sum_{\sigma \in \mathcal{N}(\sigma_P^{a,\,b})} \sum_{\zeta \in \mathcal{E}^{A,\,B} \cup \mathcal{B}^{A,\,B}} \mu_\beta(\sigma) r_\beta(\sigma,\, \zeta)[\widetilde{h}(\sigma) - \widetilde{h}(\zeta)] = o(e^{-\beta\Gamma}). \tag{4.144}$$

Indeed, the left-hand side can be written as

$$\sum_{Q \in \mathfrak{S}_M:\, P \prec Q} \sum_{\sigma \in \mathcal{C}_{P,Q}^{a,\,b} \cap \mathcal{N}(\sigma_P^{a,\,b}),\, \zeta \in \mathcal{C}_{P,Q}^{a,\,b}:\, \zeta \sim \sigma} \mu_\beta(\sigma) r_\beta(\sigma,\, \zeta)[\widetilde{h}(\sigma) - \widetilde{h}(\zeta)]$$
$$+ \sum_{Q' \in \mathfrak{S}_M:\, Q' \prec P} \sum_{\sigma \in \mathcal{C}_{Q',P}^{a,\,b} \cap \mathcal{N}(\sigma_P^{a,\,b}),\, \zeta \in \mathcal{C}_{Q',P}^{a,\,b}:\, \zeta \sim \sigma} \mu_\beta(\sigma) r_\beta(\sigma,\, \zeta)[\widetilde{h}(\sigma) - \widetilde{h}(\zeta)].$$

Since we constructed the test function $\widetilde{h}$ between $\sigma_P^{a,\,b}$ and $\sigma_Q^{a,\,b}$ ($P \prec Q$) and between $\sigma_{Q'}^{a,\,b}$ and $\sigma_P^{a,\,b}$ ($Q' \prec P$) in the same manner, the two summations above cancel out with each other, and thus we obtain (4.144).

Finally, for the last statement of the lemma, it suffices to see that if $\sigma \in \mathcal{N}(\mathcal{R}_i^{A,\,B})$ and $\zeta \notin \mathcal{N}(\mathcal{R}_i^{A,\,B})$ with $\sigma \sim \zeta$ then $H(\zeta) \geq \Gamma$, and thus

$$\mu_\beta(\sigma) r_\beta(\sigma,\, \zeta) = \mu_\beta(\zeta) \leq \frac{1}{Z_\beta} e^{-\beta\Gamma} = O(e^{-\beta\Gamma}),$$

where the last equality holds by Theorem 4.0.1. This proves the last statement of the lemma since the number of summands in (4.143) does not depend on β, and since we have $0 \leq \widetilde{h} \leq 1$ (cf. Remark 4.7.3). □

Next, we turn to the edge typical configurations.

Lemma 4.7.9. *The following statements hold.*

(1) If $\sigma \in \mathcal{O}^A \setminus (\widehat{\mathcal{R}}^{A,\,B}_{\mathfrak{m}_K} \cup \mathcal{N}(\mathcal{S}(A)))$, we have $\psi_1(\sigma) = o(e^{-\Gamma\beta})$.

(2) If $\sigma \in \overline{\mathcal{I}}^A \setminus (\widehat{\mathcal{R}}^{A,\,B}_{\mathfrak{m}_K} \cup \mathcal{N}(\mathcal{S}(A)))$, it holds that

$$\sum_{\zeta \in \mathcal{N}(\sigma)} \psi_1(\zeta) = 0, \tag{4.145}$$

and $|\psi_1(\zeta)| \le Ce^{-\Gamma\beta}$ for all $\zeta \in \mathcal{N}(\sigma)$ where C is a constant independent of β.

Proof. (1) By part (1) of Proposition 4.6.12 and the definition of $\widetilde{h}$, we calculate

$$\begin{aligned}\psi_1(\sigma) &= \sum_{\zeta \in \mathcal{E}^A} \frac{\mathfrak{e}_A}{q\mathfrak{c}} e^{-\Gamma\beta} r^A(\sigma,\, \Pi^A(\zeta))[\mathfrak{h}^A(\sigma) - \mathfrak{h}^A(\Pi^A(\zeta))] + O(e^{-(\Gamma+1)\beta}) \\ &= \frac{\mathfrak{e}_A}{q\mathfrak{c}} e^{-\Gamma\beta} \times |\mathscr{V}^A| \cdot (-L^A\mathfrak{h}^A)(\sigma) + O(e^{-(\Gamma+1)\beta}).\end{aligned}$$

Since $L^A\mathfrak{h}^A = 0$ on $\mathcal{O}^A \setminus (\widehat{\mathcal{R}}^{A,\,B}_{\mathfrak{m}_K} \cup \mathcal{N}(\mathcal{S}(A)))$ by the elementary property of equilibrium potentials (cf. (3.19)), we may conclude that $\psi_1(\sigma) = O(e^{-(\Gamma+1)\beta}) = o(e^{-\Gamma\beta})$.

(2) First, we prove (4.145). Note that $\widetilde{h}$ is constant on $\mathcal{N}(\sigma)$. Thus,

$$\sum_{\zeta \in \mathcal{N}(\sigma)} \psi_1(\zeta) = \sum_{\zeta \in \mathcal{N}(\sigma)} \sum_{\zeta' \in \mathcal{O}^A} \mu_\beta(\zeta) r_\beta(\zeta,\, \zeta')[\widetilde{h}(\zeta) - \widetilde{h}(\zeta')].$$

By part (2) of Proposition 4.6.12 and the definition of $\widetilde{h}$, this is equal to

$$\begin{aligned}&\sum_{\zeta' \in \mathcal{O}^A} \frac{\mathfrak{e}_A}{q\mathfrak{c}} e^{-\Gamma\beta} \times r^A(\sigma,\, \zeta')[\mathfrak{h}^A(\sigma) - \mathfrak{h}^A(\zeta')] + O(e^{-(\Gamma+1)\beta}) \\ &= \frac{\mathfrak{e}_A}{q\mathfrak{c}} e^{-\Gamma\beta} \times |\mathscr{V}^A| \cdot (-L^A\mathfrak{h}^A)(\sigma) + o(e^{-\Gamma\beta}).\end{aligned}$$

Since $L^A \mathfrak{h}^A = 0$ on $\overline{\mathcal{I}}^A \setminus (\widehat{\mathcal{R}}^{A,\,B}_{\mathfrak{m}_K} \cup \mathcal{N}(\mathcal{S}(A)))$, we conclude that

$$\sum_{\zeta \in \mathcal{N}(\sigma)} \psi_1(\zeta) = o(e^{-\Gamma\beta})$$

and (4.145) is now proved.

Finally, for the last statement, the last display implies that for all $\zeta \in \mathcal{N}(\sigma)$,

$$\begin{aligned} |\psi_1(\zeta)| &= \Big| \sum_{\zeta' \in \mathcal{O}^A} \frac{\mathfrak{e}_A}{q\mathfrak{c}} e^{-\Gamma\beta} \times r^A(\sigma,\, \zeta')[\mathfrak{h}^A(\sigma) - \mathfrak{h}^A(\zeta')] \Big| + O(e^{-(\Gamma+1)\beta}) \\ &\le \sum_{\zeta' \in \mathcal{O}^A} \frac{\mathfrak{e}_A}{q\mathfrak{c}} r^A(\sigma,\, \zeta') e^{-\Gamma\beta} + O(e^{-(\Gamma+1)\beta}) \le Ce^{-\Gamma\beta}, \end{aligned}$$

where the first inequality holds since $0 \le \mathfrak{h}^A \le 1$ and the second inequality holds by Proposition 4.6.9, (4.114), and the fact that the number of such $\zeta' \in \mathcal{O}^A$ with $\sigma \sim \zeta'$ does not depend on β. This concludes the proof. $\square$

Lemma 4.7.10. *It holds that*

$$\sum_{\sigma \in \widehat{\mathcal{R}}^{A,\,B}_{\mathfrak{m}_K}} \psi_1(\sigma) = o(e^{-\Gamma\beta}),$$

and that $|\psi_1(\sigma)| \le Ce^{-\Gamma\beta}$ *for all* $\sigma \in \widehat{\mathcal{R}}^{A,\,B}_{\mathfrak{m}_K}$ *where* C *is a constant independent of* β*.*

Proof. First, we consider the first statement. Proposition 4.6.10 and the definition of $\widetilde{h}$ on $\widehat{\mathcal{R}}^{A,\,B}_{\mathfrak{m}_K}$ imply that $\psi_1(\sigma) = 0$ for all $\sigma \in \widehat{\mathcal{R}}^{A,\,B}_{\mathfrak{m}_K} \setminus \mathcal{N}(\mathcal{R}^{A,\,B}_{\mathfrak{m}_K})$. Hence, it suffices to prove that

$$\sum_{\sigma \in \mathcal{N}(\mathcal{R}^{A,\,B}_{\mathfrak{m}_K})} \psi_1(\sigma) = o(e^{-\Gamma\beta}). \tag{4.146}$$

Since $\widetilde{h}$ is constant on $\mathcal{N}(\mathcal{R}^{A,\,B}_{\mathfrak{m}_K})$, the left-hand side can be decomposed into

$$\Big[\sum_{\sigma\in\mathcal{N}(\mathcal{R}^{A,\,B}_{\mathfrak{m}_K}),\,\zeta\in\mathcal{E}^A}+\sum_{\sigma\in\mathcal{N}(\mathcal{R}^{A,\,B}_{\mathfrak{m}_K}),\,\zeta\in\mathcal{B}^{A,\,B}}\Big]\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)[\widetilde{h}(\sigma)-\widetilde{h}(\zeta)]. \tag{4.147}$$

Let us analyze the first summation of (4.147). By part (2) of Proposition 4.6.12, this equals

$$\sum_{\sigma\in\mathcal{R}^{A,\,B}_{\mathfrak{m}_K}}\sum_{\zeta\in\mathcal{O}^A}\frac{\mathfrak{e}_A}{q\mathfrak{c}}e^{-\Gamma\beta}\times r^A(\sigma,\,\zeta)[\mathfrak{h}^A(\sigma)-\mathfrak{h}^A(\zeta)]+O(e^{-(\Gamma+1)\beta}).$$

By the property of capacities (e.g., [16, (7.1.39)]) and Proposition 4.6.10, we have

$$\mathfrak{e}_A^{-1}=|\mathscr{V}^A|\mathrm{cap}^A(\mathcal{S}(A),\,\mathcal{R}^{A,\,B}_{\mathfrak{m}_K})=-\sum_{\sigma\in\mathcal{R}^{A,\,B}_{\mathfrak{m}_K}}\sum_{\zeta:\,\{\sigma,\,\zeta\}\in\mathscr{E}^A}r^A(\sigma,\,\zeta)\{\mathfrak{h}^A(\sigma)-\mathfrak{h}^A(\zeta)\}. \tag{4.148}$$

Summing up, we obtain

$$\sum_{\sigma\in\mathcal{N}(\mathcal{R}^{A,\,B}_{\mathfrak{m}_K}),\,\zeta\in\mathcal{E}^A}\psi_1(\sigma)=-\frac{1}{q\mathfrak{c}}e^{-\Gamma\beta}+o(e^{-\Gamma\beta}). \tag{4.149}$$

Next, we analyze the second summation of (4.147).

$$\sum_{a\in A,\,b\in B}\ \sum_{P,\,Q\in\mathfrak{S}_M:\,P\prec Q,\,|P|=\mathfrak{m}_K}\ \sum_{\sigma\in\mathcal{N}(\sigma^{a,\,b}_{P,Q}),\,\zeta\in\mathcal{B}^{a,\,b}}\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)[\widetilde{h}(\sigma)-\widetilde{h}(\zeta)]. \tag{4.150}$$

By Theorem 4.0.1, (4.3), and the results in Section 3.5.3, this becomes (recall the 2D constant $\kappa^{\rm 2D}$ from (3.31))

$$|A||B|\times 2M\times\frac{2\mathfrak{b}(1+o(1))}{q\mathfrak{c}(M-2\mathfrak{m}_K)}e^{-2KL\beta}\times\frac{1}{2\kappa^{\rm 2D}}e^{-\Gamma^{\rm 2D}\beta}=\frac{1+o(1)}{q\mathfrak{c}}e^{-\Gamma\beta}, \tag{4.151}$$

where the identity follows from the definition of $\mathfrak{b}$ in (4.13). Combining this with (4.147) and (4.149), we can prove the first statement of the lemma.

For the second statement, from the discussion before (4.146) it is inferred that we only need to prove for $\sigma \in \mathcal{N}(\mathcal{R}_{\mathfrak{m}_K}^{A,B})$. For such $\sigma \in \mathcal{N}(\mathcal{R}_{\mathfrak{m}_K}^{A,B})$, the previous proof implies that

$$\psi_1(\sigma) = \Big[\sum_{\zeta \in \mathcal{E}^A} + \sum_{\zeta \in \mathcal{B}^{A,B}} \Big] \mu_\beta(\sigma) r_\beta(\sigma, \zeta) [\mathfrak{h}^A(\sigma) - \mathfrak{h}^A(\zeta)] + O(e^{-(\Gamma+1)\beta}),$$

where we used the fact that $0 \le \widetilde{h} \le 1$. By (4.148) and Proposition 4.6.9, the first summation in the right-hand side is bounded by $Ce^{-\Gamma\beta}$. By (4.150) and (4.151), the second summation in the right-hand side is also bounded by $Ce^{-\Gamma\beta}$. Therefore, we conclude the proof of the second statement. □

Lemma 4.7.11. *It holds that*

$$\sum_{\sigma \in \mathcal{N}(\mathcal{S}(A))} \psi_1(\sigma) = \frac{1+o(1)}{q\mathfrak{c}} e^{-\Gamma\beta} \quad \text{and} \quad \sum_{\sigma \in \mathcal{N}(\mathcal{S}(B))} \psi_1(\sigma) = o(e^{-\Gamma\beta}).$$

Moreover, it holds that $|\psi_1(\sigma)| \le Ce^{-\Gamma\beta}$ *for all* $\sigma \in \mathcal{N}(\mathcal{S}(A)) \cup \mathcal{N}(\mathcal{S}(B))$ *where* C *is a constant independent of* β.

Proof. We concentrate on the claim for $\mathcal{N}(\mathcal{S}(A))$, since the corresponding claim for $\mathcal{N}(\mathcal{S}(B))$ can be proved in the exact same way.

By the property of capacities (e.g., [16, (7.1.39)]) as above, we can write that

$$\mathfrak{e}_A^{-1} = |\mathscr{V}^A| \mathrm{cap}^A(\mathcal{S}(A), \mathcal{R}_{\mathfrak{m}_K}^{A,B}) = \sum_{\sigma \in \mathcal{S}(A)} \sum_{\zeta :\, \{\sigma, \zeta\} \in \mathscr{E}^A} r^A(\sigma, \zeta) \{\mathfrak{h}^A(\sigma) - \mathfrak{h}^A(\zeta)\}.$$

Therefore, by the definition of $\widetilde{h}$ and part (2) of Proposition 4.6.12,

$$\begin{aligned}&\sum_{\sigma\in\mathcal{N}(\mathcal{S}(A))}\psi_1(\sigma)\\&=\sum_{\sigma\in\mathcal{S}(A)}\sum_{\zeta:\,\{\sigma,\zeta\}\in\mathscr{E}^A}\frac{\mathfrak{e}_A}{q\mathfrak{c}}e^{-\Gamma\beta}\cdot r^A(\sigma,\,\zeta)[\mathfrak{h}^A(\sigma)-\mathfrak{h}^A(\zeta)]+O(e^{-(\Gamma+1)\beta})\\&=\frac{1}{q\mathfrak{c}}e^{-\Gamma\beta}+o(e^{-\Gamma\beta}).\end{aligned}$$

This proves the first statement. As before, the fact that $|\psi_1|\le Ce^{-\Gamma\beta}$ on $\mathcal{N}(\mathcal{S}(A))$ is straightforward from the observations made in the proof. □

Finally, we present a proof of Proposition 3.2.9 by combining all computations above.

Proof of Proposition 3.2.9. It remains to prove that $\widetilde{h}$ satisfies part (1) since we already verified in the previous subsection that it satisfies part (2). By the discussion at the beginning of the subsection, it suffices to prove (4.142). By the definition of ψ given in (4.141) and the series of Lemmas 4.7.5-4.7.11, and the fact that $0\le h\le 1$, we have

$$\sum_{\sigma\in\mathcal{X}}h(\sigma)\psi(\sigma)=\sum_{\sigma\in\mathcal{N}(\mathcal{S}(A))}h(\sigma)\psi_1(\sigma)+o(e^{-\Gamma\beta})=\sum_{\sigma\in\mathcal{N}(\mathcal{S}(A))}\psi_1(\sigma)+o(e^{-\Gamma\beta}),$$

where the second identity follows from Lemmas 4.7.4. Thus, by applying Lemma 4.7.11, we can complete the proof of (4.142). □

4.8 Remarks on open boundary condition

Thus far, we have only considered the models under periodic boundary conditions. In this section, we consider the same models under open boundary conditions. The proofs for the open boundary case differ slightly to those of the periodic case; however, the fundamentals of the proofs are essentially identical. Hence, we do not repeat the detail but focus solely on the technical points producing the different forms of the main results.

Energy Barrier

We start by explaining that for the open boundary case, the energy barrier is given by

$$\Gamma = KL + K + 1. \tag{4.152}$$

One can observe that the canonical path explained in Figure 4.3 becomes an optimal path (note that we should start from a corner of box in this case) with height $KL + K + 1$ between ground states. This proves that the energy barrier Γ is at most $KL+K+1$. Hence, it remains to prove the corresponding lower bound, i.e., of the fact that $\Gamma \geq KL + K + 1$. Rigorous proof of this has been developed in [69] for the 2D model, and the same argument also applies to the 3D model as well using the arguments given in Section 4.5.

Sub-exponential prefactor

As mentioned earlier, the large deviation-type results (Theorems 4.1.4 and 4.1.6) hold under open boundary conditions without modification, except for the value of Γ. On the other hand, for the precise estimates (Theorems 4.8.1 and 4.1.9), the prefactor κ must be appropriately modified.

For simplicity, we assume that $q = 2$ and analyze the transition from **1** to **2**. To heuristically investigate the speed of this transition in the open boundary case via a comparison to the periodic one, it suffices to check the bulk part of the transition, because the edge part is negligible (as $K \to \infty$) as in the periodic boundary case. The bulk transition must start from a configuration filled with $\mathfrak{m}_K$ lines of spin 2 at either the bottom or top of the lattice box Λ. In the periodic case, there are M choices for these starting clusters (of spins 2) of size $KL \times \mathfrak{m}_K$; thus, we can observe that the speed of the transition is slowed by a factor of $M/2$ under this restriction. Now, let us suppose that we are at a configuration such that several floors of spin 2 are located at the bottom of the lattice, as in Figure 4.3. When we expand this cluster of spin 2 in the periodic case, there are 2 (namely, up and down) possible choices for the next floor to be filled; on the other hand, there is only one (namely, up) possible choice in the open boundary case. This further slows down the transition by a factor of 2. Next, when we expand the floor at the top of the cluster of spin 2, we may again look at the bulk part of the spin updates (cf. Definition 3.4.14). Thus, we suppose that there are two lines filled with spin 2 on that floor. There are L possible choices of the location in the periodic case, but just two possible choices in the open case. Thus, this gives us a factor of $L/2$. Moreover, we may choose one of two directions of growth of lines in the periodic case, which gives us additional factor of 2. Finally, there are K possible ways to form a protuberance in the periodic case; however, we now have only two (at the corners) possible choices. This further slows down the transition by a factor of $K/2$. Once the protuberance has been formed, we have only one direction in which to expand it, whereas we have two directions in the periodic case. This slows down the transition by a factor of 2. Summing up, the transition on the bulk is slowed by a factor of

$$\frac{M}{2} \times 2 \times \frac{L}{2} \times 2 \times \frac{K}{2} \times 2 = KLM.$$

Turning this into a rigorous argument (via the same logic applied to the periodic case), we obtain the following Eyring–Kramers formula with a modified (compared to the periodic case) prefactor. Recall that we assumed $K \le L \le M$.

Theorem 4.8.1. *Suppose that we impose open boundary conditions on the model. Then, there exists a constant* $\kappa' = \kappa'(K, L, M) > 0$ *such that, for all* $\boldsymbol{s}, \boldsymbol{s'} \in \mathcal{S}$,

$$\mathbb{E}_{\boldsymbol{s}}[\tau_{\breve{\boldsymbol{s}}}] = (1 + o(1)) \cdot \frac{\kappa'}{q-1} e^{\Gamma\beta} \quad \text{and} \quad \mathbb{E}_{\boldsymbol{s}}[\tau_{\boldsymbol{s'}}] = (1 + o(1)) \cdot \kappa' e^{\Gamma\beta}.$$

Moreover, the constant κ' *satisfies*

$$\lim_{K\to\infty} KLM \cdot \kappa'(K,\, L,\, M) = \begin{cases} 1/8 & \text{if } K < L < M, \\ 1/16 & \text{if } K = L < M \text{ or } K < L = M, \\ 1/48 & \text{if } K = L = M. \end{cases}$$

The constant κ' *can be defined in terms of new bulk and edge constants* $\mathfrak{b}'(n)$ *and* $\mathfrak{e}'(n)$*, in the exact same manner as done in Section 4.2.*

Then, Theorem 4.1.9 also holds for open boundary conditions with modified limiting Markov chain $Y'(\cdot)$ with rate $r_{Y'}(\boldsymbol{s},\, \boldsymbol{s'}) = (\kappa')^{-1}$ for all $\boldsymbol{s},\, \boldsymbol{s'} \in \mathcal{S}$.

Chapter 5

Large-volume limit

In this chapter, we consider the Ising/Potts models in the *large-volume regime*, i.e., the case when the side length grows to infinity. We analyze, at a highly accurate level, the energy landscape of the Ising/Potts models on a two-dimensional square or hexagonal lattice of side length L with periodic boundary conditions.

Lattices

Fix a large positive integer L and denote by Λ_L^{sq} and Λ_L^{hex} square and hexagonal lattices (cf. Figure 5.1) of size L with periodic boundary conditions, respectively. There is no ambiguity in the definition of Λ_L^{sq}, but a further explanation of Λ_L^{hex} is required. To define Λ_L^{hex}, we initially select $2L^2$ vertices from infinite hexagonal lattice, as shown in Figure 5.1-(left). Then, we identify the points at the boundary naturally, as illustrated in the figure. This setting will become intuitively clear when we introduce the dual lattice in the sequel.

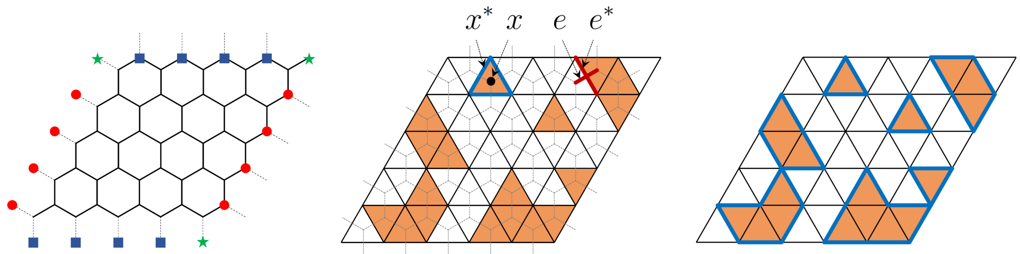


Figure 5.1: **(Left)** A hexagonal lattice $\Lambda = \Lambda_5^{\text{hex}}$ with $2 \times 5^2 = 50$ vertices which are the end points of bold edges. Under the periodic boundary condition, each vertex at the boundary highlighted by the red circle (resp. blue square) is identified with another one with a red circle (resp. blue square) at the same horizontal level (resp. same diagonal line with slope $\pi/3$). **(Middle)** The dual lattice Λ^* of the hexagonal lattice, which is a triangular lattice. The vertex x of Λ is identified with the triangular face x^* (the one highlighted by the blue bold boundary) in Λ^*. The edge e of Λ is identified with its dual edge e^* of Λ^*. In this and the figure on the right, if the spin at a certain vertex is 1 (resp. 2), we show the corresponding triangular face in white (resp. orange). Specifically, in this figure we consider the Ising case $q = 2$, and we have $\sigma(x) = 2$. **(Right)** Edges in $\mathfrak{A}^*(\sigma)$ are denoted by blue bold edges and hence $\mathfrak{A}^*(\sigma)$ is a collection of edges at the boundaries of the monochromatic clusters. Given that the Hamiltonian of σ can be computed as $|\mathfrak{A}^*(\sigma)|$, as we observed in (5.4), $H(\sigma)$ is just the sum of the perimeters of the orange (or white, equivalently) clusters.

Spin configuration

We henceforth let $\Lambda = \Lambda_L^{\mathrm{sq}}$ or Λ_L^{hex}. As before, we define the set of spins as

$$\Omega = \Omega_q = \{1,\, 2,\, \ldots,\, q\} \tag{5.1}$$

and write

$$\mathcal{X} = \mathcal{X}_L = \Omega^\Lambda \tag{5.2}$$

the space of spin configurations[1].

Visualization via dual lattice

To visualize spin configurations, it is convenient to consider the dual lattice Λ^* of Λ. If $\Lambda = \Lambda_L^{\mathrm{sq}}$, the dual lattice Λ^* is again a periodic square lattice of side length L. On the other hand, if $\Lambda = \Lambda_L^{\mathrm{hex}}$, the dual lattice Λ^* is a rhombus-shaped periodic triangular lattice with side length L, as shown in Figure 5.1-(middle). Note that the periodic boundary condition of the triangular lattice inherited from that of the hexagonal lattice simply identifies four boundaries of the rhombus in a routine manner (as in $\mathbb{Z}_L^2$).

Since we can identify a site of Λ with a face of Λ^* containing it, we can regard the spins assigned at the sites of Λ as those assigned to the faces of Λ^*. Thus, by assigning different colors to each set of spins, we can readily visualize the spin configurations on the dual lattice. For instance, in Figure 5.1-(middle, right), the triangles shown in white and orange correspond to the vertices of spins 1 and 2, respectively. This visualization is conceptually more convenient when analyzing the energy of spin configurations, as we explain in the next subsection.

[1] As in (5.2), we omit subscripts or superscripts L highlighting the dependency of the corresponding object to L, as soon as there is no risk of confusion by doing so.

Ising and Potts models

The Ising and Potts models are defined through the same Hamiltonian (3.2). Recall also the corresponding Gibbs distribution defined in Definition 2.0.2.

Computing the Hamiltonian via dual-lattice representation

We can identify an edge e in Λ with the unique edge e^* in the dual lattice Λ^* intersecting with e (cf. Figure 5.1-(middle)), and we can identify each vertex x in Λ with the unique face x^* in the dual lattice Λ^* containing x. As noted, we regard each spin in $\Omega = \{1, 2, \ldots, q\}$ as a color such that each face x^* in the dual lattice is shown in the color corresponding to the spin at x. Thus, we can identify $\sigma \in \mathcal{X}$ with a q-coloring on the faces of the dual lattice Λ^*. In this coloring representation of σ, each maximal monochromatic connected[2] component is called a (monochromatic) *cluster* of σ.

We now explain a convenient formulation to understand the Hamiltonian of a spin configuration $\sigma \in \mathcal{X}$ with the setting explained above. We refer to Figure 5.1-(right) for an illustration. Define $\mathfrak{A}(\sigma)$ as the collection of edges $e = \{x, y\}$ in Λ such that $\sigma(x) \neq \sigma(y)$. Then, define

$$\mathfrak{A}^*(\sigma) = \{e^* : e \in \mathfrak{A}(\sigma)\}, \tag{5.3}$$

such that according to the definition of the Hamiltonian, we have

$$H(\sigma) = |\mathfrak{A}(\sigma)| = |\mathfrak{A}^*(\sigma)|. \tag{5.4}$$

The crucial observation is that the dual edge e^* belongs to $\mathfrak{A}^*(\sigma)$ if and only if e^* belongs to the boundary of a cluster of σ. Hence, as in Figure 5.1-(right), we can readily compute the energy $H(\sigma)$ as

$$H(\sigma) = \frac{1}{2} \sum_{A^*:\,\text{cluster of } \sigma} (\text{perimeter of } A^*), \tag{5.5}$$

[2]Of course, two faces sharing only a vertex are not connected.

where the factor 1/2 appears since each dual edge $e^* \in \mathfrak{A}^*(\sigma)$ belongs to the perimeter of exactly two clusters.

Heat-bath Glauber dynamics

Next, we introduce a heat-bath Glauber dynamics associated with the Gibbs distribution $\mu_\beta(\cdot)$. We consider herein the continuous-time Metropolis–Hastings dynamics $\{\sigma_\beta(t)\}_{t\geq 0}$ on $\mathcal{X}$, whose jump rate from $\sigma \in \mathcal{X}$ to $\zeta \in \mathcal{X}$ is given by

$$c_\beta(\sigma,\, \zeta) = \begin{cases} e^{-\beta \max\{H(\zeta)-H(\sigma),\,0\}} & \text{if } \zeta = \sigma^{x,\,a} \neq \sigma \text{ for some } x \in \Lambda \text{ and } a \in \Omega, \\ 0 & \text{otherwise,} \end{cases} \tag{5.6}$$

where $\sigma^{x,\,a} \in \mathcal{X}$ denotes the configuration obtained from σ by flipping the spin at site x to a. This dynamics is standard in the study of the metastability of the Ising/Potts model on lattices; see e.g., [16, 71, 72] and the references therein. For $\sigma,\, \zeta \in \mathcal{X}$, we write

$$\sigma \sim \zeta \quad \text{if and only if} \quad c_\beta(\sigma,\, \zeta) > 0. \tag{5.7}$$

Note that $\sigma_\beta(\cdot)$ jumps only through single-spin flips. We use $\mathbb{P}_\sigma^\beta$ to indicate the law of the Markov process $\sigma_\beta(\cdot)$ starting from $\sigma \in \mathcal{X}$, and $\mathbb{E}_\sigma^\beta$ as the corresponding expectation.

From the definitions of $\mu_\beta(\cdot)$ and $c_\beta(\cdot,\, \cdot)$, we can directly check the following detailed balance condition:

$$\mu_\beta(\sigma)c_\beta(\sigma,\, \zeta) = \mu_\beta(\zeta)c_\beta(\zeta,\, \sigma) = \begin{cases} \min\{\mu_\beta(\sigma),\, \mu_\beta(\zeta)\} & \text{if } \sigma \sim \zeta, \\ 0 & \text{otherwise.} \end{cases} \tag{5.8}$$

Hence, the Markov process $\sigma_\beta(\cdot)$ is reversible with respect to its invariant measure $\mu_\beta(\cdot)$.

5.1 Main result

In this section, we explain the main results obtained in this article for the Ising/Potts model explained in the previous section. We assume hereafter that $L \geq 8$ to avoid unnecessary technical difficulties.

5.1.1 Hamiltonian and energy barrier

First, we explain certain results regarding the Hamiltonian $H(\cdot)$ of the Ising/Potts model. As before, we collect the *ground states* as

$$\mathcal{S} = \{\mathbf{1},\, \mathbf{2},\, \dots,\, \boldsymbol{q}\} \quad \text{and} \quad \mathcal{S}(A) = \{\boldsymbol{a} \in \mathcal{S} : a \in A\}$$

for each $A \subseteq \Omega$. Also, recall the definition of the energy barrier in Section 3.1.

Theorem 5.1.1. *For both $\Lambda = \Lambda_L^{\mathrm{sq}}$ and Λ_L^{hex}, we have $\Gamma = 2L+2$. Moreover, there is no valley of depth larger than Γ in the sense that*

$$\min_{\boldsymbol{s} \in \mathcal{S}} \Phi(\sigma,\, \boldsymbol{s}) - H(\sigma) < \Gamma \quad \textit{for all } \sigma \in \mathcal{X} \setminus \mathcal{S}.$$

This theorem has been proved for the square lattice [69], and we prove this theorem for the hexagonal lattice in Section 5.4.

5.1.2 Concentration of the Gibbs distribution

We next investigate the Gibbs distribution μ_β. We can readily observe from definition that if L is fixed and $\beta \to \infty$, the Gibbs distribution μ_β is concentrated on the ground set $\mathcal{S}$. However, if we consider the large-volume regime for which both L and β tend to ∞ together, the non-ground states can have non-negligible masses owing to the entropy effect; that is, there are sufficiently many configurations with high energy that can dominate the mass of the ground states. With the careful combinatorial analysis carried out in

Section 5.2, we can accurately quantify this competition between energy and entropy; consequently, we establish a zero-one law-type result by finding a sharp threshold determining whether the Gibbs distribution μ_β is concentrated on $\mathcal{S}$. Before explaining this result, we explicitly declare the regime that we consider.

Assumption. *The inverse temperature $\beta = \beta_L$ depends on L and we consider the large-volume, low-temperature regime, in the sense that $\beta_L \to \infty$ as $L \to \infty$.*

The following theorem will be proved in Section 5.2.

Theorem 5.1.2. *Let us define the constant γ_0 by*

$$\gamma_0 = \begin{cases} 1/2 & \text{for the square lattice,} \\ 2/3 & \text{for the hexagonal lattice.} \end{cases} \tag{5.9}$$

Then, the following estimates hold.

(1) Suppose that $L^{\gamma_0} \ll e^\beta$. Then, we have $Z_\beta = q + o(1)$ and

$$\mu_\beta(\mathcal{S}) = 1 - o(1).$$

(2) On the other hand, suppose that $e^\beta \ll L^{\gamma_0}$. Then, we have

$$\mu_\beta(\mathcal{S}) = o_L(1).$$

Henceforth, the constant γ_0 always refers to that defined in (5.9). This theorem implies that a drastic change in the valley structure of the Gibbs distribution μ_β occurs at $\beta/\log L = \gamma_0$. Specifically, if $\beta/\log L \geq \gamma$ for some $\gamma > \gamma_0$, most of the mass is concentrated on the ground states, while if $\beta/\log L \leq \gamma$ for $\gamma < \gamma_0$, the mass of the ground states is negligible.

The second regime can be investigated further. Define, for each $i \geq 0$,

$$\mathcal{X}_i = \mathcal{X}_{i,\,L} = \{\sigma \in \mathcal{X} : H(\sigma) = i\}, \tag{5.10}$$

such that $\mathcal{X}_0 = \mathcal{S}$ denotes the set of ground states. For any interval $I \subseteq \mathbb{R}$, we write

$$\mathcal{X}_I = \bigcup_{i \in I \cap \mathbb{Z}} \mathcal{X}_i.$$

Then, we have the following refinement of case (2) of Theorem 5.1.2 which will be proved in Section 5.2 as well.

Theorem 5.1.3. *Suppose that* $e^\beta \ll L^{\gamma_0}$ *and fix a constant* $\alpha \in (0,\,1)$. *Then, the following statements hold.*

(1) Suppose that $L^{\gamma_0(1-\alpha)} \ll e^\beta$. *Then, for every* $c > 0$, *we have*

$$\mu_\beta\big(\mathcal{X}_{[0,\,cL^{2\alpha}]}\big) = 1 - o(1).$$

(2) Suppose that $L^{\gamma_0(1-\alpha)} \gg e^\beta$. *Then, for every* $c > 0$, *we have*

$$\mu_\beta\big(\mathcal{X}_{[0,\,cL^{2\alpha}]}\big) = o(1).$$

In view of Theorem 5.1.1, it is natural to define the valley $\mathcal{V}_{\boldsymbol{a}}$ containing each $\boldsymbol{a} \in \mathcal{S}$ as the connected component of

$$\{\sigma \in \mathcal{X} : H(\sigma) < 2L + 2\}$$

containing $\boldsymbol{a}$, where the connectedness of a set $\mathcal{A} \subseteq \mathcal{X}$ here refers to the path-connectedness. Since Theorem 5.1.3 implies that

$$\mu_\beta\big(\mathcal{X}_{[0,\,2L+1]}\big) = \begin{cases} 1 - o(1) & \text{if } L^{\gamma_0/2} \ll e^\beta, \\ o(1) & \text{if } L^{\gamma_0/2} \gg e^\beta, \end{cases}$$

we can conclude that the valleys $\mathcal{V}_{\boldsymbol{a}}$, $\boldsymbol{a} \in \mathcal{S}$, contain almost all probability mass if $\beta/\log L \geq \gamma$ for some $\gamma > \frac{\gamma_0}{2}$. In contrast, if $\beta/\log L \leq \gamma$ for some $\gamma < \frac{\gamma_0}{2}$, the Gibbs distribution is concentrated on the complement of these valleys and the Glauber dynamics therefore spends most of the time on this complement. Hence, in the latter regime (as long as β exceeds the critical temperature $\beta_c(q) = \log(1+\sqrt{q})$ of the Ising/Potts model [4]), we deduce that the metastable set must lie upon configurations with higher energy; this is the onset at which the entropy starts to play a significant role.

5.1.3 Eyring–Kramers formula

The next main result of this chapter is the following Eyring–Kramers formula for the MH dynamics. We define the constant κ_0 by

$$\kappa_0 = \begin{cases} 1/8 & \text{for the square lattice,} \\ 1/12 & \text{for the hexagonal lattice.} \end{cases} \tag{5.11}$$

Theorem 5.1.4 (Eyring–Kramers formula)**.** *Suppose that $\beta = \beta_L$ satisfies $L^3 \ll e^\beta$ for the square lattice and $L^{10} \ll e^\beta$ for the hexagonal lattice. Then, for all $\boldsymbol{a}$, $\boldsymbol{b} \in \mathcal{S}$, we have*

$$\mathbb{E}_{\boldsymbol{a}}[\tau_{\mathcal{S}\setminus\{\boldsymbol{a}\}}] = \frac{\kappa_0 + o(1)}{q-1} e^{\Gamma\beta} \quad \textit{and} \quad \mathbb{E}_{\boldsymbol{a}}[\tau_{\boldsymbol{b}}] = (\kappa_0 + o(1)) e^{\Gamma\beta}, \tag{5.12}$$

where $\Gamma = 2L + 2$ is the energy barrier obtained in Theorem 5.1.1.

The proof of Theorem 5.1.4 is given in Sections 5.6 through 5.8. An outline of the proof of this theorem is briefly explained in the next subsection.

Remark 5.1.5. We conjecture that this result holds for all $\beta = \beta_L$ satisfying $L^{\gamma_0/2} \ll e^\beta$, under which the invariant measure is concentrated on the valleys around ground states. The sub-optimality of the lower bound (of constant order) on β stems from several technical issues arising in the proof (cf. Sections

5.7 and 5.8), and we surmise that additional innovative ideas are required to determine the optimal bound.

Remark 5.1.6. The condition on β is relatively tight ($L^3 \ll e^\beta$) for the square lattice, whereas the condition for the hexagonal lattice is slightly loose ($L^{10} \ll e^\beta$). This arises because the analysis of dead-ends is much more complicated for the hexagonal lattice owing to its complicated local geometry. This will be highlighted in Sections 5.4.2 and 5.4.3.

Remark 5.1.7. One can also obtain the Markov chain convergence of the trace process of the accelerated process $\{\sigma_\beta(e^{\Gamma\beta}t)\}_{t\geq 0}$ on the set $\mathcal{S}$ to the Markov process on $\mathcal{S}$ with uniform rate $r(\boldsymbol{a}, \boldsymbol{b}) = \dfrac{1}{\kappa_0}$ for all $\boldsymbol{a}, \boldsymbol{b} \in \mathcal{S}$. The proof of this result, using Theorem 5.6.1, is identical to that of Theorems 3.1.4 and 3.1.5, and is not repeated here.

In the remainder of this chapter, we explain the proof of the theorems explained above in detail only for the hexagonal lattice, as the proof for the square lattice is similar to that for the hexagonal lattice and in fact much simpler; the geometry of the hexagonal lattice is far more complex and requires careful consideration with additional complicated arguments. Moreover, the analysis of the square lattice can be helped considerably by the computations carried out in Chapter 3 that considered the small-volume regime (where L is fixed and β tends to infinity).

5.1.4 Outline of proof of Theorem 5.1.4

The first step in the proof of Theorem 5.1.4 is devoted to analyzing the energy landscape of the current model. In particular, we must fully characterize all configurations which can be visited by a typical trajectory of a metastable transition. In the bulk of these typical trajectories, the dynamics is found to behave in a simple manner. The dynamics should fill the sites line by line while it can visit numerous dead-end configurations in the course of the transition. On the other hand, in the edges of typical trajectories (i.e., trajectories near ground states), we cannot expect such simple behavior, and the analysis becomes very complicated. We remark that one study [11, 12, 13] successfully handles this problem for a two-dimensional fixed square lattice model and that another (Chapter 4) reveals that the same problem for a three-dimensional fixed square model is far more difficult to be analyzed explicitly. The main difference and difficulty with regard to our current problem compared to these occur at the bulk part of the typical trajectories; we encounter a large amount of dead-ends.

Once we understand the energy landscape, we can construct a suitable test function and a test flow on top of the characterized structure of the energy landscape to apply the potential-theoretic approach developed in earlier work [19] to prove Theorem 5.1.4. Construction of these test objects is far more complex when compared to the fixed lattice case in Chapter 3 mainly because configurations with energy higher than $2L + 2$ play a role here because the number of such configurations explodes in the limit $\beta \to \infty$.

5.1.5 Outlook of the remainder of the chapter

The remainder of the chapter is organized as follows. In Section 5.2, we analyze the Gibbs distribution μ_β to prove Theorems 5.1.2 and 5.1.3. In Section 5.3, we provide some preliminary observations to investigate the energy landscape in a more detailed manner. We then analyze the energy landscape of the Hamiltonian in detail in Sections 5.4 and 5.5. As a by-product of our deep analysis, Theorem 5.1.1 will be proved at the end of Section 5.4. Then, we finally prove the Eyring–Kramers formula, i.e., Theorem 5.1.4 in remaining sections.

5.2 Sharp threshold for the Gibbs distribution

In this section, we prove Theorems 5.1.2 and 5.1.3. We remark that we will now implicitly assume that the underlying lattice is the hexagonal one, unless otherwise specified. We shall briefly discuss the square lattice type in Section 5.2.5.

5.2.1 Lemma on graph decomposition

We begin with a lemma on graph decomposition, which is crucial when estimating the number of configurations having a specific energy level.

Notation 5.2.1. For a graph $G = (V, E)$ and a set $E_0 \subseteq E$ of edges, we denote by $G[E_0] = (V[E_0], E_0)$ the subgraph induced by the edge set E_0 where the vertex set $V[E_0]$ is the collection of end points of the edges in E_0. The edge set $E_0 \subseteq E$ is said to be connected if the induced graph $G[E_0]$ is a connected graph.

Lemma 5.2.2. *Let $G = (V, E)$ be a graph such that every connected component has at least three edges. Then, we can decompose*

$$E = E_1 \cup \cdots \cup E_n$$

such that E_i is connected and $|E_i| \in \{3, 4, 5, 6\}$ for all $i = 1, \ldots, n$.

Proof. It suffices to prove the lemma for a connected graph G with at least three edges, since we can apply this result to each connected component to complete the proof for general case. Henceforth, we therefore assume that G is a connected graph with at least three edges. Then, the proof is proceeded by induction on the cardinality $|E|$.

First, there is nothing to prove if $|E| \leq 6$ since we can take $n = 1$ and $E_1 = E$. Next, let us fix $k \geq 7$ and assume that the lemma holds if

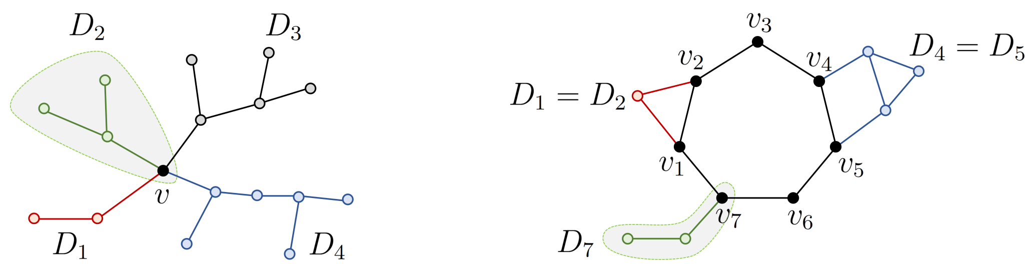


Figure 5.2: The left and right figures illustrate **(Case 1)** and **(Case 2)** in the proof of Lemma 5.2.2, respectively. Note that we have $D_3 = D_6 = \emptyset$ in the right figure.

$3 \le |E| \le k-1$. Let $G = (V, E)$ be a connected graph with $|E| = k$. We will find $E' \subseteq E$ such that

$$|E'|,\ |E \setminus E'| \ge 3 \text{ and both } E' \text{ and } E \setminus E' \text{ are connected.} \tag{5.13}$$

Once finding such an E', it suffices to apply the induction hypothesis to the sets E' and $E \setminus E'$ to complete the proof.

(Case 1: G does not have a cycle; i.e., G is a tree) If every vertex of G has a degree of at most 2, then G is a line graph, and we can thus easily divide E into two connected subsets E' and $E \setminus E'$ satisfying (5.13).

Next, we suppose that a vertex $v \in V$ has a degree of at least 3. Since G is a tree, we can decompose E into connected $D_1, D_2, \dots, D_m$ with $m = \deg(v) \ge 3$, such that the edges in D_i and D_j $(i \ne j)$ possibly intersect only at v (cf. Figure 5.2-(left)). We impose the condition $|D_1| \le \cdots \le |D_m|$ for convenience.

If $|D_k| \ge 3$ for $k = 1$ or 2, it suffices to take $E' = D_k$. If $|D_1|, |D_2| \le 2$ but $|D_1| + |D_2| \ge 3$, we take $E' = D_1 \cup D_2$. Finally, if $|D_1| = |D_2| = 1$, we take

$$E' = \begin{cases} D_1 \cup D_2 \cup \{\text{the edge in } D_3 \text{ having } v \text{ as an end point}\} & \text{if } m = 3, \\ D_1 \cup D_2 \cup D_3 & \text{if } m \ge 4. \end{cases}$$

(Case 2: G has a cycle) Suppose that $(v_1, v_2, \ldots, v_n)$ is a cycle in G in the sense that $\{v_i, v_{i+1}\} \in E$ for all $i \in [\![1, n]\!]$ (with the convention $v_{n+1} = v_1$). We denote by E_0 the edges belonging to this cycle, i.e.,

$$E_0 = \big\{\{v_i, v_{i+1}\} : i \in [\![1, n]\!]\big\}.$$

If $E = E_0$, i.e., G is a ring graph, we can easily divide E into two connected subsets E' and $E \setminus E'$ satisfying (5.13) and hence suppose that $E \setminus E_0 \neq \emptyset$. For each $i \in [\![1, n]\!]$, we denote by D_i the connected component of $E \setminus E_0$ containing the vertex v_i so that we have as in Figure 5.2-(right) so that

$$E = E_0 \cup \Big(\bigcup_{i=1}^{n} D_i\Big).$$

Note that we may have $D_i = D_j$ for some $i \neq j$. Since we assumed $E \setminus E_0 \neq \emptyset$, we can assume without loss of generality that $D_1 \neq \emptyset$. If $|D_1| \geq 3$, we take $E' = D_1$. Otherwise, we take $E' = D_1 \cup \{\{v_1, v_2\}, \{v_1, v_n\}\}$.

This completes the proof of (5.13) and we are done. □

Remark 5.2.3. We remark that the set $\{3, 4, 5, 6\}$ appearing in the previous lemma cannot be replaced with $\{3, 4, 5\}$. For example, in **(Case 1)** of the proof (cf. Figure 5.2-(left)), the graph with $m = 3$ and $|E_1| = |E_2| = |E_3| = 2$ provides such a counterexample.

5.2.2 Counting of configurations with fixed energy

The crucial lemma in the analysis of the Gibbs distribution is the following upper and lower bounds for the number of configurations belonging to the set $\mathcal{X}_i$, which denotes the collection of configurations with energy i (cf. (5.10)).

Lemma 5.2.4. *There exists $\theta > 1$ such that the following estimates hold.*

(1) (Upper bound) For all $i \in \mathbb{N}$, we have

$$|\mathcal{X}_i| \le q^{i+1} \times \sum_{\substack{n_3, n_4, n_5, n_6 \ge 0: \\ 3n_3+4n_4+5n_5+6n_6=i}} \binom{\theta L^2}{n_3}\binom{\theta L^2}{n_4}\binom{\theta L^2}{n_5}\binom{\theta L^2}{n_6}.$$

(2) (Lower bound) For all $1 \le j < \lfloor \frac{L^2}{2} \rfloor$, we have

$$|\mathcal{X}_{3j}| \ge 4^j \binom{\lfloor \frac{L^2}{2} \rfloor}{j}.$$

Proof. (1) As the assertion is obvious for $i = 0$ where $|\mathcal{X}_0| = q$, we assume $i \neq 0$ so that $i \ge 3$ (since $\mathcal{X}_1$ and $\mathcal{X}_2$ are empty). Denote by $E(\Lambda^*)$ the collection of edges of the dual lattice Λ^* and let $\mathcal{E}_i$ be the collection of $E_0 \subseteq E(\Lambda^*)$ such that $|E_0| = i$. Then, we can regard $\mathfrak{A}^*(\cdot)$ defined in (5.3) as a map from $\mathcal{X}_i$ to $\mathcal{E}_i$.

For $\sigma \in \mathcal{X}$, it is immediate that the graph $G[\mathfrak{A}^*(\sigma)]$ (cf. Notation 5.2.1) has no vertex of degree 1, since if there exists such a vertex, then there is no possible coloring on the six faces of Λ^* surrounding the vertex which realizes $\mathfrak{A}^*(\sigma)$. Therefore, each vertex of $G[\mathfrak{A}^*(\sigma)]$ has degree at least two. This implies that each connected component of $G[\mathfrak{A}^*(\sigma)]$ has a cycle and hence has at least three edges. Thus, by Lemma 5.2.2, we can decompose an element of $\mathfrak{A}^*(\mathcal{X}_i)$ by connected components of sizes 3, 4, 5, or 6. Note that there exists a fixed integer $\theta > 1$ such that there are at most θL^2 connected subgraphs of Λ^* with at most 6 edges (for all L). Combining the observations above allows us to conclude that

$$|\mathfrak{A}^*(\mathcal{X}_i)| \le \sum_{\substack{n_3, n_4, n_5, n_6 \ge 0: \\ 3n_3+4n_4+5n_5+6n_6=i}} \binom{\theta L^2}{n_3}\binom{\theta L^2}{n_4}\binom{\theta L^2}{n_5}\binom{\theta L^2}{n_6}. \tag{5.14}$$

Next, we will show that

$$|(\mathfrak{A}^*)^{-1}(\eta)| \le q^{i+1} \quad \text{for all } \eta \in \mathfrak{A}^*(\mathcal{X}_i). \tag{5.15}$$

Indeed, since $\eta \in \mathfrak{A}^*(\mathcal{X}_i)$ has i edges, it divides (the faces of) Λ^* into at most $i+1$ connected components, where each component must be a monochromatic cluster in each $\sigma \in (\mathfrak{A}^*)^{-1}(\eta)$. Therefore, there are at most q^{i+1} (indeed, $q \times (q-1)^i$) ways to paint these monochromatic clusters and we obtain (5.15). Part (1) follows directly from (5.14) and (5.15).
(2) If we take an independent set[3] A of size j from Λ (i.e., we take j mutually disconnected triangle faces in Λ^*), and assign spins 1 and 2 to A and $\Lambda \setminus A$, respectively, then the energy of the corresponding configuration is $3j$ by (5.5). If we select such j vertices one by one, then each selection of a vertex reduces at most four possibilities of the next choice (specifically the selected one and the three adjacent vertices). Since the selection does not depend on the order, there are at least

$$\frac{2L^2(2L^2-4)\cdots(2L^2-4j+4)}{j!} \ge 4^j \binom{\lfloor \frac{L^2}{2} \rfloor}{j}$$

ways of selecting such an independent set of size j. This concludes the proof of part (2). □

5.2.3 Lemma on concentration

In this subsection, we establish a counting lemma which is useful in the proof of Theorems 5.1.2 and 5.1.3. Here, we regard $\beta = \beta_L$ to be dependent of L.

Lemma 5.2.5. *Suppose that $e^\beta \ll L^{2/3}$ and moreover two sequences $(g_1(L))_{L\in\mathbb{N}}$*

[3]Here, a set is called *independent* if it consists of lattice vertices among which any two vertices are not connected by a lattice edge.

and $(g_2(L))_{L\in\mathbb{N}}$ *satisfy*

$$1 \ll g_1(L) \ll L^2 e^{-3\beta} \ll g_2(L).$$

Then, we have

$$\mu_\beta\big(\mathcal{X}_{[g_1(L),\, g_2(L)]}\big) = 1 - o(1).$$

Proof. It is enough to show that

$$\mu_\beta\Big(\bigcup_{i<g_1(L)} \mathcal{X}_i\Big) = o(1) \quad \text{and} \quad \mu_\beta\Big(\bigcup_{i>g_2(L)} \mathcal{X}_i\Big) = o(1). \tag{5.16}$$

To prove the first one, it suffices to prove that

$$\sum_{i<g_1(L)} |\mathcal{X}_i| e^{-\beta i} \ll \sum_{i\geq g_1(L)} |\mathcal{X}_i| e^{-\beta i}. \tag{5.17}$$

By part (1) of Lemma 5.2.4, we have

$$\sum_{i<g_1(L)} |\mathcal{X}_i| e^{-\beta i} \leq q \times \sum_{\substack{n_3,\, n_4,\, n_5,\, n_6 \geq 0: \\ 3n_3+4n_4+5n_5+6n_6 < g_1(L)}} \binom{\theta L^2}{n_3}\binom{\theta L^2}{n_4}\binom{\theta L^2}{n_5}\binom{\theta L^2}{n_6} \cdot (qe^{-\beta})^{3n_3+4n_4+5n_5+6n_6}.$$

Let L be large enough so that $qe^{-\beta} < 1$. Then, the summation at the right-hand side is bounded from above by

$$\begin{aligned}
&\sum_{\substack{n_3,n_4,n_5,n_6\geq 0:\\ 3n_3+3n_4+3n_5+3n_6<g_1(L)}} \binom{\theta L^2}{n_3}\binom{\theta L^2}{n_4}\binom{\theta L^2}{n_5}\binom{\theta L^2}{n_6}(qe^{-\beta})^{3n_3+3n_4+3n_5+3n_6}\\
&= \sum_{i<\frac{g_1(L)}{3}} \sum_{\substack{n_3,n_4,n_5,n_6\geq 0:\\ n_3+n_4+n_5+n_6=i}} \binom{\theta L^2}{n_3}\binom{\theta L^2}{n_4}\binom{\theta L^2}{n_5}\binom{\theta L^2}{n_6}(qe^{-\beta})^{3i}\\
&= \sum_{i<\frac{g_1(L)}{3}} \binom{4\theta L^2}{i}(qe^{-\beta})^{3i},
\end{aligned} \tag{5.18}$$

where at the last equality we used a combinatorial identity of the form

$$\sum_{x+y+z+w=k} \binom{a}{x}\binom{b}{y}\binom{c}{z}\binom{d}{w} = \binom{a+b+c+d}{k}. \tag{5.19}$$

We can further bound the last summation in (5.18) from above by

$$\begin{aligned}
\sum_{i<\frac{g_1(L)}{3}} \frac{(4\theta L^2)^i}{i!}(qe^{-\beta})^{3i} &\leq \frac{g_1(L)+3}{3}\cdot\frac{(4\theta L^2)^{\frac{g_1(L)}{3}}\cdot(qe^{-\beta})^{g_1(L)}}{\lfloor\frac{g_1(L)}{3}\rfloor!}\\
&\leq g_1(L)\cdot\Big(\frac{CL^2e^{-3\beta}}{g_1(L)}\Big)^{\frac{g_1(L)}{3}}
\end{aligned}$$

using $g_1(L) \ll L^2e^{-3\beta}$ and an elementary bound $n! \geq n^n/e^n$. Summing up, we get

$$\sum_{i<g_1(L)} |\mathcal{X}_i|e^{-\beta i} \leq qg_1(L)\cdot\Big(\frac{CL^2e^{-3\beta}}{g_1(L)}\Big)^{\frac{g_1(L)}{3}}. \tag{5.20}$$

Next, let $\widetilde{g}_1(L) = \lfloor g_1(L)^{2/3}(L^2e^{-3\beta})^{1/3}\rfloor$ so that we have $g_1(L) \ll \widetilde{g}_1(L) \ll L^2e^{-3\beta}$. Then, by part (2) of Lemma 5.2.4, we have

$$\sum_{i\geq g_1(L)} |\mathcal{X}_i|e^{-\beta i} \geq |\mathcal{X}_{3\widetilde{g}_1(L)}|e^{-3\beta\widetilde{g}_1(L)} \geq 4^{\widetilde{g}_1(L)}\binom{\lfloor\frac{L^2}{2}\rfloor}{\widetilde{g}_1(L)} \times e^{-3\beta\widetilde{g}_1(L)}.$$

By Stirling's formula and $\widetilde{g}_1(L) \ll L^2 e^{-3\beta} \ll L^2$, this is bounded from below by, for all large enough L,

$$\frac{1}{2}(4e)^{\widetilde{g}_1(L)} \frac{(\frac{L^2}{3})^{\widetilde{g}_1(L)}}{\widetilde{g}_1(L)^{\widetilde{g}_1(L)}\sqrt{2\pi\widetilde{g}_1(L)}} \cdot e^{-3\beta\widetilde{g}_1(L)} \geq \Big(\frac{L^2 e^{-3\beta}}{\widetilde{g}_1(L)}\Big)^{\widetilde{g}_1(L)} \gg \Big(\frac{L^2 e^{-3\beta}}{\widetilde{g}_1(L)}\Big)^{g_1(L)}. \tag{5.21}$$

Therefore by (5.20) and (5.21), we can reduce the proof of (5.17) into

$$\frac{L^2 e^{-3\beta}}{\widetilde{g}_1(L)} \gg \Big(\frac{L^2 e^{-3\beta}}{g_1(L)}\Big)^{1/3}.$$

This follows from the definition of $\widetilde{g}_1(L)$ and the fact that $g_1(L) \ll L^2 e^{-3\beta}$. This proves the first statement in (5.16).

Next, to prove the second estimate of (5.16), it suffices to prove

$$\sum_{i > g_2(L)} |\mathcal{X}_i| e^{-\beta i} \ll 1$$

since the partition function Z_β has a trivial lower bound $Z_\beta \geq q$ (by only considering the ground states). By a similar computation leading to (5.20), we get

$$\sum_{i > g_2(L)} |\mathcal{X}_i| e^{-\beta i} \leq q \sum_{i > \frac{g_2(L)}{6}} \frac{(4\theta L^2)^i}{i!} (qe^{-\beta})^{3i}. \tag{5.22}$$

Here, Taylor's theorem on the function $x \mapsto e^x$ implies that for $x > 0$ and $M \in \mathbb{N}$,

$$\sum_{i > M} \frac{x^i}{i!} \leq \max_{t \in [0,\, x]} |e^t| \times \frac{x^{M+1}}{(M+1)!} = \frac{e^x x^{M+1}}{(M+1)!}. \tag{5.23}$$

Therefore, the right-hand side of (5.22) is bounded from above by

$$e^{CL^2 e^{-3\beta}} \times \frac{(CL^2 e^{-3\beta})^{\frac{g_2(L)}{6}}}{(\frac{g_2(L)}{6})^{\frac{g_2(L)}{6}}} \leq \Big[\, 6C (e^{6C})^{\frac{L^2 e^{-3\beta}}{g_2(L)}} \times \frac{L^2 e^{-3\beta}}{g_2(L)} \Big]^{\frac{g_2(L)}{6}}.$$

As $L^2 e^{-3\beta} \ll g_2(L)$, this expression vanishes as $L \to \infty$. This concludes the proof. □

5.2.4 Proof of Theorems 5.1.2 and 5.1.3

Now, we are ready to prove Theorems 5.1.2 and 5.1.3. Note that the constant γ_0 is 2/3 since we consider the hexagonal lattice.

Proof of Theorem 5.1.2. (1) It suffices to prove that, for some constant $C > 0$,

$$\sum_{\sigma \in \mathcal{X} \setminus \mathcal{S}} e^{-\beta H(\sigma)} = \sum_{i=3}^{3L^2} |\mathcal{X}_i| e^{-\beta i} \ll 1, \tag{5.24}$$

where the identity follows from the observation that the minimum non-zero value of the Hamiltonian is 3 and the maximum is $3L^2$. By part (1) of Lemma 5.2.4, we have (for $qe^{-\beta} < 1$)

$$\sum_{i=3}^{3L^2} |\mathcal{X}_i| e^{-\beta i} \le q \times \sum_{i=3}^{3L^2} \sum_{\substack{n_3, n_4, n_5, n_6 \ge 0: \\ 3n_3+4n_4+5n_5+6n_6=i}} \binom{\theta L^2}{n_3} \binom{\theta L^2}{n_4} \binom{\theta L^2}{n_5} \binom{\theta L^2}{n_6} \cdot (qe^{-\beta})^{3n_3+4n_4+5n_5+6n_6},$$

which is further bounded by

$$q \times \sum_{\substack{n_3, n_4, n_5, n_6 \ge 0: \\ n_3+n_4+n_5+n_6 \ge 1}} \binom{\theta L^2}{n_3} \binom{\theta L^2}{n_4} \binom{\theta L^2}{n_5} \binom{\theta L^2}{n_6} \cdot (qe^{-\beta})^{3n_3+3n_4+3n_5+3n_6}.$$

Summing up and applying (5.19), we get

$$\sum_{\sigma \in \mathcal{X} \setminus \mathcal{S}} e^{-\beta H(\sigma)} \le q \sum_{i=1}^{\infty} \binom{4\theta L^2}{i} (qe^{-\beta})^{3i} \le q \sum_{i=1}^{\infty} \frac{(4\theta q^3 L^2 e^{-3\beta})^i}{i!}.$$

Again applying Taylor's theorem on the function $x \mapsto e^x$ (cf. (5.23)) for

$x = 4\theta q^3 L^2 e^{-3\beta}$, the last summation is bounded by

$$e^{4\theta q^3 L^2 e^{-3\beta}} \times (4\theta q^3 L^2 e^{-3\beta}).$$

This completes the proof of (5.24) since we have $L^2 e^{-3\beta} \ll 1$ by assumption.

(2) We have $e^\beta \ll L^{2/3}$ and therefore as in Lemma 5.2.5 we can take two sequences $(g_1(L))_{L\in\mathbb{N}}$ and $(g_2(L))_{L\in\mathbb{N}}$ satisfying

$$1 \ll g_1(L) \ll L^2 e^{-3\beta} \ll g_2(L).$$

Then, by Lemma 5.2.5, the measure μ_β is concentrated on $\mathcal{X}_{[g_1(L),\, g_2(L)]}$ and therefore $\mu_\beta(\mathcal{S}) = o(1)$. □

Proof of Theorem 5.1.3. (1) Since $L^{\frac{2}{3}(1-\alpha)} \ll e^\beta$, we have $L^2 e^{-3\beta} \ll cL^{2\alpha}$ for any $c > 0$. Thus, we can complete the proof by recalling Lemma 5.2.5 with any $g_1(L)$ such that $1 \ll g_1(L) \ll L^2 e^{-3\beta}$ (which is possible since we assumed that $e^\beta \ll L^{\gamma_0}$) and $g_2(L) = cL^{2\alpha}$.

(2) We can take $g_1(L) = cL^{2\alpha}$ (and any $g_2(L)$ such that $L^2 e^{-3\beta} \ll g_2(L)$) to get $\mu_\beta(\mathcal{X}_{[cL^{2\alpha},\, g_2(L)]}) = 1 - o(1)$. This completes the proof. □

5.2.5 Remarks on the square lattice case

For the square lattice case, a slightly different version of Lemma 5.2.2 is required. More precisely, we need a version which is obtained from Lemma 5.2.2 after replacing set $\{3, 4, 5, 6\}$ with $\{4, 5, \ldots, 9\}$. This modification comes from the fact that the minimal cycle in the dual graph Λ^* has three edges in the hexagonal lattice but has *four* edges in the square lattice case (cf. proof of Lemma 5.2.4). The proof of this lemma is similar to that of Lemma 5.2.2, and we will not repeat the proof. As a consequence of this modification, the upper and lower bounds appearing in Lemma 5.2.4 should be replaced with

$$|\mathcal{X}_i| \le q^{i+1} \times \sum_{\substack{n_4,\, n_5,\, \dots,\, n_9 \ge 0: \\ 4n_4+5n_5+\cdots+9n_9=i}} \binom{\theta L^2}{n_4}\binom{\theta L^2}{n_5}\cdots\binom{\theta L^2}{n_9}$$

and $|\mathcal{X}_{4j}| \ge 5^j \binom{\lfloor \frac{L^2}{5} \rfloor}{j}$ for $1 \le j < \lfloor \frac{L^2}{5} \rfloor$, respectively. The constant γ_0 for the square lattice differs from that for the hexagonal lattice due to this modification.

5.3 Preliminaries for the energy landscape

In this section, we introduce several preliminary notation and results which are useful in the subsequent analysis of the energy landscape.

5.3.1 Strip, bridge and cross

In this subsection, we provide some crucial notation regarding the structure of the dual lattice Λ^*. We refer to Figure 5.3 for illustrations of the notation defined below and we consistently refer to this figure.

Definition 5.3.1 (Strip, bridge, cross and semibridge)**.** We define the crucial concepts here.

(1) We denote by a *strip* the $2L$ consecutive triangles in Λ^* as illustrated in Figure 5.3-(left). We may regard each strip as a discrete torus $\mathbb{T}_{2L}$ via the obvious manner.

(2) There are three possible directions for strips. We call these three directions as *horizontal*, *vertical*, and *diagonal*, and these are highlighted by black, blue, and red lines in Figure 5.3-(left), respectively. For each $\ell \in \mathbb{T}_L = \{1, 2, \dots, L\}$, the ℓ-th strip of horizontal, vertical, and diag-

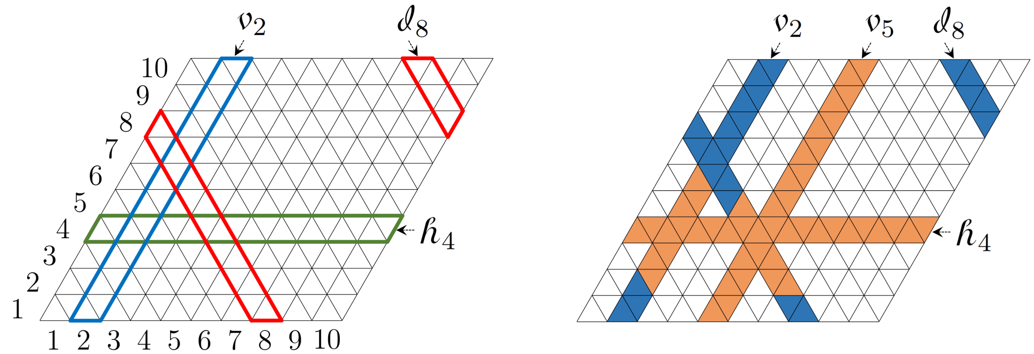


Figure 5.3: **(Left)** Strips $\mathscr{h}_4$, $\mathscr{v}_2$, and $\mathscr{d}_8$. **(Right)** *Here and in the following figures, white, orange, and blue indicate spins a, b, and c, respectively.* Strips $\mathscr{h}_4$ and $\mathscr{v}_5$ are b-bridges and thus form a b-cross. Strips $\mathscr{v}_2$ and $\mathscr{d}_8$ are $\{b,\, c\}$-semibridges.

onal directions are denoted by $\mathscr{h}_\ell$, $\mathscr{v}_\ell$, and $\mathscr{d}_\ell$, respectively, as in Figure 5.3-(left).

(3) A strip $\mathscr{s}$ is called a *bridge* of $\sigma \in \mathcal{X}$ if all the spins of σ in $\mathscr{s}$ are identical. If this spin is a, we call $\mathscr{s}$ an *a-bridge* of σ. Furthermore, we can specify the direction of a bridge by calling it a *horizontal*, *vertical*, or *diagonal bridge* of σ. Finally, the union of two bridges of different directions (of spin a) is called a *cross* (an *a-cross*). We refer to Figure 5.3-(right).

(4) A strip $\mathscr{s}$ is called a *semibridge* of $\sigma \in \mathcal{X}$, if the strip $\mathscr{s}$ in σ consists of exactly two spins, and moreover if the sites in $\mathscr{s}$ with either of these spins are consecutive. If a semibridge consists of two spins a and b, we say that it is an $\{a,\, b\}$-semibridge. We refer to Figure 5.3-(right).

5.3.2 Low-dimensional decomposition of energy

For each strip $\mathscr{s}$, the energy of configuration σ on the strip $\mathscr{s}$ is defined as

$$\Delta H_{\mathscr{s}}(\sigma) = \sum_{\{x,\, y\} \subseteq \mathscr{s}:\, x \sim y} \mathbb{1}\{\sigma(x) \neq \sigma(y)\}$$

so that by the definition of the Hamiltonian H, we have the following decomposition

$$H(\sigma) = \frac{1}{2} \sum_{\ell \in \mathbb{T}_L} \left[\Delta H_{\mathscr{h}_\ell}(\sigma) + \Delta H_{\mathscr{v}_\ell}(\sigma) + \Delta H_{\mathscr{d}_\ell}(\sigma) \right], \tag{5.25}$$

where the term $1/2$ appears since each edge is counted twice. The following simple fact is worth mentioning explicitly.

Lemma 5.3.2. *Suppose that a strip $\mathscr{s}$ is not a bridge of σ. Then, we have*

$$\Delta H_{\mathscr{s}}(\sigma) \geq 2,$$

and furthermore $\Delta H_{\mathscr{s}}(\sigma) = 2$ if and only if $\mathscr{s}$ is a semibridge of σ.

Proof. The proof is straightforward by identifying a strip $\mathscr{s}$ with $\mathbb{T}_{2L}$ as in Definition 5.3.1-(1). □

The next lemma provides an elementary lower bound on the number of bridges based on the energy of the configurations. Let us denote by $B_a(\sigma)$ the number of a-bridges in $\sigma \in \mathcal{X}$.

Lemma 5.3.3. *For $\sigma \in \mathcal{X}$, there are at least $3L - H(\sigma)$ bridges. Moreover, if σ has exactly $3L - H(\sigma)$ bridges then all strips are either bridges or semibridges.*

Proof. By (5.25) and Lemma 5.3.2, we have

$$H(\sigma) \geq \frac{1}{2} \times 2 \times \left[3L - \sum_{a \in \Omega} B_a(\sigma) \right] = 3L - \sum_{a \in \Omega} B_a(\sigma). \tag{5.26}$$

This proves that there are at least $3L - H(\sigma)$ bridges. Moreover, by Lemma 5.3.2, a strip which is not a bridge should be a semibridge in order to have the equality in the bound (5.26). This completes the proof. □

5.4 Energy barrier

This section provides the first level of investigation of the energy landscape which suffices to prove Theorem 5.1.1; that is, the energy barrier between ground states is $2L+2$. A deeper analysis of the energy landscape required to prove the Eyring–Kramers formula will be carried out in Section 5.5.

We collect here notation heavily used in the remainder of the article.

Notation 5.4.1. Here, the letters $\mathscr{h}$, $\mathscr{v}$, $\mathscr{d}$ stand for *horizontal*, *vertical*, and *diagonal*, respectively.

(1) Recall $\mathfrak{S}_L$ from Notation 3.4.11. For each $P \in \mathfrak{S}_L$, we write

$$\mathscr{h}(P) = \bigcup_{\ell \in P} \mathscr{h}_\ell, \quad \mathscr{v}(P) = \bigcup_{\ell \in P} \mathscr{v}_\ell, \quad \text{and} \quad \mathscr{d}(P) = \bigcup_{\ell \in P} \mathscr{d}_\ell.$$

(2) We regard the dual lattice Λ^* as the collection of triangles (corresponding to the sites, or vertices of Λ) and hence we say that U is a subset of Λ^* (i.e., $U \subseteq \Lambda^*$) if U is a collection of triangles in Λ^*. For example, a strip is a subset of Λ^* consisting of $2L$ triangles.

(3) For each $U \subseteq \Lambda^*$ and $a, b \in \Omega$, we write $\xi_U^{a,b} \in \mathcal{X}$ the configuration whose spins are b on the sites corresponding to the triangles in U and a on the remainder.

5.4.1 Canonical configurations

In this subsection, we define the canonical configurations between the ground states. These canonical configurations provide the backbone of the saddle structure. We shall see in the sequel that the saddle structure is completed by attaching dead-end structures or bypasses at this backbone. We define canonical configurations in several steps. The first step is devoted to defining the regular configurations which are indeed special forms of canonical configurations.

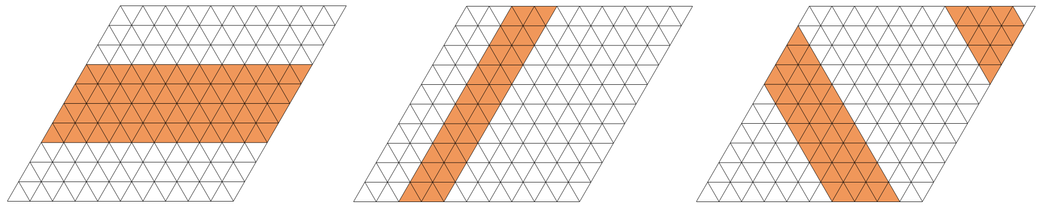


Figure 5.4: Example of regular configurations: $\xi^{a,\,b}_{\mathfrak{h}([\![4,\,7]\!])}$ (left), $\xi^{a,\,b}_{\mathfrak{v}([\![3,\,4]\!])}$ (middle), and $\xi^{a,\,b}_{\mathfrak{d}([\![7,\,9]\!])}$ (right).

Definition 5.4.2 (Regular configurations)**.** Fix $a,\, b \in \Omega$. We recall Notation 5.4.1.

- A configuration of the form $\xi^{a,\,b}_{\mathfrak{h}(P)}$, $\xi^{a,\,b}_{\mathfrak{v}(P)}$, or $\xi^{a,\,b}_{\mathfrak{d}(P)}$ for some $P \in \mathfrak{S}_L$ is called a *horizontal, vertical, or diagonal regular configuration* between $\boldsymbol{a}$ and $\boldsymbol{b}$, respectively. We refer to Figure 5.4 for illustrations.

- For $n \in [\![0,\, L]\!]$, we define

$$\mathcal{R}^{a,\,b}_n = \bigcup_{P\in\mathfrak{S}_L:\,|P|=n} \left\{\xi^{a,\,b}_{\mathfrak{h}(P)},\, \xi^{a,\,b}_{\mathfrak{v}(P)},\, \xi^{a,\,b}_{\mathfrak{d}(P)}\right\} \quad \text{and} \quad \mathcal{R}^{a,\,b} = \bigcup_{n=0}^{L} \mathcal{R}^{a,\,b}_n.$$

  Then for a proper partition $(A,\, B)$, we write

$$\mathcal{R}^{A,\,B}_n = \bigcup_{a\in A}\bigcup_{b\in B} \mathcal{R}^{a,\,b}_n \quad \text{and} \quad \mathcal{R}^{A,\,B} = \bigcup_{a\in A}\bigcup_{b\in B} \mathcal{R}^{a,\,b}.$$

Canonical configurations are now defined as those obtained by adding suitable protuberances at a monochromatic cluster of a regular configuration. To carry this out rigorously, we initially define the canonical sets.

Definition 5.4.3 (One-dimensional canonical sets)**.** We say that $U \subseteq \mathfrak{s}$ for some strip $\mathfrak{s}$ is an *1D canonical set* if $U \neq \emptyset,\, \mathfrak{s}$ and either U is connected (we remark again that two triangles sharing only a vertex are not connected) as in the two left figures below, or $|U|$ is even and U can be decomposed into

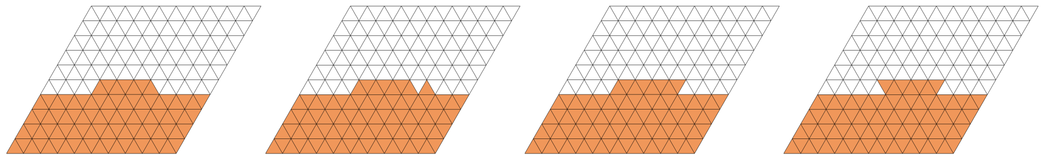
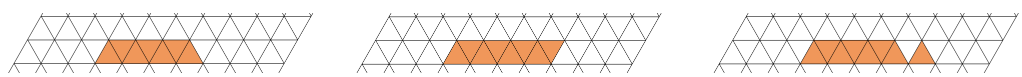


Figure 5.5: Canonical sets and configurations. For the first three figures, the sets of orange triangles are canonical sets between $\mathscr{h}(P)$ and $\mathscr{h}(P')$ where $P = [\![1,\, 4]\!]$ and $P' = [\![1,\, 5]\!]$. If we assign spins a and b at white and orange triangles, respectively, the configurations corresponding to the first, second, and third figures then belong to $\mathcal{C}^{a,\,b}_{\mathscr{h}(P,\,P'),\,o}$, $\mathcal{C}^{a,\,b}_{\mathscr{h}(P,\,P'),\,e}$, and $\mathcal{C}^{a,\,b}_{\mathscr{h}(P,\,P'),\,e}$, respectively. *Note that the set of orange triangles in the rightmost figure is not a canonical set since the condition* (5.27) *is violated.*

two disjoint, connected components U_1 and U_2 such that $|U_2| = 1$ and that U_1 and U_2 share a vertex in Λ^* as in the rightmost figure below.



We now define the general canonical sets.

Definition 5.4.4 (Canonical sets)**.** Fix $a,\, b \in \Omega$, $\mathscr{s} \in \{\mathscr{h},\, \mathscr{v},\, \mathscr{d}\}$, and $P,\, P' \in \mathfrak{S}_L$ such that $P \prec P'$. Let $P' \setminus P = \{\ell\}$. We now define the canonical sets between $\mathscr{s}(P)$ and $\mathscr{s}(P')$. We refer to Figure 5.5.

(1) A set $\mathfrak{p} \subseteq \mathscr{s}_\ell$ is called a *protuberance* attached to $\mathscr{s}(P)$ if $\mathfrak{p}$ is an 1D canonical set. Moreover, for $|P| \in [\![1,\, L-2]\!]$, it holds that

$$\big|\{x \in \mathfrak{p} : x \text{ shares a side with some } y \in \mathscr{s}(P)\}\big| \geq \frac{|\mathfrak{p}|}{2}. \tag{5.27}$$

(2) The set $\mathscr{s}(P) \cup \mathfrak{p}$, where $\mathfrak{p}$ is a protuberance attached to $\mathscr{s}(P)$, is called a *canonical set* between $\mathscr{s}(P)$ and $\mathscr{s}(P')$.

We are now finally able to define the canonical configurations. In the following definition, the letters o and e in the subscripts denote *odd* and *even*, respectively.

Definition 5.4.5 (Canonical configurations)**.** We define the canonical configurations (we refer to Figure 5.5 for an illustrations).

(1) Fix $a,\, b\in\Omega$, $\mathscr{s}\in\{\mathscr{h},\, \mathscr{v},\, \mathscr{d}\}$ and $P,\, P'\in\mathfrak{S}_L$ with $P\prec P'$. We say that a configuration $\sigma\in\mathcal{X}$ is a canonical configuration between two regular configurations $\xi^{a,\,b}_{\mathscr{s}(P)}$ and $\xi^{a,\,b}_{\mathscr{s}(P')}$ if

$$\sigma=\xi^{a,\,b}_{A}\ \text{for some canonical set } A \text{ between } \mathscr{s}(P) \text{ and } \mathscr{s}(P').$$

We denote by $\widetilde{\mathcal{C}}^{a,\,b}_{\mathscr{s}(P,\,P')}$ the collection of canonical configurations between $\xi^{a,\,b}_{\mathscr{s}(P)}$ and $\xi^{a,\,b}_{\mathscr{s}(P')}$.

(a) For each $\sigma=\xi^{a,\,b}_{A}\in\widetilde{\mathcal{C}}^{a,\,b}_{\mathscr{s}(P,\,P')}$, we can decompose A into $\mathscr{s}(P)$ and the protuberance attached to it (cf. Definition 5.4.4). We denote this protuberance as $\mathfrak{p}^{a,\,b}(\sigma)$[4].

(b) We write

$$\begin{aligned}
\mathcal{C}^{a,\,b}_{\mathscr{s}(P,\,P')}&=\widetilde{\mathcal{C}}^{a,\,b}_{\mathscr{s}(P,\,P')}\cup\big\{\xi^{a,\,b}_{\mathscr{s}(P)},\,\xi^{a,\,b}_{\mathscr{s}(P')}\big\},\\
\mathcal{C}^{a,\,b}_{\mathscr{s}(P,\,P'),\,o}&=\big\{\sigma\in\widetilde{\mathcal{C}}^{a,\,b}_{\mathscr{s}(P,\,P')}:|\mathfrak{p}^{a,\,b}(\sigma)|\text{ is odd}\big\},\\
\mathcal{C}^{a,\,b}_{\mathscr{s}(P,\,P'),\,e}&=\big\{\sigma\in\widetilde{\mathcal{C}}^{a,\,b}_{\mathscr{s}(P,\,P')}:|\mathfrak{p}^{a,\,b}(\sigma)|\text{ is even}\big\}.
\end{aligned}$$

(2) For $n\in[\![0,\,L-1]\!]$ and $a,\,b\in\Omega$, we define

$$\mathcal{C}^{a,\,b}_{n}=\bigcup_{\mathscr{s}\in\{\mathscr{h},\,\mathscr{v},\,\mathscr{d}\}}\ \bigcup_{P\prec P':\,|P|=n}\mathcal{C}^{a,\,b}_{\mathscr{s}(P,\,P')},$$

and define $\mathcal{C}^{a,\,b}_{n,\,o}$ and $\mathcal{C}^{a,\,b}_{n,\,e}$ in the same manner. The configurations belonging to $\mathcal{C}^{a,\,b}_{n}$ for some $n\in[\![0,\,L-1]\!]$ are called *canonical configurations* between $\boldsymbol{a}$ and $\boldsymbol{b}$.

[4]Note that if $\sigma\in\widetilde{\mathcal{C}}^{a,\,b}_{\mathscr{s}(P,\,P')}$, then we also have $\sigma\in\widetilde{\mathcal{C}}^{b,\,a}_{\mathscr{s}(\mathbb{T}_L\setminus P',\,\mathbb{T}_L\setminus P)}$ and moreover $\mathfrak{p}^{b,\,a}(\sigma)=\mathscr{s}_\ell\setminus\mathfrak{p}^{a,\,b}(\sigma)$.

(3) For each proper partition $(A,\, B)$, we write

$$\mathcal{C}_{n,\,o}^{A,\,B} = \bigcup_{a\in A}\bigcup_{b\in B}\mathcal{C}_{n,\,o}^{a,\,b} \quad \text{and} \quad \mathcal{C}_{n,\,e}^{A,\,B} = \bigcup_{a\in A}\bigcup_{b\in B}\mathcal{C}_{n,\,e}^{a,\,b}.$$

Remark 5.4.6 (Energy of canonical configurations). The following properties of regular and canonical configurations are straightforward from the definitions. We omit the detail of the proof. Let $a,\, b \in \Omega$.

(1) For $n \in [\![1,\, L-2]\!]$, we can decompose

$$\mathcal{C}_n^{a,\,b} = \mathcal{R}_n^{a,\,b} \cup \mathcal{R}_{n+1}^{a,\,b} \cup \mathcal{C}_{n,\,o}^{a,\,b} \cup \mathcal{C}_{n,\,e}^{a,\,b}$$

and we have

$$H(\sigma) = \begin{cases} 2L & \text{if } \sigma \in \mathcal{R}_n^{a,\,b} \cup \mathcal{R}_{n+1}^{a,\,b}, \\ 2L+1 & \text{if } \sigma \in \mathcal{C}_{n,\,o}^{a,\,b}, \\ 2L+2 & \text{if } \sigma \in \mathcal{C}_{n,\,e}^{a,\,b}. \end{cases}$$

(2) If $\sigma \in \mathcal{C}_n^{a,\,b}$ for $n = 0$ or $L-1$, we have $H(\sigma) \le 2L+1$.

In conclusion, we have $H(\sigma) \le 2L+2$ for all canonical configurations σ.

Remark 5.4.7 (Canonical paths). Fix $a,\, b \in \Omega$, $\mathscr{s} \in \{\mathscr{h},\, \mathscr{v},\, \mathscr{d}\}$, and $P,\, P' \in \mathfrak{S}_L$ with $P \prec P'$. Then, it is clear by definition that there are natural paths in $\mathcal{C}_{\mathscr{s}(P,\,P')}^{a,\,b}$ from $\xi_{\mathscr{s}(P)}^{a,\,b}$ to $\xi_{\mathscr{s}(P')}^{a,\,b}$ as in the following figure.
These paths are called *canonical paths* between $\xi_{\mathscr{s}(P)}^{a,\,b}$ and $\xi_{\mathscr{s}(P')}^{a,\,b}$. By attaching the canonical paths consecutively, one can obtain a path between $\boldsymbol{a}$ and $\boldsymbol{b}$. This path is called a *canonical path* between $\boldsymbol{a}$ and $\boldsymbol{b}$. Note that there are numerous possible canonical paths between $\boldsymbol{a}$ and $\boldsymbol{b}$, and that each canonical path is a $(2L{+}2)$-path (cf. Notation 3.4.4) by Remark 5.4.6 above. See Figure 5.7 for an illustration of the energy level of a canonical path.

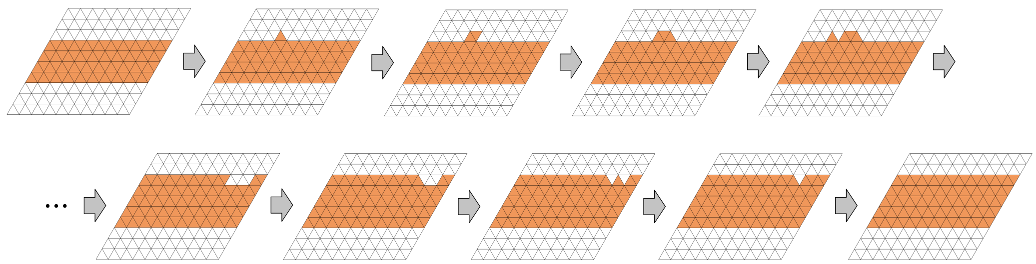


Figure 5.6: Canonical path from $\xi^{a,b}_{\mathfrak{h}(\llbracket 4,7 \rrbracket)}$ to $\xi^{a,b}_{\mathfrak{h}(\llbracket 4,8 \rrbracket)}$.

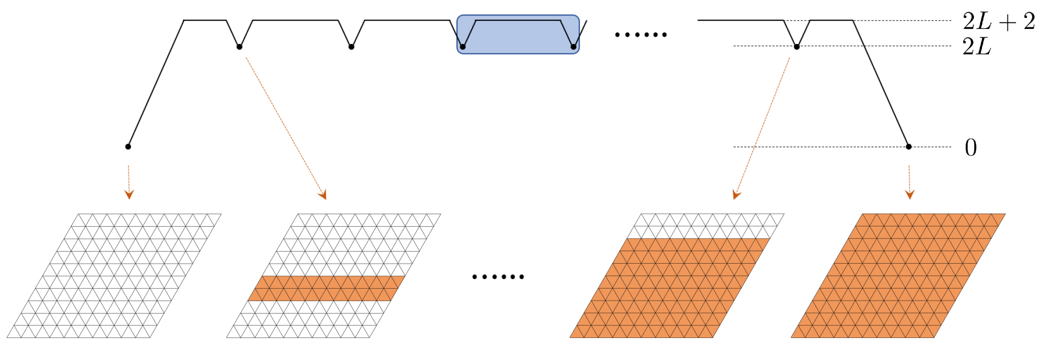


Figure 5.7: Description of the energy level of canonical paths. The transitions given in Figure 5.6 serve as an example for the blue region of the energy graph.

5.4.2 Configurations with low energy

Since the energy barrier between ground states is $2L+2$ (as will be proved in this section), the saddle structure between ground states is essentially the $\widehat{\mathcal{N}}$-neighborhood (cf. Definition 3.4.2) of canonical configurations. Therefore, to understand the saddle structure, it is crucial to characterize the configurations with energy exactly $2L+2$. This characterization is relatively simple for the square lattice (cf. Proposition 3.9.3 and Lemma 3.9.5), as dead-ends are attached only at the very end of the canonical paths. However, this characterization is highly non-trivial for the hexagonal lattice, as we shall see that a complicated dead-end structure is attached at each regular configuration. This and the next subsections are devoted to the study of this structure.

A configuration σ is called *cross-free* if it does not have a cross (cf. Definition 5.3.1-(3)). The purpose of the current subsection is to characterize all the cross-free configurations σ such that $H(\sigma) \le 2L+2$. First, we prove that a cross-free configuration σ has energy of at least $2L$ and moreover that the energy is exactly $2L$ if and only if σ is a regular configuration (cf. Definition 5.4.2).

Proposition 5.4.8. *Suppose that a cross-free configuration $\sigma \in \mathcal{X}$ satisfies $H(\sigma) \le 2L$. Then, σ is a regular configuration; i.e., $\sigma \in \mathcal{R}_n^{a,b}$ for some $a, b \in \Omega$ and $n \in [\![1, L-1]\!]$. In particular, we have $H(\sigma) = 2L$.*

Proof. We fix a cross-free configuration $\sigma \in \mathcal{X}$ with $H(\sigma) \le 2L$. By Lemma 5.3.3, σ has at least L bridges. Since these bridges must be of the same direction, there are exactly L bridges of the same direction (say, horizontal), and by the second assertion of Lemma 5.3.3, all the vertical and diagonal strips must be semibridges of the same form. We can conclude that σ is a regular configuration by combining the observations above. □

It now remains to characterize cross-free configurations with energy $2L+1$ or $2L+2$. The following lemma is useful for these characterizations.

Lemma 5.4.9. *Suppose that a cross-free configuration $\sigma \in \mathcal{X}$ satisfies $H(\sigma) \leq 2L+2$, has $k \in \{L-2,\, L-1\}$ horizontal bridges, and has at least one vertical or diagonal semibridge. Then, the following statements hold for the configuration σ.*

(1) There exist two spins $a,\, b \in \Omega$ such that all horizontal bridges are either a- or b-bridges.

(2) Following (1), define two sets P_a and P_b by

$$P_c = \{\ell \in \mathbb{T}_L : \hbar_\ell \text{ is a } c\text{-bridge}\};\ c \in \{a,\, b\}. \tag{5.28}$$

Suppose that $P_a,\, P_b \neq \emptyset$. Then, we have $P_a,\, P_b \in \mathfrak{S}_L$ and moreover

(a) if $k = L-2$, then all non-bridge strips are $\{a,\, b\}$-semibridges and $H(\sigma) = 2L+2$,

(b) if $k = L-1$ and $H(\sigma) \leq 2L+1$, then all non-bridge strips are $\{a,\, b\}$-semibridges.

Remark 5.4.10. The conclusion $P_a,\, P_b \in \mathfrak{S}_L$ holds even when either P_a or P_b is empty, but its proof will be given later in Lemma 5.4.15.

Proof of Lemma 5.4.9. (1) The conclusion is immediate since if the vertical or diagonal semibridge of σ (which exists given the assumption of the lemma) is an $\{a,\, b\}$-semibridge for some $a,\, b \in \Omega$, then each horizontal bridge must be either an a- or a b-bridge.

(2) Suppose first that no a-bridge is adjacent to a b-bridge. Then as $P_a,\, P_b \neq \emptyset$ and $k \leq L-1$, we may take one connected subset C_a of P_a so that $|C_a| \leq L-2$. Then, the two strips adjacent to C_a must not be b-bridges, so that they are not bridges. Then since $k \geq L-2$, we conclude that $C_a = P_a$ and all the strips which are not adjacent to C_a are b-bridges. This implies that $P_a,\, P_b \in \mathfrak{S}_L$.

Next, suppose that some a-bridge is adjacent to a b-bridge. Without loss of generality, we assume that $1 \in P_a$ and $L \in P_b$. Let $m = \max\{i \in [\![1,\, L-1]\!] :$

$i \in P_a\}$ and we claim that $P_a = [\![1,\, m]\!]$. There is nothing to prove if $m = 1$ or 2, since the claim holds immediately. Suppose $m \geq 3$ and there exists $i \in [\![2,\, m-1]\!]$ such that $i \notin P_a$. Then, there exists a triangle in the i-th horizontal strip at which the spin is not a. The vertical and diagonal strips containing this triangle have energy at least 4, because $1 \in P_a$, $m \in P_a$, and $L \in P_b$. All the vertical and diagonal strips other than these two have energy at least 2 (since the configuration σ is cross-free). Since at least one of the horizontal strip must be a non-bridge and has energy at least 2, we can conclude from (5.25) that

$$H(\sigma) \geq \frac{1}{2}\big[2 + [4 + 2(L-1)] + [4 + 2(L-1)]\big] = 2L + 3.$$

This yield a contradiction and thus we can conclude that $P_a = [\![1,\, m]\!] \in \mathfrak{S}_L$. The proof of $P_b \in \mathfrak{S}_L$ is the same.

(2-a) For this case, we first note that there are $L-2$ bridges. If $H(\sigma) \leq 2L+1$, by Lemma 5.3.3, there are at least $3L - H(\sigma) \geq L-1$ bridges and we get a contradiction. Hence, we have $H(\sigma) = 2L+2$ and there are $3L - H(\sigma)$ bridges; hence, by the second assertion of Lemma 5.3.3 all the non-bridge strips are semibridges. It is clear that indeed, they must be $\{a,\, b\}$-semibridges.

(2-b) The proof for this part is almost identical to (2-a) and we omit the detail. □

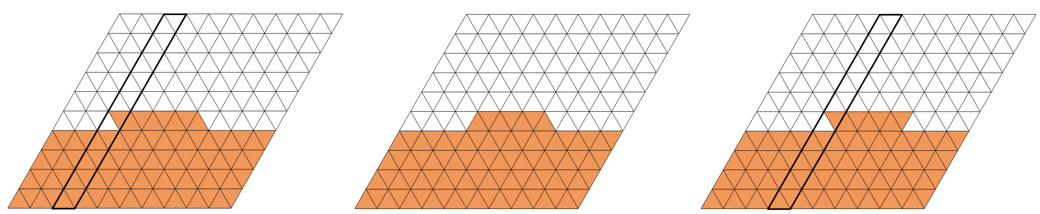
Next, we characterize all of the cross-free configurations with energy $2L+1$. Indeed, they must be canonical configurations.

Proposition 5.4.11. *Suppose that a cross-free configuration $\sigma \in \mathcal{X}$ satisfies $H(\sigma) = 2L + 1$. Then, $\sigma \in \mathcal{C}_{n,o}^{a,\,b}$ for some $a,\, b \in \Omega$ and $n \in [\![0,\, L-1]\!]$. Moreover, if $n = 0$ (resp. $n = L-1$), then $|\mathfrak{p}^{a,\,b}(\sigma)| = 2L-1$ (resp. $|\mathfrak{p}^{a,\,b}(\sigma)| = 1$).*

Proof. By Lemma 5.3.3, the configuration σ has at least $L-1$ bridges. Since σ is cross-free, these bridges are of the same direction, say horizontal. If there are L horizontal bridges, then all the vertical and diagonal strips are of the same form and thus the energy of σ should be a multiple of L in view of (5.25). It contradicts $H(\sigma) = 2L + 1$, and hence there are exactly $L - 1 = 3L - H(\sigma)$ bridges. By the second assertion of Lemma 5.3.3, *all the non-bridge strips are semibridges.* At this point, by Lemma 5.4.9, there exist $a, b \in \Omega$ such that all the horizontal bridges are either a- or b-bridges. Define P_a and P_b as in Lemma 5.4.9 and write $\{\ell\} = \mathbb{T}_L \setminus (P_a \cup P_b)$.

Suppose first that either P_a or P_b is empty, say $P_b = \emptyset$ and $P_a = \mathbb{T}_L \setminus \{\ell\}$. Then as all strips are either bridges or semibridges, we conclude that $\hbar_\ell$ is an $\{a, c\}$-semibridge for some $c \neq a$. As σ is cross-free, we must have $|\mathfrak{p}^{a,c}(\sigma)| = 2L - 1$. The other case $P_a = \emptyset$ can be handled identically.

Next, suppose that $P_a, P_b \neq \emptyset$ so that we can apply case (2-b) of Lemma 5.4.9, which implies that $\hbar_\ell$ is an $\{a, b\}$-semibridge. As illustrated in the figure below, since all the vertical and diagonal strips are semibridge, we can deduce that the set of triangles in $\hbar_\ell$ with spin b should be an odd protuberance (cf. Definition 5.4.5) between $\xi^{a,b}_{\hbar(P)}$ and $\xi^{a,b}_{\hbar(P')}$. Note that for the other cases, a vertical strip with a black bold boundary is not a semibridge.



Therefore, we can conclude that $\sigma \in \mathcal{C}^{a,b}_{n,o}$ for some $n \in [\![1, L-2]\!]$. $\square$

Now, it remains to characterize the cross-free configurations with energy $2L+2$. To this end, we introduce six different types of cross-free configurations with energy $2L + 2$ in the following definition.

Definition 5.4.12 (Cross-free configurations with energy $2L + 2$)**.** The following types characterize the cross-free configurations with energy $2L + 2$. We refer to Figure 5.8 below for illustrations and to (5.25) for the verification of the fact that these configurations (except **(MB)**) have energy $2L + 2$.

- **(ODP)** One-sided Double Protuberances: two odd protuberances are attached to one side of a regular configuration.
- **(TDP)** Two-sided Double Protuberances: two odd protuberances are attached to different sides of a regular configuration.
- **(SP)** Superimposed Protuberances: an odd protuberance is attached to a regular configuration, and another smaller odd protuberance is attached to the first odd protuberance.
- **(EP)** Even Protuberance: an even protuberance is attached to a regular configuration.
- **(PP)** Peculiar Protuberance: a protuberance of a third spin and of size 1 is attached to a regular configuration.
- **(MB)** Monochromatic Bridges: all bridges are parallel and of the same spin, where more refined characterization of this type will be given in Lemma 5.4.15.

Now, we are finally ready to characterize cross-free configurations with energy $2L+2$.

Proposition 5.4.13. *Suppose that a cross-free configuration $\sigma \in \mathcal{X}$ satisfies $H(\sigma) = 2L+2$. Then, σ is of one of the six types introduced in Definition 5.4.12.*

Proof. By Lemma 5.3.3, σ has at least $L-2$ bridges. Since σ is cross-free, these bridges are of the same direction, say horizontal. Then, as in the proof of Proposition 5.4.11, we can observe that the number of horizontal bridges cannot be L and thus the number of horizontal bridges should be either $L-1$ or $L-2$.

(Case 1: σ has $L-1$ horizontal bridges) If there is no vertical or diagonal semibridge, we must have $\Delta H_{\mathfrak{v}_\ell}(\sigma)$, $\Delta H_{\mathfrak{d}_\ell}(\sigma) \geq 3$ for all $\ell \in \mathbb{T}_L$ and therefore

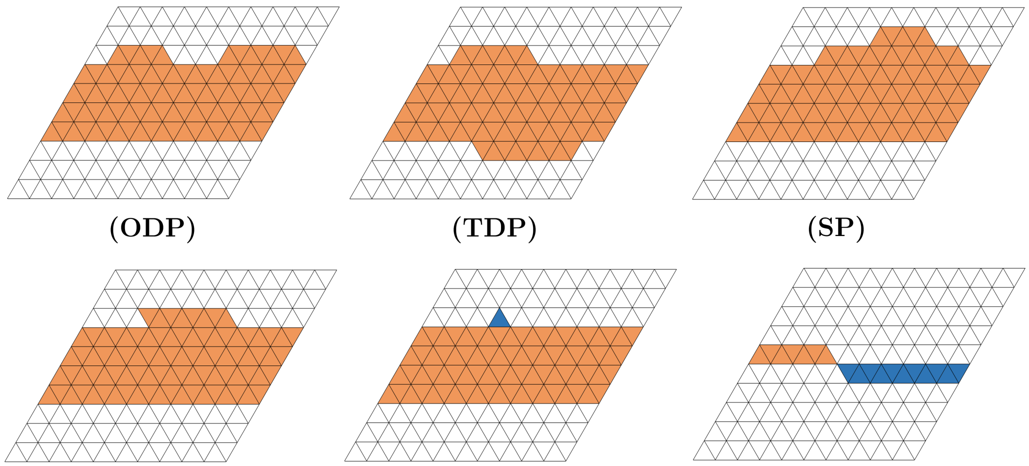


Figure 5.8: Six types of cross-free configurations with energy $2L+2$ introduced in Definition 5.4.12. We refer to Figures 5.9 and 5.10 for more refined characterizations of type **(MB)**.

by (5.25), we get $H(\sigma) \geq 3L$ which yields a contradiction. Hence, there exists at least one vertical or diagonal semibridge and thus by Lemma 5.4.9, there exist $a,\, b \in \Omega$ such that all the horizontal bridges are a- or b-bridges. Let us define P_a and P_b as in Lemma 5.4.9 and let $\{\ell_0\} = \mathbb{T}_L \setminus (P_a \cup P_b)$. If $P_a = \emptyset$ or $P_b = \emptyset$, then σ is of type **(MB)** by definition. Now, we assume that $P_a,\, P_b \neq \emptyset$.

Case 1-1: The strip $\hbar_{\ell_0}$ contains a triangle with a spin which is not a or b. If there are two or more such triangles, then there are at least three vertical or diagonal strips containing these triangles with energy at least 3. Since all the other vertical and diagonal strips have energy at least 2, we can conclude from (5.25) that

$$H(\sigma) \geq \frac{1}{2}\big[2 + 3 \times 3 + (2L-3) \times 2\big] > 2L+2$$

which yields a contradiction. Therefore, the strip $\hbar_{\ell_0}$ contains *exactly one* *triangle* with spin which is not a or b. The vertical and diagonal strips containing this triangle have energy at least 3. Thus, if the strip $\hbar_{\ell_0}$ has energy at least 3, we similarly get a contradiction since we should have

$$H(\sigma) \geq \frac{1}{2}\big[3 + 2 \times 3 + (2L-2) \times 2\big] > 2L + 2.$$

Therefore, the strip $\hbar_{\ell_0}$ has energy 2. This implies that all the triangles in this strip other than the one with spin c have the same spin, which is either a or b. Hence, σ is of type **(PP)**.

Case 1-2: The strip $\hbar_{\ell_0}$ consists of spins a and b only. By (5.25), the energy of this strip is at most 4, and hence is either 2 or 4 (since it cannot be an odd integer). If the energy of this strip is 2, i.e., it is an $\{a,\, b\}$-semibridge by Lemma 5.3.2, we can check with the argument given in the proof of Proposition 5.4.11 based on Figure 5.8 that the only possible form of configuration σ is of type **(EP)**. On the other hand, if the energy of this strip is 4, then in view of (5.25), all the vertical and diagonal bridges must have energy 2 and thus must be semibridges. Since this strip $\hbar_{\ell_0}$ of energy 4 is divided into four connected components where two of them are of spin a and the remaining two are of spin b, by the same argument given in Proposition 5.4.11 based on Figure 5.8, we can readily check that σ is of type **(ODP)**.

(Case 2: σ has $L-2$ horizontal bridges) By the second statement of Lemma 5.3.3, we can still apply Lemma 5.4.9, and we can follow the same argument with **(Case 1)** above to handle the case where P_a or P_b is empty. Hence, let us suppose that $P_a,\, P_b \neq \emptyset$ and write $\mathbb{T}_L \setminus (P_a \cup P_b) = \{\ell_1,\, \ell_2\}$. By (2) of Lemma 5.4.9, we have $P_a,\, P_b \in \mathfrak{S}_L$ and hence we can assume without loss of generality that $P_a = [\![1,\, m]\!]$ so that

$$\{\ell_1,\, \ell_2\} \in \big\{\{L,\, m+1\},\, \{m+1,\, m+2\},\, \{L-1,\, L\}\big\}.$$

Note from (2-a) of Lemma 5.4.9 that

$$\text{all the non-bridge strips of } \sigma \text{ are } \{a,\, b\}\text{-semibridges.} \tag{5.29}$$

If $\{\ell_1,\, \ell_2\} = \{L,\, m+1\}$, by the same argument with Proposition 5.4.11, strips $\hbar_{\ell_1}$ and $\hbar_{\ell_2}$ should be aligned as in the middle one of Figure 5.8 in order to achieve (5.29), and we can conclude that σ is of type **(TDP)**. A similar argument indicates that if $\{\ell_1,\, \ell_2\} = \{m+1,\, m+2\}$ or $\{L-1,\, L\}$, the configuration σ should be of type **(SP)** to fulfill (5.29).

Hence, we demonstrated that for any cases, σ is one of the six types given in Definition 5.4.12. □

Remark 5.4.14. A careful reading of the proof of the previous proposition reveals that, if σ is of type **(MB)** then it has either $L-1$ or $L-2$ parallel bridges.

In the next lemmas, we investigate in more depth configurations of type **(MB)**, since the definition of this type is vague and thus a more detailed understanding is crucially required to analyze the energy landscape of $\mathcal{N}$-neighborhoods of the ground states. In the analyses carried out below, we will omit elementary details in the characterization of possible forms, since these cases are always reduced to a small number of sub-cases that should be tediously checked individually.

Lemma 5.4.15. *Suppose that $\sigma \in \mathcal{X}$ is of type* **(MB)** *with parallel bridges of spin $a \in \Omega$. Then, exactly one between ($\star$) and ($\star\star$) given below holds.*

- ($\star$) *There exists a $(2L+2)$-path $(\omega_n)_{n=0}^{N}$ from σ to $\boldsymbol{a}$ so that $N \le 4L$ and each configuration ω_n has at least $L-2$ a-bridges.*
- ($\star\star$) *The configuration σ is isolated in the sense that $\widehat{\mathcal{N}}(\sigma) = \{\sigma\}$.*

Proof. It is immediate that ($\star$) and ($\star\star$) cannot hold simultaneously. Hence, it suffices to prove that σ satisfies ($\star$) or ($\star\star$). Without loss of generality, we

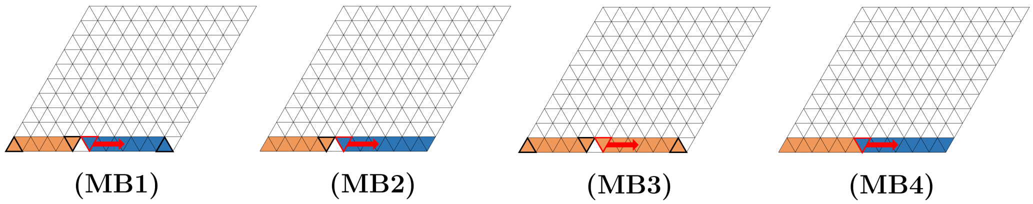


Figure 5.9: Types **(MB1)-(MB4)**: We can update the triangles according to the indicated arrow starting from the one with the red bold boundary to reach $\boldsymbol{a}$. One can change the starting triangle to those with a black bold boundary and then modify the order of updates.

assume that the parallel a-bridges are horizontal, and define P_a as in (5.28) so that we have $|P_a| = L-1$ or $L-2$ by Remark 5.4.14.

(Case 1: $|P_a| = L-1$**)** Without loss of generality, write $\mathbb{T}_L \setminus P_a = \{1\}$. If there are two adjacent triangles in $\hbar_1$ with spin a, we can find an a-cross and therefore we get a contradiction to the fact that σ is cross-free. Hence, the strip $\hbar_1$ cannot have consecutive triangles with spin a. Moreover, since all the vertical and diagonal strips have energy at least 2, by (5.25), we have $\Delta H_{\hbar_1}(\sigma) \le 4$. From this, we can readily deduce that σ should be of one of the four types **(MB1)-(MB4)** as in Figure 5.9.
We now demonstrate that $(\star)$ holds for all these types. For types **(MB1)-(MB3)**, we select any triangle adjacent to a triangle with spin a, and for type **(MB4)**, we select a triangle adjacent to a triangle with different spin. Then, we update the spins in $\hbar_1$ to a successively from the selected triangle to obtain the configuration $\boldsymbol{a}$ (cf. Figure 5.9). This procedure provides a $(2L+2)$-path connecting σ and $\boldsymbol{a}$ of length at most $2L$. It is immediate that all the configurations visited by this path have at least $2L-1$ a-bridges and hence we can verify the condition $(\star)$ for these types.

(Case 2: $|P_a| = L-2$**)** Write $\mathbb{T}_L \setminus P_a = \{\ell_1, \ell_2\}$. By the second statement of Lemma 5.3.3, all the strips which are not bridges must be semibridges. Moreover, if $\hbar_{\ell_i}$ for some $i \in \{1, 2\}$ is a $\{b, c\}$-semibridge for some $b, c \in$

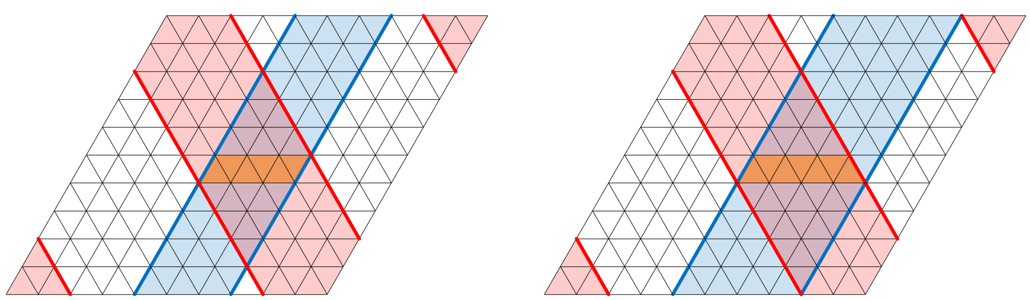
$\Omega\setminus\{a\}$, then we can find a vertical or diagonal strip which is not a semibridge (the one which contains the adjacent triangles of spins b and c in $\hbar_{\ell_i}$) and thus we obtain a contradiction. Therefore, there exist $b_1 \neq a$ and $b_2 \neq a$ so that $\hbar_{\ell_i}$ is an $\{a,\, b_i\}$-semibridge for each $i \in \{1,\, 2\}$. We denote by *b_i-protuberance in $\hbar_{\ell_i}$* the set of triangles in $\hbar_{\ell_i}$ which have spin b_i.

(Claim) *Two strips $\hbar_{\ell_1}$ and $\hbar_{\ell_2}$ are adjacent.*

To prove this claim, suppose the contrary that $\hbar_{\ell_1}$ and $\hbar_{\ell_2}$ are not adjacent. We denote by $m_i \in [\![1,\, 2L-1]\!]$ the number of spins b_i in $\hbar_{\ell_i}$ for $i = 1,\, 2$. Then since each b_i-protuberance in $\hbar_{\ell_i}$ has perimeter $m_i + 2$, we can deduce from (5.5) that $H(\sigma) = (m_1+2)+(m_2+2)$. Since we assumed that $H(\sigma) = 2L+2$, we get

$$m_1 + m_2 = 2L - 2. \tag{5.30}$$

Let us first assume that m_2 is even, as in the figure on the left below (where ℓ_2 is assumed to be 5 and spin b_i is denoted by orange).



Since the vertical strips contained in blue region must be $\{a,\, b_2\}$-semibridges, set A of triangles in strip $\hbar_{\ell_1}$ contained in these blue region should be of spin a. By the same reasoning, the set B of triangles in strip $\hbar_{\ell_1}$ contained in the red region should be of spin a. Since $|A| = m_2$, $|B| = m_2 + 2$, and $|A \cap B| \leq m_2 - 3$ provided that $\hbar_{\ell_1}$ and $\hbar_{\ell_2}$ are not adjacent, we get

$$m_1 \leq |\hbar_{\ell_1}\setminus(A\cup B)| = 2L-|A|-|B|+|A\cap B| \leq 2L-m_2-(m_2+2)+(m_2-3) = 2L-m_2-5.$$

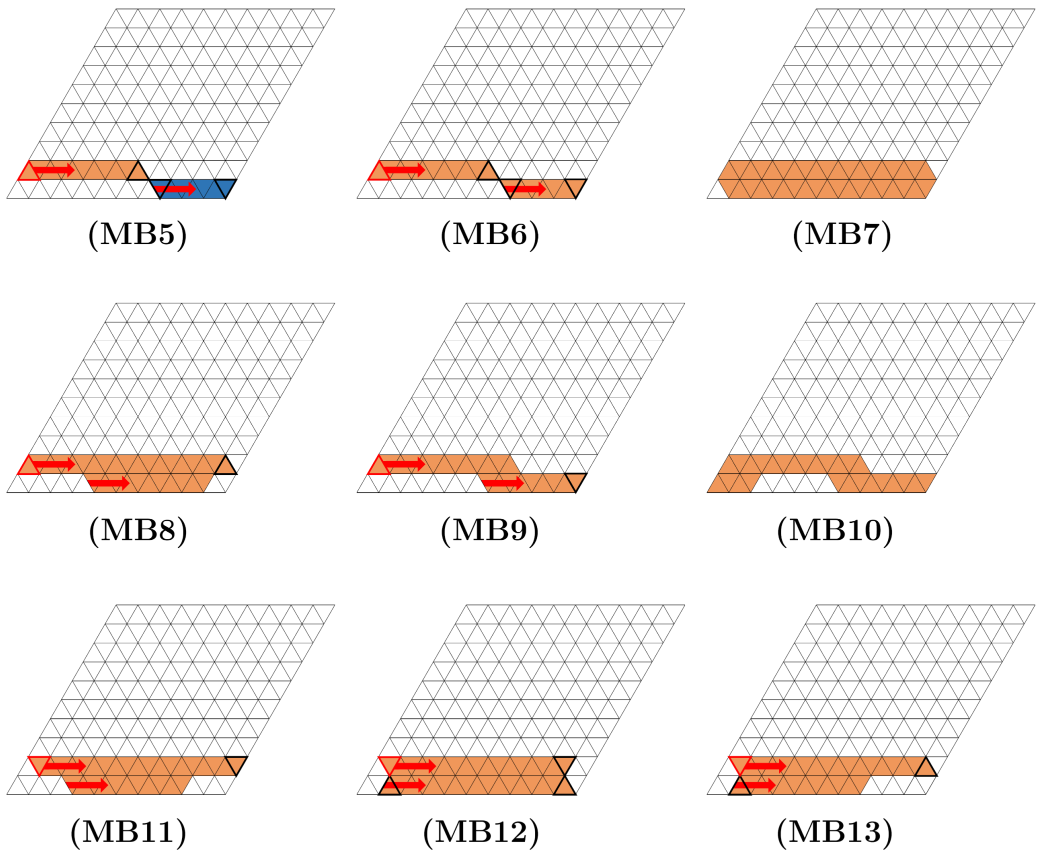


Figure 5.10: Types **(MB5)**-**(MB13)**: We refer to the last part of the proof regarding the explanation of these figures.

This contradicts (5.30). We can handle the case when m_2 is odd as in the figure on the right above in the same manner. In this case, we have $|A| = |B| = m_2 + 1$ and $|A \cap B| \le m_2 - 4$, and we can conclude $m_1 \le 2L - m_2 - 6$ to get a contradiction to (5.30). Thus, the proof is completed.

Thanks to this claim, we can now assume without loss of generality that $\ell_1 = 1$ and $\ell_2 = 2$. We then show that there are nine possible types as in the following figure.

To justify this classification, we first consider the case when $b_1 \ne b_2$. Then, the b_1-protuberance in $\hbar_1$ and the b_2-protuberance in $\hbar_2$ must not be adjacent to each other, since otherwise there exists a vertical or diagonal non-semibridge strip. Since σ is a cross-free configuration, we can readily conclude that σ should be of type **(MB5)**.

Next, we consider the case $b_1 = b_2 = b$ and we assume without loss of generality that the size of the b-protuberance in $\hbar_2$ is not smaller than that in $\hbar_1$. We can then divide the analysis into three sub-cases according to the shape of the b-protuberance in $\hbar_2$:

(1) it has an odd number of triangles and its lower side is longer than its upper side,

(2) it has an odd number of triangles and its upper side is longer than its lower side, or

(3) it has an even number of triangles.

Without loss of generality we assume that the b-protuberance in $\hbar_2$ is located at the leftmost part of the lattice as in Figure 5.10. For case (1), we can observe that the protuberance of b in $\hbar_1$ also has an odd number of triangles and its upper side should be longer than its lower side, since otherwise there will be a non-semibridge strip. According to five different types of locations of this protuberance in the strip $\hbar_1$, we get the types **(MB6)**-**(MB10)**, as illustrated in Figure 5.10. For case (2), we can similarly observe that the protuberance of b in $\hbar_1$ also have odd number of triangles and it should be aligned as in **(MB11)** or **(MB12)**. (In **(MB12)**, the sizes of the b-protuberances of $\hbar_1$ and $\hbar_2$ are identical.) Finally, for case (3), the b-protuberance in $\hbar_1$ should consist of an even number of triangles and should be aligned precisely as in **(MB13)**. (In particular, it must be right-aligned.)

We have now fully characterized the configurations of type **(MB)**, and it only remains to investigate the path-connectivity of types **(MB6)-(MB13)** to the configuration $\boldsymbol{a}$. We consider three cases separately.

- **(MB10)**: Any update in this type of configuration increases the energy. Thus, those of this type satisfy ($\star\star$).

- **(MB7)**: First, we flip a spin a in $\hbar_2$ to spin b, so that we obtain a canonical configuration in $\mathcal{C}_1^{a,b}$ with protuberance size $2L - 1$ (cf. Definition 5.4.5). Then, we can follow a canonical path (cf. Remark 5.4.7) from there to reach the configuration $\boldsymbol{a}$. The path associated with these updates is a $(2L+2)$-path of length $4L$. Moreover, a-bridges in $\hbar(\llbracket 3, L \rrbracket)$ are conserved along the path, and we can conclude that the configurations of this type satisfy $(\star)$.

- **(MB5)**, **(MB6)**, **(MB8)**, **(MB9)**, **(MB11)-(MB13)**: We update spins b to a in the order indicated in Figure 5.10 to obtain the configuration $\boldsymbol{a}$. More precisely, for types **(MB5)**, **(MB6)**, **(MB8)**, and **(MB9)**, we update the triangles according to the indicated arrow starting from the one with red bold boundary to reach $\boldsymbol{a}$. For types **(MB11)-(MB13)**, we first update the triangle with red bold boundary, then update one of the triangles with black bold boundary, and then update the remaining spins b to a according to the arrow to reach $\boldsymbol{a}$. In all the aforementioned types, one can select the starting triangle as the ones with black bold boundary. We remark that for **(MB13)**, if there are same number of orange triangles in $\hbar_1$ and $\hbar_2$, then the black triangle at $\hbar_2$ is no longer available as a starting triangle. For **(MB8)**, the red or black triangle might not be available as a starting triangle if the b-protuberance in $\hbar_1$ is aligned to the right or the left. Then, as in the previous case, we can readily observe that the path associated with these updates satisfies all the requirements in $(\star)$, and thus the configurations of these types satisfy $(\star)$.

This completes the proof. □

We can deduce the following lemma from a careful inspection of the proof of the previous lemma.

Lemma 5.4.16. *Let $\sigma \in \mathcal{X}$ be a configuration of type* **(MB)** *except* **(MB7)** *with parallel bridges of spin $a \in \Omega$, and let $\zeta \in \mathcal{X}$ be a configuration satisfying*

$\sigma \sim \zeta$ such that either $H(\zeta) \le 2L+1$ or ζ has a cross[5]*. Then, there exists a $(2L+1)$-path of length less than $4L$ connecting ζ and $\boldsymbol{a}$. In particular, $\zeta \in \mathcal{N}(\boldsymbol{a})$.*

Proof. We can notice from Figures 5.9 and 5.10 that such a ζ exists only when σ is of type **(MB1)-(MB3)**, **(MB5)**, **(MB6)**, **(MB8)**, **(MB9)**, or **(MB11)-(MB13)**, and moreover ζ is obtained from σ by one of the following ways:

(1) Updating the spin at a triangle highlighted by (either black or red) bold boundary in Figures 5.9 and 5.10 into a.

(2) For type **(MB3)**, ζ can be obtained by flipping spin a at the strip $\hbar_1$ to b. For this case, ζ is a canonical configuration with $2L-1$ triangles of b at a strip.

(3) For type **(MB8)** such that the strip $\hbar_1$ contains only one triangle with spin b, the configuration ζ can additionally obtained by flipping that spin b to spin a. We note that ζ is of the same type as in case (2) above.

For case (1), if ζ is obtained from σ by flipping the spin at a triangle with red boundary, then we can continue to update according to the order indicated in the figure to reach $\boldsymbol{a}$. Then, the path corresponding to the sequence of updates provides a $(2L+1)$-path of length less than $4L$ connecting ζ and $\boldsymbol{a}$. The case when ζ is obtained from σ by flipping a spin at a triangle with black boundary can be handled in a similar way. For cases (2) and (3), since ζ is a canonical configuration, it is connected to $\boldsymbol{a}$ via a canonical path (cf. Remark 5.4.7) which is a $(2L+1)$-path of length $2L-1$. □

Remark 5.4.17. If we consider the Ising case, then type **(PP)** is unavailable and also the analysis of type **(MB)** becomes much simpler.

[5] In fact, if ζ has a cross, then we can prove that $H(\zeta) \le 2L+1$.

As a byproduct of the characterization carried out in the current section, we derive a rough bound on the number of cross-free configurations which will be required in subsequent computations. For sequence $(a_L)_{L=1}^{\infty}$, we write $a_L = O(f(L))$ if there exists a constant $C > 0$ such that $|a_L| \leq Cf(L)$ for all L.

Lemma 5.4.18. *The number of cross-free configuration with energy less than or equal to* $2L + 2$ *is* $O(L^6)$.

Proof. Since we obtain a full characterization of cross-free configurations in Propositions 5.4.8, 5.4.11, and 5.4.13, the conclusion of the lemma follows directly from elementary counting. □

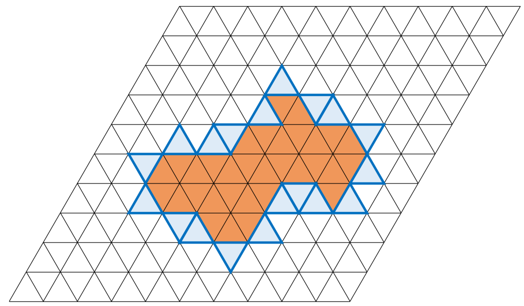
5.4.3 Dead-ends

In this subsection, we summarize the geometry of the energy landscape near canonical configurations. As a consequence, we are able to obtain the full characterization of dead-ends (cf. Definition 5.4.22) encountered by the process during the transitions between ground states.

First, we first introduce some notation.

- For configuration $\sigma \in \mathcal{X}$ and $c \in \Omega$, we say that a subset C of Λ^* is a c-cluster if it is a monochromatic cluster consisting of spin c.

- The *boundary* of a set $A \subseteq \Lambda^*$ refers to the collection of triangles in $\Lambda^* \setminus A$ adjacent to triangles in A. An example is given by the following figure; if A is the collection of orange triangles, the blue triangles are the boundary of A.



- For a configuration $\sigma \in \mathcal{X}$, we say that a triangle $x \in \Lambda^*$ is a boundary triangle of σ if x belongs to a boundary of a certain cluster of σ. Since a non-boundary triangle x of σ has the same spin with its three adjacent triangles, we can observe that

  $$\text{flipping the spin at a non-boundary triangle } x \text{ of } \sigma \text{ increases the energy by 3,} \tag{5.31}$$

  while flipping the spin at a boundary triangle increases the energy by at most 2 (or decreases the energy by as much as 3).

- Let $\sigma \in \mathcal{X}$ be a configuration satisfying $H(\sigma) \leq 2L + 2$. If $\zeta \in \mathcal{X}$ is obtained by a flip of the spin of σ (i.e., $\sigma \sim \zeta$) and $H(\zeta) \leq 2L + 2$, we write $\sigma \approx \zeta$ and the corresponding flip is called a *good flip*.

We now characterize all the configurations connected to a canonical configuration σ and having energy at most $2L + 2$. We decompose our investigation into three cases: $\sigma \in \mathcal{R}_n^{a,\,b}$ (Lemma 5.4.19), $\sigma \in \mathcal{C}_{n,\,o}^{a,\,b}$ (Lemma 5.4.20), and $\sigma \in \mathcal{C}_{n,\,e}^{a,\,b}$ (Lemma 5.4.21). To that end, we define the following collections for $a,\, b \in \Omega$.

- $\mathcal{P}_n^{a,\,b}$, $n \in [\![2,\, L-2]\!]$: the collection of configurations of type **(PP)** which can be obtained by a good flip of a configuration in $\mathcal{R}_n^{a,\,b}$.

- $\mathcal{Q}_n^{a,\,b}$, $n \in [\![1,\, L-2]\!]$: the collection of configurations of type **(ODP)**, **(TDP)**, or **(SP)** which can be obtained by a good flip of a configuration in $\mathcal{C}_{n,\,o}^{a,\,b}$.

- $\widehat{\mathcal{R}}_n^{a,\,b}$, $n \in [\![2,\, L-2]\!]$: the collection of configurations ζ such that

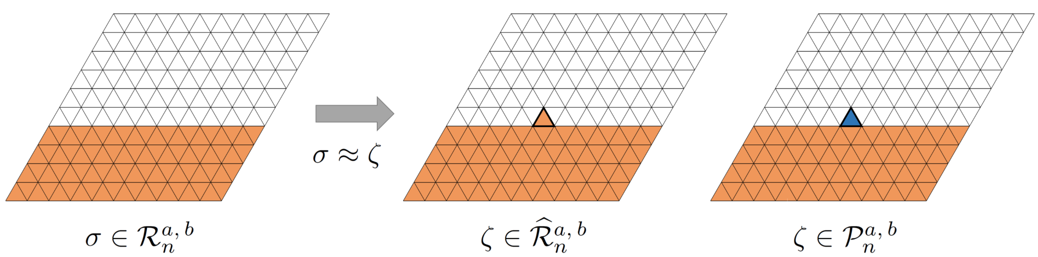
  $$\text{either } \zeta \in \mathcal{C}_{n,\,o}^{a,\,b} \text{ with } |\mathfrak{p}^{a,\,b}(\zeta)| = 1, \ \text{ or } \zeta \in \mathcal{C}_{n-1,\,o}^{a,\,b} \text{ with } |\mathfrak{p}^{a,\,b}(\zeta)| = 2L-1.$$

  Namely, $\widehat{\mathcal{R}}_n^{a,\,b}$ is the collection of canonical configurations obtained by a good flip of a regular configuration in $\mathcal{R}_n^{a,\,b}$.

We now start the characterization. We fix $a,\, b \in \Omega$ in the remainder of the current section.

Lemma 5.4.19. *Suppose that $\sigma \in \mathcal{R}_n^{a,\,b}$ with $n \in [\![2,\, L-2]\!]$ and $\zeta \in \mathcal{X}$ satisfies $\sigma \approx \zeta$. Then, we have either $\zeta \in \widehat{\mathcal{R}}_n^{a,\,b}$ or $\zeta \in \mathcal{P}_n^{a,\,b}$. In particular, we have $\widehat{\mathcal{R}}_n^{a,\,b} = \mathcal{N}(\mathcal{R}_n^{a,\,b}) \setminus \mathcal{R}_n^{a,\,b}$.*

Proof. Let us fix $\sigma \in \mathcal{R}_n^{a,\,b}$. Since $H(\sigma) = 2L$ and $H(\zeta) \le 2L+2$, by (5.31), the configuration ζ is obtained from σ by flipping a boundary triangle. First, we assume that we flip a spin at a boundary triangle of the b-cluster of σ (which has spin a) to c to get ζ. As one can check from the figure below, we get $\zeta \in \widehat{\mathcal{R}}_n^{a,\,b}$ (in particular, $\zeta \in \mathcal{C}_{n,\,o}^{a,\,b}$ with $|\mathfrak{p}^{a,\,b}(\zeta)| = 1$) or $\zeta \in \mathcal{P}_n^{a,\,b}$ if $c = a$ or $c \notin \{a,\, b\}$, respectively.



The case when we flip a boundary triangle of the a-cluster is identical to the previous case and we can conclude the proof of the first statement. For the second statement, first we observe that if $\xi \sim \zeta$ for some $\zeta \in \widehat{\mathcal{R}}_n^{a,\,b}$ and $H(\xi) < 2L+2$, then we must have $\xi \in \mathcal{R}_n^{a,\,b}$. Since the configuration of type **(PP)** has energy $2L+2$, the second assertion of the lemma is direct from the first one. $\square$

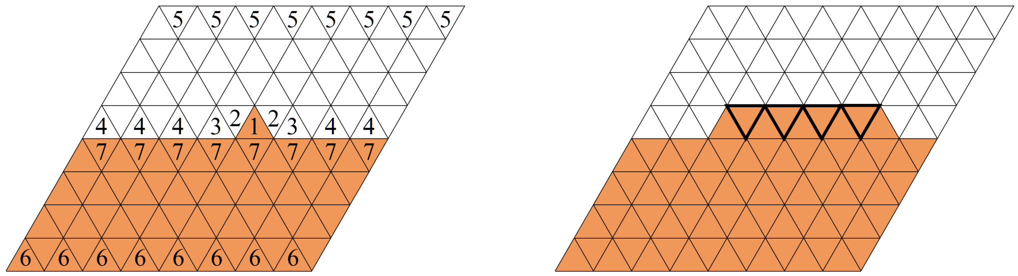


Figure 5.11: Good flip of a configuration in $\mathcal{C}_{n,\,o}^{a,\,b}$. **(Left)** $|\mathfrak{p}^{a,\,b}(\sigma)| = 1$ or $2L-1$. **(Right)** $3 \le |\mathfrak{p}^{a,\,b}(\sigma)| \le 2L-3$.

Thanks to Lemma 5.4.19, we will hereafter discard the notation $\widehat{\mathcal{R}}_n^{a,\,b}$ and use $\mathcal{N}(\mathcal{R}_n^{a,\,b}) \setminus \mathcal{R}_n^{a,\,b}$ instead.

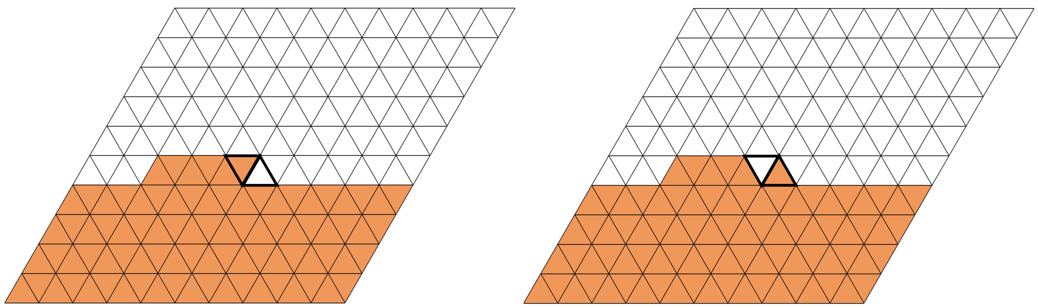
Lemma 5.4.20. *Suppose that $\sigma \in \mathcal{C}_{n,\,o}^{a,\,b}$ with $n \in [\![2,\,L-2]\!]$ and $\zeta \in \mathcal{X}$ satisfies $\sigma \approx \zeta$. Then, we have either $\zeta \in \mathcal{R}_n^{a,\,b} \cup \mathcal{R}_{n+1}^{a,\,b} \cup \mathcal{C}_{n,\,e}^{a,\,b}$, $\zeta \in \mathcal{P}_n^{a,\,b} \cup \mathcal{P}_{n+1}^{a,\,b}$, or $\zeta \in \mathcal{Q}_n^{a,\,b}$. In particular, if $3 \le |\mathfrak{p}^{a,\,b}(\sigma)| \le 2L-3$, we have either $\zeta \in \mathcal{C}_{n,\,e}^{a,\,b}$ or $\zeta \in \mathcal{Q}_n^{a,\,b}$.*

Proof. We fix $\sigma \in \mathcal{C}_{n,\,o}^{a,\,b}$ and first consider the case $|\mathfrak{p}^{a,\,b}(\sigma)| = 1$. By (5.31), we can notice that we must flip a boundary triangle of σ to obtain ζ. We can group the boundary triangles of σ into seven types as in Figure 5.11-(left). If we flip the triangle of type 1, we get $\zeta \in \mathcal{R}_n^{a,\,b}$ or $\zeta \in \mathcal{P}_n^{a,\,b}$. If a flip of the spin of a triangle in types 2-7 is a good flip, the spin must be flipped to either a or b. Hence, we get a configuration in $\mathcal{C}_{n,\,e}^{a,\,b}$ (resp. in $\mathcal{Q}_n^{a,\,b}$) if we flip the spin at a triangle of types 2 or 3 (resp. types 4-7). The case $|\mathfrak{p}^{a,\,b}(\sigma)| = 2L-1$ can be handled in the exact same way with this case and we get either $\zeta \in \mathcal{R}_{n+1}^{a,\,b}$, $\zeta \in \mathcal{P}_{n+1}^{a,\,b}$, $\zeta \in \mathcal{C}_{n,\,e}^{a,\,b}$, or $\zeta \in \mathcal{Q}_n^{a,\,b}$.

Next, we consider the case $3 \le |\mathfrak{p}^{a,\,b}(\sigma)| \le 2L-3$. The proof is similar to the previous case. In particular, the flip of triangles of types 2-7 are of the identical nature. The only difference appears in the flip of a triangle of type 1, i.e., a triangle in the protuberance of spin b. For this case, we have to flip triangle denoted by bold black boundary in Figure 5.11-(right) to get a configuration belonging to $\mathcal{C}_{n,e}^{a,b}$ or $\mathcal{Q}_{n}^{a,b}$. ☐

Lemma 5.4.21. *Suppose that $\sigma \in \mathcal{C}_{n,e}^{a,b}$ with $n \in [\![2, L-2]\!]$ and $\zeta \in \mathcal{X}$ satisfies $\sigma \approx \zeta$. Then, $\zeta \in \mathcal{C}_{n,o}^{a,b}$.*

Proof. There are essentially two cases (depending on whether the protuberance is connected or not) to be considered as in the figure below.



Since the configuration σ already has energy $2L+2$, the good flip must not increase the energy, and therefore should flip the spin at one of the triangles with bold black boundary in the figure above either from a to b or from b to a. Since the configuration obtained from this any of such flips belongs to $\mathcal{C}_{n,o}^{a,b}$, the proof is completed. ☐

The non-canonical configurations appearing in the preceding three lemmas are defined now as the dead-ends.

Definition 5.4.22 (Dead-ends)**.** For $a, b \in \Omega$, define

$$\mathcal{D}^{a,b} = \Big[\bigcup_{n=2}^{L-2} \mathcal{P}_n^{a,b}\Big] \cup \Big[\bigcup_{n=2}^{L-3} \mathcal{Q}_n^{a,b}\Big].$$

It is clear that $\sigma \in \mathcal{D}^{a,b}$ implies $H(\sigma) = 2L+2$. We say that a configuration σ belonging to $\mathcal{D}^{a,b}$ is a *dead-end* between $\boldsymbol{a}$ and $\boldsymbol{b}$. For each proper partition (A, B), we write

$$\mathcal{D}^{A,B} = \bigcup_{a' \in A} \bigcup_{b' \in B} \mathcal{D}^{a',b'}.$$

Next, we perform further investigations of the dead-end configurations, after which we can explain why these configurations are called dead-ends (cf. Remark 5.4.26).

Lemma 5.4.23. *Suppose that* $\sigma \in \mathcal{P}_n^{a,\,b}$ *with* $n \in [\![2,\, L-2]\!]$ *and* $\zeta \in \mathcal{X}$ *satisfies* $\sigma \approx \zeta$*. Then, we have either* $\zeta \in \mathcal{N}(\mathcal{R}_n^{a,\,b})$ *(two choices) or* $\zeta \in \mathcal{P}_n^{a,\,b}$ *(*$q-3$ *choices).*

Proof. A good flip of a configuration $\sigma \in \mathcal{P}_n^{a,\,b}$ must flip the spin at the peculiar protuberance. By flipping this spin to a or b, we obtain a configuration in $\mathcal{N}(\mathcal{R}_n^{a,\,b})$. Otherwise, the result is a configuration in $\mathcal{P}_n^{a,\,b}$, and we are done. □

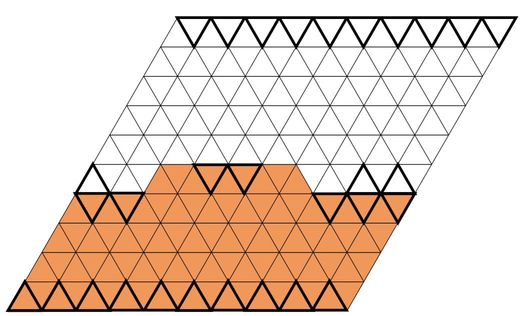
Lemma 5.4.24. *Suppose that* $\sigma \in \mathcal{Q}_n^{a,\,b}$ *with* $n \in [\![2,\, L-3]\!]$ *is obtained from* $\xi \in \mathcal{C}_{n,\,o}^{a,\,b}$ *by flipping a spin. Suppose also that* $\zeta \in \mathcal{X}$ *satisfies* $\sigma \approx \zeta$*.*

(1) If $|\mathfrak{p}^{a,\,b}(\xi)| \neq 1,\, 2L-1$*, we have* $\zeta = \xi$*.*

(2) If $|\mathfrak{p}^{a,\,b}(\xi)| = 1$ *(so that* $\xi \in \mathcal{N}(\mathcal{R}_n^{a,\,b})$*), there are exactly two possible configurations for* ζ*, which are both in* $\mathcal{N}(\mathcal{R}_n^{a,\,b}) \setminus \mathcal{R}_n^{a,\,b}$*.*

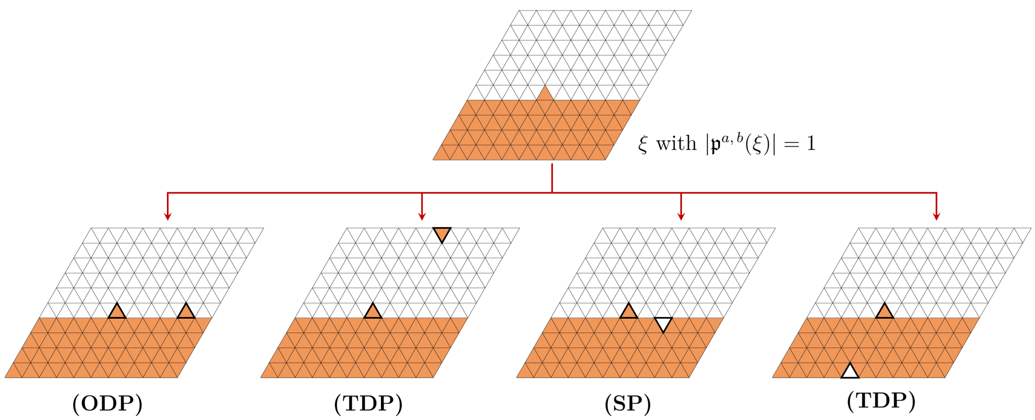
(3) If $|\mathfrak{p}^{a,\,b}(\xi)| = 2L-1$ *(so that* $\xi \in \mathcal{N}(\mathcal{R}_{n+1}^{a,\,b})$*), there are exactly two possible configurations for* ζ*, which are both in* $\mathcal{N}(\mathcal{R}_{n+1}^{a,\,b}) \setminus \mathcal{R}_{n+1}^{a,\,b}$*.*

Proof. If $|\mathfrak{p}^{a,\,b}(\xi)| \neq 1,\, 2L-1$. we can notice from the figure below that σ is obtained from ξ by flipping the spin at one of the triangles with a bold boundary either from a to b or b to a.



Then, it is direct from that a good flip of σ must flip back this updated spin, since otherwise the energy will be further increased to at least $2L+3$. Hence, we obtain $\zeta = \xi$.

Next, we consider the case $|\mathfrak{p}^{a,b}(\xi)| = 1$. Then, as in the figure below, σ should be obtained by adding a protuberance of spin a or b of size one to ξ, and there are four different types.



Therefore, σ has two protuberances of size one denoted by the bold boundary, and a good flip must remove one of them. Thus, there are exactly two possible configurations ζ_1, ζ_2 for ζ and it is immediate that $\zeta_1, \zeta_2 \in \mathcal{N}(\mathcal{R}_n^{a,b}) \setminus \mathcal{R}_n^{a,b}$. The proof for the case $|\mathfrak{p}^{a,b}(\xi)| = 2L-1$ is nearly identical to the case $|\mathfrak{p}^{a,b}(\xi)| = 1$, and we omit the details here. □

Finally, we provide a summary of the preceding results.

Proposition 5.4.25. *Let* $\sigma \in \bigcup_{n=2}^{L-3} \mathcal{C}_n^{a,b}$ *or* $\sigma \in \mathcal{D}^{a,b}$ *and suppose that* $\zeta \in \mathcal{X}$ *satisfies* $\zeta \approx \sigma$. *Then,* ζ *is either a canonical configuration*[6] *or a dead-end in* $\mathcal{D}^{a,b}$.

Proof. This proposition is a direct consequence of Lemmas 5.4.19, 5.4.20, 5.4.21, 5.4.23, and 5.4.24. □

[6]Indeed, we have $\zeta \in [\bigcup_{n=2}^{L-3} \mathcal{C}_n^{a,b}] \cup \mathcal{N}(\mathcal{R}_2^{a,b}) \cup \mathcal{N}(\mathcal{R}_{L-2}^{a,b})$.

Remark 5.4.26. Now, we are able to explain why the configurations in $\mathcal{D}^{a,b}$ are called dead-end configurations. According to the definition of $\mathcal{D}^{a,b}$, a dead-end σ is adjacent to either $\mathcal{N}(\mathcal{R}_n^{a,b})$ for some $n \in [\![2,\, L-2]\!]$ or $\xi \in \mathcal{C}_{n,o}^{a,b}$ such that $|\mathfrak{p}^{a,b}(\xi)| \in [\![3,\, 2L-3]\!]$ for some $n \in [\![2,\, L-3]\!]$. Let $\sigma \approx \zeta$. Then, for the former case, by Lemmas 5.4.23 and 5.4.24-(2)(3), ζ is either another dead-end configuration adjacent to $\mathcal{N}(\mathcal{R}_n^{a,b})$ or a configuration in $\mathcal{N}(\mathcal{R}_n^{a,b})$. Hence, these ones indeed serve as *dead-ends* attached to $\mathcal{N}(\mathcal{R}_n^{a,b})$ (consisting of canonical configurations only according to Lemma 5.4.19). For the latter case, $\zeta = \xi$ by Lemma 5.4.24-(1); therefore, $\{\sigma\}$ is a single *dead-end* attached to the canonical configuration ξ.

5.4.4 Energy barrier

Now, we are ready to prove Theorem 5.1.1. First, we establish the upper bound.

Proposition 5.4.27. *For any $a,\, b \in \Omega$, we have $\Phi(\boldsymbol{a},\, \boldsymbol{b}) \le 2L+2$.*

Proof. Let $P_0 = \emptyset$ and let $P_n = \{1,\, \dots,\, n\} \subseteq \mathbb{T}_L$ for $n \in [\![1,\, L]\!]$ so that $P_0 \prec P_1 \prec \cdots \prec P_L$. Since $\xi_{\hslash(P_0)}^{a,b} = \boldsymbol{a}$ and $\xi_{\hslash(P_L)}^{a,b} = \boldsymbol{b}$, it suffices to show that $\Phi(\xi_{\hslash(P_n)}^{a,b},\, \xi_{\hslash(P_{n+1})}^{a,b}) \le 2L+2$ for all $n \in [\![0,\, L-1]\!]$. This follows from Remark 5.4.7. □

Next, we turn to the matching lower bound which is the crucial part in the proof.

Proposition 5.4.28. *For any $a,\, b \in \Omega$, we have $\Phi(\boldsymbol{a},\, \boldsymbol{b}) \ge 2L+2$.*

Proof. Suppose the contrary so that there exists a $(2L+1)$-path $(\omega_n)_{n=0}^N$ in $\mathcal{X}$ with $\omega_0 = \boldsymbol{a}$, $\omega_N = \boldsymbol{b}$. For each $n \in [\![0,\, N]\!]$, define $u(n)$ as the number of b-bridges in ω_n so that we have $u(0) = 0$ and $u(N) = 3L$. Now, we define

$$n^* = \min\{n \in [\![0,\, N]\!] : u(n) \ge 2\}, \tag{5.32}$$

so that we have a trivial bound $n^* \geq 3$. Notice that a spin flip at a certain triangle can only affect the three strips containing that triangle and hence

$$|u(n+1) - u(n)| \leq 3 \quad \text{for all } n \in [\![0,\, L-1]\!]. \tag{5.33}$$

From this observation, we know that $u(n^*) \in [\![2,\, 4]\!]$. On the other hand, by Lemma 5.3.3, we have at least $3L - (2L+1) = L-1$ bridges, and hence there exists a bridge with a spin that is not b. This implies that ω_{n^*} does not have a cross. Then, we must have $u(n^*) - u(n^*-1) = 1$ and therefore we have $u(n^*) = 2$.

By Propositions 5.4.8 and 5.4.11, we have either $\omega_{n^*} \in \mathcal{R}_2^{a',\,b}$ or $\omega_{n^*} \in \mathcal{C}_{2,\,o}^{a',\,b}$ for some $a' \in \Omega \backslash \{b\}$. If $\omega_{n^*} \in \mathcal{R}_2^{a',\,b}$, then by Lemma 5.4.19 and the minimality assumption of n^*, we must have $\omega_{n^*-1} \in \mathcal{C}_{1,\,o}^{a',\,b}$. Then, since $H(\omega_{n^*-2}) \leq 2L+1$, we can deduce from Lemma 5.4.20 that $\omega_{n^*-2} \in \mathcal{R}_2^{a',\,b}$ which contradicts the minimality of n^* in (5.32). On the other hand, if $\omega_{n^*} \in \mathcal{C}_{2,\,o}^{a',\,b}$, then since $H(\omega_{n^*-1}) \leq 2L+1$, we can infer from Lemma 5.4.20 that $\omega_{n^*-1} \in \mathcal{R}_2^{a',\,b} \cup \mathcal{R}_3^{a',\,b}$, and therefore we again get a contradiction to the minimality of n^*. Since we got a contradiction for both cases, the proof is completed. $\square$

Now, we can conclude the proof of Theorem 5.1.1.

Proof of Theorem 5.1.1. By Propositions 5.4.27 and 5.4.28, it suffices to prove that $\Phi(\sigma,\, \mathcal{S}) - H(\sigma) < 2L+2$ for all $\sigma \notin \mathcal{S}$. The proof of this bound is identical to Lemma 3.9.4 and we refer to the detailed proof therein. $\square$

5.5 Saddle structure

In order to conduct an Eyring–Kramers-type quantitative analysis of metastability, we need a more detailed understanding of the energy landscape. We acquire this in the current section by completely analyzing the saddle structure between the ground states. We remark that the flavor of the discussion given in this section is similar to that in Section 3.4, but the detail is quite different because we are considering the hexagonal lattice with a complicated dead-end structure, and also we are working in the large-volume regime.

5.5.1 Typical configurations

Definition 5.5.1 (Typical configurations)**.** Let $(A,\, B)$ be a proper partition of Ω.

(1) For $a,\, b\in\Omega$, we define the collection of *bulk typical configurations* between $\boldsymbol{a}$ and $\boldsymbol{b}$ as

$$\mathcal{B}^{a,\,b}=\bigcup_{n=2}^{L-3}\mathcal{C}_n^{a,\,b}\cup\mathcal{D}^{a,\,b}. \tag{5.34}$$

Then, we define the collection of bulk configurations between $\mathcal{S}(A)$ and $\mathcal{S}(B)$ as

$$\mathcal{B}^{A,\,B}=\bigcup_{a'\in A}\bigcup_{b'\in B}\mathcal{B}^{a',\,b'}.$$

(2) For $a,\, b\in\Omega$, we write

$$\begin{aligned}\mathcal{B}_\Gamma^{a,\,b}&=\{\sigma\in\mathcal{B}^{a,\,b}:H(\sigma)=\Gamma\}=\bigcup_{n=2}^{L-3}\mathcal{C}_{n,\,e}^{a,\,b}\cup\mathcal{D}^{a,\,b},\\ \mathcal{B}_\Gamma^{A,\,B}&=\{\sigma\in\mathcal{B}^{A,\,B}:H(\sigma)=\Gamma\}=\bigcup_{a'\in A}\bigcup_{b'\in B}\mathcal{B}_\Gamma^{a',\,b'}.\end{aligned}$$

Then, we define (cf. Definition 3.4.2)

$$\mathcal{E}^A=\widehat{\mathcal{N}}\big(\mathcal{S}(A);\,\mathcal{B}_\Gamma^{A,\,B}\big)\quad\text{and}\quad\mathcal{E}^B=\widehat{\mathcal{N}}\big(\mathcal{S}(B);\,\mathcal{B}_\Gamma^{A,\,B}\big). \tag{5.35}$$

The collection of *edge typical configurations* between $\mathcal{S}(A)$ and $\mathcal{S}(B)$ is defined as

$$\mathcal{E}^{A,\,B}=\mathcal{E}^A\cup\mathcal{E}^B.$$

In the remainder of the current section, we fix a proper partition $(A,\, B)$ of Ω.

Remark 5.5.2. In fact, all canonical configurations are indeed typical configurations. To see this, we let $c_1,\, c_2 \in \Omega$ and demonstrate that $\mathcal{C}_n^{c_1,\, c_2} \subseteq \mathcal{B}^{A,\, B} \cup \mathcal{E}^{A,\, B}$ for all $n \in [\![0,\, L-1]\!]$. First, if $c_1,\, c_2 \in A$ or $c_1,\, c_2 \in B$, then by Remark 5.4.7, it is straightforward that $\mathcal{C}_n^{c_1,\, c_2} \subseteq \mathcal{E}^A$ or $\mathcal{C}_n^{c_1,\, c_2} \subseteq \mathcal{E}^B$, respectively. Next, we assume that c_1 and c_2 belong to different sets, say $c_1 \in A$ and $c_2 \in B$. We divide these into two cases.

(1) In the bulk part, for $n \in [\![2,\, L-3]\!]$ we have $\mathcal{C}_n^{c_1,\, c_2} \subseteq \mathcal{B}^{A,\, B}$ which is immediate from the definition (5.34).

(2) Remarks 5.4.6 and 5.4.7 imply that all the canonical configurations in $\mathcal{C}_0^{c_1,\, c_2} \cup \mathcal{C}_1^{c_1,\, c_2}$ are connected by a Γ-path in $\mathcal{C}_0^{c_1,\, c_2} \cup \mathcal{C}_1^{c_1,\, c_2}$ to $\boldsymbol{c_1} \in \mathcal{S}(A)$. As we clearly have $(\mathcal{C}_0^{c_1,\, c_2} \cup \mathcal{C}_1^{c_1,\, c_2}) \cap \mathcal{B}_\Gamma^{A,\, B} = \emptyset$, the definition of $\mathcal{E}^A$ implies that $\mathcal{C}_0^{c_1,\, c_2} \cup \mathcal{C}_1^{c_1,\, c_2} \subseteq \mathcal{E}^A$. Similarly, we have $\mathcal{C}_{L-2}^{c_1,\, c_2} \cup \mathcal{C}_{L-1}^{c_1,\, c_2} \subseteq \mathcal{E}^B$.

Proposition 5.5.3. *The following properties hold.*

(1) We have $\mathcal{E}^A \cap \mathcal{B}^{A,\, B} = \mathcal{N}(\mathcal{R}_2^{A,\, B})$ *and* $\mathcal{E}^B \cap \mathcal{B}^{A,\, B} = \mathcal{N}(\mathcal{R}_{L-2}^{A,\, B})$.

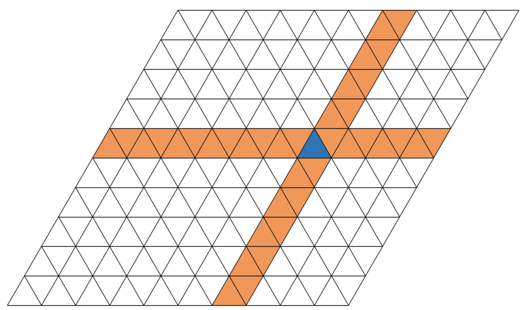
(2) It holds that $\mathcal{E}^{A,\, B} \cup \mathcal{B}^{A,\, B} = \widehat{\mathcal{N}}(\mathcal{S})$.

This proposition explains why we defined the typical configurations as in Definition 5.5.1. In particular, since $\widehat{\mathcal{N}}(\mathcal{S})$ is the collection of all configurations connected to the ground states by a Γ-path, we can observe from part (2) of the previous proposition that the sets $\mathcal{E}^{A,\, B}$ and $\mathcal{B}^{A,\, B}$ are properly defined to explain the saddle structure between $\mathcal{S}(A)$ and $\mathcal{S}(B)$.

The proof of Proposition 5.5.3 is identical to that in Proposition 3.4.17, since the proof therein is robust against the microscopic features of the model. It suffices to replace Lemma 3.9.5 for the square lattice with Lemmas 5.4.19, 5.4.20, and 5.4.21 for the hexagonal lattice. It should also be mentioned that in Proposition 3.4.17, it was asserted that $\mathcal{E}^A \cap \mathcal{B}^{A,\, B} = \mathcal{R}_2^{A,\, B}$ and

$\mathcal{E}^B \cap \mathcal{B}^{A,\,B} = \mathcal{R}_{L-2}^{A,\,B}$ (instead of $\mathcal{N}(\mathcal{R}_2^{A,\,B})$ and $\mathcal{N}(\mathcal{R}_{L-2}^{A,\,B})$) since in that case it holds that $\mathcal{N}(\mathcal{R}_i^{A,\,B}) = \mathcal{R}_i^{A,\,B}$ for all $i \in [\![2,\, L-2]\!]$.

The following proposition is the hexagonal version of Proposition 3.4.17 and asserts that $\mathcal{E}^A$ and $\mathcal{E}^B$ are disjoint. We provide a proof since it is technically more difficult than that of Proposition 3.4.17. A union of two strips of different directions is called a b-*semicross* of $\sigma \in \mathcal{X}$ if all the spins at these two strips are b, except for the one at the intersection, which is not b, as shown in the following figure.



Proposition 5.5.4. *Let $(A,\, B)$ be a proper partition. Each configuration in $\mathcal{E}^A$ does not have a b-cross for all $b \in B$. In particular, it holds that $\mathcal{E}^A \cap \mathcal{E}^B = \emptyset$.*

Proof. Suppose on the contrary that $\sigma \in \mathcal{E}^A$ has a b-cross for some $b \in B$. Then since $\sigma \in \mathcal{E}^A$, we can find a Γ-path $(\omega_n)_{n=0}^N$ in $\mathcal{X} \setminus \mathcal{B}_\Gamma^{A,\,B}$ with $\omega_0 \in \mathcal{S}(A)$ and $\omega_N = \sigma$. For $n \in [\![0,\, N]\!]$, define $u(n)$ as the number of b-bridges in ω_n so that

$$u(0) = 0,\;\; u(N) \geq 2,\;\; \text{and } |u(n+1) - u(n)| \leq 3 \text{ for all } n \in [\![0,\, N-1]\!], \quad (5.36)$$

as in the proof of Proposition 5.4.28. Define

$$n_0 = \max\{n \geq 1 : u(n-1) \leq 1 \text{ and } u(n) \geq 2\}$$

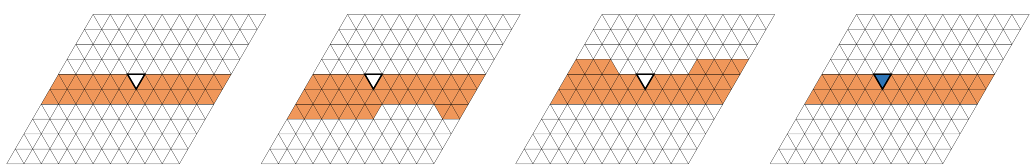
so that, summing up,

$$(\omega_n)_{n=0}^{N} \text{ is a } \Gamma\text{-path in } \mathcal{X} \setminus \mathcal{B}_{\Gamma}^{A,\,B} \quad \text{and} \quad u(n) \geq 2 \text{ for all } n \geq n_0. \tag{5.37}$$

We divide the proof into two cases.

(Case 1: $u(n_0) - u(n_0 - 1) \geq 2$) In this case, a single spin update from ω_{n_0-1} to ω_{n_0} creates at least two b-bridges. This is possible only when we update the triangle at the intersection of a b-semicross to obtain a b-cross. Since $u(n_0 - 1) \in \{0, 1\}$, the configuration ω_{n_0-1} cannot have a b-cross. Moreover, the existence of a b-semicross implies that there is no c-bridge for all $c \in \Omega \setminus \{b\}$. Hence, ω_{n_0-1} has at most one bridge and its energy is at least $3L - 1$ by Lemma 5.3.3. This contradicts the fact that (ω_n) is a Γ-path.

(Case 2: $u(n_0) - u(n_0 - 1) = 1$) Here, we must have $u(n_0 - 1) = 1$ and $u(n_0) = 2$. Since ω_{n_0-1} has exactly one b-bridge, it is cross-free. Moreover, since a single spin update from ω_{n_0-1} to ω_{n_0} should create the second b-bridge, we can apply Propositions 5.4.8, 5.4.11, and 5.4.13 to assert that there are only four possible forms of ω_{n_0-1} as in the figure below.



$\mathcal{N}(\mathcal{R}_2^{a,b}) \setminus \mathcal{R}_2^{a,b}$ **(PP)** **(TDP)** **(SP)**

Note that we have to update the spin at a triangle with bold boundary to b to get ω_{n_0},and hence we have $\omega_{n_0} \in \mathcal{R}_2^{a,\,b} \cup \mathcal{C}_{2,\,o}^{a,\,b}$. Note that ω_{n_0} does not have a b-cross so that $n_0 < N$. Now, we consider four sub-cases.

- $\omega_{n_0} \in \mathcal{R}_2^{a,\,b}$: We can conclude from Lemmas 5.4.19, 5.4.20, 5.4.23, and 5.4.24-(2) along with (5.37) that $\omega_n \in \mathcal{N}(\mathcal{R}_2^{a,\,b})$ for all $n \geq n_0$. This contradicts the fact that ω_N has a b-cross.

- $\omega_{n_0} \in \mathcal{C}_{2,o}^{a,b}$ with $|\mathfrak{p}^{a,b}(\omega_{n_0})| \in [\![3,\, 2L-3]\!]$: Since $\omega_{n_0} \approx \omega_{n_0+1}$, by Lemma 5.4.20, we get $\omega_{n_0+1} \in \mathcal{C}_{2,e}^{a,b} \cup \mathcal{Q}_2^{a,b} \subseteq \mathcal{B}_\Gamma^{A,B}$. This contradicts (5.37).

- $\omega_{n_0} \in \mathcal{C}_{2,o}^{a,b}$ with $|\mathfrak{p}^{a,b}(\omega_{n_0})| = 1$: The same logic used in the case $\omega_{n_0} \in \mathcal{R}_2^{a,b}$ leads to the same conclusion.

- $\omega_{n_0} \in \mathcal{C}_{2,o}^{a,b}$ with $|\mathfrak{p}^{a,b}(\omega_{n_0})| = 2L-1$: By the same logic applied to the case $\omega_{n_0} \in \mathcal{R}_2^{a,b}$, we get $\omega_n \in \mathcal{N}(\mathcal{R}_3^{a,b})$ for all $n \geq n_0$. This again contradicts the fact that ω_N has a b-cross.

Since we get a contradiction in all cases, the first assertion of the proposition is proved. For the second assertion, we first observe from the first part of the proposition that $\mathcal{E}^A \cap \mathcal{S}(B) = \emptyset$. Then, by the definitions of $\mathcal{E}^A$ and $\mathcal{E}^B$, it also holds that $\mathcal{E}^A \cap \mathcal{E}^B = \emptyset$. □

5.5.2 Structure of edge configurations

We fix a proper partition $(A,\, B)$ throughout this subsection and investigate the structure of the sets $\mathcal{E}^A$ and $\mathcal{E}^B$ more deeply, as in Section 3.4.4.

We start by decomposing $\mathcal{E}^A = \mathcal{I}^A \cup \mathcal{O}^A$ where

$$\mathcal{O}^A = \{\sigma \in \mathcal{E}^A : H(\sigma) = \Gamma\} \quad \text{and} \quad \mathcal{I}^A = \{\sigma \in \mathcal{E}^A : H(\sigma) < \Gamma\}.$$

Further, we take a representative set $\mathcal{I}^A_{\text{rep}} \subseteq \mathcal{I}^A$ in such a way that each $\sigma \in \mathcal{I}^A$ satisfies $\sigma \in \mathcal{N}(\zeta)$ for exactly one $\zeta \in \mathcal{I}^A_{\text{rep}}$. With this notation, we can further decompose the set $\mathcal{E}^A$ into

$$\mathcal{E}^A = \mathcal{O}^A \cup \Big(\bigcup_{\zeta \in \mathcal{I}^A_{\text{rep}}} \mathcal{N}(\zeta) \Big).$$

For convenience of the notation, we can assume that $\mathcal{S}(A),\, \mathcal{R}_2^{A,B} \subseteq \mathcal{I}^A_{\text{rep}}$ so that configurations in $\mathcal{N}(\boldsymbol{a})$ with $\boldsymbol{a} \in \mathcal{S}(A)$ and in $\mathcal{N}(\sigma)$ with $\sigma \in \mathcal{R}_2^{A,B}$ are represented by $\boldsymbol{a}$ and σ, respectively[7].

We now assign a graph structure to $\mathcal{E}^A$ based on this decomposition. More precisely, we introduce a graph $\mathscr{G}^A = (\mathscr{V}^A,\, E(\mathscr{V}^A))$ where the vertex set is defined by $\mathscr{V}^A = \mathcal{O}^A \cup \mathcal{I}^A_{\text{rep}}$ and the edge set is defined by $\{\sigma,\, \sigma'\} \in E(\mathscr{V}^A)$ for $\sigma,\, \sigma' \in \mathscr{V}^A$ if and only if

$$\begin{cases} \sigma,\, \sigma' \in \mathcal{O}^A \text{ and } \sigma \sim \sigma' \ \text{ or} \\ \sigma \in \mathcal{O}^A,\ \sigma' \in \mathcal{I}^A_{\text{rep}} \text{ and } \sigma \sim \zeta \text{ for some } \zeta \in \mathcal{N}(\sigma'). \end{cases}$$

Next, we construct a continuous-time Markov chain $\{Z^A(t)\}_{t\ge 0}$ on $\mathscr{V}^A$ with rate $r^A : \mathscr{V}^A \times \mathscr{V}^A \to \mathbb{R}$ defined by

$$r^A(\sigma,\, \sigma') = \begin{cases} 1 & \text{if } \sigma,\, \sigma' \in \mathcal{O}^A, \\ |\{\zeta \in \mathcal{N}(\sigma) : \zeta \sim \sigma'\}| & \text{if } \sigma \in \mathcal{I}^A_{\text{rep}},\ \sigma' \in \mathcal{O}^A, \\ |\{\zeta \in \mathcal{N}(\sigma') : \zeta \sim \sigma\}| & \text{if } \sigma \in \mathcal{O}^A,\ \sigma' \in \mathcal{I}^A_{\text{rep}}, \end{cases} \tag{5.38}$$

and $r^A(\sigma,\, \sigma') = 0$ if $\{\sigma,\, \sigma'\} \notin E(\mathscr{V}^A)$. Since the rate $r^A(\cdot,\, \cdot)$ is symmetric, the Markov chain $Z^A(\cdot)$ is reversible with respect to the uniform distribution on $\mathscr{V}^A$.

Notation 5.5.5. We denote by $L^A(\cdot)$, $h^A_{\cdot,\,\cdot}(\cdot)$, $\text{cap}^A(\cdot,\, \cdot)$, and $D^A(\cdot)$ the generator, equilibrium potential, capacity, and Dirichlet form, respectively, of the Markov chain $Z^A(\cdot)$.

Configurations in $\mathcal{E}^A$

In the following series of lemmas, we study several essential features of the configurations in $\mathcal{E}^A$.

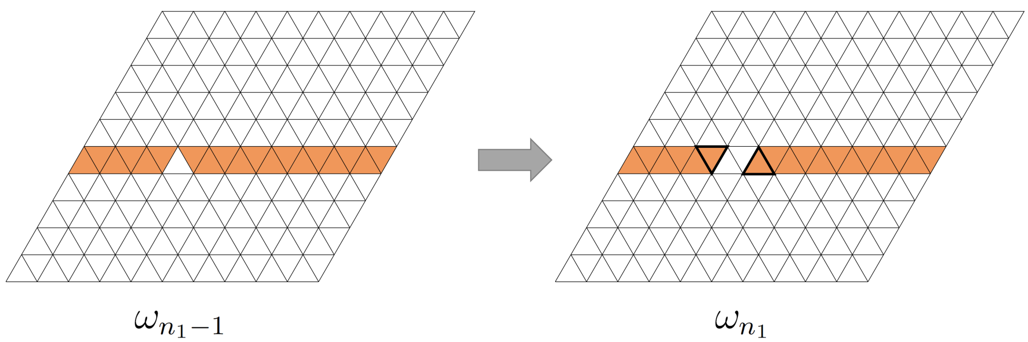
Lemma 5.5.6. *Suppose that $\sigma \in \mathcal{E}^A$ has an a-cross for some $a \in A$. Then, we have that $h^A_{\mathcal{S}(A),\, \mathcal{R}_2^{a,\, b}}(\sigma) = 1$ (cf. Notation 5.5.5).*

[7] We note from Lemma 5.4.19 that $\mathcal{N}$-neighborhoods of two different $\sigma,\, \sigma' \in \mathcal{R}_2^{A,\, B}$ are indeed disjoint.

Proof. We fix $\sigma \in \mathcal{E}^A$ which has an a-cross for some $a \in A$. It suffices to prove that any Γ-path from σ to $\mathcal{R}_2^{A,\,B}$ in $\mathcal{X} \setminus \mathcal{B}_\Gamma^{A,\,B}$ must visit $\mathcal{N}(\mathcal{S}(A))$. Suppose the contrary that there exists a Γ-path $(\omega_n)_{n=0}^N$ in $\mathcal{X} \setminus [\mathcal{N}(\mathcal{S}(A)) \cup \mathcal{B}_\Gamma^{A,\,B}]$ connecting $\omega_0 \in \mathcal{R}_2^{A,\,B}$ and $\omega_N = \sigma$. Let

$$n_1 = \min\{n \geq 1 : \omega_n \text{ has an } a\text{-cross}\} \in [\![1,\, N]\!],$$

so that ω_{n_1-1} is clearly cross-free. Hence, we are able to apply Propositions 5.4.8, 5.4.11, and 5.4.13 to conclude that ω_{n_1-1} is either of type **(MB)** or satisfies $\omega_{n_1-1} \in \mathcal{C}_{0,\,o}^{a,\,b}$ with $|\mathfrak{p}^{a,\,b}(\omega_{n_1-1})| = 2L-1$. For the former case, ω_{n_1-1} is clearly not of type **(MB7)** since ω_{n_1} must have a cross, and thus by Lemma 5.4.16, we have $\omega_{n_1} \in \mathcal{N}(\boldsymbol{a})$, leading to a contradiction. For the latter case, since ω_{n_1} has an a-cross, the configurations ω_{n_1-1} and ω_{n_1} must be of the following form.



Thus, we update each spin b in ω_{n_1} to spin a in a consecutive manner as in the proof of Lemma 5.4.15 (where we start the update from a triangle highlighted by a bold boundary), to obtain a $(\Gamma-1)$-path from ω_{n_1} to $\boldsymbol{a}$. Hence, we have $\omega_{n_1} \in \mathcal{N}(\boldsymbol{a})$ and we get a contradiction in this case as well. $\square$

Lemma 5.5.7. *Fix $a \in A$ and suppose that $\sigma \in \mathcal{N}(\boldsymbol{a})$ and that there exists $\zeta \in \mathcal{O}^A$ such that $\sigma \sim \zeta$ and $h^A_{\mathcal{S}(A),\,\mathcal{R}_2^{a,\,b}}(\zeta) \neq 1$. Then, the following statements hold.*

(1) There exists a $(\Gamma-1)$-path from σ to $\boldsymbol{a}$ of length less than $4L$.

(2) We have

$$\left|\{\sigma \in \mathcal{N}(\boldsymbol{a}) : \exists \zeta \in \mathcal{O}^A \text{ with } \sigma \sim \zeta \text{ and } h^A_{\mathcal{S}(A),\, \mathcal{R}_2^{a,\,b}}(\zeta) \neq 1\}\right| = O(L^8).$$

Proof. (1) By Proposition 5.5.4 and Lemma 5.5.6, ζ is a cross-free configuration of energy Γ. Thus, by Proposition 5.4.13, ζ is of type **(ODP)**, **(TDP)**, **(SP)**, **(EP)**, **(PP)** or **(MB)**. For the first five types, since $\sigma \in \mathcal{N}(\boldsymbol{a})$, we can readily infer that the only possible cases are $\sigma \in \mathcal{R}_1^{a,\,c}$ or $\sigma \in \mathcal{C}_{1,\,o}^{a,\,c}$ with $|\mathfrak{p}^{a,\,c}(\sigma)| = 1$ for some $c \in \Omega \setminus \{a\}$. Then, we clearly have a $(\Gamma-1)$-path from σ to $\boldsymbol{a}$ of length $2L$ or $2L+1$ which is indeed a canonical path (cf. Remarks 5.4.6 and 5.4.7). Next we assume that ζ is of type **(MB)**. If ζ is of type **(MB7)**, then clearly we have $\sigma \in \mathcal{C}_{1,\,o}^{c,\,c'}$ for some c, $c' \in \Omega$, which contradicts $\sigma \in \mathcal{N}(\boldsymbol{a})$ by Lemmas 5.4.19 and 5.4.20. Otherwise, the statement of part (1) is direct from Lemma 5.4.16.

(2) Since ζ is a cross-free configuration of energy Γ, Lemma 5.4.18 implies that there are $O(L^6)$ possibilities for ζ. As there are $O(L^2)$ ways of flipping a spin, we get a (loose) bound $O(L^8)$ for the number of possible configurations for σ. ∎

Lemma 5.5.8. *Let $\zeta \in \mathcal{I}^A_{\text{rep}} \setminus (\mathcal{S}(A) \cup \mathcal{R}_2^{A,\,B} \cup \mathcal{C}_{1,\,o}^{A,\,B})$ and let $\sigma \in \mathcal{N}(\zeta)$. Then, σ has an a-cross for some $a \in A$. If $\xi \in \mathcal{O}^A$ satisfies $\xi \sim \sigma$, then ξ also has an a-cross.*

Proof. By Propositions 5.4.8 and 5.4.11, σ cannot be a cross-free configuration. Since σ cannot have a b-cross for $b \in B$ by Proposition 5.5.4, it must have an a-cross for some $a \in A$. For the second part of the lemma, since $\xi \sim \sigma$, the configuration ξ should be cross-free if it does not have an a-cross. If ξ is cross-free, then by Proposition 5.4.13, ξ is of type **(ODP)**, **(TDP)**, **(SP)**, **(EP)**, **(PP)** or **(MB)**. The first five types are impossible since σ has a cross. If ξ is of type **(MB)** other than **(MB7)**, then Lemma 5.4.16 implies that $\sigma \in \mathcal{N}(\boldsymbol{a})$ which contradicts $\zeta \notin \mathcal{S}(A)$. Finally, if ξ is of type **(MB7)**, then σ cannot have a cross, and thus we have a contradiction. This concludes the proof. $\square$

Estimate of jump rate

The following proposition explains the reason why we introduced the Markov chain $Z^A(\cdot)$.

Proposition 5.5.9. *Define a projection map* $\Pi^A : \mathcal{E}^A \to \mathscr{V}^A$ *by*

$$\Pi^A(\sigma) = \begin{cases} \zeta & \text{if } \sigma \in \mathcal{N}(\zeta) \text{ for some } \zeta \in \mathcal{I}^A_{\text{rep}}, \\ \sigma & \text{if } \sigma \in \mathcal{O}^A. \end{cases}$$

Suppose that $L^{2/3} \ll e^\beta$. *Then, the following statements hold.*

(1) For $\sigma_1, \sigma_2 \in \mathcal{O}^A$ *with* $\sigma_1 \sim \sigma_2$, *we have*

$$\frac{1}{q} e^{-\Gamma\beta} r^A\big(\,\Pi^A(\sigma_1),\, \Pi^A(\sigma_2)\,\big) = (1+o(1)) \times \mu_\beta(\sigma_1) c_\beta(\sigma_1,\, \sigma_2).$$

(2) For $\sigma_1 \in \mathcal{O}^A$ *and* $\sigma_2 \in \mathcal{I}^A$ *with* $\sigma_1 \sim \sigma_2$, *we have*

$$\frac{1}{q} e^{-\Gamma\beta} r^A\big(\,\Pi^A(\sigma_1),\, \Pi^A(\sigma_2)\,\big) = (1+o(1)) \times \sum_{\zeta \in \mathcal{N}(\sigma_2)} \mu_\beta(\sigma_1) c_\beta(\sigma_1,\, \zeta).$$

Proof. (1) By definition, we have $r^A\big(\Pi^A(\sigma_1),\, \Pi^A(\sigma_2)\big) = 1$ and the conclusion thus follows immediately from (5.8) and part (1) of Theorem 5.1.2.

(2) For this case, by definition we can write

$$\frac{1}{q} e^{-\Gamma\beta} r^A\big(\Pi^A(\sigma_1),\, \Pi^A(\sigma_2)\big) = \frac{1}{q} e^{-\Gamma\beta} \times \big|\{\zeta \in \mathcal{N}(\sigma_2) : \zeta \sim \sigma_1\}\big|.$$

By part (1) of Theorem 5.1.2 and (5.8), the right-hand side equals

$$
\begin{aligned}
&(1+o(1)) \times \mu_\beta(\sigma_1) \times \big|\{\zeta \in \mathcal{N}(\sigma_2) : \zeta \sim \sigma_1\}\big| \\
&= (1+o(1)) \times \sum_{\zeta \in \mathcal{N}(\sigma_2):\, \zeta \sim \sigma_1} \mu_\beta(\sigma_1) c_\beta(\sigma_1,\, \zeta),
\end{aligned}
$$

where we implicitly used the fact that $\min\{\mu_\beta(\sigma_1),\, \mu_\beta(\sigma_2)\} = \mu_\beta(\sigma_1)$ at the identity. This proves part (2). □

An auxiliary constant

Finally, we define a constant

$$
\mathfrak{e}_A = \frac{1}{|\mathscr{V}^A| \mathrm{cap}^A\big(\mathcal{S}(A),\, \mathcal{R}_2^{A,\,B}\big)}. \tag{5.39}
$$

Proposition 5.5.10. *We have* $\mathfrak{e}_A \le L^{-1}$.

Proof. As in the proof of Proposition 4.6.9, the proof is completed by applying Thomson principle along with a test flow defined along a canonical path from $\mathcal{R}_2^{A,\,B}$ to $\mathcal{S}(A)$. We do not tediously repeat the proof and refer the readers to Proposition 4.6.9 for more detailed explanation of this method. □

To conclude this section, it should be noted that we can repeat the same constructions on the other set $\mathcal{E}^B$ and obviously the same conclusions also hold for this set as well.

5.6 Capacity estimates

In the remainder of the article, we focus on the proof of the Eyring–Kramers formula (Theorem 5.1.4) based on our careful investigation of the energy landscape carried out in the previous section.

Theorem 5.6.1 (Capacity estimate for hexagonal lattice)**.** *Suppose that* $\beta = \beta_L$ *satisfies* $L^{10} \ll e^{\beta}$ *and let* $(A,\, B)$ *be a proper partition. Then, it holds that*

$$\mathrm{Cap}_\beta\big(\mathcal{S}(A),\, \mathcal{S}(B)\big) = \Big[\frac{12|A|(q-|A|)}{q} + o(1)\Big] e^{-\Gamma\beta}. \tag{5.40}$$

Remark 5.6.2 (Capacity estimate for square lattice). For the square lattice, we have the same form of capacity estimate under the condition $L^3 \ll e^{\beta}$, where the only difference is that the constant 12 on the right-hand side of (5.40) should be replaced by 8.

The proof of this theorem will be given in Sections 5.7 and 5.8. At this moment, let us conclude the proof of Theorem 5.1.4 by assuming Theorem 5.6.1.

Proof of Theorem 5.1.4. First, we consider the formula in (5.12). Employing once again the magic formula (3.24), we can write

$$\mathbb{E}_{\boldsymbol{a}}[\tau_{\mathcal{S}\setminus\{\boldsymbol{a}\}}] = \frac{\sum_{\sigma\in\mathcal{X}} \mu_\beta(\sigma) h_{\boldsymbol{a},\,\mathcal{S}\setminus\{\boldsymbol{a}\}}(\sigma)}{\mathrm{Cap}_\beta(\boldsymbol{a},\, \mathcal{S}\setminus\{\boldsymbol{a}\})} \quad \text{for } \boldsymbol{a}\in\mathcal{S}. \tag{5.41}$$

Since

$$\Big|\sum_{\sigma\in\mathcal{S}} \mu_\beta(\sigma) h_{\boldsymbol{a},\,\mathcal{S}\setminus\{\boldsymbol{a}\}}(\sigma) - \mu_\beta(\boldsymbol{a})\Big| \le \mu_\beta(\mathcal{X}\setminus\mathcal{S}) = o(1)$$

by part (1) of Theorem 5.1.2, we can conclude that the numerator on the right-hand side of (5.41) is $1/q + o(1)$. Since the denominator is $[12(q-1)/q + o(1)]e^{-\Gamma\beta}$ by Theorem 5.6.1 with $A = \{a\}$ and $B = \Omega\setminus\{a\}$, we can prove the first formula in (5.12).

Now, let us turn to the second formula of (5.12). By the symmetry of the model, we have $\mathbb{P}_{\boldsymbol{a}}[\sigma_\beta(\tau_{\mathcal{S}\setminus\{\boldsymbol{a}\}}) = \boldsymbol{b}] = 1/(q-1)$. If $\sigma_\beta(\tau_{\mathcal{S}\setminus\{\boldsymbol{a}\}}) \neq \boldsymbol{b}$, we can refresh the dynamics from $t = \tau_{\mathcal{S}\setminus\{\boldsymbol{a}\}}$. Then, by the strong Markov property, we obtain a geometric random variable (with success probability $1/(q-1)$)

structure and thus deduce that

$$\mathbb{E}_{\boldsymbol{a}}[\tau_{\boldsymbol{b}}] = (q-1)\mathbb{E}_{\boldsymbol{a}}[\tau_{\mathcal{S}\setminus\{\boldsymbol{a}\}}].$$

For a more rigorous and formal proof of this argument, we refer the readers to Section 3.2.4. Hence, the first and second formulas in (5.12) are equivalent to each other and we conclude the proof. □

5.7 Upper bound for capacities

Notation 5.7.1. In this and the subsequent sections, we fix a proper partition $(A,\, B)$. Then, we define the constants $\mathfrak{b} = \mathfrak{b}(L,\, A,\, B)$ and $\mathfrak{c} = \mathfrak{c}(L,\, A,\, B)$ as

$$\mathfrak{b} = \frac{(5L-3)(L-4)}{60L^2|A|(q-|A|)} \quad \text{and} \quad \mathfrak{c} = \mathfrak{b} + \mathfrak{e}_A + \mathfrak{e}_B \tag{5.42}$$

where the constants $\mathfrak{e}_A$ and $\mathfrak{e}_B$ are defined in (5.39). Then, by (5.42) and Proposition 5.5.10,

$$\mathfrak{c} = \mathfrak{b} + \mathfrak{e}_A + \mathfrak{e}_B = \frac{1}{12|A|(q-|A|)}(1+o(1)). \tag{5.43}$$

The purpose of the current section is to establish a suitable test function in order to use the Dirichlet principle to get a sharp upper bound of $\mathrm{Cap}_\beta(\mathcal{S}(A),\, \mathcal{S}(B))$. The corresponding computation for the square lattice in the $\beta \to \infty$ regime was carried out in Section 3.5, where the discontinuity of the test function along the boundary of $\widehat{\mathcal{N}}(\mathcal{S})$ and the set $\widehat{\mathcal{N}}(\mathcal{S})^c$ was easily handled since energy is the only dominating factor of the system (as L is fixed). For the current model, we need to be very careful when controlling the discontinuity of the test function along this boundary, because the number of configurations with higher energy also increases as L tends to ∞. This difficulty imposes a sub-optimal condition on β (i.e., $L^{10} \ll e^\beta$).

5.7.1 Construction of test function

The following definition (Definition 5.7.3) constructs our test function which approximates the equilibrium potential $h_{\mathcal{S}(A),\,\mathcal{S}(B)}$ between $\mathcal{S}(A)$ and $\mathcal{S}(B)$ in view of Theorem 3.2.5.

Notation 5.7.2. The following notation will be used in the remainder of the article.

(1) We simply write $\mathfrak{h}^A = h^A_{\mathcal{S}(A),\,\mathcal{R}_2^{a,\,b}} : \mathscr{V}^A \to [0,\,1]$ (cf. Notation 5.5.5) and naturally extend $\mathfrak{h}^A$ to a function on $\mathcal{E}^A$ by letting $\mathfrak{h}^A(\sigma) = \mathfrak{h}^A(\zeta)$ if $\sigma \in \mathcal{N}(\zeta)$ for some $\zeta \in \mathcal{I}^A_{\text{rep}}$.

(2) Recall the notation $\|\sigma\|_a$ from (3.121).

Definition 5.7.3. We now define a function $f = f^{A,\,B} : \mathcal{X} \to \mathbb{R}$. Recall Notation 5.7.1 and 5.7.2.

(1) **Construction on $\mathcal{E}^{A,\,B} = \mathcal{E}^A \cup \mathcal{E}^B$:** We define (cf. (5.39))

$$f(\sigma) = \begin{cases} 1 - \dfrac{\mathfrak{e}_A}{\mathfrak{c}}[1 - \mathfrak{h}^A(\sigma)] & \text{if } \sigma \in \mathcal{E}^A, \\ \dfrac{\mathfrak{e}_B}{\mathfrak{c}}[1 - \mathfrak{h}^B(\sigma)] & \text{if } \sigma \in \mathcal{E}^B. \end{cases}$$

(2) **Construction on $\mathcal{B}^{A,\,B}$:** Let $a \in A$ and $b \in B$. By (5.34), it suffices to consider the following cases.

- $\sigma \in \mathcal{N}(\mathcal{R}_n^{a,\,b})$ with $n \in [\![2,\,L-2]\!]$:

$$f(\sigma) = \frac{1}{\mathfrak{c}}\Big[\frac{L-2-n}{L-4}\mathfrak{b} + \mathfrak{e}_B\Big].$$

- $\sigma \in \mathcal{C}_n^{a,\,b}$ with $n \in [\![2,\,L-3]\!]$ and $|\mathfrak{p}^{a,\,b}(\sigma)| \in [\![2,\,2L-2]\!]$ (the case $|\mathfrak{p}^{a,\,b}(\sigma)| \in \{0,\,1,\,2L-1,\,2L\}$ is considered above):

$$f(\sigma) = \frac{1}{\mathfrak{c}}\Big[\frac{(5L-3)(L-2-n) - (3 - \mathfrak{d}(\sigma))}{(5L-3)(L-4)}\mathfrak{b} + \mathfrak{e}_B\Big]$$

if $|\mathfrak{p}^{a,\,b}(\sigma)| = 2$,

$$f(\sigma) = \frac{1}{\mathfrak{c}}\Big[\frac{(5L-3)(L-3-n)+(3-\mathfrak{d}(\sigma))}{(5L-3)(L-4)}\mathfrak{b}+\mathfrak{e}_B\Big]$$

if $|\mathfrak{p}^{a,\,b}(\sigma)| = 2L-2$, and

$$f(\sigma) = \frac{1}{\mathfrak{c}}\Big[\frac{(5L-3)(L-2-n)-\frac{5m-3}{2}}{(5L-3)(L-4)}\mathfrak{b}+\mathfrak{e}_B\Big]$$

if $|\mathfrak{p}^{a,\,b}(\sigma)| = m \in [\![3,\, 2L{-}3]\!]$. Here, $\mathfrak{d}(\sigma) = \mathbb{1}\{\sigma : \mathfrak{p}^{a,\,b}(\sigma) \text{ is disconnected}\}$.

- $\sigma \in \mathcal{D}^{a,\,b}$: By the definition of $\mathcal{D}^{a,\,b}$, we can find a canonical configuration ζ in $\mathcal{B}^{a,\,b}$ such that $\zeta \sim \sigma$. If this ζ is unique, we set $f(\sigma) = f(\zeta)$. In view of Lemmas 5.4.23 and 5.4.24, it is also possible that there are two such canonical configurations ζ_1 and ζ_2, but in such a case we have $\zeta_1,\, \zeta_2 \in \mathcal{N}(\mathcal{R}_n^{A,\,B})$ for some $n \in [\![2,\, L-2]\!]$ and therefore $f(\zeta_1) = f(\zeta_2)$ by the definition above. We set $f(\sigma) = f(\zeta_1) = f(\zeta_2)$ in this case.

We note at this point that parts (1) and (2) do not collide on the set $\mathcal{E}^{A,\,B} \cap \mathcal{B}^{A,\,B} = \mathcal{N}(\mathcal{R}_2^{A,\,B}) \cup \mathcal{N}(\mathcal{R}_{L-2}^{A,\,B})$ (cf. Proposition 5.5.3-(1)), since both definitions assign the same value $(\mathfrak{b}+\mathfrak{e}_B)/\mathfrak{c}$ (resp. $\mathfrak{e}_B/\mathfrak{c}$) on $\mathcal{N}(\mathcal{R}_2^{A,\,B})$ (resp. $\mathcal{N}(\mathcal{R}_{L-2}^{A,\,B})$).

(3) **Construction on $\widehat{\mathcal{N}}(\mathcal{S})^c$:** For $\sigma \in \widehat{\mathcal{N}}(\mathcal{S})^c$, we define

$$f(\sigma) = \begin{cases} 1 & \text{if } \sum_{a\in A} \|\sigma\|_a \ge L^2, \\ 0 & \text{if } \sum_{a\in A} \|\sigma\|_a < L^2. \end{cases}$$

By Proposition 5.5.3-(2), the constructions above define f on the set $\mathcal{X}$.

In the remainder of the current section, we shall prove the following proposition.

Proposition 5.7.4. *The test function $f = f^{A,\,B}$ constructed in the previous definition belongs to $\mathfrak{C}(\mathcal{S}(A),\,\mathcal{S}(B))$ and moreover satisfies*

$$D_\beta(f) = \frac{1+o(1)}{q\mathfrak{c}} e^{-\Gamma\beta}.$$

5.7.2 Configurations with intermediate energy

The purpose of the current section is to provide some estimates for controlling the discontinuity of the test function f along the boundary of $\widehat{\mathcal{N}}(\mathcal{S})$, which will be the most difficult part in the proof of Proposition 5.7.4 and was not encountered in the small-volume regime considered in Chapter 3.

A pair of configurations $(\sigma,\,\zeta)$ in $\mathcal{X}$ is called a *nice pair* if they satisfy

$$\sigma,\,\zeta \notin \widehat{\mathcal{N}}(\mathcal{S}), \quad \sigma \sim \zeta, \quad \sum_{a\in A} \|\sigma\|_a = L^2, \quad \text{and} \quad \sum_{a\in A} \|\zeta\|_a = L^2 - 1. \tag{5.44}$$

The following counting of nice pairs is the main result of the current section.

Proposition 5.7.5. *For $i \geq 0$, denote by $U_i = U_i^{A,\,B,\,L}$ the number of nice pairs $(\sigma,\,\zeta)$ satisfying $\max\{H(\sigma),\,H(\zeta)\} = 2L + i$.*

(1) We have $U_i = 0$ for all $i \leq 2$.

(2) There exists a constant $C = C(q) > 0$ such that $U_i \leq (CL)^{3i+1}$ for all $i < (\sqrt{6} - 2)L - 1$.

To prove this proposition, first we establish an isoperimetric inequality.

Lemma 5.7.6. *Suppose that $\sigma \in \mathcal{X}$ has an a-cross for some $a \in \Omega$. Then, we have $\sum_{b\in\Omega\setminus\{a\}} \|\sigma\|_b \leq H(\sigma)^2/6$.*

Proof. We fix $b_0 \in \Omega \setminus \{a\}$ and define $\widetilde{\sigma} \in \mathcal{X}$ by

$$\widetilde{\sigma}(x) = \begin{cases} a & \text{if } \sigma(x) = a, \\ b_0 & \text{if } \sigma(x) \neq a. \end{cases}$$

Then, it is immediate that $H(\widetilde{\sigma}) \le H(\sigma)$ and $\sum_{b\in\Omega\setminus\{a\}} \|\sigma\|_b = \|\widetilde{\sigma}\|_{b_0}$. Therefore, it suffices to prove that $\|\widetilde{\sigma}\|_{b_0} \le \frac{H(\widetilde{\sigma})^2}{6}$. As $\widetilde{\sigma}$ also has an a-cross, this is a direct consequence of the isoperimetric inequality [41, Theorem 1.2]. $\square$

Proof of Proposition 5.7.5. Let (σ, ζ) be a nice pair satisfying $\max\{H(\sigma), H(\zeta)\} < \sqrt{6}L - 1$. Suppose now that $\eta \in \{\sigma, \zeta\}$ has a c-cross for some $c \in \Omega$. Then, by Lemma 5.7.6, we have

$$\sum_{c' : c' \neq c} \|\eta\|_{c'} \le \frac{H(\eta)^2}{6} < \frac{(\sqrt{6}L - 1)^2}{6} < L^2 - 1.$$

If $c \in B$, we get a contradiction to $\sum_{a\in A} \|\eta\|_a \ge L^2 - 1$, and we get a similar contradiction when $c \in A$. Thus, both σ and ζ are cross-free.

(1) Suppose that there exists a nice pair (σ, ζ) such that $H(\sigma), H(\zeta) \le \Gamma$. If the cross-free configuration $\eta \in \{\sigma, \zeta\}$ satisfies $H(\eta) < \Gamma$, we can apply Propositions 5.4.8 and 5.4.11 to conclude that $\eta \in \mathcal{R}_n^{a_1, a_2} \cup \mathcal{C}_{n,o}^{a_1, a_2}$ for some n and $a_1, a_2 \in \Omega$. Then by Remark 5.5.2, we obtain $\eta \in \widehat{\mathcal{N}}(\mathcal{S})$ which yields a contradiction. Therefore, we must have that $H(\sigma) = H(\zeta) = \Gamma$. Since $\sigma \sim \zeta$, by Proposition 5.4.13, we can notice that σ and ζ must be both of type **(PP)** or both of type **(MB)**. If they are both of type **(PP)**, then Lemma 5.4.23 implies that $\sigma, \zeta \in \widehat{\mathcal{N}}(\mathcal{S})$. If they are both of type **(MB)**, then Lemma 5.4.15 implies that both σ and ζ satisfy $(\star)$ and thus $\sigma, \zeta \in \widehat{\mathcal{N}}(\mathcal{S})$. Hence, we get contradiction in both cases and the proof of part (1) is completed.

(2) Fix $2 < i < (\sqrt{6} - 2)L - 1$ and let $\eta \in \{\sigma, \zeta\}$ be the configuration with energy $2L + i$. Since η is cross-free, all the bridges of η (whose existence is guaranteed by Lemma 5.3.3) must be of the same direction. Without loss of generality, we suppose that all bridges of η are horizontal. Denote these horizontal bridges by

$$\hbar_{k_1}, \ldots, \hbar_{k_{L-\alpha}} \quad \text{where } 1 \le k_1 < \cdots < k_{L-\alpha} \le L.$$

Since $2L+i = H(\eta)$ is not a multiple of L by the condition $i < (\sqrt{6}-2)L-1 < L$, at least one horizontal strip is not a bridge and hence $\alpha \geq 1$. Write

$$\mathbb{T}_L \setminus \{k_1, \dots, k_{L-\alpha}\} = \{k'_1, \dots, k'_\alpha\} \quad \text{where } 1 \leq k'_1 < \cdots < k'_\alpha \leq L.$$

By Lemma 5.3.3, we have that

$$2L + \alpha = 3L - (L-\alpha) \leq H(\sigma) = 2L + i \quad \text{and hence } \alpha \leq i. \tag{5.45}$$

Define $\delta \in \mathbb{N}$ as

$$\delta = \sum_{\ell=1}^{\alpha} \Delta H_{\hbar_{k'_\ell}}(\eta) \geq 2\alpha, \tag{5.46}$$

where the inequality follows since $\Delta H_{\hbar_{k'_\ell}}(\eta) \geq 2$ for all $\ell \in [\![1, \alpha]\!]$ (cf. Lemma 5.3.2). Now, we count possible number of nice pairs for fixed α and δ.

(Step 1) There are $\binom{L}{\alpha}$ ways to choose the positions of strips $\hbar_{k_1}, \dots, \hbar_{k_{L-\alpha}}$.

(Step 2) Number of possible spin configurations on $\hbar_{k_1} \cup \cdots \cup \hbar_{k_{L-\alpha}}$: If these horizontal bridges have three different spins, then all the vertical and diagonal strips have energy at least 3, and hence by (5.25) we get

$$H(\eta) \geq \frac{1}{2}(0 + 3L + 3L) = 3L. \tag{5.47}$$

This contradicts $H(\eta) < \sqrt{6}L$. If all these bridges are of the same spin, there are q possible choices. If all these bridges consist of two spins, there exist $1 \leq u < v \leq L-\alpha$ and $a_1, a_2 \in \Omega$ such that

$$\hbar_{k_\ell} \text{ is an } \begin{cases} a_1\text{-bridge} & \text{if } u \leq \ell < v, \\ a_2\text{-bridge} & \text{otherwise,} \end{cases} \tag{5.48}$$

since otherwise all the vertical and diagonal strips have energy at least 4 and we get a contradiction as in (5.47). Now, we will see which values of (u, v)

are available. By counting the number of spins in $\hbar_{k_1} \cup \cdots \cup \hbar_{k_{L-\alpha}}$ we should have

$$\|\eta\|_{a_1} \geq 2L(v-u) \quad \text{and} \quad \|\eta\|_{a_2} \geq 2L(L-\alpha-v+u).$$

On the other hand, by (5.44), we have $\|\eta\|_{a_1},\ \|\eta\|_{a_2} \leq L^2+1$. Summing these up, we get $\frac{L}{2} - \alpha \leq v-u \leq \frac{L}{2}$. Therefore, there are at most

$$q \times (q-1) \times L \times (\alpha+1) \leq 2\alpha L q^2$$

ways of assigning spins on $\hbar_{k_1} \cup \cdots \cup \hbar_{k_{L-\alpha}}$ satisfying (5.48). Summing up, there are at most $q + 2\alpha L q^2 \leq 3\alpha L q^2$ possible choices on these strips.

(Step 3) Number of possible spin configurations on $\hbar_{k'_1} \cup \cdots \cup \hbar_{k'_\alpha}$: Write $\delta_\ell = \Delta H_{\hbar_{k'_\ell}}(\eta)$ for $\ell \in [\![1,\, \alpha]\!]$ so that $\delta_1 + \cdots + \delta_\alpha = \delta$. Since each strip $\hbar_{k'_\ell}$ has energy δ_ℓ, it should be divided into δ_ℓ monochromatic clusters. There are $\binom{2L}{\delta_\ell}$ ways of dividing $\hbar_{k'_\ell} \simeq \mathbb{T}_{2L}$ into δ_ℓ connected clusters, and there are at most q^{δ_ℓ} ways to assign spins to these clusters. Hence, given α and δ, the number of possible spin choices on $\hbar_{k'_1} \cup \cdots \cup \hbar_{k'_\alpha}$ is at most

$$\sum_{\delta_1,\, \dots,\, \delta_\alpha \geq 0:\, \delta_1+\cdots+\delta_\alpha=\delta} \binom{2L}{\delta_1} \cdots \binom{2L}{\delta_\alpha} q^{\delta_1+\cdots+\delta_\alpha} = \binom{2\alpha L}{\delta} q^{\delta}. \tag{5.49}$$

(Step 4) Since η is one of $\{\sigma,\, \zeta\}$ with bigger energy, we next count the number of possible other configurations. This configuration is obtained from η by an update which does not increase the energy. Since updating a spin in a bridge always increases the energy, we have to update a spin in strips $\hbar_{k'_\ell}$, $\ell \in [\![1,\, \alpha]\!]$. For each strip, $\hbar_{k'_\ell}$ has δ_ℓ monochromatic clusters as observed in the previous step, and thus there are at most $2\delta_\ell$ updatable triangles in this strip (which are located at the edge of each monochromatic cluster). Hence, we have in total 2δ updatable triangles. Since each spin in the triangle can be updated to at most three spins in order not to increase the energy, there are at most 6δ possible ways of updates.

Summing **(Step 1)-(Step 4)** up, the number of possible nice pairs for given α and δ is bounded from above by

$$3 \times \binom{L}{\alpha} \times 3\alpha L q^2 \times \binom{2\alpha L}{\delta} q^\delta \times 6\delta,$$

where the first factor 3 reflects three possible directions for parallel bridges. Since $\Delta H_{\mathfrak{v}_\ell}(\eta),\, \Delta H_{\mathfrak{d}_\ell}(\eta) \geq 2$ for all $\ell \in \mathbb{T}_L$ by Lemma 5.3.2, we can deduce from (5.25) that

$$\delta = \sum_{\ell=1}^{\alpha} \Delta H_{\mathfrak{h}_{k'_\ell}}(\eta) \leq 2H(\eta) - 4L = 2i.$$

Combining with (5.46), we get $\delta \in [\![2\alpha,\, 2i]\!]$. Thus, we can finally bound the number of nice pairs by

$$\sum_{\alpha=1}^{i} \sum_{\delta=2\alpha}^{2i} 3 \times \binom{L}{\alpha} \times 3\alpha L q^2 \times \binom{2\alpha L}{\delta} q^\delta \times 6\delta. \tag{5.50}$$

Since $i < (\sqrt{6} - 2)L - 1$, the following bounds hold for $\alpha \leq i$:

$$\binom{L}{\alpha} \leq \binom{L}{i}, \quad 3\alpha L q^2 \leq 3iLq^2, \quad \text{and} \quad \binom{2\alpha L}{\delta} q^\delta \times 6\delta \leq 12i \binom{2iL}{2i} q^{2i}.$$

Therefore, we can bound the summation (5.50) from above by

$$i \times 2i \times 3 \times \binom{L}{i} \times 3iLq^2 \times 12i \binom{2iL}{2i} q^{2i} \leq 216 L i^4 q^{2i+2} \binom{L}{i} \binom{2iL}{2i}.$$

By Stirling's formula and the bound $\binom{L}{i} \leq \frac{L^i}{i!}$, the right-hand side of the last formula can be bounded from above by

$$CLi^4 q^{2i} \times \frac{L^i}{i!} \times (eL)^{2i} \leq C(eqL)^{3i+1}$$

for some constant $C > 0$. This concludes the proof. □

5.7.3 Computation of Dirichlet form

In turn, we calculate the Dirichlet form $D_\beta(f)$ of the test function $f = f^{A,\,B}$. To this end, we decompose $D_\beta(f)$ as

$$\Big[\sum_{\{\sigma,\,\zeta\}\subseteq\widehat{\mathcal{N}}(\mathcal{S})} + \sum_{\sigma\in\widehat{\mathcal{N}}(\mathcal{S})}\sum_{\zeta\in\widehat{\mathcal{N}}(\mathcal{S})^c} + \sum_{\{\sigma,\,\zeta\}\subseteq\widehat{\mathcal{N}}(\mathcal{S})^c}\Big]\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)[f(\zeta)-f(\sigma)]^2 \quad (5.51)$$

and we shall estimate three summations separately. We recall that we are imposing the condition $L^{10} \ll e^\beta$ on β. We write for each $\mathcal{A} \subseteq \mathcal{X}$,

$$E(\mathcal{A}) = \big\{\{\sigma,\,\zeta\} \subseteq \mathcal{A} : \sigma \sim \zeta\big\}. \quad (5.52)$$

Lemma 5.7.7. *We have*

$$\sum_{\{\sigma,\,\zeta\}\subseteq\widehat{\mathcal{N}}(\mathcal{S})} \mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)[f(\zeta)-f(\sigma)]^2 = \frac{1+o(1)}{q\mathfrak{c}}e^{-\Gamma\beta}. \quad (5.53)$$

Proof. By Propositions 5.5.3 and 5.5.4, we can decompose the left-hand side of (5.53) as

$$\Big[\sum_{\{\sigma,\,\zeta\}\in E(\mathcal{B}^{a,\,b})} + \sum_{\{\sigma,\,\zeta\}\in E(\mathcal{E}^A)} + \sum_{\{\sigma,\,\zeta\}\in E(\mathcal{E}^B)}\Big]\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)[f(\zeta)-f(\sigma)]^2, \quad (5.54)$$

since the test function f is constant on $\mathcal{E}^A \cap \mathcal{B}^{A,\,B} = \mathcal{N}(\mathcal{R}_2^{A,\,B})$ and $\mathcal{E}^B \cap \mathcal{B}^{A,\,B} = \mathcal{N}(\mathcal{R}_{L-2}^{A,\,B})$ as remarked in Definition 5.7.3.

Let us consider the first summation of (5.54). Suppose that $\sigma \in \mathcal{D}^{A,\,B}$. If $\sigma \in \mathcal{P}_n^{A,\,B}$ for some $n \in [\![2,\,L-2]\!]$, $a \in A$, and $b \in B$, then Lemma 5.4.23 and Definition 5.7.3-(2) assert that $f(\sigma) = f(\zeta)$. If $\sigma \in \mathcal{Q}_n^{a,\,b}$ for some $n \in [\![2,\,L-3]\!]$, $a \in A$, and $b \in B$, then Lemma 5.4.24 and Definition 5.7.3-(2) imply that $f(\sigma) = f(\zeta)$. The similar conclusion holds for the case $\zeta \in \mathcal{D}^{A,\,B}$

by the same logic and hence the summand vanishes if either $\sigma \in \mathcal{D}^{A,\,B}$ or $\zeta \in \mathcal{D}^{A,\,B}$. Thus, we can write the first summation of (5.54) as

$$\sum_{a\in A}\sum_{b\in B}\sum_{n=2}^{L-3}\sum_{\mathscr{s}\in\{\mathscr{h},\,\mathscr{v},\,\mathscr{d}\}}\sum_{P\prec P':\,|P|=n}\sum_{\{\sigma,\,\zeta\}\in E(\mathcal{C}^{a,\,b}_{\mathscr{s}(P,P')})}\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)[f(\zeta)-f(\sigma)]^2.$$

By Lemmas 5.4.19, 5.4.20, 5.4.21, and the definition of f, the last summation on $\{\sigma,\,\zeta\}$ can be rearranged as

$$\sum_{\sigma\in\mathcal{C}^{a,\,b}_{\mathscr{s}(P,P'),o},\,\zeta\in\mathcal{C}^{a,\,b}_{\mathscr{s}(P,P'),e}:\,\sigma\sim\zeta}\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)[f(\zeta)-f(\sigma)]^2.$$

We now decompose this summation into three parts according to the value of $|\mathfrak{p}^{a,\,b}(\zeta)|$. First suppose that $|\mathfrak{p}^{a,\,b}(\zeta)|\neq 2,\,2L-2$. Then, by the definition of f, (5.8), and Theorem 5.1.2-(1), the summation under this restriction equals

$$4L\times\sum_{m=3}^{2L-4}\frac{1}{Z_\beta}e^{-\Gamma\beta}\times\frac{\mathfrak{b}^2}{\mathfrak{c}^2}\frac{25/4}{(5L-3)^2(L-4)^2}=\frac{50\mathfrak{b}^2L(L-3)(1+o(1))}{q\mathfrak{c}^2(5L-3)^2(L-4)^2}\times e^{-\Gamma\beta}.$$

Next we suppose that $|\mathfrak{p}^{a,\,b}(\zeta)|=2$. Then the summation under this restriction can be decomposed into

$$\Bigg[\sum_{\substack{\zeta:\,|\mathfrak{p}^{a,\,b}(\zeta)|=2,\\ \mathfrak{p}^{a,\,b}(\zeta)\text{ connected}}}+\sum_{\substack{\zeta:\,|\mathfrak{p}^{a,\,b}(\zeta)|=2,\\ \mathfrak{p}^{a,\,b}(\zeta)\text{ disconnected}}}\Bigg]\sum_{\sigma:\,|\mathfrak{p}^{a,\,b}(\sigma)|\in\{1,\,3\}}\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)[f(\zeta)-f(\sigma)]^2.$$

By the definition of f, (5.8), and part (1) of Theorem 5.1.2, the last display equals $(1+o(1))$ times

$$\begin{aligned}&2L\times\frac{1}{q}e^{-\Gamma\beta}\times\frac{\mathfrak{b}^2}{\mathfrak{c}^2}\frac{9+9}{(5L-3)^2(L-4)^2}+L\times\frac{1}{q}e^{-\Gamma\beta}\times\frac{\mathfrak{b}^2}{\mathfrak{c}^2}\frac{4+4+16}{(5L-3)^2(L-4)^2}\\&=\frac{60\mathfrak{b}^2L(1+o(1))}{q\mathfrak{c}^2(5L-3)^2(L-4)^2}e^{-\Gamma\beta}.\end{aligned}$$

For the case $|\mathfrak{p}^{a,\,b}(\zeta)| = 2L-2$, we get the same result with the case $|\mathfrak{p}^{a,\,b}(\zeta)| = 2$ by an identical argument. Gathering the computations above and applying the definition (5.42) of $\mathfrak{b}$, we can conclude that the first summation of (5.54) is $(1+o(1))$ times

$$\begin{aligned}&\sum_{a\in A}\sum_{b\in B}\sum_{n=2}^{L-3}\sum_{\mathscr{s}\in\{\mathscr{h},\,\mathscr{v},\,\mathscr{d}\}}\sum_{P\prec P':\,|P|=n}\frac{50\mathfrak{b}^2L(L-3)+60\mathfrak{b}^2L+60\mathfrak{b}^2L}{q\mathfrak{c}^2(5L-3)^2(L-4)^2}e^{-\Gamma\beta}\\&=|A|(q-|A|)\times\frac{60\mathfrak{b}^2L^2}{q\mathfrak{c}^2(5L-3)(L-4)}e^{-\Gamma\beta}=\frac{\mathfrak{b}}{q\mathfrak{c}^2}e^{-\Gamma\beta}.\end{aligned}\tag{5.55}$$

Next, we turn to the second summation of (5.54). We decompose this summation as

$$\begin{aligned}&\sum_{\{\sigma_1,\,\sigma_2\}\subseteq\mathcal{O}^A}\mu_\beta(\sigma_1)r_\beta(\sigma_1,\,\sigma_2)[f(\sigma_2)-f(\sigma_1)]^2\\&+\sum_{\sigma_1\in\mathcal{O}^A}\sum_{\sigma_2\in\mathcal{I}^A_{\mathrm{rep}}}\sum_{\zeta\in\mathcal{N}(\sigma_2)}\mu_\beta(\sigma_1)r_\beta(\sigma_1,\,\zeta)[f(\zeta)-f(\sigma_1)]^2.\end{aligned}$$

By Proposition 5.5.9, this equals $(1+o(1))$ times

$$\Big[\sum_{\{\sigma_1,\,\sigma_2\}\subseteq\mathcal{O}^A}+\sum_{\sigma_1\in\mathcal{O}^A}\sum_{\sigma_2\in\mathcal{I}^A_{\mathrm{rep}}}\Big]\frac{e^{-\Gamma\beta}}{q}r^A(\sigma_1,\,\sigma_2)[f(\sigma_2)-f(\sigma_1)]^2.$$

By the definition of f, this can be written as

$$\begin{aligned}&(1+o(1))\frac{\mathfrak{e}_A^2}{\mathfrak{c}^2}\sum_{\{\sigma_1,\,\sigma_2\}\subseteq\mathscr{V}^A}\frac{e^{-\Gamma\beta}}{q}r^A(\sigma_1,\,\sigma_2)[\mathfrak{h}^A(\sigma_2)-\mathfrak{h}^A(\sigma_1)]^2\\&=(1+o(1))\frac{e^{-\Gamma\beta}\mathfrak{e}_A^2}{q\mathfrak{c}^2}\times|\mathscr{V}^A|\mathrm{cap}^A\big(\mathcal{S}(A),\,\mathcal{R}_2^{A,\,B}\big)=(1+o(1))\frac{\mathfrak{e}_A}{q\mathfrak{c}^2}e^{-\Gamma\beta}.\end{aligned}\tag{5.56}$$

In conclusion, we get

$$\sum_{\{\sigma,\,\zeta\}\in E(\mathcal{E}^A)}\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)[f(\zeta)-f(\sigma)]^2=(1+o(1))\frac{\mathfrak{e}_A}{q\mathfrak{c}^2}e^{-\Gamma\beta}.$$

By an entirely same computation, the summation $\sum_{\{\sigma,\zeta\}\in E(\mathcal{E}^B)}$ yields $(1+o(1))\frac{\mathfrak{e}_B}{q\mathfrak{c}^2}e^{-\Gamma\beta}$. Gathering these results with (5.55), we can finally conclude that (5.54) equals

$$(1+o(1))\times\frac{\mathfrak{b}+\mathfrak{e}_A+\mathfrak{e}_B}{q\mathfrak{c}^2}e^{-\Gamma\beta}=\frac{1+o(1)}{q\mathfrak{c}}e^{-\Gamma\beta},$$

as desired. This completes the proof. □

Lemma 5.7.8. *We have*

$$\sum_{\sigma\in\widehat{\mathcal{N}}(\mathcal{S})}\sum_{\zeta\in\widehat{\mathcal{N}}(\mathcal{S})^c}\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)[f(\zeta)-f(\sigma)]^2=o(e^{-\Gamma\beta}). \tag{5.57}$$

Proof. If $\sigma\in\widehat{\mathcal{N}}(\mathcal{S})$ and $\zeta\in\widehat{\mathcal{N}}(\mathcal{S})^c$, we have that $H(\sigma)\le 2L+2<H(\zeta)$ and therefore by (5.8), we can rewrite the left-hand side of (5.57) as

$$\Big[\sum_{\sigma\in\mathcal{E}^A}+\sum_{\sigma\in\mathcal{E}^B}+\sum_{\sigma\in\mathcal{B}^{a,\,b}\setminus\mathcal{E}^{a,\,b}}\Big]\sum_{\zeta\in\widehat{\mathcal{N}}(\mathcal{S})^c}\mu_\beta(\zeta)[f(\zeta)-f(\sigma)]^2. \tag{5.58}$$

Let us consider the first summation.

- $\sigma\in\mathcal{E}^A$ has a cross and $\zeta\in\widehat{\mathcal{N}}(\mathcal{S})^c$ is adjacent to σ: By Proposition 5.5.4 and Lemma 5.5.6, σ has an a-cross for some $a\in A$ and $h^A_{\mathcal{S}(A),\,\mathcal{R}_2^{a,\,b}}(\sigma)=1$ so that $f(\sigma)=1$ by the definition of f on $\mathcal{E}^A$. Moreover, by Lemma 5.7.6, we have

  $$\sum_{b\in B}\|\sigma\|_b\le\sum_{b\in\Omega\setminus\{a\}}\|\sigma\|_b\le\frac{H(\sigma)^2}{6}\le\frac{2(L+1)^2}{3}.$$

  Since $\zeta\sim\sigma$, we have $\sum_{b\in B}\|\zeta\|_b\le L^2$ and thus $f(\zeta)=1$ by the definition of f. Hence, we have $f(\sigma)=f(\zeta)$ and we can neglect this case.

- $\sigma\in\mathcal{E}^A$ is cross-free and $\zeta\in\widehat{\mathcal{N}}(\mathcal{S})^c$ is adjacent to σ: By Lemma 5.4.18, the number of such σ is $O(L^6)$. Since there are at most $2qL^2$ possible $\zeta \in \widehat{\mathcal{N}}(\mathcal{S})^c$ with $\sigma \sim \zeta$, we obtain

$$\begin{aligned}\sum_{\sigma \in \mathcal{E}^A} \sum_{\zeta \in \widehat{\mathcal{N}}(\mathcal{S})^c} \mu_\beta(\zeta)[f(\zeta) - f(\sigma)]^2 &\le O(L^6) \times qL^2 \times Ce^{-(\Gamma+1)\beta} \\ &= O(L^8 e^{-(\Gamma+1)\beta}).\end{aligned}$$

By the same logic, the second summation of (5.58) is $O(L^8 e^{-(\Gamma+1)\beta})$ as well.

For the third summation of (5.58), we note that[8]

$$\mathcal{B}^{A,B} \setminus \mathcal{E}^{A,B} \subseteq \bigcup_{n=3}^{L-3} \mathcal{R}_n^{A,B} \cup \bigcup_{n=2}^{L-3} \mathcal{C}_{n,o}^{A,B} \cup \bigcup_{n=2}^{L-3} \mathcal{C}_{n,e}^{A,B} \cup \mathcal{D}^{A,B}. \tag{5.59}$$

Since $|f(\zeta) - f(\sigma)| \le 1$, we have

$$\sum_{\zeta \in \widehat{\mathcal{N}}(\mathcal{S})^c:\, \zeta \sim \sigma} \mu_\beta(\zeta)[f(\zeta) - f(\sigma)]^2 \le \sum_{\zeta \in \widehat{\mathcal{N}}(\mathcal{S})^c:\, \zeta \sim \sigma} \mu_\beta(\zeta),$$

and moreover by a direct computation, we get[9]

$$\sum_{\zeta \in \widehat{\mathcal{N}}(\mathcal{S})^c:\, \zeta \sim \sigma} \mu_\beta(\zeta) = \begin{cases} O(L^2 e^{-(\Gamma+1)\beta}) & \text{if } \sigma \in \mathcal{R}_n^{A,B}, \\ O(Le^{-(\Gamma+1)\beta}) + O(L^2 e^{-(\Gamma+2)\beta}) & \text{if } \sigma \in \mathcal{C}_{n,o}^{A,B}, \\ O(Le^{-(\Gamma+1)\beta}) + O(L^2 e^{-(\Gamma+3)\beta}) & \text{if } \sigma \in \mathcal{C}_{n,e}^{A,B}, \\ O(Le^{-(\Gamma+1)\beta}) + O(L^2 e^{-(\Gamma+3)\beta}) & \text{if } \sigma \in \mathcal{D}^{A,B}. \end{cases}$$

Since

$$\sum_{n=3}^{L-3} |\mathcal{R}_n^{A,B}| = O(L^2) \quad \text{and} \quad \sum_{n=2}^{L-3} \big(|\mathcal{C}_{n,o}^{A,B}| + |\mathcal{C}_{n,e}^{A,B}|\big) + |\mathcal{D}^{A,B}| = O(L^4),$$

[8] This is not an equality; consider e.g., $\xi \in \mathcal{C}_{2,o}^{a,b}$ with $|\mathfrak{p}^{a,b}(\xi)| = 1$ for some $a \in A$ and $b \in B$.

[9] It is enough to find the order of the number of configurations adjacent to σ with energy $\Gamma + 1$, $\Gamma + 2$, or $\Gamma + 3$. We omit tedious and elementary verification.

we can combine the computations above along with (5.59) to conclude that (as $L \ll e^{\beta}$)

$$\sum_{\sigma \in \mathcal{B}^{a,\, b} \setminus \mathcal{E}^{a,\, b}} \sum_{\zeta \in \widehat{\mathcal{N}}(\mathcal{S})^c} \mu_\beta(\sigma) r_\beta(\sigma,\, \zeta)[f(\zeta) - f(\sigma)]^2 = O(L^5 e^{-(\Gamma+1)\beta}).$$

We can now complete the proof by gathering all the results so far since

$$\sum_{\sigma \in \widehat{\mathcal{N}}(\mathcal{S})} \sum_{\zeta \in \widehat{\mathcal{N}}(\mathcal{S})^c} \mu_\beta(\sigma) r_\beta(\sigma,\, \zeta)[f(\zeta) - f(\sigma)]^2 = e^{-\Gamma\beta} \times O(L^8 e^{-\beta}) = o_L(e^{-\Gamma\beta}).$$

□

Lemma 5.7.9. *We have*

$$\sum_{\{\sigma,\zeta\} \subseteq \widehat{\mathcal{N}}(\mathcal{S})^c} \mu_\beta(\sigma) r_\beta(\sigma,\, \zeta)[f(\zeta) - f(\sigma)]^2 = o_L(e^{-\Gamma\beta}). \tag{5.60}$$

Proof. By Proposition 5.7.5-(1) and the definition of f on $\widehat{\mathcal{N}}(\mathcal{S})^c$, the left-hand side of (5.60) can be written as

$$\sum_{i=3}^{3L^2-2L} \sum_{\substack{\{\sigma,\zeta\} \subseteq \widehat{\mathcal{N}}(\mathcal{S})^c: \\ \sigma \sim \zeta,\, \max\{H(\sigma), H(\zeta)\} = 2L+i, \\ \sum_{a \in A} \|\sigma\|_a = L^2 \text{ and } \sum_{a \in A} \|\zeta\|_a = L^2 - 1}} \frac{1}{Z_\beta} e^{-(2L+i)\beta}. \tag{5.61}$$

By Theorem 5.1.2-(1) and Proposition 5.7.5-(2), the summation for $3 \le i < (\sqrt{6} - 2)L - 1$ is bounded by

$$CL \times \sum_{i=3}^{\infty} (CL)^{3i} e^{-(2L+i)\beta} \le L e^{2\beta} e^{-\Gamma\beta} \sum_{i=3}^{\infty} (CL^3 e^{-\beta})^i \le CL^{10} e^{-\beta} e^{-\Gamma\beta},$$

which equals $o(e^{-\Gamma\beta})$. We emphasize that *this is the location where the condition $L^{10} \ll e^{\beta}$ is crucially used.*

Next, by Lemma 5.2.4, there exists a positive integer θ such that

$$|\mathcal{X}_{2L+i}| \leq q^{2L+i+1} \sum_{\substack{n_3,n_4,n_5,n_6 \geq 0: \\ 3n_3+4n_4+5n_5+6n_6=2L+i}} \binom{\theta L^2}{n_3}\binom{\theta L^2}{n_4}\binom{\theta L^2}{n_5}\binom{\theta L^2}{n_6},$$

and thus by Theorem 5.1.2-(1), the summation (5.61) for $i \geq (\sqrt{6}-2)L - 1$ is bounded from above by

$$2qL^2 \sum_{j=\lfloor\sqrt{6}L\rfloor}^{3L^2} q^{j+1} \sum_{\substack{n_3,n_4,n_5,n_6 \geq 0: \\ 3n_3+4n_4+5n_5+6n_6=j}} \binom{\theta L^2}{n_3}\binom{\theta L^2}{n_4}\binom{\theta L^2}{n_5}\binom{\theta L^2}{n_6} e^{-\beta j},$$

where the factor $2qL^2$ comes from the trivial bound on the number of possible ζ (resp. σ) given σ (resp. ζ). Using $\binom{\alpha}{\beta}\binom{\gamma}{\delta} \leq \binom{\alpha+\gamma}{\beta+\delta}$, we bound this by

$$2q^2L^2 \sum_{j=\lfloor\sqrt{6}L\rfloor}^{3L^2} (qe^{-\beta})^j \sum_{\substack{n_3,n_4,n_5,n_6 \geq 0: \\ 3n_3+4n_4+5n_5+6n_6=j}} \binom{4\theta L^2}{n_3+n_4+n_5+n_6}. \tag{5.62}$$

Since $n_3+n_4+n_5+n_6 \leq \frac{1}{3}(3n_3+4n_5+5n_5+6n_6) = \frac{j}{3} \leq L^2$, and since $\theta > 1$, the last summation is bounded from above by

$$\sum_{\substack{n_3,n_4,n_5,n_6 \geq 0: \\ 3n_3+4n_4+5n_5+6n_6=j}} \binom{4\theta L^2}{\lfloor \frac{j}{3} \rfloor} \leq \binom{4\theta L^2}{\lfloor \frac{j}{3} \rfloor} \times CL^6 \leq CL^6(4\theta L^2)^{j/3}$$

for some positive constant C. Hence, (5.62) is bounded from above by

$$CL^8 \sum_{j>\sqrt{6}L-1} (qe^{-\beta})^j (4\theta L^2)^{j/3} = CL^8 \sum_{j>\sqrt{6}L-1} (CL^{2/3}e^{-\beta})^j.$$

Since $L^{2/3}e^{-\beta} \ll e^{-\frac{14}{15}\beta}$ by the condition $L^{10} \ll e^{\beta}$, we can further bound the right-hand side by

$$CL^8(Ce^{-\frac{14}{15}\beta})^{\sqrt{6}L-1} = o_L(e^{-\Gamma\beta})$$

since $\dfrac{14}{15}\sqrt{6} > 2$. □

Finally, we can now conclude the proof of Proposition 5.7.4.

Proof of Proposition 5.7.4. The fact that $f \in \mathfrak{C}(\mathcal{S}(A),\, \mathcal{S}(B))$ is immediate from the construction of f on $\mathcal{E}^{A,\,B}$. The estimate of $D_\beta(f)$ follows from the decomposition (5.51) and Lemmas 5.7.7, 5.7.8, and 5.7.9. □

Remark 5.7.10. A careful reading of the proof reveals that Lemmas 5.7.7, 5.7.8, and 5.7.9 hold under the conditions $L^{2/3} \ll e^\beta$ (the optimal condition in view of Theorem 5.1.2), $L^8 \ll e^\beta$, and $L^{10} \ll e^\beta$, respectively. This shows that the sub-optimality of our result comes essentially from our ignorance of the behavior of the process $\sigma_\beta(\cdot)$ outside $\widehat{\mathcal{N}}(\mathcal{S})$.

5.8 Lower bound for capacities

The purpose of this section is to establish a suitable test flow to apply the generalized Thomson principle (Theorem 3.2.8). This yields the lower bound for the capacity compensating for the upper bound obtained in the previous section. At the end of the current section, the proof of Theorem 5.6.1 will finally be presented. We note that Notation 5.7.1 will be consistently used in the current section as well.

5.8.1 Construction of test flow

In view of Theorem 3.2.8, the test flow should approximate the flow $c\Psi_{h_{\mathcal{S}(A),\,\mathcal{S}(B)}}$ where $h_{\mathcal{S}(A),\mathcal{S}(B)}$ denotes the equilibrium potential between $\mathcal{S}(A)$ and $\mathcal{S}(B)$.

We provide this approximation below. Since we already know the approximation of $h_{\mathcal{S}(A),\,\mathcal{S}(B)}$ from Definition 5.7.3, the construction of the test flow follows naturally from it.

Definition 5.8.1 (Test flow)**.** Recall the test function $f = f^{A,\,B}$ constructed in Definition 5.7.3. We define the test flow $\psi = \psi^{A,\,B}$ by (cf. Notation 5.7.2)

$$\psi(\sigma,\,\zeta) = \begin{cases} \mu_\beta(\sigma) r_\beta(\sigma,\,\zeta)[f(\sigma) - f(\zeta)] & \text{if } \sigma,\,\zeta \in \mathcal{B}^{A,\,B}, \\ \dfrac{\mathfrak{e}_A}{Z_\beta \mathfrak{c}} e^{-\Gamma\beta} \times [\mathfrak{h}^A(\sigma) - \mathfrak{h}^A(\zeta)] & \text{if } \sigma,\,\zeta \in \mathcal{E}^A \text{ with } \sigma \sim \zeta, \\ \dfrac{\mathfrak{e}_B}{Z_\beta \mathfrak{c}} e^{-\Gamma\beta} \times [\mathfrak{h}^B(\zeta) - \mathfrak{h}^B(\sigma)] & \text{if } \sigma,\,\zeta \in \mathcal{E}^B \text{ with } \sigma \sim \zeta, \\ 0 & \text{otherwise.} \end{cases}$$

The well-definedness of the definitions on $\mathcal{N}(\mathcal{R}_2^{A,\,B})$ and on $\mathcal{N}(\mathcal{R}_{L-2}^{A,\,B})$ should be carefully addressed. This can be checked by noting that, for $\sigma,\,\zeta \in \mathcal{N}(\mathcal{R}_2^{A,\,B})$ (resp. $\mathcal{N}(\mathcal{R}_{L-2}^{A,\,B})$), the definitions of ψ on $\mathcal{B}^{A,\,B}$ and $\mathcal{E}^{A,\,B}$ both imply that $\psi(\sigma,\,\zeta) = 0$, since we have $f(\sigma) = f(\zeta)$ as mentioned in Definition 5.7.3 and $\mathfrak{h}^A(\sigma) = \mathfrak{h}^A(\zeta)$ (resp. $\mathfrak{h}^B(\sigma) = \mathfrak{h}^B(\zeta)$), as mentioned in Notation 5.7.2.

In the remainder of the current section, we shall prove the following proposition.

Proposition 5.8.2. *For the test flow $\psi = \psi^{A,\,B}$ constructed in the previous definition, it holds that*

$$\frac{1}{\|\psi\|^2} \Big[\sum_{\sigma \in \mathcal{X}} h^\beta_{\mathcal{S}(A),\,\mathcal{S}(B)}(\sigma)(\operatorname{div}\psi)(\sigma) \Big]^2 = \frac{1 + o(1)}{q\mathfrak{c}} e^{-\Gamma\beta}. \tag{5.63}$$

The proof of this proposition is divided into two steps. First, we have to compute the flow norm $\|\psi\|^2$. This can be done by a direct computation with our explicit construction of the test flow ψ and will be presented in Section 5.8.2. Then, it remains to compute the summation appearing in the left-hand side (5.63). To that end, we have to suitably estimate $h_{\mathcal{S}(A),\,\mathcal{S}(B)}(\sigma)$ and then compute the divergence term $(\operatorname{div}\psi)(\sigma)$. This will be done in Section 5.8.3. Finally, in Section 5.8.4, we shall conclude the proof of Proposition 5.8.2 as well as the proof of Theorem 5.6.1.

The main issue in the large-volume regime in the construction of the test function carried out in the previous section is the construction on $\widehat{\mathcal{N}}(\mathcal{S})^c$. However, in the test flow, we do not encounter this sort of difficulty as we simply assign zero flow on this remainder set. Instead, an additional difficulty, compared to the small-volume regime, appears in the control of $h_{\mathcal{S}(A),\,\mathcal{S}(B)}(\sigma)$.

5.8.2 Flow norm of ψ

Proposition 5.8.3. *For $L^{2/3} \ll e^\beta$, it holds that*

$$\|\psi\|^2 = \frac{1+o(1)}{q\mathfrak{c}} e^{-\Gamma\beta}.$$

Proof. The strategy is to compare the flow norm with the Dirichlet form of f. Since $\psi \equiv 0$ on $\mathcal{B}^{A,\,B} \cap \mathcal{E}^A$ and $\mathcal{B}^{A,\,B} \cap \mathcal{E}^A$ as mentioned in Definition 5.8.1, we can write

$$\|\psi\|^2 = \Big[\sum_{\{\sigma,\zeta\}\subseteq\mathcal{B}^{a,\,b}} + \sum_{\{\sigma,\zeta\}\subseteq\mathcal{E}^A} + \sum_{\{\sigma,\zeta\}\subseteq\mathcal{E}^B} \Big] \frac{\psi(\sigma,\,\zeta)^2}{\mu_\beta(\sigma) r_\beta(\sigma,\,\zeta)}. \tag{5.64}$$

Let us consider three summations separately.

- By the definition of ψ on $\mathcal{B}^{A,\,B}$, we can write the first summation as

$$\sum_{\{\sigma,\zeta\}\subseteq\mathcal{B}^{a,\,b}} \mu_\beta(\sigma) r_\beta(\sigma,\,\zeta) [f^{A,\,B}(\sigma) - f^{A,\,B}(\zeta)]^2. \tag{5.65}$$

- By the definition of ψ on $\mathcal{E}^A$, the second summation equals

$$\sum_{\{\sigma,\,\zeta\}\subseteq\mathcal{E}^A}\frac{1}{\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)}\times\frac{\mathfrak{e}_A^2}{Z_\beta^2\mathfrak{c}^2}e^{-2\Gamma\beta}\times[\mathfrak{h}^A(\sigma)-\mathfrak{h}^A(\zeta)]^2.$$

  Note from Notation 5.7.2 that $\{\sigma,\,\zeta\}\subseteq\mathcal{E}^A$ with $\mathfrak{h}^A(\sigma)\neq\mathfrak{h}^A(\zeta)$ implies $\max\{H(\sigma),\,H(\zeta)\}=\Gamma$. Thus, by (5.8), we can rewrite the last summation as

$$\begin{aligned}&\sum_{\{\sigma,\,\zeta\}\subseteq\mathcal{E}^A}\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)\times\frac{\mathfrak{e}_A^2}{\mathfrak{c}^2}[\mathfrak{h}^A(\sigma)-\mathfrak{h}^A(\zeta)]^2\\&=\sum_{\{\sigma,\,\zeta\}\subseteq\mathcal{E}^A}\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)[f(\sigma)-f(\zeta)]^2.\end{aligned}\tag{5.66}$$

  Similarly, the third summation equals

$$\sum_{\{\sigma,\,\zeta\}\subseteq\mathcal{E}^B}\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)[f(\sigma)-f(\zeta)]^2.\tag{5.67}$$

Gathering (5.54), (5.55), (5.56), and (5.67), we can conclude that

$$\|\psi\|^2=\sum_{\{\sigma,\,\zeta\}\subseteq\widehat{\mathcal{N}}(\mathcal{S})}\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)[f(\sigma)-f(\zeta)]^2.$$

The right-hand side is $\dfrac{1+o(1)}{q\mathfrak{c}}e^{-\Gamma\beta}$ by Lemma 5.7.7 and the proof is completed. $\square$

5.8.3 Divergence of ψ

Next, we compute the summation appearing in (5.63). More precisely, we wish to prove the following proposition in this section.

Proposition 5.8.4. *Suppose that $L^{10} \ll e^{\beta}$. Then, we have that*

$$\sum_{\sigma\in\mathcal{X}} h_{\mathcal{S}(A),\,\mathcal{S}(B)}(\sigma)(\operatorname{div}\psi)(\sigma) = \frac{1}{q\mathfrak{c}}e^{-\Gamma\beta} + o(e^{-\Gamma\beta}). \tag{5.68}$$

The proof is divided into several lemmas. We first look at the divergence term $(\operatorname{div}\psi)(\sigma)$. We deduce that this divergence is zero at most of the bulk configurations.

Lemma 5.8.5. *We have* $(\operatorname{div}\psi)(\sigma) = 0$ *if*

(1) $\sigma \in \mathcal{D}^{A,\,B}$,

(2) $\sigma \in \mathcal{C}^{a,\,b}_{n,\,e}$ *for some* $a \in A$, $b \in B$ *and* $n \in [\![2,\, L-3]\!]$, *and*

(3) $\sigma \in \mathcal{C}^{a,\,b}_{n,\,o}$ *with* $|\mathfrak{p}^{a,\,b}(\sigma)| \in [\![3,\, 2L-3]\!]$ *for some* $a \in A$, $b \in B$ *and* $n \in [\![2,\, L-3]\!]$.

Proof. (1) By the definition of f on $\mathcal{D}^{a,\,b}$ in Definition 5.7.3, we have $f(\sigma) = f(\zeta)$ for all $\zeta \sim \sigma$ with $\zeta \in \widehat{\mathcal{N}}(\mathcal{S})$. Recalling the definition of ψ in Definition 5.8.1, we have $\psi(\sigma,\,\zeta) = 0$ for all $\sigma \in \mathcal{D}^{a,\,b}$ and $\zeta \sim \sigma$, and we are done.

(2) For $\sigma \in \mathcal{C}^{a,\,b}_{n,\,e}$ with $n \in [\![2,\, L-3]\!]$, by Lemma 5.4.21 and (5.8), we can write

$$(\operatorname{div}\psi)(\sigma) = \frac{1}{Z_\beta}e^{-\Gamma\beta} \times \sum_{\zeta\in\mathcal{C}^{a,\,b}_{n,o}:\,\zeta\sim\sigma} [f(\sigma) - f(\zeta)].$$

The last summation can be computed as

$$\begin{cases} \frac{\mathfrak{b}}{\mathfrak{c}} \times \big[\frac{\frac{5}{2}-\frac{5}{2}}{(5L-3)(L-4)}\big] = 0 & \text{if } |\mathfrak{p}^{a,\,b}(\sigma)| \in [\![4,\, 2L-4]\!], \\ \frac{\mathfrak{b}}{\mathfrak{c}} \times \big[\frac{3-3}{(5L-3)(L-4)}\big] = 0 & \text{if } |\mathfrak{p}^{a,\,b}(\sigma)| = 2 \text{ and } \mathfrak{p}^{a,\,b}(\sigma) \text{ is connected}, \\ \frac{\mathfrak{b}}{\mathfrak{c}} \times \big[\frac{4-2-2}{(5L-3)(L-4)}\big] = 0 & \text{if } |\mathfrak{p}^{a,\,b}(\sigma)| = 2 \text{ and } \mathfrak{p}^{a,\,b}(\sigma) \text{ is disconnected}, \end{cases}$$

and we can similarly handle the case $|\mathfrak{p}^{a,\,b}(\sigma)| = 2L-2$. This proves part (2).

(3) For $\sigma \in \mathcal{C}_{n,\,o}^{a,\,b}$ with $|\mathfrak{p}^{a,\,b}(\sigma)| \in [\![3,\,2L-3]\!]$ and $n \in [\![2,\,L-3]\!]$, by Lemma 5.4.20 and (5.8), we can write

$$(\operatorname{div}\psi)(\sigma) = \frac{1}{Z_\beta} e^{-\Gamma\beta} \times \sum_{\zeta \in \mathcal{C}_{n,e}^{a,\,b} \cup \mathcal{Q}_n^{a,\,b}:\,\zeta\sim\sigma} [f(\sigma) - f(\zeta)].$$

For $\zeta \in \mathcal{Q}_n^{a,\,b}$, the summation vanishes by Lemma 5.4.24 and Definition 5.7.3-(2). For $\zeta \in \mathcal{C}_{n,\,e}^{a,\,b}$, the last summation is calculated as

$$\frac{\mathfrak{b}}{\mathfrak{c}} \times \Big[\frac{\frac{5}{2} \times 4 - \frac{5}{2} \times 4}{(5L-3)(L-4)}\Big] = 0. \tag{5.69}$$

This concludes the proof. □

In the previous lemma, it has been shown that the divergence of ψ is zero on all bulk configurations except in $\mathcal{N}(\mathcal{R}_n^{A,\,B})$ with $n \in [\![2,\,L-2]\!]$. We next show that the divergences on these sets are canceled out with each other.

Lemma 5.8.6. *Let $\zeta \in \mathcal{R}_n^{A,\,B}$ for some $n \in [\![2,\,L-2]\!]$. Then, we have*

$$\sum_{\sigma \in \mathcal{N}(\zeta)} (\operatorname{div}\psi)(\sigma) = 0.$$

Proof. Let $a \in A$, $b \in B$ and $n \in [\![2,\,L-2]\!]$ and then fix $\zeta \in \mathcal{R}_n^{a,\,b}$.

First, by definitions of f and ψ, we can readily deduce that $\psi(\zeta,\,\xi) = 0$ for all $\xi \in \mathcal{X}$ and therefore we immediately have $(\operatorname{div}\psi)(\zeta) = 0$. Next let $\sigma \in \mathcal{N}(\zeta) \setminus \{\zeta\}$ so that, by Lemma 5.4.19,

$$\begin{cases} \sigma \in \mathcal{C}_{n,\,o}^{a,\,b} \text{ with } |\mathfrak{p}^{a,\,b}(\sigma)| = 1 \text{ or} \\ \sigma \in \mathcal{C}_{n-1,\,o}^{a,\,b} \text{ with } |\mathfrak{p}^{a,\,b}(\sigma)| = 2L-1. \end{cases} \tag{5.70}$$

(Case 1: $n \in [\![3,\,L-3]\!]$**)** By (5.8) and explicit definitions of f and ψ, we can check through elementary computations that

$$(\mathrm{div}\,\psi)(\sigma)=\begin{cases}\dfrac{1}{Z_\beta}\dfrac{10\mathfrak{b}e^{-\Gamma\beta}}{\mathfrak{c}(5L-3)(L-4)} & \text{if } \sigma\in\mathcal{C}^{a,\,b}_{n,\,o},\ |\mathfrak{p}^{a,\,b}(\sigma)|=1,\\ -\dfrac{1}{Z_\beta}\dfrac{10\mathfrak{b}e^{-\Gamma\beta}}{\mathfrak{c}(5L-3)(L-4)} & \text{if } \sigma\in\mathcal{C}^{a,\,b}_{n-1,\,o},\ |\mathfrak{p}^{a,\,b}(\sigma)|=2L-1.\end{cases} \tag{5.71}$$

Hence, we have

$$\sum_{\sigma\in\mathcal{N}(\zeta)}(\mathrm{div}\,\psi)(\sigma)=0+\Big[\frac{1}{Z_\beta}\frac{10\mathfrak{b}e^{-\Gamma\beta}}{\mathfrak{c}(5L-3)(L-4)}-\frac{1}{Z_\beta}\frac{10\mathfrak{b}e^{-\Gamma\beta}}{\mathfrak{c}(5L-3)(L-4)}\Big]\times 2L=0.$$

(Case 2: $n=2$ or $L-2$) First, we let $n=2$. By the same computation above, we can check

$$(\mathrm{div}\,\psi)(\sigma)=\frac{1}{Z_\beta}\frac{10\mathfrak{b}e^{-\Gamma\beta}}{\mathfrak{c}(5L-3)(L-4)}\quad \text{if } \sigma\in\mathcal{C}^{a,\,b}_{2,\,o}\text{ with } |\mathfrak{p}^{a,\,b}(\sigma)|=1. \tag{5.72}$$

On the other hand, by the definition of ψ on $\mathcal{E}^A$, we can write

$$\sum_{\sigma\in\mathcal{C}^{a,\,b}_{1,\,o}\cap\mathcal{N}(\zeta)}(\mathrm{div}\,\psi)(\sigma)=\sum_{\sigma\in\mathcal{C}^{a,\,b}_{1,\,o}\cap\mathcal{N}(\zeta)}\ \sum_{\xi\in\mathcal{O}^A:\,\xi\sim\sigma}\psi(\sigma,\,\xi)=\sum_{\sigma\in\mathcal{N}(\zeta)}\ \sum_{\xi\in\mathcal{O}^A:\,\xi\sim\sigma}\psi(\sigma,\,\xi),$$

where the first equality holds since, for $\sigma\in\mathcal{C}^{a,\,b}_{1,\,o}\cap\mathcal{N}(\zeta)$, we have $\psi(\sigma,\,\xi)=0$ unless $\xi\in\mathcal{O}^A$, and the second equality holds since the configurations in $\mathcal{C}^{a,\,b}_{2,\,o}\cup\{\zeta\}$ is not connected with $\mathcal{O}^A$. By (5.8), we can write

$$\begin{aligned}\sum_{\sigma\in\mathcal{N}(\zeta)}\ \sum_{\xi\in\mathcal{O}^A:\,\xi\sim\sigma}\psi(\sigma,\,\xi)&=\sum_{\sigma\in\mathcal{N}(\zeta)}\ \sum_{\xi\in\mathcal{O}^A:\,\xi\sim\sigma}\frac{\mathfrak{e}_A}{Z_\beta\mathfrak{c}}e^{-\Gamma\beta}[\mathfrak{h}^A(\sigma)-\mathfrak{h}^A(\xi)]\\ &=\frac{\mathfrak{e}_A}{Z_\beta\mathfrak{c}}e^{-\Gamma\beta}\sum_{\xi\in\mathcal{O}^A}r^A(\zeta,\,\xi)[\mathfrak{h}^A(\zeta)-\mathfrak{h}^A(\xi)]\\ &=-\frac{\mathfrak{e}_A}{Z_\beta\mathfrak{c}}e^{-\Gamma\beta}\times(L^A\mathfrak{h}^A)(\zeta),\end{aligned}$$

where the second equality follows from Notation (5.7.2) and the definition of

r^A (cf. (5.38)). By the property of capacities (e.g. [16, Lemmas 7.7 and 7.12]) and the definition of $\mathfrak{e}_A$ (cf. (5.39)), we get

$$\sum_{\zeta\in\mathcal{R}_2^{a,\,b}}(L^A\mathfrak{h}^A)(\zeta)=|\mathscr{V}^A|\mathrm{cap}^A\big(\mathcal{S}(A),\,\mathcal{R}_2^{A,\,B}\big)=\frac{1}{\mathfrak{e}_A},\tag{5.73}$$

and therefore by symmetry, we get

$$(L^A\mathfrak{h}^A)(\zeta)=\frac{1}{|\mathcal{R}_2^{A,\,B}|\mathfrak{e}_A}=\frac{1}{3L|A|(q-|A|)\mathfrak{e}_A},$$

where the factor 3 comes from three possible directions. By gathering the computations above, we can conclude that

$$\sum_{\sigma\in\mathcal{C}_{1,\,o}^{a,\,b}\cap\mathcal{N}(\zeta)}(\mathrm{div}\,\psi)(\sigma)=\frac{1}{Z_\beta\mathfrak{c}}e^{-\Gamma\beta}\times\frac{1}{3L|A|(q-|A|)}.\tag{5.74}$$

By (5.72) and (5.74), Theorem 5.1.2-(1), and by recalling the definitions (5.42) of $\mathfrak{b}$ and $\mathfrak{c}$, we finally get

$$\sum_{\sigma\in\mathcal{N}(\zeta)}(\mathrm{div}\,\psi)(\sigma)=\frac{1}{Z_\beta}\frac{10\mathfrak{b}e^{-\Gamma\beta}}{\mathfrak{c}(5L-3)(L-4)}\times 2L-\frac{1}{Z_\beta\mathfrak{c}}e^{-\Gamma\beta}\times\frac{1}{3L|A|(q-|A|)}=0.$$

Since the proof for the case $n=L-2$ is identical, the proof is completed. □

Next, we turn to the divergences of ψ on the edge typical configurations.

Lemma 5.8.7. *For all* $\sigma\in\mathcal{O}^A\cup\mathcal{O}^B$*, we have* $(\mathrm{div}\,\psi)(\sigma)=0$.

Proof. We only consider the case $\sigma\in\mathcal{O}^A$ since the proof for $\mathcal{O}^B$ is identical. By definition of ψ, we can write

$$\begin{aligned}(\mathrm{div}\,\psi)(\sigma)=\sum_{\zeta\in\mathcal{E}^A:\,\zeta\sim\sigma}\psi(\sigma,\,\zeta)&=\sum_{\zeta\in\mathcal{E}^A:\,\zeta\sim\sigma}\frac{\mathfrak{e}_A}{Z_\beta\mathfrak{c}}e^{-\Gamma\beta}\times\big[\,\mathfrak{h}^A(\sigma)-\mathfrak{h}^A(\zeta)\,\big]\\&=-\frac{\mathfrak{e}_A}{Z_\beta\mathfrak{c}}e^{-\Gamma\beta}\times(L^A\mathfrak{h}^A)(\sigma).\end{aligned}$$

Since $\mathcal{O}^A \subseteq \mathcal{E}^A \setminus (\mathcal{S}(A) \cup \mathcal{R}_2^{A,\,B})$, we have $(L^A \mathfrak{h}^A)(\sigma) = (L^A h^A_{\mathcal{S}(A),\,\mathcal{R}_2^{a,\,b}})(\sigma) = 0$ by the elementary property of equilibrium potentials. This completes the proof. □

Lemma 5.8.8. *For $a \in A$, $b \in B$, and $\sigma \in \mathcal{C}^{a,\,b}_{1,\,o} \cup \mathcal{C}^{a,\,b}_{L-2,\,o}$ with $|\mathfrak{p}^{a,\,b}(\sigma)| \in [\![3,\,2L-3]\!]$, we have $(\mathrm{div}\,\psi)(\sigma) = 0$.*

Proof. By symmetry, we may assume $\sigma \in \mathcal{C}^{a,\,b}_{1,\,o}$ and $|\mathfrak{p}^{a,\,b}(\sigma)| \in [\![3,\,2L-3]\!]$. Then as $\mathcal{N}(\sigma) = \{\sigma\}$, we may write

$$
\begin{aligned}
(\mathrm{div}\,\psi)(\sigma) = \sum_{\zeta \in \mathcal{E}^A:\,\zeta \sim \sigma} \psi(\sigma,\,\zeta) &= \sum_{\zeta \in \mathcal{O}^A:\,\zeta \sim \sigma} \frac{\mathfrak{e}_A}{Z_\beta \mathfrak{c}} e^{-\Gamma\beta} \times \big[\mathfrak{h}^A(\sigma) - \mathfrak{h}^A(\zeta)\big] \\
&= -\frac{\mathfrak{e}_A}{Z_\beta \mathfrak{c}} e^{-\Gamma\beta} \times (L^A \mathfrak{h}^A)(\sigma).
\end{aligned}
$$

Since $\sigma \notin \mathcal{S}(A) \cup \mathcal{R}_2^{A,\,B}$, we again have $(L^A \mathfrak{h}^A)(\sigma) = (L^A h^A_{\mathcal{S}(A),\,\mathcal{R}_2^{a,\,b}})(\sigma) = 0$ and the proof is completed. □

Lemma 5.8.9. *We have $(\mathrm{div}\,\psi)(\sigma) = 0$ for all $\sigma \in \mathcal{N}(\zeta)$ with $\zeta \in \mathcal{I}^A_{\mathrm{rep}} \setminus (\mathcal{S}(A) \cup \mathcal{R}_2^{A,\,B} \cup \mathcal{C}^{A,\,B}_{1,\,o})$.*

Proof. For all $\xi \in \widehat{\mathcal{N}}(\mathcal{S})$ with $\sigma \sim \xi$, by Lemma 5.5.8, both σ and ξ have an a-cross for some $a \in A$. Therefore, we have by Lemma 5.5.6 that $\mathfrak{h}^A(\sigma) = \mathfrak{h}^A(\xi) = 1$ and therefore we have $\psi(\sigma,\,\xi) = 0$. This concludes the proof. □

Lemma 5.8.10. *We have*

$$
\sum_{\sigma \in \mathcal{N}(\mathcal{S}(A))} (\mathrm{div}\,\psi)(\sigma) = \frac{1}{Z_\beta \mathfrak{c}} e^{-\Gamma\beta} \quad \textit{and} \quad \sum_{\sigma \in \mathcal{N}(\mathcal{S}(B))} (\mathrm{div}\,\psi)(\sigma) = -\frac{1}{Z_\beta \mathfrak{c}} e^{-\Gamma\beta}.
$$

Proof. We focus only on the first one since the proof for the second one is identical. As in the previous proof, we can write

$$
\begin{aligned}
\sum_{\sigma \in \mathcal{N}(\mathcal{S}(A))} (\mathrm{div}\,\psi)(\sigma) &= \sum_{\sigma \in \mathcal{S}(A)} \sum_{\zeta \in \mathcal{E}^A:\,\zeta \sim \sigma} \frac{\mathfrak{e}_A}{Z_\beta \mathfrak{c}} e^{-\Gamma\beta} \times \big[\,\mathfrak{h}^A(\sigma) - \mathfrak{h}^A(\zeta)\,\big] \\
&= -\frac{\mathfrak{e}_A}{Z_\beta \mathfrak{c}} e^{-\Gamma\beta} \times \sum_{\sigma \in \mathcal{S}(A)} (L^A \mathfrak{h}^A)(\sigma).
\end{aligned}
\tag{5.75}
$$

By the same reasoning with (5.73), we have that

$$\sum_{\sigma\in\mathcal{S}(A)}(L^A\mathfrak{h}^A)(\sigma)=-|\mathscr{V}^A|\mathrm{cap}^A\big(\mathcal{S}(A),\,\mathcal{R}_2^{A,\,B}\big)=-\frac{1}{\mathfrak{e}_A},$$

and injecting this to (5.75) completes the proof. □

Since we only have the control on the summation of divergences in the $\mathcal{N}$-neighborhoods of ground states or regular configurations, we need the following flatness result on the equilibrium potential $h^{\beta}_{\mathcal{S}(A),\,\mathcal{S}(B)}$ on these $\mathcal{N}$-neighborhoods to control the summation at the left-hand side of (5.68).

Lemma 5.8.11. *There exists $C>0$ such that the following results hold.*

(1) For $\boldsymbol{s}\in\mathcal{S}$ and $\sigma\in\mathcal{N}(\boldsymbol{s})$, denote by N_σ the shortest length of $(\Gamma-1)$-paths connecting $\boldsymbol{s}$ and σ. Then, it holds that

$$\big|h_{\mathcal{S}(A),\,\mathcal{S}(B)}(\sigma)-h_{\mathcal{S}(A),\,\mathcal{S}(B)}(\boldsymbol{s})\big|\le CN_\sigma e^{-\beta}.\tag{5.76}$$

(2) For all $n\in[\![2,\,L-2]\!]$ and $\zeta\in\mathcal{R}_n^{A,\,B}$, it holds that

$$\max_{\sigma\in\mathcal{N}(\zeta)}\big|h_{\mathcal{S}(A),\,\mathcal{S}(B)}(\sigma)-h_{\mathcal{S}(A),\,\mathcal{S}(B)}(\zeta)\big|\le CL^2e^{-\beta}.$$

The proof of this lemma follows from a well-known standard renewal argument (cf. [16, Lemma 8.4]) along with rough estimate of capacities based on the Dirichlet–Thomson principles. Moreover, the proof is identical to that of Lemma 3.5.8. Thus, we omit the detail of the proof. The reason why we have the L^2-term in the right-hand side of part (2) comes from explicit computation, i.e., the number of pairs of configurations $(\xi_1,\,\xi_2)$ with $\xi_1\in\mathcal{N}(\zeta)$, $\xi_2\notin\mathcal{N}(\zeta)$, and $\xi_1\sim\xi_2$.

We next control the factor N_σ appearing in (5.76). Note that this quantitative result was not needed in small-volume regime.

Lemma 5.8.12. *In the notation of Lemma 5.8.11 with* $\boldsymbol{s} = \boldsymbol{a}$ *for some* $a \in A$*, we have* $N_\sigma < 4L$ *if* $(\operatorname{div}\psi)(\sigma) \neq 0$.

Proof. By the definition of ψ that for $\sigma \in \mathcal{N}(\boldsymbol{s})$,

$$(\operatorname{div}\psi)(\sigma) = \sum_{\zeta \in \mathcal{O}^A :\, \zeta \sim \sigma} \psi(\sigma,\, \zeta) = \sum_{\zeta \in \mathcal{O}^A} \frac{\mathfrak{e}_A}{Z_\beta \mathfrak{c}} e^{-\Gamma\beta} \times [1 - \mathfrak{h}^A(\zeta)]. \tag{5.77}$$

Therefore, $(\operatorname{div}\psi)(\sigma) \neq 0$ if and only if there exists $\zeta \in \mathcal{O}^A$ with $\mathfrak{h}^A(\zeta) \neq 1$. Therefore, the statement of lemma is a direct consequence of Lemma 5.5.7. □

Lemma 5.8.13. *There exists* $C > 0$ *such that*

$$\sum_{\sigma \in \mathcal{N}(\zeta)} |(\operatorname{div}\psi)(\sigma)| \le CL^2 e^{-\Gamma\beta} \quad \textit{for all } \zeta \in \mathcal{R}_n^{A,\,B} \textit{ with } n \in [\![2,\, L-2]\!], \tag{5.78}$$

$$\sum_{\sigma \in \mathcal{N}(\boldsymbol{s})} |(\operatorname{div}\psi)(\sigma)| \le CL^9 e^{-\Gamma\beta} \quad \textit{for all } \boldsymbol{s} \in \mathcal{S}. \tag{5.79}$$

Proof. First, suppose that $\zeta \in \mathcal{R}_n^{A,\,B}$ with $n \in [\![3,\, L-3]\!]$. Then, we have by (5.71) that

$$\sum_{\sigma \in \mathcal{N}(\zeta)} |(\operatorname{div}\psi)(\sigma)| = 8L \times \frac{1}{Z_\beta} \frac{10\mathfrak{b} e^{-\Gamma\beta}}{\mathfrak{c}(5L-3)(L-4)} \le CL^{-1} e^{-\Gamma\beta},$$

where the factor $8L$ denotes the number of $\sigma \in \mathcal{N}(\zeta) \setminus \{\zeta\}$. This proves (5.78) in this case.

Next, suppose that $\zeta \in \mathcal{R}_2^{A,\,B}$, say $\zeta \in \mathcal{R}_2^{a,\,b}$ for some $(a,\, b) \in A \times B$. In this case, as above, we again have $(\operatorname{div}\psi)(\zeta) = 0$ and for $\sigma \in \mathcal{N}(\zeta)$ with $\sigma \in \mathcal{C}_{2,\,o}^{a,\,b}$ and $|\mathfrak{p}^{a,\,b}(\sigma)| = 1$,

$$|(\operatorname{div}\psi)(\sigma)| = \frac{1}{Z_\beta} \frac{10\mathfrak{b} e^{-\Gamma\beta}}{\mathfrak{c}(5L-3)(L-4)} \le CL^{-2} e^{-\Gamma\beta}. \tag{5.80}$$

Moreover, if $\sigma \in \mathcal{N}(\zeta)$ with $\sigma \in \mathcal{C}_{1,o}^{a,b}$ and $|\mathfrak{p}^{a,b}(\sigma)| = 2L-1$, then by the definition of ψ, we have

$$|(\operatorname{div}\psi)(\sigma)| \le \sum_{\xi:\,\xi\sim\sigma} |\psi(\sigma,\,\xi)| = \sum_{\xi:\,\xi\sim\sigma} \frac{\mathfrak{c}_A}{Z_\beta \mathfrak{c}} e^{-\Gamma\beta} \times |\mathfrak{h}^A(\sigma) - \mathfrak{h}^A(\xi)|.$$

Since number of such ξ is trivially bounded by $2qL^2$, we can bound the right-hand side using Proposition 5.5.10 by

$$2qL^2 \times CL^{-1}e^{-\Gamma\beta} = 2qCLe^{-\Gamma\beta}, \tag{5.81}$$

where we used $|\mathfrak{h}^A(\sigma) - \mathfrak{h}^A(\xi)| \le 1$. Therefore by (5.80) and (5.81), we have

$$\sum_{\sigma\in\mathcal{N}(\zeta)} |(\operatorname{div}\psi)(\sigma)| \le 4L \times CL^{-2}e^{-\Gamma\beta} + 4L \times 2qCLe^{-\Gamma\beta} = O(L^2 e^{-\Gamma\beta}),$$

where the two factors $4L$ denote the number of such possible σ. This concludes (5.78) in the case $\zeta \in \mathcal{R}_2^{A,\,B}$. The case $\mathcal{R}_{L-2}^{A,\,B}$ can be proved in the same manner. Thus, we conclude the proof of (5.78).

Finally, we prove (5.79). We may assume $\boldsymbol{s} = \boldsymbol{a}$ for some $a \in A$. By the definition of ψ, we have

$$\sum_{\sigma\in\mathcal{N}(\boldsymbol{a})} |(\operatorname{div}\psi)(\sigma)| = \sum_{\sigma\in\mathcal{N}(\boldsymbol{a})} \sum_{\zeta\in\mathcal{O}^A:\,\sigma\sim\zeta} \frac{\mathfrak{c}_A}{Z_\beta \mathfrak{c}} e^{-\Gamma\beta} \times |\mathfrak{h}^A(\sigma) - \mathfrak{h}^A(\zeta)|.$$

Since the summand vanishes if $\mathfrak{h}^A(\zeta) = \mathfrak{h}^A(\sigma)$, we can bound the right-hand side by

$$\sum_{\sigma\in\mathcal{N}(\boldsymbol{a})} \sum_{\zeta\in\mathcal{O}^A:\,\sigma\sim\zeta,\,\mathfrak{h}^A(\zeta)\ne 1} \frac{\mathfrak{c}_A}{Z_\beta \mathfrak{c}} e^{-\Gamma\beta} \le \sum_{\sigma\in\mathcal{N}(\boldsymbol{a})} \sum_{\zeta\in\mathcal{O}^A:\,\sigma\sim\zeta,\,\mathfrak{h}^A(\zeta)\ne 1} CL^{-1}e^{-\Gamma\beta},$$

where the inequality is induced by Proposition 5.5.10 and Theorem 5.1.2-(1). By Lemma 5.5.7, the number of such σ so that the summand does not vanish is $O(L^8)$, and for each such σ, the corresponding ζ has at most $2qL^2$ choices.

Thus, we conclude

$$\sum_{\sigma\in\mathcal{N}(\boldsymbol{a})}|(\operatorname{div}\psi)(\sigma)|\le O(L^8)\times 2qL^2\times CL^{-1}e^{-\Gamma\beta}=O(L^9e^{-\Gamma\beta}).$$

This concludes the proof of Lemma 5.8.13. □

Now, we are ready to prove Proposition 5.8.4.

Proof of Proposition 5.8.4. It is clear from the definition of ψ that $\operatorname{div}\psi=0$ on $\widehat{\mathcal{N}}(\mathcal{S})^c$. Hence, by Lemmas 5.8.5, 5.8.7, 5.8.8, and 5.8.9, we can write the left-hand side of (5.68) as

$$\Big[\sum_{n=2}^{L-2}\sum_{\zeta\in\mathcal{R}_n^{a,\,b}}\sum_{\sigma\in\mathcal{N}(\zeta)}+\sum_{\zeta\in\mathcal{S}}\sum_{\sigma\in\mathcal{N}(\zeta)}\Big]h_{\mathcal{S}(A),\,\mathcal{S}(B)}(\sigma)(\operatorname{div}\psi)(\sigma). \tag{5.82}$$

By Lemmas 5.8.6, 5.8.10, 5.8.11, 5.8.12, and 5.8.13, this equals

$$\frac{1}{Z_\beta\mathfrak{c}}e^{-\Gamma\beta}+L^2\times O(L^2e^{-\beta})\times O(L^2e^{-\Gamma\beta})+O(Le^{-\beta})\times O(L^9e^{-\Gamma\beta})=\frac{1+o(1)}{Z_\beta\mathfrak{c}}e^{-\Gamma\beta},$$

since $L^{10}\ll e^\beta$, where the factor L^2 takes the possibility of selecting a regular configuration in $\mathcal{R}_n^{A,\,B}$, $n\in[\![2,\,L-2]\!]$ into account. By Theorem 5.1.2-(1), the proof is completed. □

5.8.4 Proof of Theorem 5.6.1

First, by gathering the previous proposition with Proposition 5.8.3, we can conclude the proof of Proposition 5.8.2.

Proof of Proposition 5.8.2. By Propositions 5.8.3 and 5.8.4, we have

$$\|\psi^{A,\,B}\|^2=\frac{1+o(1)}{q\mathfrak{c}}e^{-\Gamma\beta},\quad \sum_{\sigma\in\mathcal{X}}h_{\mathcal{S}(A),\,\mathcal{S}(B)}(\sigma)(\operatorname{div}\psi^{A,\,B})(\sigma)=\frac{1+o(1)}{q\mathfrak{c}}e^{-\Gamma\beta}.$$

Inserting these to the left-hand side of (5.63) completes the proof. ☐

Then, we can now complete the proof of the capacity estimate.

Proof of Theorem 5.6.1. By Theorem 3.2.5 and Proposition 5.7.4, we get the upper bound as

$$\mathrm{Cap}_\beta\big(\mathcal{S}(A),\,\mathcal{S}(B)\big) \le D_\beta(f^{A,\,B}) = \frac{1+o(1)}{q\mathfrak{c}}e^{-\Gamma\beta}.$$

On the other hand, by Theorem 3.2.8 and Proposition 5.8.2, we get the matching lower bound as

$$\begin{aligned}\mathrm{Cap}_\beta\big(\mathcal{S}(A),\,\mathcal{S}(B)\big) &\ge \frac{1}{\|\psi^{A,\,B}\|^2}\Big[\sum_{\sigma\in\mathcal{X}} h_{\mathcal{S}(A),\,\mathcal{S}(B)}(\sigma)(\mathrm{div}\,\psi^{A,\,B})(\sigma)\Big]^2 \\ &= \frac{1+o(1)}{q\mathfrak{c}}e^{-\Gamma\beta}.\end{aligned}$$

The proof is completed by combining these upper and lower bounds. ☐

Chapter 6

Blume–Capel model

6.1 Main results

6.1.1 Model definition

Blume–Capel model

We define the Blume–Capel model on the finite 2D lattice box $\Lambda = [\![1,\, K]\!] \times [\![1,\, L]\!]$, where K and L are fixed positive integers. For convenience, we assume that

$$5 \le K \le L. \tag{6.1}$$

We impose either open or periodic boundary conditions on Λ. If $K = L$ under the periodic boundary conditions, the lattice is indeed $\mathbb{T}_L \times \mathbb{T}_L$ as in the previous studies [26, 28, 53]. For $x,\, y \in \Lambda$, we write $x \sim y$ if they are nearest neighbors; that is, $|x - y| = 1$.

We have three spins in this model, namely -1, 0, and $+1$. We denote by $\mathcal{X} = \{-1,\, 0,\, +1\}^\Lambda$ the space of the spin configurations on Λ. Subsequently, we define the Hamiltonian $H : \mathcal{X} \to \mathbb{R}$ as

$$H(\sigma) = \sum_{x \sim y} \{\sigma(x) - \sigma(y)\}^2 - \lambda \sum_{x \in \Lambda} \sigma(x)^2 - h \sum_{x \in \Lambda} \sigma(x). \tag{6.2}$$

Here, $\sigma(x)$ is the spin of configuration $\sigma \in \mathcal{X}$ at site $x \in \Lambda$. Moreover, we assume that the *chemical potential* λ and *external field* h are both zero, so that

$$H(\sigma) = \sum_{x \sim y} \{\sigma(x) - \sigma(y)\}^2. \tag{6.3}$$

We denote by μ_β the Gibbs distribution on $\mathcal{X}$ associated with the Hamiltonian H at the inverse temperature $\beta > 0$:

$$\mu_\beta(\sigma) = \frac{1}{Z_\beta} e^{-\beta H(\sigma)}, \quad Z_\beta = \sum_{\sigma \in \mathcal{X}} e^{-\beta H(\sigma)}. \tag{6.4}$$

We denote by $\mathbf{-1}$, $\mathbf{0}$, $\mathbf{+1} \in \mathcal{X}$ the monochromatic configurations, of which all spins are -1, 0, $+1$, respectively. We write

$$\mathcal{S} = \{\mathbf{-1}, \mathbf{0}, \mathbf{+1}\}. \tag{6.5}$$

When we select spins a or b, the corresponding monochromatic configuration is denoted by $\boldsymbol{a} \in \mathcal{S}$ or $\boldsymbol{b} \in \mathcal{S}$, respectively. It is precisely on $\mathcal{S}$ that $H(\cdot)$ attains its minimum 0, and hence, $\mathcal{S}$ denotes the collection of *ground states*. The following estimates are straightforward:

$$Z_\beta = 3 + O(e^{-2\beta}) \quad \text{and} \quad \lim_{\beta \to \infty} \mu_\beta(\boldsymbol{s}) = \frac{1}{3} \text{ for all } \boldsymbol{s} \in \mathcal{S}. \tag{6.6}$$

Also, recall the continuous-time MH dynamics $\sigma_\beta(\cdot) = \sigma_\beta^{\mathrm{MH}}(\cdot)$.

Remark 6.1.1. We remark on the model symmetry. First, our model is fully symmetric with respect to the spin correspondence $-1 \leftrightarrow +1$. *However, our model is not symmetric with respect to* $-1 \leftrightarrow 0$ *or* $0 \leftrightarrow +1$. Therefore, spins -1 and $+1$ play the same role, but spin 0 does not. This is the *main difference* from the Potts model studied in Chapter 3, in which all of the spins play the same role. More specifically, we present the following differentiated features in this chapter:

- The canonical transitions occur only along *good* pairs of spins (cf. Notation 6.3.1). Thus, when analyzing the relevant configurations, care should be taken with this underlying asymmetry of the model.

- The typical configurations are defined individually for each good pair, whereas the corresponding ones are globally defined in Section 3.4.3. This is because the edge typical configurations near $\mathbf{-1}$ and $\mathbf{+1}$ possess a different structure compared to those near $\mathbf{0}$ (cf. Section 6.5; see also Remark 6.5.1).

- We cannot estimate the capacities in a unified manner owing to the model asymmetry; thus, we first construct fundamental test functions and flows in Section 6.6, which serve as the building blocks for the actual test objects. Subsequently, in Section 6.7, we construct individual test objects for each capacity (cf. Theorem 6.2.2).

6.1.2 Main results: large deviation-type results

In this subsection, we explain the large deviation-type main results on the metastable behavior.

Theorem 6.1.2 (Energy barrier)**.** *Define a constant* Γ *by*

$$\Gamma = \begin{cases} 2K+2 & \text{under periodic boundary conditions,} \\ K+1 & \text{under open boundary conditions.} \end{cases} \tag{6.7}$$

Then, it holds that

$$\Gamma_{-1,\,0} = \Gamma_{0,\,+1} = \Gamma_{-1,\,+1} = \Gamma. \tag{6.8}$$

The proof of Theorem 6.1.2 is provided in Section 6.3.2.

Large deviation-type results

Recall the concepts defined before Theorem 4.1.4.

Theorem 6.1.3 (Large deviation-type results)**.** *The following statements hold.*

(1) ***(Transition time)*** *For all* $\boldsymbol{s}$, $\boldsymbol{s'} \in \mathcal{S}$ *and* $\epsilon > 0$, *we have*

$$\lim_{\beta\to\infty} \mathbb{P}_{\boldsymbol{s}}[e^{\beta(\Gamma-\epsilon)} < \tau_{\mathcal{S}\setminus\{\boldsymbol{s}\}} \le \tau_{\boldsymbol{s'}} < e^{\beta(\Gamma+\epsilon)}] = 1, \tag{6.9}$$

$$\lim_{\beta\to\infty} \frac{1}{\beta} \log \mathbb{E}_{\boldsymbol{s}}[\tau_{\mathcal{S}\setminus\{\boldsymbol{s}\}}] = \lim_{\beta\to\infty} \frac{1}{\beta} \log \mathbb{E}_{\boldsymbol{s}}[\tau_{\boldsymbol{s'}}] = \Gamma. \tag{6.10}$$

Moreover, under $\mathbb{P}_{\boldsymbol{s}}$, *as* $\beta \to \infty$,

$$\frac{\tau_{\mathcal{S}\setminus\{\boldsymbol{s}\}}}{\mathbb{E}_{\boldsymbol{s}}[\tau_{\mathcal{S}\setminus\{\boldsymbol{s}\}}]} \rightharpoonup \mathrm{Exp}(1) \quad \textit{and} \quad \frac{\tau_{\boldsymbol{s'}}}{\mathbb{E}_{\boldsymbol{s}}[\tau_{\boldsymbol{s'}}]} \rightharpoonup \mathrm{Exp}(1), \tag{6.11}$$

where Exp(1) *represents the exponential distribution with parameter* 1.

(2) ***(Mixing time)*** *For all* $\epsilon \in (0,\, 1/2)$, *the mixing time* $t^{\mathrm{mix}}_{\beta}(\epsilon)$ *satisfies*

$$\lim_{\beta\to\infty} \frac{1}{\beta} \log t^{\mathrm{mix}}_{\beta}(\epsilon) = \Gamma.$$

(3) ***(Spectral gap)*** *There exist constants* $0 < c_1 = c_1(K,\, L) \le c_2 = c_2(K,\, L)$ *such that*

$$c_1 e^{-\beta\Gamma} \le \lambda_\beta \le c_2 e^{-\beta\Gamma}.$$

Remark 6.1.4. The connection between Theorems 6.1.2 and 6.1.3 is that the concepts discussed in Theorem 6.1.3 (the transition time, mixing time, and inverse spectral gap) have an exponential scale with respect to the inverse temperature $\beta \to \infty$, and the precise scale is the energy barrier Γ between the ground states that are determined in Theorem 6.1.2.

Remark 6.1.5. We remark that in Theorem 6.1.3, the only difference between the two boundary types (periodic and open) relates to the exact value of Γ, whereas the other features regarding the three concepts are identical. Thus, we state that they share the same *exponential features* in the study of metastability. However, crucial differences between them arise in more quantitative analyses of the metastable transitions, which are presented in Section 6.1.3. That is, the *sub-exponential prefactor* differs between the two boundary types because it depends on the number of possible metastable transition paths between the ground states. The reason for this difference is briefly discussed in Section 6.8.

The proof of Theorem 6.1.3 is provided in Section 6.3.4.

Metastable transition paths between ground states

We obtain the following theorem for the metastable transition paths. We remark that part (1) of Theorem 6.1.6 implies the same behavior of the metastable transition from $\mathbf{-1}$ to $\mathbf{+1}$ as that demonstrated in [53, Proposition 2.1], where the authors investigated the case of $\lambda = 0$ and $h > 0$.

Theorem 6.1.6 (Transition paths)**.** *We have the following asymptotics for the metastable transitions:*

(1) Starting from $\mathbf{-1}$*, the chain must visit* $\mathbf{0}$ *on its way to visiting* $\mathbf{+1}$*:*

$$\lim_{\beta\to\infty} \mathbb{P}_{\mathbf{-1}}[\tau_{\mathbf{0}} < \tau_{\mathbf{+1}}] = 1.$$

Similarly, we have $\lim_{\beta\to\infty} \mathbb{P}_{\mathbf{+1}}[\tau_{\mathbf{0}} < \tau_{\mathbf{-1}}] = 1.$

(2) Starting from $\mathbf{0}$*, the probability of hitting* $\mathbf{-1}$ *before* $\mathbf{+1}$ *is equal to the opposite case; that is,*

$$\lim_{\beta\to\infty} \mathbb{P}_{\mathbf{0}}[\tau_{\mathbf{-1}} < \tau_{\mathbf{+1}}] = \lim_{\beta\to\infty} \mathbb{P}_{\mathbf{0}}[\tau_{\mathbf{+1}} < \tau_{\mathbf{-1}}] = \frac{1}{2}.$$

Using the potential-theoretic terminology, the above theorem is equivalent to

$$\lim_{\beta\to\infty} h_{\mathbf{0},\mathbf{+1}}(\mathbf{-1}) = \lim_{\beta\to\infty} h_{\mathbf{0},\mathbf{-1}}(\mathbf{+1}) = 1 \quad \text{and} \quad \lim_{\beta\to\infty} h_{\mathbf{-1},\mathbf{+1}}(\mathbf{0}) = \frac{1}{2}.$$

We remark that part (2) of Theorem 6.1.6 is straightforward based on the symmetry of our model (cf. Remark 6.1.1). The proof of part (1) of this theorem is presented in Section 6.4.3.

6.1.3 Main results: potential-theoretic results

A crucial difference between the results in the current and preceding subsections is that the quantitative results in this subsection *are dependent on the selection of the boundary conditions.* For simplicity, *we assume open boundary conditions in this subsection.* The periodic case can be handled in a similar manner; thus, we briefly discuss the periodic case in Section 6.8.

Eyring–Kramers formula

The following result generalizes (6.10), in the sense that it characterizes the sub-exponential prefactor with respect to the exponential factor $e^{\beta\Gamma}$ that appears in the quantities in Theorem 6.1.3.

Theorem 6.1.7 (Eyring–Kramers law)**.** *Under open boundary conditions on* Λ*, there exists a constant* $\kappa = \kappa(K,\, L) > 0$ *such that the following estimates hold:*

(1) $\mathbb{E}_{\mathbf{-1}}[\tau_{\{\mathbf{0},\,\mathbf{+1}\}}] = \mathbb{E}_{\mathbf{+1}}[\tau_{\{\mathbf{-1},\,\mathbf{0}\}}] \simeq \kappa e^{\beta\Gamma}$ *and* $\mathbb{E}_{\mathbf{0}}[\tau_{\{\mathbf{-1},\,\mathbf{+1}\}}] \simeq \dfrac{\kappa}{2} e^{\beta\Gamma}$.

(2) $\mathbb{E}_{\mathbf{-1}}[\tau_{\mathbf{0}}] = \mathbb{E}_{\mathbf{+1}}[\tau_{\mathbf{0}}] \simeq \kappa e^{\beta\Gamma}$.

(3) $\mathbb{E}_{\mathbf{0}}[\tau_{\mathbf{-1}}] = \mathbb{E}_{\mathbf{0}}[\tau_{\mathbf{+1}}] \simeq 2\kappa e^{\beta\Gamma}$.

(4) $\mathbb{E}_{\mathbf{-1}}[\tau_{\mathbf{+1}}] = \mathbb{E}_{\mathbf{+1}}[\tau_{\mathbf{-1}}] \simeq 3\kappa e^{\beta\Gamma}$.

Moreover, the constant κ *satisfies (cf.* (6.1)*)*

$$\lim_{K\to\infty} \frac{\kappa(K,\, L)}{KL} = \begin{cases} 1/4 & \text{if } K < L, \\ 1/8 & \text{if } K = L. \end{cases} \tag{6.12}$$

The proof of Theorem 6.1.7 is discussed in Section 6.2.

Remark 6.1.8. The limit (6.12) provides the aforementioned prefactor estimate of the metastable transition times. According to Remark 6.1.5, it can be expected that in the periodic boundary case, a different estimate on the prefactor $\kappa = \kappa(K, L)$ will be obtained. This is indeed the case and the precise estimate in the periodic case is (6.55) provided in Section 6.8. The asymptotic factor difference between the conditions on the boundaries is KL, which is fundamentally owing to the number of possible paths for the canonical transitions (cf. Definition 6.3.3). We refer to Section 6.8 for a more detailed explanation of this comparison.

Remark 6.1.9. A notable feature that only the open boundary model possesses is that *we can explicitly compute the constant* κ, which is provided in Definition 6.2.1. More specifically, the edge constant $\mathfrak{e} = \mathfrak{e}(K)$ can be completely characterized, which is described in Section 6.9 by *solving the symmetric recurrence formulas (cf.* (6.61) *and* (6.62)*).* This is not the case in the periodic boundary case; we can clearly characterize the asymptotic limit (6.55), but we cannot obtain such an explicit formula for the edge constant $\mathfrak{e}' = \mathfrak{e}'(K, L)$ (note that $\mathfrak{e}'$ depends on both K and L). We overcome this drawback in the periodic case by providing a sufficient upper bound on $\mathfrak{e}'$ (cf. (6.57)).

Remark 6.1.10. We compare the precise asymptotics obtained in Theorem 6.1.7 to those obtained in [53, Propositions 2.4 and 2.5] and [28, Theorems 5 and 6] for the case of $\lambda = 0$ and $h > 0$. The main observable difference is that the asymptotics are dependent on the lattice size $K \times L$, which was not the case in previous studies. This is because in our setting, canonical metastable transitions (cf. Definition 6.3.3) occur by updating the spins of the entire lattice line by line; each spin update of a line constitutes a positive portion of the expected transition time. Hence, the exact lattice size is relevant in this case. However, in the case of $\lambda = 0$ and $h > 0$, the essence of the metastable transition is the construction of a specific form of critical saddle configurations. Following the formulation, the process rapidly proceeds to the target ground state. Hence, the lattice only needs to be sufficiently large to contain such critical configurations and the exact size is irrelevant to the sharp transition time.

Remark 6.1.11. An interesting phenomenon occurs in [53, Propositions 2.4 and 2.5] for the case of $\lambda = 0$ and $h > 0$, which is that the time scale of the expected transition time $\mathbb{E}_{\mathbf{-1}}[\tau_{\mathbf{0}}]$ is larger than the time scale of $\mathbb{E}_{\mathbf{-1}}[\tau_{\mathbf{+1}}]$ and $\mathbb{E}_{\mathbf{0}}[\tau_{\mathbf{+1}}]$. This is owing to the fact that the main contribution to the quantity $\mathbb{E}_{\mathbf{-1}}[\tau_{\mathbf{0}}]$ originates from the event that the process (starting from $\mathbf{-1}$) first hits $\mathbf{+1}$ and subsequently arrives at $\mathbf{0}$, which means that the valley with respect to $\mathbf{+1}$ is much deeper than the others. This is not the case in our model, because the valley depths are all equal to Γ according to Theorem 6.1.2. Hence, we determine that all of the relevant expected transition times share the same time scale, which is $e^{\beta\Gamma}$.

Markov chain model reduction

Again, recall the accelerated process $\widetilde{\sigma}_\beta(t)$, $t \geq 0$ and the accelerated trace process $Y_\beta(t)$, $t \geq 0$ defined as in Section 3.1.2. We define the limiting Markov chain $\{Y(t)\}_{t\geq 0}$ on $\mathcal{S}$ as the continuous-time Markov chain that is associated with the transition rate

$$r_Y(\boldsymbol{s},\, \boldsymbol{s'}) = \begin{cases} \kappa^{-1} & \text{if } \{\boldsymbol{s},\, \boldsymbol{s'}\} = \{\mathbf{-1},\, \mathbf{0}\} \text{ or } \{\mathbf{0},\, \mathbf{+1}\}, \\ 0 & \text{otherwise.} \end{cases} \tag{6.13}$$

Theorem 6.1.12 (Markov chain reduction)**.** *Under open boundary conditions on Λ, the following statements hold.*

(1) For $\boldsymbol{s} \in \mathcal{S}$, the law of the Markov chain $Y_\beta(\cdot)$ starting from $\boldsymbol{s}$ converges to the law of the limiting Markov chain $Y(\cdot)$ starting from $\boldsymbol{s}$ in the limit $\beta \to \infty$.

(2) The accelerated process spends negligible time outside $\mathcal{S}$; that is,

$$\lim_{\beta\to\infty} \sup_{\boldsymbol{s}\in\mathcal{S}} \mathbb{E}_{\boldsymbol{s}}\Big[\int_0^t \mathbb{1}\{\widetilde{\sigma}_\beta(u) \notin \mathcal{S}\}du\Big] = 0.$$

The proof of Theorem 6.1.12 is discussed in Section 6.2.

6.2 Outline of proofs

In this section, we provide an outline of the proofs of the main theorems presented in Section 6.1. Henceforth, *we assume that the lattice Λ is given open boundary conditions;* that is, $\Lambda = [\![1,\, K]\!] \times [\![1,\, L]\!] \subseteq \mathbb{Z}^2$, except in Section 6.8, where we briefly discuss the case of periodic boundaries. The basic story of the proofs is as explained in Section 3.2.

We define the following constants that characterize the constant κ that appears in Theorem 6.1.7.

Definition 6.2.1. We define the constants $\mathfrak{b}$, $\mathfrak{e}$, and κ.

- The bulk and edge constants $\mathfrak{b} = \mathfrak{b}(K,\, L)$ and $\mathfrak{e} = \mathfrak{e}(K)$ are defined as

$$\mathfrak{b} = \begin{cases} \dfrac{K(L-4)}{4} & \text{if } K < L \\ \dfrac{K(L-4)}{8} & \text{if } K = L \end{cases} \quad \text{and} \quad \mathfrak{e} = \begin{cases} 1/(4\mathfrak{c}_K) & \text{if } K < L, \\ 1/(8\mathfrak{c}_K) & \text{if } K = L, \end{cases} \tag{6.14}$$

  where $\mathfrak{c}_K$ is the constant defined in (6.59).

- The constant $\kappa = \kappa(K,\, L)$ is defined as

$$\kappa = \mathfrak{b} + 2\mathfrak{e}. \tag{6.15}$$

We thus obtain the following theorem, which provides the main capacity estimate.

Theorem 6.2.2 (Capacity estimates)**.** *The following estimates hold for the relevant capacities:*

(1) $\mathrm{Cap}_\beta(\mathbf{-1},\, \{\mathbf{0},\, \mathbf{+1}\}) = \mathrm{Cap}_\beta(\mathbf{+1},\, \{\mathbf{-1},\, \mathbf{0}\}) \simeq \dfrac{1}{3\kappa} e^{-\beta\Gamma}.$

(2) $\mathrm{Cap}_\beta(\mathbf{-1},\, \mathbf{0}) = \mathrm{Cap}_\beta(\mathbf{+1},\, \mathbf{0}) \simeq \dfrac{1}{3\kappa} e^{-\beta\Gamma}.$

(3) $\mathrm{Cap}_\beta(\mathbf{0},\, \{\mathbf{-1},\, \mathbf{+1}\}) \simeq \dfrac{2}{3\kappa} e^{-\beta\Gamma}.$

(4) $\mathrm{Cap}_\beta(\mathbf{-1},\, \mathbf{+1}) \simeq \dfrac{1}{6\kappa} e^{-\beta\Gamma}.$

The fact that theses capacity estimates readily provide the proof of the Eyring–Kramers formulas are now routine; we refer the readers to Section 3.2.4 and omit the details. Thus, it suffices to prove Theorem 6.2.2, which can be done by applying the strategies explained in Section 3.2.

The remainder of this chapter is organized as follows. In Section 6.3, we define several basic concepts that are crucial to understanding the natural metastable transitions between the ground states. During this process, we prove Theorems 6.1.2 and 6.1.3. In Sections 6.4 and 6.5, we define and investigate the typical and gateway configurations that are the building blocks of the overall energy landscape of our model. Such thorough investigation results in the proof of Theorem 6.1.6 in Section 6.4. In Section 6.6, we construct the fundamental test functions and flows, which are the components of the actual test objects, to estimate the capacities. Thereafter, in Section 6.7, we prove the capacity estimates in Theorem 6.2.2. Finally, in Section 6.8, we discuss the periodic boundary case. Section 6.9 is devoted to investigating the auxiliary process, which is used to handle the edge typical configurations in Section 6.5.

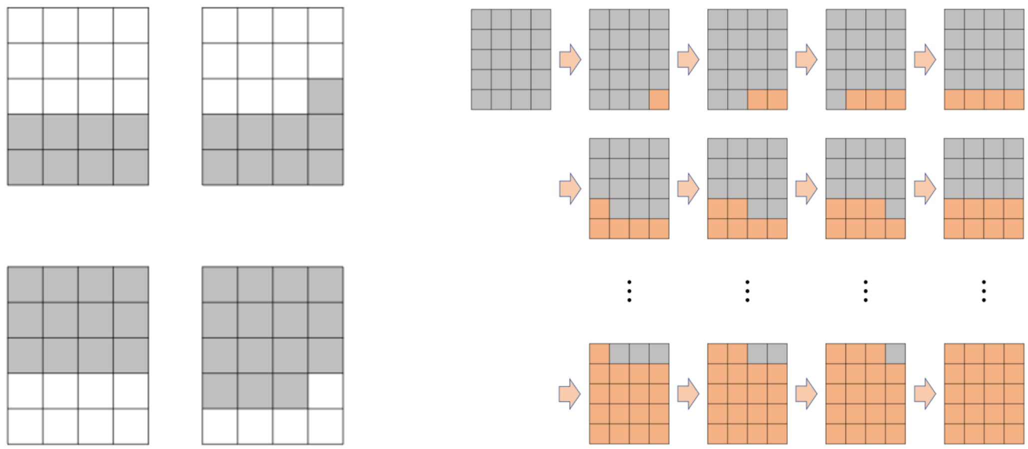


Figure 6.1: In the figures in this article, white, gray, and orange colors denote the spins −1, 0, and +1, respectively. (Left) canonical configurations for $(K,\ L) = (4,\ 5)$; ζ_2^+, $\zeta_{2,1}^{+-}$ (upper-right), ζ_3^- (lower-left), and $\zeta_{3,3}^{-+}$. (Right) a canonical path from $\mathbf{0}$ to $\mathbf{+1}$ for $(K,\ L) = (4,\ 5)$.

6.3 Canonical configurations and energy barrier

The following notation is frequently used throughout the remainder of the chapter.

Notation 6.3.1. A pair $(a,\ b)$ of spins is called *good*, if $\{a,\ b\} = \{-1,\ 0\}$ or $\{0,\ +1\}$.

Throughout the article, we use v and h to denote vertical and horizontal lengths, respectively.

6.3.1 Canonical configurations and paths

Definition 6.3.2 (Pre-canonical configurations and paths)**.** Here, we define pre-canonical configurations between $\mathbf{-1}$ and $\mathbf{0}$. We refer to Figure 6.1 (left) for an illustration.

- For $v \in [\![0,\, L]\!]$, we denote by $\zeta_v^+ \in \mathcal{X}$ the spin configuration whose spins are 0 on $[\![1,\, K]\!] \times [\![1,\, v]\!]$ and -1 on the remainder. Moreover, we denote by $\zeta_v^- \in \mathcal{X}$ the spin configuration whose spins are 0 on $[\![1,\, K]\!] \times [\![L-v+1,\, L]\!]$ and -1 on the remainder. Hence, we have $\zeta_0^+ = \zeta_0^- = \mathbf{-1}$ and $\zeta_L^+ = \zeta_L^- = \mathbf{0}$. For $v \in [\![0,\, L]\!]$, we write

$$\mathcal{R}_v = \{\zeta_v^+,\, \zeta_v^-\}. \tag{6.16}$$

- For $v \in [\![0,\, L-1]\!]$ and $h \in [\![0,\, K]\!]$, we denote by $\zeta_{v,\,h}^{++} \in \mathcal{X}$ the configuration whose spins are 0 on

$$\big[[\![1,\, K]\!] \times [\![1,\, v]\!]\big] \cup \big[[\![1,\, h]\!] \times \{v+1\}\big]$$

and -1 on the remainder. Similarly, we denote by $\zeta_{v,\,h}^{+-} \in \mathcal{X}$ the configuration whose spins are 0 on

$$\big[[\![1,\, K]\!] \times [\![1,\, v]\!]\big] \cup \big[[\![K-h+1,\, K]\!] \times \{v+1\}\big]$$

and -1 on the remainder. Namely, we obtain $\zeta_{v,\,h}^{++}$ (resp. $\zeta_{v,\,h}^{+-}$) from ζ_v^+ by attaching a protuberance of spin 0 of size h at its upper-left (resp. upper-right) corner of the cluster of spin 0. Similarly, we define $\zeta_{v,\,h}^{-+}$ and $\zeta_{v,\,h}^{--}$ by attaching a protuberance of spin 0 of size h in ζ_v^-. For $v \in [\![0,\, L-1]\!]$, we write

$$\mathcal{Q}_v = \bigcup_{h=1}^{K-1} \{\zeta_{v,\,h}^{++},\, \zeta_{v,\,h}^{+-},\, \zeta_{v,\,h}^{-+},\, \zeta_{v,\,h}^{--}\}. \tag{6.17}$$

Concisely, $\mathcal{Q}_v$ consists of the configurations which connect the ones in $\mathcal{R}_v$ and $\mathcal{R}_{v+1}$.

- We define the collection $\mathcal{C}$ of *pre-canonical configurations* as

$$\mathcal{C} = \bigcup_{v=0}^{L} \mathcal{R}_v \cup \bigcup_{v=0}^{L-1} \mathcal{Q}_v.$$

- Finally, a sequence $(\omega_n)_{n=0}^{KL}$ of configurations is a *pre-canonical path* if it satisfies the following conditions; see Figure 6.1 (right).
  - $\omega_{Kv} = \zeta_v^+$ for all $v \in [\![0,\, L]\!]$ *(Type 1)* or $\omega_{Kv} = \zeta_v^-$ for all $v \in [\![0,\, L]\!]$ *(Type 2)*.
  - *(Type 1)* For each $v \in [\![0,\, L-1]\!]$, $\omega_{Kv+h} = \zeta_{v,\,h}^{++}$ for all $h \in [\![0,\, K]\!]$ or $\omega_{Kv+h} = \zeta_{v,\,h}^{+-}$ for all $h \in [\![0,\, K]\!]$.
  - *(Type 2)* For each $v \in [\![0,\, L-1]\!]$, $\omega_{Kv+h} = \zeta_{v,\,h}^{-+}$ for all $h \in [\![0,\, K]\!]$ or $\omega_{Kv+h} = \zeta_{v,\,h}^{--}$ for all $h \in [\![0,\, K]\!]$.

We can readily verify that a pre-canonical path is indeed a path. Moreover, pre-canonical paths characterize all the possible paths from $\mathbf{-1}$ to $\mathbf{0}$ in $\mathcal{C}$ if $K < L$. However, more possible paths exist if $K = L$; that is, the transposed pre-canonical paths.

Based on this observation, we define canonical configurations and paths between the ground states as follows:

Definition 6.3.3 (Canonical configurations and paths)**.** For two spins a and b, we denote by $\mathcal{X}^{a,\,b} \subseteq \mathcal{X}$ the collection of configurations of which all spins are either a or b. Then, we define the natural one-to-one correspondence $\Xi^{a,\,b} : \mathcal{X}^{-1,\,0} \to \mathcal{X}^{a,\,b}$ which maps spins -1 and 0 to a and b, respectively.

Now, we fix a good pair $(a,\, b)$ (cf. Notation 6.3.1). Then, we divide into the cases of $K < L$ and $K = L$.

- **(Case** $K < L$**)** We define the collection $\mathcal{C}^{a,\,b}$ of *canonical configurations* between $\boldsymbol{a}$ and $\boldsymbol{b}$ as

$$\mathcal{C}^{a,\,b} = \Xi^{a,\,b}(\mathcal{C}).$$

By symmetry, using $\Xi^{b,\,a}$ instead of $\Xi^{a,\,b}$ yields the same result, so that $\mathcal{C}^{a,\,b} = \mathcal{C}^{b,\,a}$. Then, we define (cf. (6.16) and (6.17))

$$\mathcal{R}_v^{a,\,b} = \Xi^{a,\,b}(\mathcal{R}_v);\ v \in [\![0,\,L]\!], \quad \mathcal{Q}_v^{a,\,b} = \Xi^{a,\,b}(\mathcal{Q}_v);\ v \in [\![0,\,L-1]\!].$$

- **(Case** $K = L$**)** We define a transpose operator $\Theta : \mathcal{X} \to \mathcal{X}$ by, for $\sigma \in \mathcal{X}$,

$$(\Theta(\sigma))(k,\,\ell) = \sigma(\ell,\,k);\ k \in [\![1,\,K]\!] \text{ and } \ell \in [\![1,\,L]\!].$$

Then, we define the collection $\mathcal{C}^{a,\,b}$ of *canonical configurations* between $\boldsymbol{a}$ and $\boldsymbol{b}$ as

$$\mathcal{C}^{a,\,b} = \Xi^{a,\,b}(\mathcal{C}) \cup (\Theta \circ \Xi^{a,\,b})(\mathcal{C}).$$

We enlarge the collection of canonical configurations in this case, because the transposed configurations also have the same energy due to the condition $K = L$. Again, we have $\mathcal{C}^{a,\,b} = \mathcal{C}^{b,\,a}$. Moreover, we define

$$\mathcal{R}_v^{a,\,b} = \Xi^{a,\,b}(\mathcal{R}_v) \cup (\Theta \circ \Xi^{a,\,b})(\mathcal{R}_v);\ v \in [\![0,\,L]\!],$$
$$\mathcal{Q}_v^{a,\,b} = \Xi^{a,\,b}(\mathcal{Q}_v) \cup (\Theta \circ \Xi^{a,\,b})(\mathcal{Q}_v);\ v \in [\![0,\,L-1]\!].$$

A sequence $(\omega_n)_{n=0}^{KL}$ of configurations is a *canonical path* from $\boldsymbol{a}$ to $\boldsymbol{b}$ if there exists a pre-canonical path $(\widetilde{\omega}_n)_{n=0}^{KL}$ such that $\omega_n = \Xi^{a,\,b}(\widetilde{\omega}_n)$ for all $n \in [\![0,\,KL]\!]$ (or additionally $\omega_n = (\Theta \circ \Xi^{a,\,b})(\widetilde{\omega}_n)$ for all $n \in [\![0,\,KL]\!]$ if $K = L$).

Remark 6.3.4. It holds that $H(\sigma) \le \Gamma$ for all $\sigma \in \mathcal{C}^{-1,\,0} \cup \mathcal{C}^{0,\,+1}$ and

$$H(\sigma) = \begin{cases} \Gamma - 1 & \text{if } \sigma \in \mathcal{R}_v^{-1,\,0} \cup \mathcal{R}_v^{0,\,+1} \text{ for } v \in [\![1,\,L-1]\!], \\ \Gamma & \text{if } \sigma \in \mathcal{Q}_v^{-1,\,0} \cup \mathcal{Q}_v^{0,\,+1} \text{ for } v \in [\![1,\,L-2]\!]. \end{cases}$$

These facts imply that canonical paths are Γ-paths.

Remark 6.3.5. One may be tempted to define similar objects between $\mathbf{-1}$

and $\mathbf{+1}$ by choosing $(a,\, b) = (-1,\, +1)$ or $(+1,\, -1)$. However, the resulting configurations have too high energy to be considered in our investigation. To explain this, recall $\Xi^{-1,\,+1} : \mathcal{X}^{-1,\,0} \to \mathcal{X}^{-1,\,+1}$ from Definition 6.3.3. Then, we can deduce that

$$H(\sigma) = \begin{cases} 4\Gamma - 4 & \text{if } \sigma \in \Xi^{-1,\,+1}(\mathcal{R}_v) \text{ for } v \in [\![1,\, L-1]\!], \\ 4\Gamma & \text{if } \sigma \in \Xi^{-1,\,+1}(\mathcal{Q}_v) \text{ for } v \in [\![1,\, L-2]\!], \end{cases}$$

where $4\Gamma - 4 > \Gamma$. Hence, we cannot connect $\mathbf{-1}$ and $\mathbf{+1}$ by a direct canonical Γ-path, and thus it is natural to expect that *Γ-paths between $\mathbf{-1}$ and $\mathbf{+1}$ must visit at least a certain neighborhood of $\mathbf{0}$.* Rigorously, this is exactly part (1) of Theorem 6.1.6.

6.3.2 Proof of Theorem 6.1.2

Based on the canonical configurations, we are now ready to prove that the energy barrier of the dynamics is exactly Γ.

Proof of Theorem 6.1.2. First, we claim that for two spins a and b,

$$\Gamma_{a,\,b} = \Phi(\boldsymbol{a},\, \boldsymbol{b}) \le \Gamma. \tag{6.18}$$

Indeed, the canonical paths between $\mathbf{-1}$ and $\mathbf{0}$ assert that $\Gamma_{-1,\,0} = \Phi(\mathbf{-1},\, \mathbf{0}) \le \Gamma$. Similarly, the canonical paths between $\mathbf{0}$ and $\mathbf{+1}$ imply $\Gamma_{0,\,+1} \le \Gamma$. Hence,

$$\Gamma_{-1,\,+1} = \Phi(\mathbf{-1},\, \mathbf{+1}) \le \max\{\Phi(\mathbf{-1},\, \mathbf{0}),\, \Phi(\mathbf{0},\, \mathbf{+1})\} \le \Gamma.$$

Thus, we get (6.18). Therefore, to conclude the proof of Theorem 6.1.2, it suffices to prove that for distinct spins a and b,

$$\Gamma_{a,\,b} = \Phi(\boldsymbol{a},\, \boldsymbol{b}) \ge \Gamma. \tag{6.19}$$

To provide a simple proof of (6.19), we recall the MH dynamics of the 2D

Potts model for $q = 3$ with zero external field defined in Chapter 3. In this model, everything is defined in the same way as in Section 6.1.1, except that the Hamiltonian is given by (3.2). Comparing this to our Hamiltonian (6.3), we can easily notice that

$$H(\sigma) \geq H_{\text{Potts}}(\sigma);\ \sigma \in \mathcal{X}. \tag{6.20}$$

Moreover, it is proved in [69, Theorem 2.1] that the energy barrier $\Phi_{\text{Potts}}(\boldsymbol{s},\, \boldsymbol{s'})$, $\boldsymbol{s},\, \boldsymbol{s'} \in \mathcal{S}$, of the Potts dynamics is exactly Γ. Therefore, as the energy landscapes of the two models are identical, we deduce from (6.20) that

$$\Phi(\boldsymbol{s},\, \boldsymbol{s'}) \geq \Phi_{\text{Potts}}(\boldsymbol{s},\, \boldsymbol{s'}) = \Gamma;\ \boldsymbol{s},\, \boldsymbol{s'} \in \mathcal{S}.$$

This is exactly (6.19), and thus we conclude the proof of Theorem 6.1.2. □

6.3.3 Neighborhoods and configurations with small energy

Recall the concept of neighborhoods defined in Definition 3.4.2, with the energy barrier Γ as in Theorem 6.1.2, and also Lemma 3.8.1.

We verified in Section 6.3.2 that the energy barrier is exactly Γ. Now, we fully characterize the spin configurations with energy less than Γ. This result is an analogue of Proposition 3.9.3 and can be proved in a similar manner; thus, we omit the proof. We refer to Figure 6.2 for some examples of such configurations.

Proposition 6.3.6. *Suppose that $\sigma \in \mathcal{X}$ satisfies $H(\sigma) < \Gamma$. Then, exactly one of* **(T1)** *or* **(T2)** *below holds.*

- **(T1)** *There exist a good pair $(a,\, b)$ and $v \in [\![2,\, L-2]\!]$ such that $\sigma \in \mathcal{R}_v^{a,\, b}$. In particular, $\mathcal{N}(\sigma)$ is a singleton, i.e., $\mathcal{N}(\sigma) = \{\sigma\}$.*

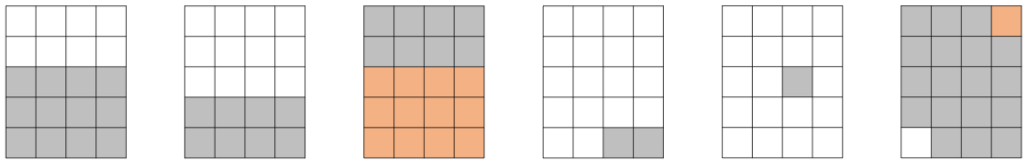


Figure 6.2: Configurations with energy smaller than Γ; type **(T1)** (the first three) and type **(T2)** (the last three).

- **(T2)** *The configuration* σ *belongs to* $\mathcal{N}(\boldsymbol{a})$ *for exactly one spin* a*, so that* $\mathcal{N}(\sigma) = \mathcal{N}(\boldsymbol{a})$*.*

6.3.4 Proof of Theorem 6.1.3

In this subsection, we prove Theorem 6.1.3. To this end, we need the following result regarding the valley depths of the entire energy landscape.

Lemma 6.3.7. *We have the following upper bounds for the depths of the valleys:*

(1) For all $\sigma \in \mathcal{X}$ *and* $\boldsymbol{s} \in \mathcal{S}$*, it holds that* $\Phi(\sigma, \boldsymbol{s}) - H(\sigma) \le \Gamma$*.*

(2) For all $\sigma \in \mathcal{X} \setminus \mathcal{S}$*, it holds that* $\Phi(\sigma, \mathcal{S}) - H(\sigma) < \Gamma$*.*

Proof. The same assertions for the Metropolis dynamics on the Potts model are proved in [69, Theorem 2.1]. Because the same arguments work for our Blume–Capel model as well, we omit the proof. □

Remark 6.3.8. An alternative proof can be found in Lemma 3.9.4 which provides an explicit path that guarantees the upper bounds stated in Lemma 6.3.7.

Based on the previous lemma, we give a formal proof of Theorem 6.1.3.

Proof of Theorem 6.1.3. By the general theory developed in [69, 70], Theorem 6.1.2 and Lemma 6.3.7 are sufficient to conclude the assertions on the transition time, mixing time, and spectral gap given in Theorem 6.1.3. □

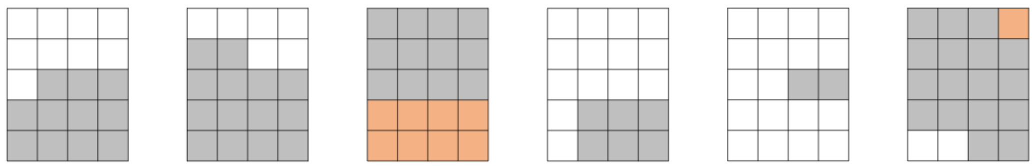


Figure 6.3: Typical configurations; bulk ones (the first three) and edge ones (the last three).

6.4 Typical and gateway configurations

In this section, we define the concepts of typical and gateway configurations and investigate their several basic properties. The concepts are analogues of those defined in Section 3.4. We note that even though the results are similar, we still thoroughly review the notation here because *there indeed exist technical differences due to the non-symmetry of the Blume–Capel model (cf. Remark 6.1.1).*

6.4.1 Typical configurations

Definition 6.4.1 (Typical configurations)**.** Here, we define typical configurations. We refer to Figure 6.3 for a visualization.

- Fix a good pair (a, b). The collection of *bulk typical configurations* between $\boldsymbol{a}$ and $\boldsymbol{b}$ is defined as

$$\mathcal{B}^{a,\,b} = \bigcup_{v=2}^{L-2} \mathcal{R}_v^{a,\,b} \cup \bigcup_{v=2}^{L-3} \mathcal{Q}_v^{a,\,b}. \tag{6.21}$$

  Moreover, we define (cf. Remark 6.3.4)

$$\mathcal{B}_\Gamma^{a,\,b} = \bigcup_{v=2}^{L-3} \mathcal{Q}_v^{a,\,b} = \{\sigma \in \mathcal{B}^{a,\,b} : H(\sigma) = \Gamma\}.$$

  Clearly, we have $\mathcal{B}^{a,\,b} = \mathcal{B}^{b,\,a}$ and $\mathcal{B}_\Gamma^{a,\,b} = \mathcal{B}_\Gamma^{b,\,a}$.

- For a spin a, the collection of *edge typical configurations* near $\boldsymbol{a}$ is defined as
$$\mathcal{E}^a = \widehat{\mathcal{N}}(\boldsymbol{a};\, \mathcal{B}_\Gamma^{-1,\,0} \cup \mathcal{B}_\Gamma^{0,\,+1}). \tag{6.22}$$

- Finally, the collection of *typical configurations* is defined as
$$\mathcal{T} = \mathcal{B}^{-1,\,0} \cup \mathcal{B}^{0,\,+1} \cup \mathcal{E}^{-1} \cup \mathcal{E}^{0} \cup \mathcal{E}^{+1}. \tag{6.23}$$

Then, we summarize the following properties for the typical configurations. Rigorous verifications can be found in Section 3.9 and thus we do not repeat them.

Proposition 6.4.2. *The following properties hold for the typical configurations.*

(1) The collections $\mathcal{E}^{-1}$, $\mathcal{E}^{0}$, and $\mathcal{E}^{+1}$ are disjoint.

(2) We have
$$\mathcal{E}^{-1} \cap \mathcal{B}^{-1,\,0} = \mathcal{R}_2^{-1,\,0}, \quad \mathcal{E}^{0} \cap \mathcal{B}^{-1,\,0} = \mathcal{R}_{L-2}^{-1,0},$$
$$\mathcal{E}^{+1} \cap \mathcal{B}^{0,\,+1} = \mathcal{R}_{L-2}^{0,\,+1}, \quad \mathcal{E}^{0} \cap \mathcal{B}^{0,\,+1} = \mathcal{R}_2^{0,\,+1}.$$

(3) We have $\mathcal{E}^{-1} \cap \mathcal{B}^{0,\,+1} = \mathcal{E}^{+1} \cap \mathcal{B}^{-1,\,0} = \emptyset$.

(4) Recall the definition (6.23) *of $\mathcal{T}$. Then, $\widehat{\mathcal{N}}(\mathcal{S}) = \mathcal{T}$.*

Remark 6.4.3 (Edge structure of typical configurations). Based on Proposition 6.4.2, we have the following decomposition of $E(\widehat{\mathcal{N}}(\mathcal{S})) = E(\mathcal{T})$ (see Figure 6.4 for the full energy landscape):

$$E(\widehat{\mathcal{N}}(\mathcal{S})) = E(\mathcal{B}^{-1,\,0}) \cup E(\mathcal{B}^{0,\,+1}) \cup E(\mathcal{E}^{-1}) \cup E(\mathcal{E}^{0}) \cup E(\mathcal{E}^{+1}).$$

To prove this fact, we check that the members constituting $\mathcal{T}$ (cf. (6.23)) are *separated*, in the sense that for members $\mathcal{A}$ and $\mathcal{A}'$,

$$\{\sigma,\, \sigma'\} \in E(\mathcal{A} \cup \mathcal{A}') \quad \text{implies} \quad \sigma,\, \sigma' \in \mathcal{A} \text{ or } \sigma,\, \sigma' \in \mathcal{A}'.$$

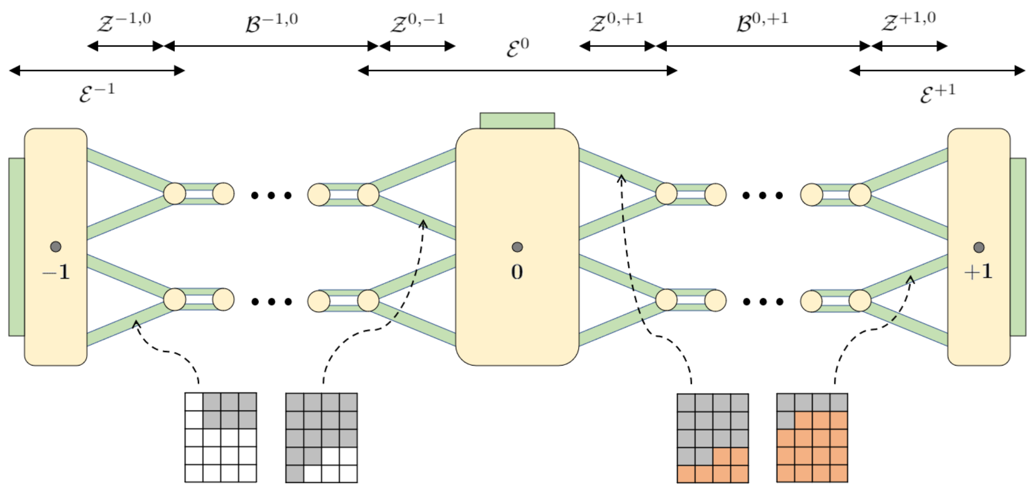


Figure 6.4: Energy landscape of $\widehat{\mathcal{N}}(\mathcal{S})$ for the case of $K < L$. Green regions represent the configurations with energy exactly Γ, and yellow regions represent the ones with energy less than Γ.

Indeed, $\mathcal{E}^a$ for spins a are separated by part (1) of Proposition 6.4.2. The collections $\mathcal{B}^{-1,0}$ and $\mathcal{B}^{0,+1}$ are clearly separated.

To check that a bulk collection $\mathcal{B}^{a,b}$ and an edge collection $\mathcal{E}^{a'}$ are separated, it suffices to prove that if $\sigma \in \mathcal{B}^{a,b}$ and $\sigma' \in \mathcal{E}^{a'} \setminus \mathcal{B}^{a,b}$ with $\sigma \sim \sigma'$, then $\sigma \in \mathcal{E}^{a'}$. To this end, as $\sigma' \notin \mathcal{B}^{a,b}$, we must have $\sigma \in \mathcal{R}_2^{a,b}$ or $\sigma \in \mathcal{R}_{L-2}^{a,b}$. For the former case, as $\mathcal{R}_2^{a,b} \subseteq \mathcal{E}^a$, by part (1) of Proposition 6.4.2 we obtain $a = a'$ and thus $\sigma \in \mathcal{E}^{a'}$. For the latter case, as $\mathcal{R}_{L-2}^{a,b} \subseteq \mathcal{E}^b$, we obtain $b = a'$ and thus $\sigma \in \mathcal{E}^{a'}$.

6.4.2 Gateway configurations

Here, we define gateway configurations of the dynamics. We again refer to Figure 6.4 for a visualization of the role and examples of gateway configurations.

Definition 6.4.4 (Gateway configurations)**.** As for the typical configurations, we define gateway configurations between $\boldsymbol{a}$ and $\boldsymbol{b}$ for good pairs (a, b).

Thus, we fix a good pair $(a,\,b)$. We define $\mathcal{Z}^{a,\,b}$ as

$$\begin{aligned}\{\sigma\in\mathcal{X}:\,&\exists\text{a path }(\omega_n)_{n=0}^{N}\text{ in }\mathcal{X}\setminus\mathcal{B}_{\Gamma}^{a,\,b}\text{ with }N\geq 1\text{ such that}\\ &\omega_0\in\mathcal{R}_2^{a,\,b},\ \omega_N=\sigma,\ \text{and }H(\omega_n)=\Gamma\text{ for all }n\in[\![1,\,N]\!]\}.\end{aligned}\tag{6.24}$$

Note that $\mathcal{Z}^{a,\,b}\neq\mathcal{Z}^{b,\,a}$. Then, we define the collection of *gateway configurations* between $\boldsymbol{a}$ and $\boldsymbol{b}$ as

$$\mathcal{G}^{a,\,b}=\mathcal{Z}^{a,\,b}\cup\mathcal{B}^{a,\,b}\cup\mathcal{Z}^{b,\,a},\tag{6.25}$$

which is indeed a decomposition of $\mathcal{G}^{a,\,b}$. As $\mathcal{B}^{a,\,b}=\mathcal{B}^{b,\,a}$, we have $\mathcal{G}^{a,\,b}=\mathcal{G}^{b,\,a}$.

Then, we have the following properties for the gateway configurations.

Lemma 6.4.5. *Fix a good pair $(a,\,b)$ and suppose that $\sigma,\,\zeta\in\mathcal{X}$ satisfy*

$$\sigma\in\mathcal{G}^{a,\,b},\ \zeta\notin\mathcal{G}^{a,\,b},\ \sigma\sim\zeta,\ \text{and }H(\zeta)\leq\Gamma.$$

Then, we have either $\zeta\in\mathcal{N}(\boldsymbol{a})$ and $\sigma\in\mathcal{Z}^{a,\,b}$ or $\zeta\in\mathcal{N}(\boldsymbol{b})$ and $\sigma\in\mathcal{Z}^{b,\,a}$.

Proof. This lemma can be proved in an identical manner to Lemma 3.9.10. □

6.4.3 A lemma and proof of Theorem 6.1.6

In this subsection, we prove Theorem 6.1.6. Before providing the proof, we give an elementary estimate on equilibrium potentials, which is a generalization of Lemma 3.5.8. This lemma is used in the proof of Theorem 6.1.6 and later in Section 6.7 to estimate the test flow. We refer to Lemmas 3.5.8 and 4.7.4 for the proof.

Lemma 6.4.6. *For disjoint and non-empty subsets $\mathcal{A}$ and $\mathcal{B}$ of $\mathcal{S}$, there exists $C=C(K,\,L)>0$ such that for all $\boldsymbol{s}\in\mathcal{S}$,*

$$\max_{\zeta\in\mathcal{N}(\boldsymbol{s})}\left|\mathbb{P}_{\zeta}[\tau_{\mathcal{A}}<\tau_{\mathcal{B}}]-\mathbb{P}_{\boldsymbol{s}}[\tau_{\mathcal{A}}<\tau_{\mathcal{B}}]\right|\leq Ce^{-\beta}.\tag{6.26}$$

Then, we provide a proof of Theorem 6.1.6.

Proof of Theorem 6.1.6. Part (2) is obvious from the model symmetry. Thus, to conclude the proof, we prove part (1). We first prove that

$$\lim_{\beta\to\infty} \mathbb{P}_{\mathbf{-1}}[\tau_{\mathcal{N}(\mathbf{0})} < \tau_{\mathbf{+1}}] = 1. \tag{6.27}$$

We denote by τ^* the hitting time of the set $\{\sigma \in \mathcal{X} : H(\sigma) \geq \Gamma + 1\}$. Then, [70, Theorem 3.2] implies that

$$\mathbb{P}_{\mathbf{-1}}[\tau^* > e^{\beta(\Gamma+1/2)}] = 1 - o(1).$$

Hence, by part (1) of Theorem 6.1.3 with $\epsilon = 1/2$, we have

$$\begin{aligned}\mathbb{P}_{\mathbf{-1}}[\tau_{\mathbf{+1}} < \tau^*] = 1 - \mathbb{P}_{\mathbf{-1}}[\tau_{\mathbf{+1}} \geq \tau^*] &= 1 - o(1) - \mathbb{P}_{\mathbf{-1}}[\tau_{\mathbf{+1}} \geq \tau^* > e^{\beta(\Gamma+1/2)}] \\ &\geq 1 - o(1) - \mathbb{P}_{\mathbf{-1}}[\tau_{\mathbf{+1}} > e^{\beta(\Gamma+1/2)}] \\ &= 1 - o(1).\end{aligned}$$

Therefore, it suffices to prove that a Γ-path from $\mathbf{-1}$ to $\mathbf{+1}$ must visit $\mathcal{N}(\mathbf{0})$. To this end, we fix a Γ-path $(\omega_n)_{n=0}^N$ with $\omega_0 = \mathbf{-1} \in \mathcal{E}^{-1}$ and $\omega_N = \mathbf{+1} \in \mathcal{E}^{+1}$. Then, by Proposition 6.4.2 and Remark 6.4.3, starting from $\mathbf{-1} \in \mathcal{E}^{-1}$, this path must successively visit $\mathcal{E}^{-1} \cap \mathcal{B}^{-1,0} = \mathcal{R}_2^{-1,0}$, $\mathcal{B}^{-1,0}$, $\mathcal{B}^{-1,0} \cap \mathcal{E}^0 = \mathcal{R}_2^{0,-1}$, $\mathcal{E}^0$, $\mathcal{E}^0 \cap \mathcal{B}^{0,+1} = \mathcal{R}_2^{0,+1}$, $\mathcal{B}^{0,+1}$, and $\mathcal{B}^{0,+1} \cap \mathcal{E}^{+1} = \mathcal{R}_2^{+1,0}$ to finally arrive at $\mathbf{+1} \in \mathcal{E}^{+1}$. Thus, the following time is well defined:

$$n_0 = \max\{n : \omega_n \in \mathcal{R}_2^{0,-1}\}.$$

Then, by the definition of gateway configurations, we have $\omega_{n_0+1} \in \mathcal{Z}^{0,-1}$. Then, by defining

$$n_1 = \min\{n > n_0 : \omega_n \notin \mathcal{G}^{0,-1}\},$$

we have $\omega_{n_1} \in \mathcal{N}(\mathbf{0})$ by Lemma 6.4.5, which concludes the proof of (6.27).

Moreover, Lemma 6.4.6 with $\mathcal{A} = \{\mathbf{0}\}$, $\mathcal{B} = \{\mathbf{+1}\}$, and $\boldsymbol{s} = \mathbf{0}$ implies that

$$\max_{\sigma \in \mathcal{N}(\mathbf{0})} \mathbb{P}_\sigma[\tau_{\mathbf{0}} < \tau_{\mathbf{+1}}] = 1 - o(1).$$

This is equivalent to

$$\lim_{\beta \to \infty} \max_{\sigma \in \mathcal{N}(\mathbf{0})} \mathbb{P}_\sigma[\tau_{\mathbf{0}} < \tau_{\mathbf{+1}}] = 1. \tag{6.28}$$

Therefore, we conclude the proof of the first assertion of part (1) with (6.27) and (6.28) by the casual argument using the strong Markov property. The second assertion follows identically. □

6.5 Edge typical configurations

In this section, we focus on the edge typical configurations defined in Definition 6.4.1, which have much more complex geometry than the bulk typical configurations. This section is an analogue of Section 3.4.4, but *we provide here a much more detailed and quantitative analysis on the behavior of the edge typical configurations.*

6.5.1 Projected graph

We consistently refer to Figure 6.5 for an illustration of the notions defined in this subsection. For each spin a, we decompose $\mathcal{E}^a = \mathcal{I}^a \cup \mathcal{O}^a$ where

$$\mathcal{O}^a = \{\sigma \in \mathcal{E}^a : H(\sigma) = \Gamma\} \quad \text{and} \quad \mathcal{I}^a = \{\sigma \in \mathcal{E}^a : H(\sigma) < \Gamma\}.$$

By Proposition 6.3.6, we notice that

$$\mathcal{I}^a = \mathcal{N}(\boldsymbol{a}) \cup \Big[\bigcup_{b\colon (a,b) \text{ is good}} \mathcal{R}_2^{a,b} \Big]. \tag{6.29}$$

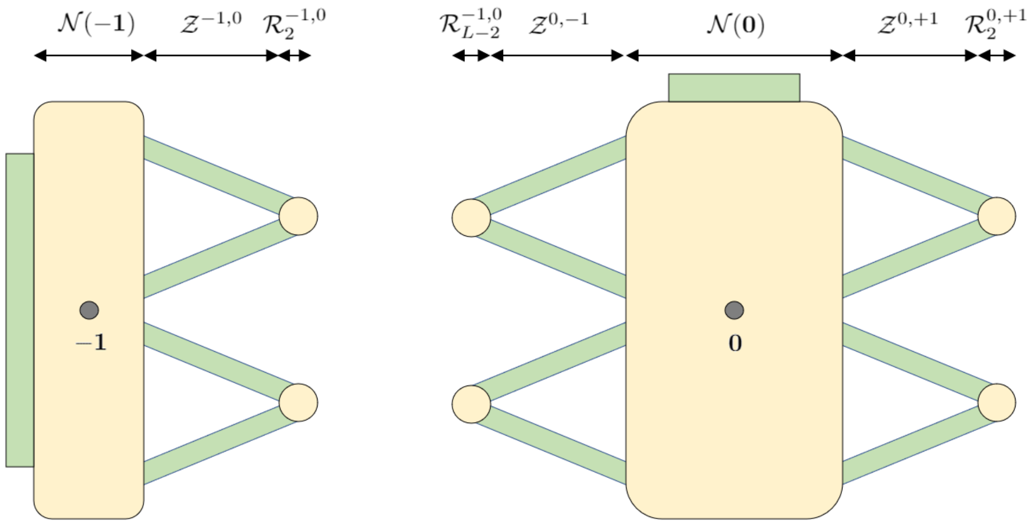


Figure 6.5: Edge typical configurations in the case of $K < L$. (Left) structure of $\mathcal{E}^{-1}$. (Right) structure of $\mathcal{E}^{0}$.

We further define

$$\mathcal{I}_\circ^a = \{\boldsymbol{a}\} \cup \Big[\bigcup_{b:\,(a,b)\text{ is good}} \mathcal{R}_2^{a,\,b} \Big], \tag{6.30}$$

so that each $\sigma \in \mathcal{I}^a$ satisfies $\sigma \in \mathcal{N}(\zeta)$ for exactly one $\zeta \in \mathcal{I}_\circ^a$. Hence, we get the following alternative decomposition of $\mathcal{E}^a$:

$$\mathcal{E}^a = \mathcal{O}^a \cup \Big[\bigcup_{\zeta \in \mathcal{I}_\circ^a} \mathcal{N}(\zeta) \Big]. \tag{6.31}$$

We chose the set of representatives $\mathcal{I}_\circ^a$ because configurations belonging to the same $\mathcal{N}$-neighborhood are not distinguished in the study of metastability, in the sense of Lemma 6.4.6.

Remark 6.5.1. We remark on the display (6.29). In details, we have

$$\mathcal{I}^{-1} = \mathcal{N}(-\mathbf{1}) \cup \mathcal{R}_2^{-1,\,0} \quad \text{and} \quad \mathcal{I}^{+1} = \mathcal{N}(+\mathbf{1}) \cup \mathcal{R}_{L-2}^{0,\,+1},$$

whereas

$$\mathcal{I}^0 = \mathcal{N}(\mathbf{0}) \cup \mathcal{R}_{L-2}^{-1,0} \cup \mathcal{R}_2^{0,+1}.$$

Hence, the structures of $\mathcal{E}^{-1}$ and $\mathcal{E}^{+1}$ are exactly the same, but they differ from the structure of $\mathcal{E}^0$. Figure 6.5 illustrates this difference.

Now, we define a graph structure on $\mathcal{O}^a \cup \mathcal{I}_\circ^a$.

Definition 6.5.2. We fix spin a and introduce a graph structure and a Markov chain on $\mathcal{O}^a \cup \mathcal{I}_\circ^a$.

- **(Graph)** Vertex set $\mathscr{V}^a$ is defined by

$$\mathscr{V}^a = \mathcal{O}^a \cup \mathcal{I}_\circ^a. \tag{6.32}$$

  Then, the edge set $E(\mathscr{V}^a)$ is defined as follows: $\{\sigma, \sigma'\} \in E(\mathscr{V}^a)$ if and only if either $\sigma, \sigma' \in \mathcal{O}^a$ and $\sigma \sim \sigma'$, or $\sigma \in \mathcal{O}^a$, $\sigma' \in \mathcal{I}_\circ^a$, and $\sigma \sim \zeta$ for some $\zeta \in \mathcal{N}(\sigma')$.

- **(Markov chain)** We define a transition rate $r^{\boldsymbol{a}} : \mathscr{V}^a \times \mathscr{V}^a \to [0, \infty)$ as follows: If $\{\sigma, \sigma'\} \notin E(\mathscr{V}^a)$, then $r^{\boldsymbol{a}}(\sigma, \sigma') = 0$. If $\{\sigma, \sigma'\} \in E(\mathscr{V}^a)$, then

$$r^{\boldsymbol{a}}(\sigma, \sigma') = \begin{cases} 1 & \text{if } \sigma, \sigma' \in \mathcal{O}^a, \\ |\{\zeta \in \mathcal{N}(\sigma) : \zeta \sim \sigma'\}| & \text{if } \sigma \in \mathcal{I}_\circ^a,\ \sigma' \in \mathcal{O}^a, \\ |\{\zeta \in \mathcal{N}(\sigma') : \zeta \sim \sigma\}| & \text{if } \sigma \in \mathcal{O}^a,\ \sigma' \in \mathcal{I}_\circ^a. \end{cases} \tag{6.33}$$

  Then, we define $\{Z^a(t)\}_{t \geq 0}$ as the continuous-time Markov chain on $\mathscr{V}^a$ with transition rate $r^{\boldsymbol{a}}(\cdot, \cdot)$. As the rate is symmetric, the Markov chain $Z^a(\cdot)$ is reversible with respect to its invariant distribution, which is the uniform distribution on $\mathscr{V}^a$.

Next, we prove that the process $Z^a(\cdot)$ approximates the Metropolis dynamics on the edge typical configurations.

Proposition 6.5.3. *For each spin a, define a projection map $\Pi^{\boldsymbol{a}} : \mathcal{E}^a \to \mathscr{V}^a$ by*

$$\Pi^{\boldsymbol{a}}(\sigma) = \begin{cases} \sigma & \text{if } \sigma \in \mathcal{O}^a, \\ \zeta & \text{if } \sigma \in \mathcal{N}(\zeta) \text{ for some } \zeta \in \mathcal{I}^a_{\mathfrak{o}}. \end{cases}$$

Then, there exists a constant $C = C(K,\, L) > 0$ such that

(1) for $\sigma_1,\, \sigma_2 \in \mathcal{O}^a$, we have

$$\left| \frac{1}{3} e^{-\beta\Gamma} r^{\boldsymbol{a}}(\Pi^{\boldsymbol{a}}(\sigma_1),\, \Pi^{\boldsymbol{a}}(\sigma_2)) - \mu_\beta(\sigma_1) r_\beta(\sigma_1,\, \sigma_2) \right| \le C e^{-\beta(\Gamma+1)},$$

(2) for $\sigma_1 \in \mathcal{O}^a$ and $\sigma_2 \in \mathcal{I}^a_{\mathfrak{o}}$, we have

$$\left| \frac{1}{3} e^{-\beta\Gamma} r^{\boldsymbol{a}}(\Pi^{\boldsymbol{a}}(\sigma_1),\, \Pi^{\boldsymbol{a}}(\sigma_2)) - \sum_{\zeta \in \mathcal{N}(\sigma_2)} \mu_\beta(\sigma_1) r_\beta(\sigma_1,\, \zeta) \right| \le C e^{-\beta(\Gamma+1)}.$$

Proof. As the proof is identical to that of Proposition 3.4.22, we omit the details. □

6.5.2 Approximation to auxiliary process

In this subsection, we prove that the auxiliary process analyzed in Section 6.9.1 successfully represents the Markov chain $Z^a(\cdot)$. First, we handle the case of $K < L$.

Lemma 6.5.4. *Suppose that $K < L$. Fix a good pair $(a,\, b)$ and recall the projected auxiliary process in Section 6.9.2. Then, there exists a surjective mapping $\Phi^{a,\,b} : \mathscr{V}^a \to V_K$ which satisfies:*

(1) for each $\{\sigma,\, \sigma'\} \in E(\mathscr{V}^a)$ with $\{\sigma,\, \sigma'\} \cap \mathcal{Z}^{a,\,b} = \emptyset$, we have $\Phi^{a,\,b}(\sigma) = \Phi^{a,\,b}(\sigma')$,

(2) for each $\{\sigma,\, \sigma'\} \in E(\mathscr{V}^a)$ with $\{\sigma,\, \sigma'\} \cap \mathcal{Z}^{a,\,b} \neq \emptyset$, we have $\{\Phi^{a,\,b}(\sigma),\, \Phi^{a,\,b}(\sigma')\} \in E(V_K)$ and $r^{\boldsymbol{a}}(\sigma,\, \sigma') = r_K(\Phi^{a,\,b}(\sigma),\, \Phi^{a,\,b}(\sigma'))$,

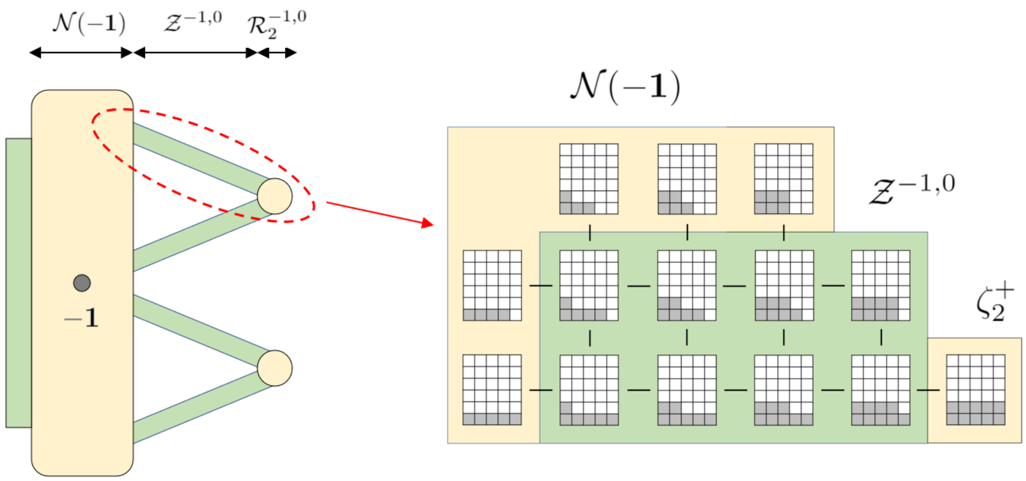


Figure 6.6: Visualization of Lemma 6.5.4 for $(K,\, L) = (5,\, 6)$.

(3) for each $\{x,\, y\} \in E(V_K)$*, there exist exactly* ***four*** *edges* $\{\sigma,\, \sigma'\} \in E(\mathscr{V}^a)$ *such that* $\{\Phi^{a,\,b}(\sigma),\, \Phi^{a,\,b}(\sigma')\} = \{x,\, y\}$.

Proof. First, we assume that $(a,\, b) = (-1,\, 0)$. We refer to Figure 6.6 to provide insight of the proof given here. We have $\mathcal{R}_2^{-1,\,0} = \{\zeta_2^+,\, \zeta_2^-\}$ (cf. Definition 6.3.3). First, we focus on the landscape between $\mathcal{N}(-\mathbf{1})$ and ζ_2^+.

There are two possible $\sigma \in \mathcal{Z}^{-1,\,0}$ with $\sigma \sim \zeta_2^+$; that is, $\zeta_{1,\,K-1}^{++}$ and $\zeta_{1,\,K-1}^{+-}$. we first consider $\zeta_{1,\,K-1}^{++}$. All the possible paths from $\zeta_{1,\,K-1}^{++}$ to $\mathcal{N}(-\mathbf{1})$ are illustrated in Figure 6.6 (right) for the case of $K = 5$ and $L = 6$. Rigorously, we temporarily denote by $\xi_h \in \mathcal{X}$, $h \in [\![1,\, K-1]\!]$ the configuration which has spins 0 on

$$\big[[\![1,\, K-1]\!] \times \{1\}\big] \cup \big[[\![1,\, h]\!] \times \{2\}\big]$$

and spins -1 on the remainder. Then, we define $\Phi_1^{-1,\,0} : \{-\mathbf{1}\} \cup \bigcup_{h=1}^{K-1} \{\zeta_{1,\,h}^{++},\, \xi_h\} \cup \{\zeta_2^+\} \to V_K$ by $\Phi_1^{-1,\,0}(\zeta_2^+) = 0$, $\Phi_1^{-1,\,0}(-\mathbf{1}) = \mathfrak{d}$, and for $h \in [\![1,\, K-1]\!]$,

$$\Phi_1^{-1,\,0}(\zeta_{1,\,h}^{++}) = (0,\, K-h), \quad \Phi_1^{-1,\,0}(\xi_h) = (1,\, K-h).$$

Then from Figures 6.6 and 6.7, it is straightforward that $\Phi_1^{-1,\,0}$ is bijective and that it preserves the edge structure.

If we consider $\zeta_{1,\,K-1}^{+-}$, we deduce as in the previous case another separated landscape of configurations between $\mathbf{-1}$ and $\zeta_{1,\,K-1}^{+-}$. Then, we can define a similar bijective function $\Phi_2^{-1,\,0}$ defined on the relevant configurations to V_K that preserves the edge structure.

Similarly, by examining the landscape between $\mathbf{-1}$ and ζ_2^-, we obtain two more bijective functions $\Phi_3^{-1,\,0}$ and $\Phi_4^{-1,\,0}$ that preserve the edge structure. Moreover, it is clear that the union of $\mathrm{dom}\Phi_i^{-1,\,0}$, the domain of $\Phi_i^{-1,\,0}$, for $i \in [\![1,\,4]\!]$ is indeed $\{\mathbf{-1}\} \cup \mathcal{Z}^{-1,\,0} \cup \mathcal{R}_2^{-1,\,0}$.

Now, we define $\Phi^{-1,\,0} : \mathscr{V}^{-1} \to V_K$ by

$$\Phi^{-1,\,0}(\sigma) = \begin{cases} \Phi_i^{-1,\,0}(\sigma) & \text{if } \sigma \in \mathrm{dom}\Phi_i^{-1,\,0}, \\ \mathfrak{d} & \text{if } \sigma \notin \{\mathbf{-1}\} \cup \mathcal{Z}^{-1,\,0} \cup \mathcal{R}_2^{-1,\,0}. \end{cases}$$

In this way, the function $\Phi^{-1,\,0}$ is well defined because the only possible intersection among $\mathrm{dom}\Phi_i^{-1,\,0}$, $i \in [\![1,\,4]\!]$ is $\{\mathbf{-1}\}$, on which $\Phi_i^{-1,\,0}$ is uniformly defined as $\mathfrak{d}$.

Finally, we prove the assertions. $\Phi^{-1,\,0}$ is clearly surjective as each $\Phi_i^{-1,\,0}$ is bijective. For part (1), if $\{\sigma,\,\sigma'\} \in E(\mathscr{V}^{-1})$ with $\{\sigma,\,\sigma'\} \cap \mathcal{Z}^{-1,\,0} = \emptyset$ then we have $\sigma,\,\sigma' \in \mathcal{E}^{-1} \setminus (\mathcal{Z}^{-1,\,0} \cup \mathcal{R}_2^{-1,\,0})$, so that $\Phi^{-1,\,0}(\sigma) = \Phi^{-1,\,0}(\sigma') = \mathfrak{d}$. Part (2) is obvious from the bijective functions $\Phi_i^{-1,\,0}$. As we have four such bijections, part (3) is now verified.

The other good pairs $(a,\,b)$ can be dealt with in a similar way; thus, we do not repeat the tedious proof. □

Next, we deal with the case of $K = L$.

Lemma 6.5.5. *Suppose that $K = L$ and fix a good pair $(a,\,b)$. Then, there exists a surjective mapping $\Phi^{a,\,b} : \mathscr{V}^a \to V_K$ which satisfies:*

(1) for each $\{\sigma,\,\sigma'\} \in E(\mathscr{V}^a)$ with $\{\sigma,\,\sigma'\} \cap \mathcal{Z}^{a,\,b} = \emptyset$, we have $\Phi^{a,\,b}(\sigma) = \Phi^{a,\,b}(\sigma')$,

(2) for each $\{\sigma,\, \sigma'\} \in E(\mathscr{V}^a)$ *with* $\{\sigma,\, \sigma'\} \cap \mathcal{Z}^{a,\,b} \neq \emptyset$*, we have* $\{\Phi^{a,\,b}(\sigma),\, \Phi^{a,\,b}(\sigma')\} \in E(V_K)$ *and* $r^{\boldsymbol{a}}(\sigma,\, \sigma') = r_K(\Phi^{a,\,b}(\sigma),\, \Phi^{a,\,b}(\sigma'))$,

(3) for each $\{x,\, y\} \in E(V_K)$*, there exist exactly* ***eight*** *edges* $\{\sigma,\, \sigma'\} \in E(\mathscr{V}^a)$ *such that* $\{\Phi^{a,\,b}(\sigma),\, \Phi^{a,\,b}(\sigma')\} = \{x,\, y\}$.

Proof. First, we assume that $(a,\, b) = (-1,\, 0)$. The only difference to Lemma 6.5.4 is that we now have $\mathcal{R}_2^{-1,\,0} = \{\zeta_2^+,\, \zeta_2^-,\, \Theta(\zeta_2^+),\, \Theta(\zeta_2^-)\}$, where Θ is the operator defined in Definition 6.3.3. Thus, the corresponding number of edges are exactly doubled compared to Lemma 6.5.4. The rest of the proof is identical. □

6.6 Construction of fundamental test functions and flows

6.6.1 Fundamental test objects

In this subsection, we construct two fundamental test functions which are the main ingredients of the actual test functions to approximate the capacities via the Dirichlet principle (cf. Theorem 3.2.5). More specifically, we construct two real test functions, namely, $g^{-1,\,0}$ and $g^{+1,\,0}$ on $\mathcal{X}$. Concisely, $g^{-1,\,0}$ (resp. $g^{+1,\,0}$) describes the dynamical transitions from $\mathbf{-1}$ (resp. $\mathbf{+1}$) to $\mathbf{0}$ in the sense of equilibrium potentials. Then, we define two fundamental test flows according to (3.35).

Definition 6.6.1 (Test function $g^{-1,\,0}$)**.** Here, we construct the function $g^{-1,\,0} : \mathcal{X} \to \mathbb{R}$ which describes the metastable transition from $\mathbf{-1}$ to $\mathbf{0}$. For the construction, we recall (6.23) and define $g^{-1,\,0}$ on the members of $\mathcal{T}$ separately, and then define on $\mathcal{X} \setminus \mathcal{T}$.

- $\mathcal{B}^{-1,\,0}$**:** For $\sigma \in \mathcal{B}^{-1,\,0}$, where the number of spins 0 in σ is $z \in [\![2K,\ K(L-$

2)⟧, we define

$$g^{-1,0}(\sigma) = \frac{1}{\kappa}\Big[\frac{K(L-2)-z}{K(L-4)}\mathfrak{b} + \mathfrak{e}\Big].$$

- $\mathcal{E}^{-1}$**:** We define (cf. Proposition 6.5.3, Lemmas 6.5.4 and 6.5.5)

$$g^{-1,0}(\sigma) = 1 - \frac{\mathfrak{e}}{\kappa} \cdot h^K_{0,\mathfrak{d}}\big((\Phi^{-1,0} \circ \Pi^{\mathbf{-1}})(\sigma)\big).$$

- $\mathcal{E}^{0}$**:** We define

$$g^{-1,0}(\sigma) = \frac{\mathfrak{e}}{\kappa} \cdot h^K_{0,\mathfrak{d}}\big((\Phi^{0,-1} \circ \Pi^{\mathbf{0}})(\sigma)\big).$$

- $\mathcal{B}^{0,+1} \cup \mathcal{E}^{+1} \cup (\mathcal{X} \setminus \mathcal{T})$**:** We define $g^{-1,0} \equiv 0$.

Definition 6.6.2 (Test function $g^{+1,0}$)**.** We define $g^{+1,0}$ in exactly the same manner. Rigorously, we define $\Xi : \mathcal{X} \to \mathcal{X}$ by

$$(\Xi(\sigma))(x) = \begin{cases} +1 & \text{if } \sigma(x) = -1, \\ -1 & \text{if } \sigma(x) = +1, \\ 0 & \text{if } \sigma(x) = 0. \end{cases}$$

Then, we define $g^{+1,0}(\sigma) = g^{-1,0}(\Xi(\sigma))$.

Definition 6.6.3 (Test flows $\phi^{-1,0}$ and $\phi^{+1,0}$)**.** We define $\phi^{-1,0} = \Psi_{g^{-1,0}}$ and $\phi^{+1,0} = \Psi_{g^{+1,0}}$ (cf. (3.35)) on the typical configurations and zero on the remainder.

Remark 6.6.4. To check that the functions are well defined, it suffices to recognize that $g^{-1,0}$ is defined as $1 - \mathfrak{e}/\kappa$ on $\mathcal{R}_2^{-1,0} = \mathcal{B}^{-1,0} \cap \mathcal{E}^{-1}$ and $\mathfrak{e}/\kappa$ on $\mathcal{R}_{L-2}^{-1,0} = \mathcal{B}^{-1,0} \cap \mathcal{E}^{0}$.

Remark 6.6.5. We remark that if $\sigma, \sigma' \in \widehat{\mathcal{N}}(\mathcal{S})$ with $\sigma \sim \sigma'$, then either $g^{-1,0}(\sigma) = g^{-1,0}(\sigma')$ or $g^{+1,0}(\sigma) = g^{+1,0}(\sigma')$ must hold. To prove this, recall from Remark 6.4.3 that

$$E(\widehat{\mathcal{N}}(\mathcal{S})) = E(\mathcal{B}^{-1,\,0}) \cup E(\mathcal{B}^{0,\,+1}) \cup E(\mathcal{E}^{-1}) \cup E(\mathcal{E}^{0}) \cup E(\mathcal{E}^{+1}).$$

By Definitions 6.6.1 and 6.6.2, we only need to consider the case of $\{\sigma,\, \sigma'\} \in E(\mathcal{E}^0)$. Then, by the proof of Lemma 6.5.4, $g^{-1,\,0}(\sigma) = g^{-1,\,0}(\sigma')$ unless $\{\sigma,\, \sigma'\} \in E(\mathcal{N}(\mathbf{0}) \cup \mathcal{Z}^{0,\,-1} \cup \mathcal{R}_2^{0,\,-1})$ and $g^{+1,\,0}(\sigma) = g^{+1,\,0}(\sigma')$ unless $\{\sigma,\, \sigma'\} \in E(\mathcal{N}(\mathbf{0}) \cup \mathcal{Z}^{0,\,+1} \cup \mathcal{R}_2^{0,\,+1})$. As

$$E(\mathcal{N}(\mathbf{0}) \cup \mathcal{Z}^{0,\,-1} \cup \mathcal{R}_2^{0,\,-1}) \cap E(\mathcal{N}(\mathbf{0}) \cup \mathcal{Z}^{0,\,+1} \cup \mathcal{R}_2^{0,\,+1}) = E(\mathcal{N}(\mathbf{0}))$$

and both functions are constantly zero on $\mathcal{N}(\mathbf{0})$, we obtain the desired result. In turn, if $\sigma,\, \sigma' \in \widehat{\mathcal{N}}(\mathcal{S})$ with $\sigma \sim \sigma'$, then we have either $\phi^{-1,\,0}(\sigma,\, \sigma') = 0$ or $\phi^{+1,\,0}(\sigma,\, \sigma') = 0$.

6.6.2 Properties of fundamental test functions

Now, we calculate the Dirichlet form of the test functions.

Proposition 6.6.6. *We have*

$$D_\beta(g^{-1,\,0}) = \frac{1+o(1)}{3\kappa} e^{-\beta\Gamma} \quad \text{and} \quad D_\beta(g^{+1,\,0}) = \frac{1+o(1)}{3\kappa} e^{-\beta\Gamma}.$$

Proof. By symmetry, it suffices to estimate $D_\beta(g^{-1,\,0})$. By definition, we write $D_\beta(g^{-1,\,0})$ as

$$\Big[\sum_{\{\sigma,\,\zeta\}\subseteq\mathcal{T}} + \sum_{\sigma\in\mathcal{T}}\sum_{\zeta\in\mathcal{X}\setminus\mathcal{T}} + \sum_{\{\sigma,\,\zeta\}\subseteq\mathcal{X}\setminus\mathcal{T}}\Big]\mu_\beta(\sigma) r_\beta(\sigma,\,\zeta)[g^{-1,\,0}(\zeta) - g^{-1,\,0}(\sigma)]^2. \quad (6.34)$$

The third summation of (6.34) vanishes because $g^{-1,\,0} \equiv 0$ on $\mathcal{X} \setminus \mathcal{T}$. For the second (double) summation of (6.34), if $\sigma \in \mathcal{T}$ and $\zeta \in \mathcal{X} \setminus \mathcal{T}$ with $\sigma \sim \zeta$, then as $\mathcal{T} = \widehat{\mathcal{N}}(\mathcal{S})$ by part (4) of Proposition 6.4.2, we have $H(\zeta) \geq \Gamma + 1$.

Hence,

$$\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)=\min\{\mu_\beta(\sigma),\,\mu_\beta(\zeta)\}=\mu_\beta(\zeta)=O(e^{-\beta(\Gamma+1)}).$$

Therefore, the second (double) summation is of scale $O(e^{-\beta(\Gamma+1)})$.

It remains to calculate the first summation of (6.34). By Remark 6.4.3 and the fact that $g^{-1,0}$ is constant on $\mathcal{B}^{0,+1}$ and on $\mathcal{E}^{+1}$, we can rewrite the summation as

$$\Big[\sum_{\{\sigma,\zeta\}\subseteq\mathcal{B}^{-1,0}}+\sum_{\{\sigma,\zeta\}\subseteq\mathcal{E}^{-1}}+\sum_{\{\sigma,\zeta\}\subseteq\mathcal{E}^{0}}\Big]\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)[g^{-1,0}(\zeta)-g^{-1,0}(\sigma)]^2. \quad (6.35)$$

We first deal with the first summation of (6.35). Recall from Definition 6.4.1 that $\mathcal{B}^{-1,0}=\bigcup_{v=2}^{L-2}\mathcal{R}_v^{-1,0}\cup\bigcup_{v=2}^{L-3}\mathcal{Q}_v^{-1,0}$. If $K<L$, then the first summation of (6.35) becomes

$$\sum_{v=2}^{L-3}\sum_{h=0}^{K-1}\mu_\beta(\zeta_{v,h}^{+\pm})r_\beta(\zeta_{v,h}^{+\pm},\,\zeta_{v,h+1}^{+\pm})[g^{-1,0}(\zeta_{v,h+1}^{+\pm})-g^{-1,0}(\zeta_{v,h}^{+\pm})]^2$$
$$+\sum_{v=2}^{L-3}\sum_{h=0}^{K-1}\mu_\beta(\zeta_{v,h}^{-\pm})r_\beta(\zeta_{v,h}^{-\pm},\,\zeta_{v,h+1}^{-\pm})[g^{-1,0}(\zeta_{v,h+1}^{-\pm})-g^{-1,0}(\zeta_{v,h}^{-\pm})]^2,$$

where the signs $\pm$ indicate shorthands for $+$ and $-$ (so that the above formula actually consists of four double summations). By (6.6) and Definition 6.6.1, this asymptotically equals (cf. (6.14))

$$4\sum_{v=2}^{L-3}\sum_{h=0}^{K-1}\frac{1}{3}e^{-\beta\Gamma}\cdot\frac{1}{\kappa^2}\frac{\mathfrak{b}^2}{K^2(L-4)^2}=\frac{4\mathfrak{b}^2}{3\kappa^2K(L-4)}e^{-\beta\Gamma}=\frac{\mathfrak{b}}{3\kappa^2}e^{-\beta\Gamma}.$$

If $K=L$, then the first summation of (6.35) must be counted twice the preceding computation due to the presence of transposed configurations obtained by the operator Θ (cf. Definition 6.3.3). Thus, the summation asymptotically equals (cf. (6.14))

$$8\sum_{v=2}^{L-3}\sum_{h=0}^{K-1}\frac{1}{3}e^{-\beta\Gamma}\cdot\frac{1}{\kappa^2}\frac{\mathfrak{b}^2}{K^2(L-4)^2}=\frac{8\mathfrak{b}^2}{3\kappa^2K(L-4)}e^{-\beta\Gamma}=\frac{\mathfrak{b}}{3\kappa^2}e^{-\beta\Gamma}.$$

Summing up, we have

$$\sum_{\{\sigma,\,\zeta\}\subseteq\mathcal{B}^{-1,\,0}}\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)[g^{-1,\,0}(\zeta)-g^{-1,\,0}(\sigma)]^2\simeq\frac{\mathfrak{b}}{3\kappa^2}e^{-\beta\Gamma}. \tag{6.36}$$

Next, we calculate the second summation of (6.35). Recalling the decomposition (6.31), we rewrite this as

$$\sum_{\{\sigma,\,\zeta\}\subseteq\mathcal{O}^{-1}}\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)[g^{-1,\,0}(\zeta)-g^{-1,\,0}(\sigma)]^2$$
$$+\sum_{\sigma\in\mathcal{O}^{-1}}\sum_{\zeta\subseteq\mathcal{I}_{\mathfrak{o}}^{-1}}\sum_{\zeta'\in\mathcal{N}(\zeta)}\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta')[g^{-1,\,0}(\zeta')-g^{-1,\,0}(\sigma)]^2.$$

By Proposition 6.5.3 and Definition 6.6.1, this is asymptotically equal to

$$\Big[\sum_{\{\sigma,\,\zeta\}\subseteq\mathcal{O}^{-1}}+\sum_{\sigma\in\mathcal{O}^{-1}}\sum_{\zeta\in\mathcal{I}_{\mathfrak{o}}^{-1}}\Big]\frac{1}{3}e^{-\beta\Gamma}r^{-\mathbf{1}}(\sigma,\,\zeta)[g^{-1,\,0}(\zeta)-g^{-1,\,0}(\sigma)]^2.$$

By Definition 6.6.1, this becomes

$$\frac{1}{3}e^{-\beta\Gamma}\sum_{\{\sigma,\,\zeta\}\in E(\mathscr{V}^{-1})}r^{-\mathbf{1}}(\sigma,\,\zeta)\cdot\frac{\mathfrak{e}^2}{\kappa^2}\big[h_{0,\mathfrak{d}}^K(\Phi^{-1,\,0}(\zeta))-h_{0,\mathfrak{d}}^K(\Phi^{-1,\,0}(\sigma))\big]^2. \tag{6.37}$$

If $K<L$, then by Lemma 6.5.4, this becomes

$$\frac{4}{3}e^{-\beta\Gamma}\sum_{\{x,y\}\in E(V_K)}r_K(x,\,y)\cdot\frac{\mathfrak{e}^2}{\kappa^2}\big[h_{0,\mathfrak{d}}^K(y)-h_{0,\mathfrak{d}}^K(x)\big]^2$$
$$=\frac{4\mathfrak{e}^2}{3\kappa^2}e^{-\beta\Gamma}\cdot|V_K|\mathrm{cap}_K(0,\,\mathfrak{d})=\frac{4\mathfrak{e}^2}{3\kappa^2}e^{-\beta\Gamma}\cdot\mathfrak{c}_K=\frac{\mathfrak{e}}{3\kappa^2}e^{-\beta\Gamma}.$$

The last two equalities hold by (6.70) and (6.14), respectively. If $K = L$, then by Lemma 6.5.5, term (6.37) equals

$$\frac{8}{3}e^{-\beta\Gamma}\sum_{\{x,\,y\}\in E(V_K)} r_K(x,\,y)\cdot\frac{\mathfrak{e}^2}{\kappa^2}\big[h^K_{0,\,\mathfrak{d}}(y)-h^K_{0,\,\mathfrak{d}}(x)\big]^2=\frac{\mathfrak{e}}{3\kappa^2}e^{-\beta\Gamma},$$

which is again by (6.70) and (6.14). Therefore, in any cases, we have that

$$\sum_{\{\sigma,\,\zeta\}\subseteq\mathcal{E}^{-1}}\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)[g^{-1,\,0}(\zeta)-g^{-1,\,0}(\sigma)]^2\simeq\frac{\mathfrak{e}}{3\kappa^2}e^{-\beta\Gamma}. \tag{6.38}$$

Similarly, we have that the third summation of (6.35) is asymptotically equal to the last displayed term. Gathering this fact, (6.35), (6.36), and (6.38), we have that the first summation of (6.34) is asymptotically equal to

$$\frac{\mathfrak{b}}{3\kappa^2}e^{-\beta\Gamma}+\frac{2\mathfrak{e}}{3\kappa^2}e^{-\beta\Gamma}=\frac{1}{3\kappa}e^{-\beta\Gamma}.$$

Therefore, we deduce that (6.34) asymptotically equals $e^{-\beta\Gamma}/(3\kappa)$, which concludes the estimate of $D_\beta(g^{-1,\,0})$. □

6.6.3 Properties of fundamental test flows

We first estimate the flow norm.

Proposition 6.6.7. *We have*

$$\|\phi^{-1,\,0}\|^2=\frac{1+o(1)}{3\kappa}e^{-\beta\Gamma}\quad\textit{and}\quad\|\phi^{+1,\,0}\|^2=\frac{1+o(1)}{3\kappa}e^{-\beta\Gamma}.$$

Proof. The formulas are straightforward from (3.35) and the last display of the proof of Proposition 6.6.6. □

Now, we deal with the divergence of the fundamental test flows. As $\phi^{-1,\,0}$ and $\phi^{+1,\,0}$ have the same structure, we focus on estimating the former test flow $\phi^{-1,\,0}$.

Lemma 6.6.8. *For $\sigma \in \mathcal{B}^{-1,0} \setminus (\mathcal{E}^{-1} \cup \mathcal{E}^{0})$, it holds that* $(\operatorname{div} \phi^{-1,0})(\sigma) = 0$.

Proof. By (6.21) and Proposition 6.4.2, we have

$$\mathcal{B}^{-1,0} \setminus (\mathcal{E}^{-1} \cup \mathcal{E}^{0}) = \bigcup_{v=3}^{L-3} \mathcal{R}_v^{-1,0} \cup \bigcup_{v=2}^{L-3} \mathcal{Q}_v^{-1,0}.$$

If $\sigma \in \mathcal{R}_v^{-1,0}$, $v \in [\![3,\, L-3]\!]$, then $\sigma \in \{\zeta_v^+,\, \zeta_v^-\}$ (or additionally in $\{\Theta(\zeta_v^+),\, \Theta(\zeta_v^-)\}$ if $K = L$). Taking $\sigma = \zeta_v^+$ for instance, $(\operatorname{div} \phi^{-1,0})(\sigma)$ equals

$$\begin{aligned}&\phi^{-1,0}(\zeta_v^+,\, \zeta_{v,1}^{++}) + \phi^{-1,0}(\zeta_v^+,\, \zeta_{v,1}^{+-}) + \phi^{-1,0}(\zeta_v^+,\, \zeta_{v-1,K-1}^{++}) + \phi^{-1,0}(\zeta_v^+,\, \zeta_{v-1,K-1}^{+-})\\ &= \frac{1}{Z_\beta} e^{-\beta\Gamma} \cdot \frac{\mathfrak{b}}{\kappa}\Big[\frac{1}{K(L-4)} + \frac{1}{K(L-4)} - \frac{1}{K(L-4)} - \frac{1}{K(L-4)}\Big] = 0.\end{aligned}$$

Same computation works for the other cases as well. If $\sigma \in \mathcal{Q}_v^{-1,0}$, $v \in [\![2,\, L-3]\!]$, then $\sigma \in \bigcup_{h=1}^{K-1} \{\zeta_{v,h}^{++},\, \zeta_{v,h}^{+-},\, \zeta_{v,h}^{-+},\, \zeta_{v,h}^{--}\}$ (or additionally in

$$\bigcup_{h=1}^{K-1} \{\Theta(\zeta_{v,h}^{++}),\, \Theta(\zeta_{v,h}^{+-}),\, \Theta(\zeta_{v,h}^{-+}),\, \Theta(\zeta_{v,h}^{--})\}$$

if $K = L$). Taking $\sigma = \zeta_{v,h}^{++}$ for instance, $(\operatorname{div} \phi^{-1,0})(\sigma)$ equals

$$\begin{aligned}&\phi^{-1,0}(\zeta_{v,h}^{++},\, \zeta_{v,h+1}^{++}) + \phi^{-1,0}(\zeta_{v,h}^{++},\, \zeta_{v,h-1}^{++})\\ &= \frac{1}{Z_\beta} e^{-\beta\Gamma} \cdot \frac{\mathfrak{b}}{\kappa}\Big[\frac{1}{K(L-4)} - \frac{1}{K(L-4)}\Big] = 0.\end{aligned}$$

Again, same computation works for the remaining cases. Thus, we conclude that $\phi^{-1,0}$ is divergence-free on $\mathcal{B}^{-1,0} \setminus (\mathcal{E}^{-1} \cup \mathcal{E}^{0})$. □

Lemma 6.6.9. *For $\sigma \in \mathcal{R}_2^{-1,0} \cup \mathcal{R}_2^{0,-1}$, it holds that* $(\operatorname{div} \phi^{-1,0})(\sigma) = 0$.

Proof. We only consider the set $\mathcal{R}_2^{-1,0}$, as the latter set can be handled similarly. We claim that

$$\sum_{\sigma\in\mathcal{R}_2^{-1,0}} (\operatorname{div}\phi^{-1,0})(\sigma) = 0, \tag{6.39}$$

which in turn implies $(\operatorname{div}\phi^{-1,0})(\sigma) = 0$ for all $\sigma \in \mathcal{R}_2^{-1,0}$ because of the model symmetry. Elements of $\mathcal{R}_2^{-1,0}$ are connected to elements of both $\mathcal{B}^{-1,0}$ and $\mathcal{E}^{-1}$, so that

$$\sum_{\sigma\in\mathcal{R}_2^{-1,0}} (\operatorname{div}\phi^{-1,0})(\sigma) = \sum_{\sigma\in\mathcal{R}_2^{-1,0}} \Big[\sum_{\zeta\in\mathcal{E}^{-1}} + \sum_{\zeta\in\mathcal{B}^{-1,0}}\Big]\phi^{-1,0}(\sigma,\,\zeta). \tag{6.40}$$

First, we consider the former double summation. By definition, this is

$$\begin{aligned}&\frac{\mathfrak{e}}{\kappa}\sum_{\sigma\in\mathcal{R}_2^{-1,0}}\sum_{\zeta\in\mathcal{E}^{-1}} \mu_\beta(\sigma) r_\beta(\sigma,\,\zeta)\big[h^K_{0,\mathfrak{d}}\big((\Phi^{-1,0}\circ\Pi^{-\mathbf{1}})(\zeta)\big) - 1\big]\\ &= -\frac{\mathfrak{e}}{Z_\beta\kappa}e^{-\beta\Gamma}\sum_{\sigma\in\mathcal{R}_2^{-1,0}}\sum_{\zeta\in\mathcal{O}^{-1}} \big[1 - h^K_{0,\mathfrak{d}}(\Phi^{-1,0}(\zeta))\big].\end{aligned}$$

By Lemmas 6.5.4, 6.5.5, and an elementary property of capacities (cf. [16, (7.1.39)]), this equals

$$\begin{cases} -\dfrac{\mathfrak{e}}{Z_\beta\kappa}e^{-\beta\Gamma}\cdot 4\mathfrak{c}_K & \text{if } K<L,\\ -\dfrac{\mathfrak{e}}{Z_\beta\kappa}e^{-\beta\Gamma}\cdot 8\mathfrak{c}_K & \text{if } K=L.\end{cases}$$

Therefore, by (6.14), we have

$$\sum_{\sigma\in\mathcal{R}_2^{-1,0}}\sum_{\zeta\in\mathcal{E}^{-1}} \phi^{-1,0}(\sigma,\,\zeta) = -\frac{1}{Z_\beta\kappa}e^{-\beta\Gamma}. \tag{6.41}$$

Next, we consider the latter double summation of (6.40). We divide into two cases.

- Suppose that $K < L$, so that $\mathcal{R}_2^{-1,\,0} = \{\zeta_2^+,\, \zeta_2^-\}$. Then, we have by Definition 6.6.3 that the summation equals

$$\begin{aligned}
&\phi^{-1,\,0}(\zeta_2^+,\, \zeta_{2,\,1}^{++}) + \phi^{-1,\,0}(\zeta_2^+,\, \zeta_{2,\,1}^{+-}) + \phi^{-1,\,0}(\zeta_2^-,\, \zeta_{2,\,1}^{-+}) + \phi^{-1,\,0}(\zeta_2^-,\, \zeta_{2,\,1}^{--}) \\
&= \frac{1}{Z_\beta} e^{-\beta\Gamma} \cdot \frac{\mathfrak{b}}{\kappa} \Big[\frac{1}{K(L-4)} + \frac{1}{K(L-4)} + \frac{1}{K(L-4)} + \frac{1}{K(L-4)} \Big] \\
&= \frac{1}{Z_\beta \kappa} e^{-\beta\Gamma}.
\end{aligned}$$

  The last equality holds by (6.14).

- Suppose that $K = L$, so that $\mathcal{R}_2^{-1,\,0} = \{\zeta_2^+,\, \zeta_2^-,\, \Theta(\zeta_2^+),\, \Theta(\zeta_2^-)\}$. Then, the above summation must be exactly doubled, so that

$$\sum_{\sigma \in \mathcal{R}_2^{-1,\,0}} \sum_{\zeta \in \mathcal{B}^{-1,\,0}} \phi^{-1,\,0}(\sigma,\, \zeta) = \frac{1}{Z_\beta \kappa} e^{-\beta\Gamma} \cdot \frac{8\mathfrak{b}}{K(L-4)} = \frac{1}{Z_\beta \kappa} e^{-\beta\Gamma},$$

  where the last equality still holds by (6.14).

Therefore, in any cases we have

$$\sum_{\sigma \in \mathcal{R}_2^{-1,\,0}} \sum_{\zeta \in \mathcal{B}^{-1,\,0}} \phi^{-1,\,0}(\sigma,\, \zeta) = \frac{1}{Z_\beta \kappa} e^{-\beta\Gamma}. \tag{6.42}$$

Combining (6.40), (6.41), and (6.42) yields (6.39), which concludes the proof. □

Lemma 6.6.10. *For $\sigma \in \mathcal{O}^{-1} \cup \mathcal{O}^0$, it holds that* $(\operatorname{div} \phi^{-1,\,0})(\sigma) = 0$.

Proof. By symmetry, we only prove $(\operatorname{div} \phi^{-1,\,0})(\sigma) = 0$ for each $\sigma \in \mathcal{O}^{-1}$. If $\sigma \in \mathcal{O}^{-1} \setminus \mathcal{Z}^{-1,\,0}$, then there is nothing to prove because by Lemmas 6.5.4 and 6.5.5, we have $g^{-1,\,0}(\sigma) = g^{-1,\,0}(\sigma') = 1$ for all $\sigma' \in \mathcal{E}^{-1}$ with $\sigma \sim \sigma'$.

Now, assume that $\sigma \in \mathcal{Z}^{-1,0}$. To this end, we may rewrite as

$$(\operatorname{div}\phi^{-1,0})(\sigma) = \sum_{\zeta\in\mathscr{V}^{-1}} \phi^{-1,0}(\sigma,\,\zeta) = \sum_{\zeta\in\mathcal{O}^{-1}} \phi^{-1,0}(\sigma,\,\zeta) + \sum_{\zeta\in\mathcal{I}_{\mathfrak{o}}^{-1}} \sum_{\zeta'\in\mathcal{N}(\zeta)} \phi^{-1,0}(\sigma,\,\zeta'). \tag{6.43}$$

The summation of $\zeta \in \mathcal{O}^{-1}$ in (6.43) becomes

$$\sum_{\zeta\in\mathcal{O}^{-1}} \frac{\mathfrak{e}}{Z_\beta \kappa} e^{-\beta\Gamma} \big[h_{0,\mathfrak{d}}^K\big((\Phi^{-1,0}\circ\Pi^{\mathbf{-1}})(\zeta)\big) - h_{0,\mathfrak{d}}^K\big((\Phi^{-1,0}\circ\Pi^{\mathbf{-1}})(\sigma)\big)\big]. \tag{6.44}$$

The double summation in (6.43) becomes

$$\sum_{\zeta\in\mathcal{I}_{\mathfrak{o}}^{-1}} \sum_{\zeta'\in\mathcal{N}(\zeta):\,\sigma\sim\zeta'} \frac{\mathfrak{e}}{Z_\beta \kappa} e^{-\beta\Gamma} \big[h_{0,\mathfrak{d}}^K\big((\Phi^{-1,0}\circ\Pi^{\mathbf{-1}})(\zeta)\big) - h_{0,\mathfrak{d}}^K\big((\Phi^{-1,0}\circ\Pi^{\mathbf{-1}})(\sigma)\big)\big]. \tag{6.45}$$

By (6.44) and (6.45), we have that (6.43) equals

$$\sum_{\zeta\in\mathscr{V}^{-1}} \frac{\mathfrak{e}}{Z_\beta \kappa} e^{-\beta\Gamma} r^{\mathbf{-1}}(\sigma,\,\zeta) \big[h_{0,\mathfrak{d}}^K((\Phi^{-1,0}(\zeta)) - h_{0,\mathfrak{d}}^K(\Phi^{-1,0}(\sigma))\big].$$

By Lemmas 6.5.4 and 6.5.5, the last displayed term equals four (if $K < L$) or eight (if $K = L$) times

$$\frac{\mathfrak{e}}{Z_\beta \kappa} e^{-\beta\Gamma} \sum_{y\in V_K} r_K(\Phi^{-1,0}(\sigma),\,y) \big[h_{0,\mathfrak{d}}^K(y) - h_{0,\mathfrak{d}}^K(\Phi^{-1,0}(\sigma))\big] = 0,$$

where the equality holds by an elementary property of stochastic generators (e.g., [16, (7.1.15)]). This conclues the proof. □

Gathering the preceding lemmas, we have the following proposition.

Proposition 6.6.11. *For* $\sigma \in \mathcal{X} \setminus (\mathcal{N}(\mathbf{-1}) \cup \mathcal{N}(\mathbf{0}))$, *we have* $(\operatorname{div}\phi^{-1,0})(\sigma) = 0$. *Similarly, for* $\sigma \in \mathcal{X} \setminus (\mathcal{N}(\mathbf{0}) \cup \mathcal{N}(\mathbf{+1}))$, *we have* $(\operatorname{div}\phi^{0,+1})(\sigma) = 0$.

Proof. We only prove the first statement. By Definition 6.6.3, the test flow $\phi^{-1,0}$ is divergence-free on $\mathcal{X} \setminus (\mathcal{B}^{-1,0} \cup \mathcal{E}^{-1} \cup \mathcal{E}^0)$. By Lemmas 6.6.8, 6.6.9, and 6.6.10, $\phi^{-1,0}$ is divergence-free on

$$\big[\mathcal{B}^{-1,0}\setminus(\mathcal{E}^{-1}\cup\mathcal{E}^{0})\big]\cup\big[\mathcal{R}_2^{-1,0}\cup\mathcal{R}_2^{0,-1}\big]\cup\big[\mathcal{O}^{-1}\cup\mathcal{O}^{0}\big].$$

By Proposition 6.4.2 and (6.29), the above set is precisely $(\mathcal{B}^{-1,0}\cup\mathcal{E}^{-1}\cup\mathcal{E}^{0})\setminus(\mathcal{N}(\mathbf{-1})\cup\mathcal{N}(\mathbf{0}))$. This observation concludes the proof. □

Finally, we provide estimates for the divergence on the remainder.

Proposition 6.6.12. *We have*

$$\sum_{\sigma\in\mathcal{N}(\mathbf{-1})}(\operatorname{div}\phi^{-1,0})(\sigma)\simeq\frac{1}{3\kappa}e^{-\beta\Gamma}\quad\textit{and}\quad\sum_{\sigma\in\mathcal{N}(\mathbf{0})}(\operatorname{div}\phi^{-1,0})(\sigma)\simeq-\frac{1}{3\kappa}e^{-\beta\Gamma}. \tag{6.46}$$

Similarly, we have

$$\sum_{\sigma\in\mathcal{N}(\mathbf{+1})}(\operatorname{div}\phi^{+1,0})(\sigma)\simeq\frac{1}{3\kappa}e^{-\beta\Gamma}\quad\textit{and}\quad\sum_{\sigma\in\mathcal{N}(\mathbf{0})}(\operatorname{div}\phi^{+1,0})(\sigma)\simeq-\frac{1}{3\kappa}e^{-\beta\Gamma}. \tag{6.47}$$

Proof. First, we focus on the first formula of (6.46). By Definition 6.6.3, this becomes

$$\sum_{\sigma\in\mathcal{N}(\mathbf{-1})}\sum_{\zeta\in\mathcal{O}^{-1}:\,\sigma\sim\zeta}\phi^{-1,0}(\sigma,\,\zeta)=\sum_{\zeta\in\mathcal{O}^{-1}}\sum_{\sigma\in\mathcal{N}(\mathbf{-1}):\,\sigma\sim\zeta}\phi^{-1,0}(\sigma,\,\zeta).$$

Substituting the exact value of $\phi^{-1,0}$ and from the fact that $\phi^{-1,0}$ is anti-symmetric, we compute this as

$$\begin{aligned}&\sum_{\zeta\in\mathcal{O}^{-1}}\sum_{\sigma\in\mathcal{N}(\mathbf{-1}):\,\sigma\sim\zeta}\frac{\mathfrak{e}}{Z_\beta\kappa}e^{-\beta\Gamma}\big[h_{0,\mathfrak{d}}^{K}(\Phi^{-1,0}(\zeta))-h_{0,\mathfrak{d}}^{K}(\Phi^{-1,0}(\mathbf{-1}))\big]\\&=\sum_{\zeta\in\mathcal{O}^{-1}}\frac{\mathfrak{e}}{Z_\beta\kappa}e^{-\beta\Gamma}r^{\mathbf{-1}}(\zeta,\,\mathbf{-1})\big[h_{0,\mathfrak{d}}^{K}(\Phi^{-1,0}(\zeta))-h_{0,\mathfrak{d}}^{K}(\Phi^{-1,0}(\mathbf{-1}))\big].\end{aligned}$$

By Lemmas 6.5.4 and 6.5.5, this becomes

$$\begin{cases} \dfrac{\mathfrak{e}}{Z_\beta \kappa} e^{-\beta\Gamma} \cdot 4\mathfrak{c}_K & \text{if } K < L, \\ \dfrac{\mathfrak{e}}{Z_\beta \kappa} e^{-\beta\Gamma} \cdot 8\mathfrak{c}_K & \text{if } K = L, \end{cases}$$

which is exactly $e^{-\beta\Gamma}/(Z_\beta\kappa)$ by (6.14). This proves the first formula of (6.46) by (6.6). The second formula of (6.46) similarly follows as

$$\sum_{\sigma \in \mathcal{N}(\mathbf{0})} (\operatorname{div} \phi^{-1,\,0})(\sigma) = -\frac{1}{Z_\beta \kappa} e^{-\beta\Gamma}.$$

Finally, the formulas in (6.47) can be proved in the same manner. □

6.7 Capacity estimates

In this section, we provide precise estimates of the relevant capacities and thereby prove Theorem 6.2.2.

6.7.1 Proof of parts (1) and (2) of Theorem 6.2.2

By symmetry, it suffices to estimate $\mathrm{Cap}_\beta(-\mathbf{1},\, \{\mathbf{0},\, +\mathbf{1}\})$ and $\mathrm{Cap}_\beta(-\mathbf{1},\, \mathbf{0})$. For both objects, we use the test function $g^{-1,\,0}$ (cf. Definition 6.6.1) and the test flow $\phi^{-1,\,0}$ (cf. Definition 6.6.3).

Proof of parts (1) and (2) of Theorem 6.2.2. First, note that

$$g^{-1,\,0} \in \mathfrak{C}(\{-\mathbf{1}\},\, \{\mathbf{0},\, +\mathbf{1}\}) \subseteq \mathfrak{C}(\{-\mathbf{1}\},\, \{\mathbf{0}\}).$$

Hence, by the Dirichlet principle and Proposition 6.6.6, we have

$$\mathrm{Cap}_\beta(-\mathbf{1},\, \{\mathbf{0},\, +\mathbf{1}\}),\, \mathrm{Cap}_\beta(-\mathbf{1},\, \mathbf{0}) \le D_\beta(g^{-1,\,0}) = \frac{1+o(1)}{3\kappa} e^{-\beta\Gamma}. \tag{6.48}$$

Next, we consider the lower bounds using the generalized Thomson principle. First, by Proposition 6.6.7, we have

$$\|\phi^{-1,0}\|^2 = \frac{1+o(1)}{3\kappa} e^{-\beta\Gamma}.$$

Next, Proposition 6.6.11 implies that $(\mathrm{div}\,\phi^{-1,0})(\sigma) = 0$ for all $\sigma \notin \mathcal{N}(\mathbf{-1}) \cup \mathcal{N}(\mathbf{0})$. Moreover, by Lemma 6.4.6, there exists a constant $C = C(K,\, L) > 0$ such that we have

$$\max_{\zeta \in \mathcal{N}(\mathbf{-1})} \big|h(\zeta) - h(\mathbf{-1})\big| \le Ce^{-\beta}, \quad \max_{\zeta \in \mathcal{N}(\mathbf{0})} \big|h(\zeta) - h(\mathbf{0})\big| \le Ce^{-\beta}$$

for both $h = h_{\mathbf{-1},\{\mathbf{0},\mathbf{+1}\}}$ and $h_{\mathbf{-1},\mathbf{0}}$. Thus, we have

$$\begin{aligned}\sum_{\sigma \in \mathcal{X}} h(\sigma)(\mathrm{div}\,\phi^{-1,0})(\sigma) &= \sum_{\sigma \in \mathcal{N}(\mathbf{-1}) \cup \mathcal{N}(\mathbf{0})} h(\sigma)(\mathrm{div}\,\phi^{-1,0})(\sigma) \\ &\simeq h(\mathbf{-1}) \sum_{\sigma \in \mathcal{N}(\mathbf{-1})} (\mathrm{div}\,\phi^{-1,0})(\sigma) + h(\mathbf{0}) \sum_{\sigma \in \mathcal{N}(\mathbf{0})} (\mathrm{div}\,\phi^{-1,0})(\sigma).\end{aligned}$$

By Proposition 6.6.12, the last formula asymptotically equals

$$\frac{1}{3\kappa} e^{-\beta\Gamma}[h(\mathbf{-1}) - h(\mathbf{0})] = \frac{1}{3\kappa} e^{-\beta\Gamma},$$

because $h_{\mathbf{-1},\{\mathbf{0},\mathbf{+1}\}}(\mathbf{-1}) = h_{\mathbf{-1},\mathbf{0}}(\mathbf{-1}) = 1$ and $h_{\mathbf{-1},\{\mathbf{0},\mathbf{+1}\}}(\mathbf{0}) = h_{\mathbf{-1},\mathbf{0}}(\mathbf{0}) = 0$. Summing up, we have

$$\frac{1}{\|\phi^{-1,0}\|^2} \Big[\sum_{\sigma \in \mathcal{X}} h(\sigma)(\mathrm{div}\,\phi^{-1,0})(\sigma) \Big]^2 \simeq \frac{1}{3\kappa} e^{-\beta\Gamma},$$

which holds for both $h = h_{\mathbf{-1},\{\mathbf{0},\mathbf{+1}\}}$ and $h_{\mathbf{-1},\mathbf{0}}$. Hence, by the generalized Thomson principle in Theorem 3.2.8, we have

$$\mathrm{Cap}_\beta(\mathbf{-1},\, \{\mathbf{0},\, \mathbf{+1}\}),\, \mathrm{Cap}_\beta(\mathbf{-1},\, \mathbf{0}) \ge \frac{1+o(1)}{3\kappa} e^{-\beta\Gamma}. \tag{6.49}$$

Therefore, by (6.48) and (6.49), we conclude the proof. □

6.7.2 Proof of part (3) of Theorem 6.2.2

In this subsection, we compute $\mathrm{Cap}_\beta(\mathbf{0},\, \{\mathbf{-1},\, \mathbf{+1}\})$.

Proof of part (3) of Theorem 6.2.2. Here, we use the test objects

$$g = 1 - g^{-1,\,0} - g^{+1,\,0} \quad \text{and} \quad \phi = -\phi^{-1,\,0} - \phi^{+1,\,0}.$$

First, Definitions 6.6.1 and 6.6.2 imply that

$$g^{-1,\,0}(\boldsymbol{s}) = \begin{cases} 1 & \text{if } \boldsymbol{s} = \mathbf{-1} \\ 0 & \text{if } \boldsymbol{s} = \mathbf{0},\, \mathbf{+1} \end{cases} \quad \text{and} \quad g^{+1,\,0}(\boldsymbol{s}) = \begin{cases} 1 & \text{if } \boldsymbol{s} = \mathbf{+1}, \\ 0 & \text{if } \boldsymbol{s} = \mathbf{-1},\, \mathbf{0}. \end{cases} \tag{6.50}$$

Thus, $g \in \mathfrak{C}(\{\mathbf{0}\},\, \{\mathbf{-1},\, \mathbf{+1}\})$. Moreover, we write

$$\begin{aligned} D_\beta(g) &= \sum_{\{\sigma,\,\zeta\} \in E(\mathcal{X})} \mu_\beta(\sigma) r_\beta(\sigma,\,\zeta) \{g(\zeta) - g(\sigma)\}^2 \\ &= \sum_{\{\sigma,\,\zeta\} \in E(\mathcal{X})} \mu_\beta(\sigma) r_\beta(\sigma,\,\zeta) \{g^{-1,\,0}(\sigma) - g^{-1,\,0}(\zeta) + g^{+1,\,0}(\sigma) - g^{+1,\,0}(\zeta)\}^2. \end{aligned}$$

By Remark 6.6.5, if $\sigma \sim \zeta$, then $g^{-1,\,0}(\sigma) = g^{-1,\,0}(\zeta)$ or $g^{+1,\,0}(\sigma) = g^{+1,\,0}(\zeta)$. This implies that the last summation equals

$$\begin{aligned} &\sum_{\{\sigma,\,\zeta\} \in E(\mathcal{X})} \mu_\beta(\sigma) r_\beta(\sigma,\,\zeta) \big[\{g^{-1,\,0}(\sigma) - g^{-1,\,0}(\zeta)\}^2 + \{g^{+1,\,0}(\sigma) - g^{+1,\,0}(\zeta)\}^2\big] \\ &= D_\beta(g^{-1,\,0}) + D_\beta(g^{+1,\,0}). \end{aligned}$$

Hence, by the Dirichlet principle and Proposition 6.6.6, we have

$$\mathrm{Cap}_\beta(\mathbf{0},\, \{\mathbf{-1},\, \mathbf{+1}\}) \le D_\beta(g) = D_\beta(g^{-1,\,0}) + D_\beta(g^{+1,\,0}) = \frac{2 + o(1)}{3\kappa} e^{-\beta\Gamma}. \tag{6.51}$$

Next, we handle the lower bound. By Remark 6.6.5, we have

$$\|\phi\|^2 = \sum_{\{\sigma,\,\zeta\}\in E(\mathcal{X})} \frac{\phi(\sigma,\,\zeta)^2}{\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)} = \sum_{\{\sigma,\,\zeta\}\in E(\mathcal{X})} \frac{\phi^{-1,\,0}(\sigma,\,\zeta)^2}{\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)} + \sum_{\{\sigma,\,\zeta\}\in E(\mathcal{X})} \frac{\phi^{+1,\,0}(\sigma,\,\zeta)^2}{\mu_\beta(\sigma)r_\beta(\sigma,\,\zeta)},$$

which is exactly $\|\phi^{-1,\,0}\|^2 + \|\phi^{+1,\,0}\|^2$. Hence, by Proposition 6.6.7, we have

$$\|\phi\|^2 = \|\phi^{-1,\,0}\|^2 + \|\phi^{+1,\,0}\|^2 = \frac{2+o(1)}{3\kappa} e^{-\beta\Gamma}.$$

Moreover, we temporarily denote by $h = h_{\mathbf{0},\,\{\mathbf{-1},\,\mathbf{+1}\}}$. Then, the same deduction as in the proof of parts (1) and (2) of Theorem 6.2.2 implies that

$$\sum_{\sigma\in\mathcal{X}} h(\sigma)(\operatorname{div}\phi^{-1,\,0})(\sigma) \simeq \frac{1}{3\kappa} e^{-\beta\Gamma}[h(\mathbf{-1}) - h(\mathbf{0})] = -\frac{1}{3\kappa} e^{-\beta\Gamma}$$

and

$$\sum_{\sigma\in\mathcal{X}} h(\sigma)(\operatorname{div}\phi^{+1,\,0})(\sigma) \simeq \frac{1}{3\kappa} e^{-\beta\Gamma}[h(\mathbf{+1}) - h(\mathbf{0})] = -\frac{1}{3\kappa} e^{-\beta\Gamma}.$$

Hence, we have

$$\sum_{\sigma\in\mathcal{X}} h(\sigma)(\operatorname{div}\phi)(\sigma) \simeq \frac{1}{3\kappa} e^{-\beta\Gamma} + \frac{1}{3\kappa} e^{-\beta\Gamma} = \frac{2}{3\kappa} e^{-\beta\Gamma}.$$

Summing up, we have

$$\frac{1}{\|\phi\|^2}\Big[\sum_{\sigma\in\mathcal{X}} h(\sigma)(\operatorname{div}\phi)(\sigma)\Big]^2 \simeq \frac{2}{3\kappa} e^{-\beta\Gamma}.$$

Hence, by the generalized Thomson principle in Theorem 3.2.8, we have

$$\mathrm{Cap}_\beta(\mathbf{0},\,\{\mathbf{-1},\,\mathbf{+1}\}) \geq \frac{2+o(1)}{3\kappa} e^{-\beta\Gamma}. \tag{6.52}$$

Therefore, by (6.51) and (6.52), we conclude the proof. □

6.7.3 Proof of part (4) of Theorem 6.2.2

Finally, we prove part (4) of Theorem 6.2.2 and thereby conclude the proof of the main theorems.

Proof of part (4) of Theorem 6.2.2. Here, we use the test objects

$$g = \frac{1}{2}(1 + g^{-1,0} - g^{+1,0}) \quad \text{and} \quad \phi = \phi^{-1,0} - \phi^{+1,0}.$$

First, (6.50) implies that $g \in \mathfrak{C}(\{\mathbf{-1}\}, \{\mathbf{+1}\})$. Moreover, as in the preceding proof, Remark 6.6.5 and Proposition 6.6.6 imply that

$$D_\beta(g) = \frac{1}{4}\big[D_\beta(g^{-1,0}) + D_\beta(g^{+1,0})\big] = \frac{1+o(1)}{6\kappa}e^{-\beta\Gamma}.$$

Hence, by the Dirichlet principle, we have

$$\mathrm{Cap}_\beta(\mathbf{-1}, \mathbf{+1}) \le D_\beta(g) = \frac{1+o(1)}{6\kappa}e^{-\beta\Gamma}. \tag{6.53}$$

Next, again using Remark 6.6.5 and Proposition 6.6.7, we first have

$$\|\phi\|^2 = \|\phi^{-1,0}\|^2 + \|\phi^{+1,0}\|^2 = \frac{2+o(1)}{3\kappa}e^{-\beta\Gamma}.$$

Moreover, we temporarily denote by $h = h_{\mathbf{-1},\mathbf{+1}}$. Then, the same deduction as above and Theorem 6.1.6 imply that

$$\sum_{\sigma\in\mathcal{X}} h(\sigma)(\mathrm{div}\,\phi^{-1,0})(\sigma) \simeq \frac{1}{3\kappa}e^{-\beta\Gamma}[h(\mathbf{-1}) - h(\mathbf{0})] \simeq \frac{1}{6\kappa}e^{-\beta\Gamma}$$

and

$$\sum_{\sigma\in\mathcal{X}} h(\sigma)(\mathrm{div}\,\phi^{+1,0})(\sigma) \simeq \frac{1}{3\kappa}e^{-\beta\Gamma}[h(\mathbf{+1}) - h(\mathbf{0})] \simeq -\frac{1}{6\kappa}e^{-\beta\Gamma}.$$

Hence, we have

$$\sum_{\sigma\in\mathcal{X}} h(\sigma)(\operatorname{div}\phi)(\sigma) = \frac{1}{6\kappa}e^{-\beta\Gamma} + \frac{1}{6\kappa}e^{-\beta\Gamma} = \frac{1}{3\kappa}e^{-\beta\Gamma}.$$

Summing up, we have

$$\frac{1}{\|\phi\|^2}\Big[\sum_{\sigma\in\mathcal{X}} h(\sigma)(\operatorname{div}\phi)(\sigma)\Big]^2 \simeq \frac{1}{6\kappa}e^{-\beta\Gamma}.$$

Hence, by the generalized Thomson principle, we have

$$\mathrm{Cap}_\beta(\mathbf{-1},\,\mathbf{+1}) \geq \frac{1+o(1)}{6\kappa}e^{-\beta\Gamma}. \tag{6.54}$$

Therefore, by (6.53) and (6.54), we conclude the proof. □

6.8 Periodic boundary conditions

In this section, we briefly discuss the model with periodic boundary conditions imposed. Thus, throughout this section, we assume that Λ *is given periodic boundary conditions;* that is, $\Lambda = \mathbb{T}_K \times \mathbb{T}_L$. Compared to the logic established thus far for the open boundary case, the storyline for the periodic boundary case is nearly the same, although certain slight technical differences exist between the two. We provide a short summary in this section.

We handle two issues here: the energy barrier between the ground states that appears in Theorem 6.1.2 and the sub-exponential prefactor that appears in Theorem 6.1.7.

Energy barrier between ground states

Recall that Theorem 6.1.2 in the periodic case is interpreted as

$$\Gamma_{-1,\,0} = \Gamma_{0,\,+1} = \Gamma_{-1,\,+1} = 2K+2.$$

It can be observed that the energy barrier in this case is twice that of the open boundary model. To explain this, we recall the canonical path defined in Definition 6.3.3. The exact same canonical path also attains the energy barrier in the periodic case. However, in the periodic case, the maximal energy of the canonical path is doubled, because the sites on the edges of Λ are also connected to the corresponding sites on the other end of Λ. Therefore, in the periodic case, we can easily determine that (cf. Remark 6.3.4)

$$H(\sigma) = \begin{cases} 2K & \text{if } \sigma \in \mathcal{R}_v^{-1,0} \cup \mathcal{R}_v^{0,+1} \text{ for } v \in [\![1,\, L-1]\!], \\ 2K+2 & \text{if } \sigma \in \mathcal{Q}_v^{-1,0} \cup \mathcal{Q}_v^{0,+1} \text{ for } v \in [\![1,\, L-2]\!], \end{cases}$$

so that the canonical paths are $(2K+2)$-paths connecting the ground states in $\mathcal{S}$. Moreover, the deduction in Section 6.3.2 can be modified slightly to verify that the energy barrier is precisely $2K+2$.

As noted in Remark 6.1.5, once the energy barrier $\Gamma = 2K+2$ is settled, the large deviation-type main results in Theorem 6.1.3 hold without any modification. Theorem 6.1.6 follows in the same manner.

Sub-exponential prefactor

As explained in Remark 6.1.5, the exact quantitative estimates of the metastable transitions differ between the two boundary conditions. The constant κ in Theorem 6.1.7, which constitutes the sub-exponential prefactor of the Eyring–Kramers law, must be modified to κ' in this case. We provide the correct versions of Theorems 6.1.7 and 6.1.12 in the periodic case.

Theorem 6.8.1. *Under periodic boundary conditions on Λ, there exists a constant $\kappa' = \kappa'(K,\, L) > 0$ such that parts (1) to (4) of Theorem 6.1.7 hold with κ' instead of κ. Moreover, the constant κ' satisfies (cf.* (6.1)*)*

$$\lim_{K\to\infty} \kappa'(K,\, L) = \begin{cases} 1/4 & \text{if } K < L, \\ 1/8 & \text{if } K = L. \end{cases} \tag{6.55}$$

Moreover, as an analogue of (6.13), we define the limiting Markov chain $\{Y'(t)\}_{t\geq 0}$ on $\mathcal{S}$ as the continuous-time Markov chain associated with the transition rate given by

$$r_{Y'}(\boldsymbol{s},\,\boldsymbol{s'}) = \begin{cases} (\kappa')^{-1} & \text{if } \{\boldsymbol{s},\,\boldsymbol{s'}\} = \{\mathbf{-1},\,\mathbf{0}\} \text{ or } \{\mathbf{0},\,\mathbf{+1}\}, \\ 0 & \text{otherwise.} \end{cases} \tag{6.56}$$

Theorem 6.8.2. *Under periodic boundary conditions on Λ, parts (1) and (2) of Theorem 6.1.12 hold with $X'(\cdot)$ instead of $X(\cdot)$.*

As can be observed from Theorems 6.8.1 and 6.8.2, the difference between the two boundary conditions lies in the constants κ and κ'. That is, according to (6.12) and (6.55), the constants κ and κ' differ by the factor KL (in the limit $K \to \infty$). We refer to Section 4.8 for a thorough heuristic explanation of this factor KL. We provide the precise definition of κ', which is an analogue of Definition 6.2.1. The constant κ' satisfies $\kappa' = \mathfrak{b}' + 2\mathfrak{e}'$, where the bulk constant $\mathfrak{b}' = \mathfrak{b}'(K,\,L)$ is defined as

$$\mathfrak{b}' = \begin{cases} \dfrac{(K+2)(L-4)}{4KL} & \text{if } K < L \\ \dfrac{(K+2)(L-4)}{8KL} & \text{if } K = L \end{cases}$$

and the edge constant $\mathfrak{e}' = \mathfrak{e}'(K,\,L)$ is defined in the same manner as $\mathfrak{e}$ which satisfies

$$\mathfrak{e}' \leq \frac{C}{KL} \quad \text{for some constant } C > 0. \tag{6.57}$$

Thus, the estimate (6.55) holds for κ'.

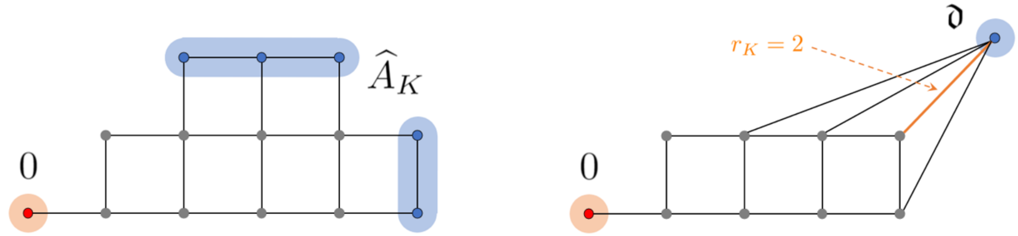


Figure 6.7: (Left) graph structure $(\widehat{V}_K,\, E(\widehat{V}_K))$. (Right) graph structure $(V_K,\, E(V_K))$.

6.9 Auxiliary process

6.9.1 Original auxiliary process

In this subsection, we define an auxiliary process which successfully represents the Metropolis dynamics on the edge typical configurations. For $K \ge 5$, we define a graph structure $(\widehat{V}_K,\, E(\widehat{V}_K))$ (see Figure 6.7 (left) for an illustration for the case of $K = 5$). First, the vertex set $\widehat{V}_K \subseteq \mathbb{R}^2$ is defined by

$$\widehat{V}_K = \{(a,\, b) \in \mathbb{R}^2 : 0 \le b \le a \le K \text{ and } b \le 2\} \setminus \{(K,\, 2)\}. \tag{6.58}$$

Then, the edge structure $E(\widehat{V}_K)$ is inherited by the Euclidean lattice. We abbreviate by $0 = (0,\, 0) \in \widehat{V}_K$ and define

$$\widehat{A}_K = \{(a,\, b) \in \widehat{V}_K : a = K \text{ or } b = 2\}.$$

Then, we define $\{\widehat{Z}_K(t)\}_{t\ge0}$ as the continuous-time random walk on the aforementioned graph whose transition rate is uniformly 1. In other words, the transition rate $\widehat{r}_K : \widehat{V}_K \times \widehat{V}_K \to [0,\, \infty)$ is given by

$$\widehat{r}_K(x,\, y) = \begin{cases} 1 & \text{if } \{x,\, y\} \in E(\widehat{V}_K), \\ 0 & \text{otherwise.} \end{cases}$$

Obviously, the process is reversible with respect to the uniform distribution on $\widehat{V}_K$.

We denote by $\widehat{h}^K_{\cdot,\cdot}(\cdot)$ and $\widehat{\mathrm{cap}}_K(\cdot,\,\cdot)$ the equilibrium potential and capacity with respect to $\widehat{Z}_K(\cdot)$, respectively. We define a constant $\mathfrak{c}_K > 0$ by

$$\mathfrak{c}_K = |\widehat{V}_K|\widehat{\mathrm{cap}}_K(0,\, \widehat{A}_K). \tag{6.59}$$

Then, we have the following asymptotic lemma.

Lemma 6.9.1. *There exists a positive constant δ with $|\delta - 0.435| < 0.0001$ such that*

$$\lim_{K\to\infty} \mathfrak{c}_K = \delta.$$

Proof. We explicitly compute the equilibrium potential $\widehat{h}^K_{0,\widehat{A}_K}(\cdot)$. For simplicity, we write $h = \widehat{h}^K_{0,\widehat{A}_K}$ and abbreviate by $h(a,\, b) = h((a,\, b))$ for $(a,\, b) \in \widehat{V}_K$. We define

$$a_i = h(K-i,\, 0);\ i \in [\![0,\, K]\!] \quad \text{and} \quad b_i = h(K-i,\, 1);\ i \in [\![0,\, K-1]\!].$$

Then, we trivially have $a_K = h(0,\, 0) = 1$,

$$a_0 = h(K,\, 0) = 0 \quad \text{and} \quad b_0 = h(K,\, 1) = 0. \tag{6.60}$$

Moreover, by the Markov property, the following recurrence relations hold:

$$3a_i = a_{i+1} + a_{i-1} + b_i;\ i \in [\![1,\, K-1]\!], \tag{6.61}$$

$$4b_i = b_{i+1} + b_{i-1} + a_i;\ i \in [\![1,\, K-2]\!], \tag{6.62}$$

$$2b_{K-1} = b_{K-2} + a_{K-1} \quad \text{and} \quad 3a_{K-1} = 1 + a_{K-2} + b_{K-1}. \tag{6.63}$$

Then, (6.61) and (6.62) induce the following relations:

$$a_{i+2} - 7a_{i+1} + 13a_i - 7a_{i-1} + a_{i-2} = 0;\ i \in [\![2,\ K-3]\!], \tag{6.64}$$

$$b_{i+2} - 7b_{i+1} + 13b_i - 7b_{i-1} + b_{i-2} = 0;\ i \in [\![2,\ K-3]\!]. \tag{6.65}$$

Hence, we solve $t^4 - 7t^3 + 13t^2 - 7t + 1 = 0$, which is equivalent to $(t+t^{-1})^2 - 7(t+t^{-1}) + 11 = 0$. This gives $t + t^{-1} = (7 \pm \sqrt{5})/2$. Thus, we define the positive constants $\alpha_1,\ \alpha_2,\ \alpha_3,\ \alpha_4 > 0$ such that $\alpha_1 > \alpha_2$ are the solutions of $t + t^{-1} = (7+\sqrt{5})/2$ and $\alpha_3 > \alpha_4$ are the solutions of $t + t^{-1} = (7-\sqrt{5})/2$. Then, there exist constants p_n and q_n, $n \in [\![1,\ 4]\!]$ such that we have, for $i \in [\![0,\ K-1]\!]$,

$$a_i = \sum_{n=1}^{4} p_n \alpha_n^i \quad \text{and} \quad b_i = \sum_{n=1}^{4} q_n \alpha_n^i. \tag{6.66}$$

Based on the last formula, (6.60) implies

$$p_1 + p_2 + p_3 + p_4 = q_1 + q_2 + q_3 + q_4 = 0, \tag{6.67}$$

and (6.61) implies, for $i \in [\![1,\ K-1]\!]$,

$$\sum_{n=1}^{4} \alpha_n^{i-1} \{p_n \alpha_n^2 - (3p_n - q_n)\alpha_n + p_n\} = 0.$$

As $K \geq 5$, this implies that

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ \alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 \\ \alpha_1^2 & \alpha_2^2 & \alpha_3^2 & \alpha_4^2 \\ \alpha_1^3 & \alpha_2^3 & \alpha_3^3 & \alpha_4^3 \end{bmatrix} \begin{bmatrix} p_1\alpha_1^2 - (3p_1 - q_1)\alpha_1 + p_1 \\ p_2\alpha_2^2 - (3p_2 - q_2)\alpha_2 + p_2 \\ p_3\alpha_3^2 - (3p_3 - q_3)\alpha_3 + p_3 \\ p_4\alpha_4^2 - (3p_4 - q_4)\alpha_4 + p_4 \end{bmatrix} = 0.$$

As the square matrix is invertible (cf. Vandermonde matrix), we must have

$p_n\alpha_n^2 - (3p_n - q_n)\alpha_n + p_n = 0$ for all $n \in [\![1, 4]\!]$, which implies that

$$3p_n - q_n = \frac{7+\sqrt{5}}{2}p_n;\ n = 1,\ 2, \quad \text{and} \quad 3p_n - q_n = \frac{7-\sqrt{5}}{2}p_n;\ n = 3,\ 4.$$

Hence, substituting (6.67) and the last display to (6.66) gives, for $i \in [\![0,\ K-1]\!]$,

$$a_i = p_1(\alpha_1^i - \alpha_2^i) + p_3(\alpha_3^i - \alpha_4^i), \quad b_i = -\frac{1+\sqrt{5}}{2}p_1(\alpha_1^i - \alpha_2^i) + \frac{-1+\sqrt{5}}{2}p_3(\alpha_3^i - \alpha_4^i). \tag{6.68}$$

Substituting the last formula to (6.63) implies

$$\begin{aligned}&(2+\sqrt{5})p_1(\alpha_1^{K-1} - \alpha_2^{K-1}) + (2-\sqrt{5})p_3(\alpha_3^{K-1} - \alpha_4^{K-1})\\ &= \frac{1+\sqrt{5}}{2}p_1(\alpha_1^{K-2} - \alpha_2^{K-2}) + \frac{1-\sqrt{5}}{2}p_3(\alpha_3^{K-2} - \alpha_4^{K-2})\end{aligned}$$

and

$$\begin{aligned}&\frac{7+\sqrt{5}}{2}p_1(\alpha_1^{K-1} - \alpha_2^{K-1}) + \frac{7-\sqrt{5}}{2}p_3(\alpha_3^{K-1} - \alpha_4^{K-1})\\ &= 1 + p_1(\alpha_1^{K-2} - \alpha_2^{K-2}) + p_3(\alpha_3^{K-2} - \alpha_4^{K-2}).\end{aligned}$$

Solving the last two equations, we can express p_1 and p_3 in terms of $\alpha_1,\ \alpha_2,\ \alpha_3,\ \alpha_4$. Substituting these to the first equation of (6.68) for $i = K-1$, we deduce that a_{K-1} equals

$$-\Big[(2-\sqrt{5}) - \frac{1-\sqrt{5}}{2}\frac{\alpha_3^{K-2} - \alpha_4^{K-2}}{\alpha_3^{K-1} - \alpha_4^{K-1}}\Big] + \Big[(2+\sqrt{5}) - \frac{1+\sqrt{5}}{2}\frac{\alpha_1^{K-2} - \alpha_2^{K-2}}{\alpha_1^{K-1} - \alpha_2^{K-1}}\Big]$$

divided by

$$\Big[(2+\sqrt{5})-\frac{1+\sqrt{5}}{2}\frac{\alpha_1^{K-2}-\alpha_2^{K-2}}{\alpha_1^{K-1}-\alpha_2^{K-1}}\Big]\Big[\frac{7-\sqrt{5}}{2}-\frac{\alpha_3^{K-2}-\alpha_4^{K-2}}{\alpha_3^{K-1}-\alpha_4^{K-1}}\Big]$$
$$-\Big[(2-\sqrt{5})-\frac{1-\sqrt{5}}{2}\frac{\alpha_3^{K-2}-\alpha_4^{K-2}}{\alpha_3^{K-1}-\alpha_4^{K-1}}\Big]\Big[\frac{7+\sqrt{5}}{2}-\frac{\alpha_1^{K-2}-\alpha_2^{K-2}}{\alpha_1^{K-1}-\alpha_2^{K-1}}\Big].$$

As $\alpha_1 > \alpha_2$ and $\alpha_3 > \alpha_4$, we have $(\alpha_2/\alpha_1)^{K-1} \to 0$ and $(\alpha_4/\alpha_3)^{K-1} \to 0$ as $K \to \infty$. Thus, we may calculate

$$\lim_{K\to\infty} a_{K-1} = \frac{-\Big[(2-\sqrt{5})-\frac{1-\sqrt{5}}{2}\frac{1}{\alpha_3}\Big]+\Big[(2+\sqrt{5})-\frac{1+\sqrt{5}}{2}\frac{1}{\alpha_1}\Big]}{\Big[(2+\sqrt{5})-\frac{1+\sqrt{5}}{2}\frac{1}{\alpha_1}\Big]\Big[\frac{7-\sqrt{5}}{2}-\frac{1}{\alpha_3}\Big]-\Big[(2-\sqrt{5})-\frac{1-\sqrt{5}}{2}\frac{1}{\alpha_3}\Big]\Big[\frac{7+\sqrt{5}}{2}-\frac{1}{\alpha_1}\Big]}$$
$$= \frac{2\sqrt{5}-\frac{1+\sqrt{5}}{2}\alpha_2+\frac{1-\sqrt{5}}{2}\alpha_4}{5\sqrt{5}+\frac{3-5\sqrt{5}}{2}\alpha_2+\frac{-3-5\sqrt{5}}{2}\alpha_4+\sqrt{5}\alpha_2\alpha_4}.$$

In the second equality, we used that $\alpha_1\alpha_2 = \alpha_3\alpha_4 = 1$. By substituting the exact values of α_i, this is asymptotically 0.5649853624. Moreover, as $0 = (0,\, 0) \in \widehat{V}_K$ is connected only to $(1,\, 0) \in \widehat{V}_K$, we have by [16, (7.1.39)] that

$$\widehat{\mathrm{cap}}_K(0,\, \widehat{A}_K) = \frac{1}{|\widehat{V}_K|}[h(0,\, 0) - h(1,\, 0)] = \frac{1-a_{K-1}}{|\widehat{V}_K|}.$$

Therefore, we have

$$\lim_{K\to\infty} \mathfrak{c}_K = \lim_{K\to\infty} |\widehat{V}_K|\widehat{\mathrm{cap}}_K(0,\, \widehat{A}_K) = 1 - \lim_{K\to\infty} a_{K-1} \approx 0.4350146376,$$

which concludes the proof. □

Remark 6.9.2. In the periodic boundary case, we need a completely different auxiliary process to estimate the structure of edge typical configurations. Namely, the desired process is a Markov chain on the collection of subtrees of a $K \times 2$-shaped ladder graph with semi-periodic boundary conditions (i.e., open on the horizontal boundaries and periodic on the vertical ones). In this case, we deduce an upper bound for the corresponding capacity, which is sufficient to obtain the bound (6.57). We refer to Proposition 4.6.9 for more information on this estimate.

6.9.2 Projected auxiliary process

Based on the original auxiliary process defined in the preceding subsection, we define a projected auxiliary process which is obtained by simply projecting the elements in $\widehat{A}_K$ to a single element $\mathfrak{d}$. Rigorously, we define a graph structure $(V_K,\, E(V_K))$ (see Figure 6.7 (right) for an illustration for the case of $K = 5$). The vertex set $V_K \subseteq \mathbb{R}^2$ is defined by

$$V_K = (\widehat{V}_K \setminus \widehat{A}_K) \cup \{\mathfrak{d}\}. \tag{6.69}$$

Then, the edge structure $E(V_K)$ is inherited by $E(\widehat{V}_K)$; we have $\{x,\, y\} \in E(V_K)$ for $\{x,\, y\} \in E(\widehat{V}_K)$, $x,\, y \in \widehat{V}_K \setminus \widehat{A}_K$, and we have $\{x,\, \mathfrak{d}\} \in E(V_K)$ for

$$x \in \widehat{V}_K \setminus \widehat{A}_K \quad \text{satisfying} \quad \exists y \in \widehat{A}_K \quad \text{with} \quad \{x,\, y\} \in E(\widehat{V}_K).$$

Then, we define $\{Z_K(t)\}_{t\geq 0}$ as the continuous-time Markov chain on $(V_K,\, E(V_K))$ whose transition rate r_K is defined by $r_K(x,\, y) = \widehat{r}_K(x,\, y)$ if $x,\, y \neq \mathfrak{d}$ and

$$r_K(x,\, \mathfrak{d}) = r_K(\mathfrak{d},\, x) = \sum_{y\in\widehat{A}_K} \widehat{r}_K(x,\, y).$$

This process is reversible with respect to the uniform distribution on V_K.

We denote by $h^K_{\cdot,\cdot}(\cdot)$, $\mathrm{cap}_K(\cdot,\, \cdot)$, $D_K(\cdot)$ the equilibrium potential, capacity, and Dirichlet form with respect to $Z_K(\cdot)$, respectively. Then, by the strong Markov property, it is immediate from the definition that

$$h^K_{0,\mathfrak{d}}(x) = \widehat{h}^K_{0,\widehat{A}_K}(x);\ x \in \widehat{V}_K \setminus \widehat{A}_K \quad \text{and} \quad h^K_{0,\mathfrak{d}}(\mathfrak{d}) = \widehat{h}^K_{0,\widehat{A}_K}(y) = 0;\ y \in \widehat{A}_K.$$

Therefore, we have (cf. (6.59))

$$|V_K|\mathrm{cap}_K(0,\,\mathfrak{d}) = |\widehat{V}_K|\widehat{\mathrm{cap}}_K(0,\,\widehat{A}_K) = \mathfrak{c}_K. \tag{6.70}$$

Chapter 7

General interaction constants

In this chapter, we consider a generalized three-state Potts model on a finite two-dimensional rectangular lattice graph $\Lambda = (V, E)$, where $V = \{0, \ldots, K-1\} \times \{0, \ldots, L-1\}$ is the vertex set and E is the edge set. Without loss of generality, we assume throughout the article that

$$K \leq L.$$

To fix ideas, we assume periodic boundary conditions; more precisely, we also include each pair of vertices lying on opposite sides of the lattice in the edge set, so that we obtain a two-dimensional torus $\mathbb{T}_K \times \mathbb{T}_L$. We say that two vertices $v, w \in V$ are nearest neighbors (or simply neighbors) and denote by $v \sim w$ when they share an edge of Λ, i.e., when $\{v, w\} \in E$. To each vertex $v \in V$ is associated a spin taking value in $\Omega := \{1, 2, 3\}$, and thus $\mathcal{X} := \Omega^V$ denotes the set of *spin configurations*. We denote by $\mathbf{1}, \mathbf{2}, \mathbf{3} \in \mathcal{X}$ those configurations in which all the vertices have spin value 1, 2, 3, respectively.

To each configuration $\sigma \in \mathcal{X}$ we associate the energy $H(\sigma) \in \mathbb{R}$ given by

$$H(\sigma) := -\sum_{i\in S} J_{ii} \sum_{\{v,w\}\in E} \mathbb{1}_{\{\sigma(v)=\sigma(w)=i\}} + \sum_{i,j\in S:\, i<j} J_{ij} \sum_{\{v,w\}\in E} \mathbb{1}_{\{\{\sigma(v),\sigma(w)\}=\{i,j\}\}}, \tag{7.1}$$

where for any $i, j \in S$, $J_{ij} > 0$ are the coupling or interaction constants. We remark that our techniques would also work if the Hamiltonian includes an external field, leading to similar results. For simplicity we decided to focus on the case of zero external field.

We assume that

$$J_{11} > J_{22} = J_{33} \quad \text{and} \quad J_{12} = J_{13}, \tag{7.2}$$

so that, intuitively, spin 1 is more stable than spins 2 and 3, and the Hamiltonian is symmetric with respect to the spin exchange $2 \leftrightarrow 3$. Then, we write

$$\gamma_1 := J_{11} - J_{22} > 0, \quad \gamma_{12} := J_{12} + J_{22} > 0 \quad \text{and} \quad \gamma_{23} := J_{23} + J_{22} > 0. \tag{7.3}$$

We assume the following conditions throughout this article. Recall the definition of function $f_h(x)$ from (7.43).

Assumption 7.0.1. *The following conditions hold.*

A. $\dfrac{2\gamma_{12} + \gamma_1}{2\gamma_1}$ *is not an integer.*

B. $f_{\gamma_1}(\gamma_{12}) = 2(K+1)\gamma_{23}$.

C. $2\gamma_{12} \geq 4\gamma_{23} + \gamma_1$.

Intuitively, condition **A** corresponds to the familiar condition $2/h \notin \mathbb{N}$, where $h > 0$ is the external field of the original Ising model, first proposed in [71, standard case]. Condition **B** implies that the energy barriers of the canonical transitions $\mathbf{2} \to \mathbf{1}$ and $\mathbf{2} \to \mathbf{3}$ are the same. It is clear that condition

C is satisfied if there exists a constant $k > 0$ sufficiently large so that $\gamma_{12} \geq k\gamma_1$ and $\gamma_{12} \geq k\gamma_{23}$. This is a natural selection of constants which will be justified in more detail in Section 7.5.3. We refer to Section 7.5.3 for more detailed explanation on each of our specific choices.

Remark 7.0.2. Condition **C** is an optimal condition on the coefficients and used in the proof of Lemma 7.2.2 only. This inequality has the following interpretation. Keeping (7.3) in mind, we can rewrite condition **C** as

$$2J_{12} - J_{11} + 3J_{22} \geq 4J_{23} + 4J_{22}. \tag{7.4}$$

By a simple algebraic computation, we can see that the left-hand side of (7.4) is the energy needed to add a protuberance to a cluster of spins 1 in the sea of spins 2, and the right-hand side of (7.4) is the energy needed to add a new spin 3 in the sea of spins 2. Thus, (7.4) suggests that the dynamics favor a single appearance of an unrelated spin (in this case, 3) over the enlargement of a cluster of spins 1. This subtle dynamical behavior constitutes a significant challenge that is not present in the ferromagnetic Ising and Potts models analyzed in, say, [13].

Recall the Gibbs distribution μ_β from Definition 2.0.2 and the MH dynamics $\sigma_\beta(\cdot)$ from (2.1).

7.1 Main results

7.1.1 Stable and metastable states

We denote by $\mathcal{X}^s$ the set of global minima of the Hamiltonian (7.1). A simple algebraic computation implies the following proposition.

Proposition 7.1.1 (Identification of $\mathcal{X}^s$). *It holds that* $\mathcal{X}^s = \{\mathbf{1}\}$.

Proof. By the definition (7.1) and the assumption (7.2), it is straightforward that

$$H(\sigma) \geq -\sum_{i\in S} J_{ii} \sum_{\{v,\,w\}\in E} \mathbb{1}_{\{\sigma(v)=\sigma(w)=i\}} \geq -J_{11} \sum_{i\in S} \sum_{\{v,\,w\}\in E} \mathbb{1}_{\{\sigma(v)=\sigma(w)=i\}}.$$

The last double summation is exactly $\sum_{\{v,\,w\}\in E} \mathbb{1}_{\{\sigma(v)=\sigma(w)\}}$, which is clearly bounded above by $|E| = 2KL$. Therefore, we conclude that $H(\sigma) \geq -2J_{11}KL$. The equality holds if and only if $\sigma(v) = \sigma(w) = 1$ for all $\{v, w\} \in E$, which is equivalent to $\sigma = \mathbf{1}$. $\square$

Next, we identify the metastable configurations. We denote by $\Omega_{\sigma,\,\sigma'}$ the set of all paths between σ and σ'. For convenience of notation, we sometimes write $\omega : \sigma \to \sigma'$ to indicate $\omega \in \Omega_{\sigma,\,\sigma'}$. For any path $\omega = (\omega_0, \ldots, \omega_n)$, we define the *height* of ω as

$$\Phi_\omega := \max_{i=0,\,\ldots,\,n} H(\omega_i). \tag{7.5}$$

For any pair of configurations $\sigma, \sigma' \in \mathcal{X}$, the *communication height* $\Phi(\sigma, \sigma')$ between σ and σ' is defined as the minimal height among all paths $\omega : \sigma \to \sigma'$, i.e.,

$$\Phi(\sigma,\, \sigma') := \min_{\omega:\sigma\to\sigma'} \Phi_\omega = \min_{\omega:\sigma\to\sigma'} \max_{\eta\in\omega} H(\eta). \tag{7.6}$$

We define the set of *optimal paths* between σ, $\sigma' \in \mathcal{X}$ as

$$\Omega^{\mathrm{opt}}_{\sigma,\,\sigma'} := \{\omega \in \Omega_{\sigma,\,\sigma'} : \Phi_\omega = \Phi(\sigma,\, \sigma')\}. \tag{7.7}$$

Accordingly, for disjoint subsets $\mathcal{A}$ and $\mathcal{B}$ of $\mathcal{X}$, we define

$$\Phi(\mathcal{A},\, \mathcal{B}) := \min_{\sigma\in\mathcal{A}} \min_{\sigma'\in\mathcal{B}} \Phi(\sigma,\, \sigma')$$

and

$$\Omega^{\mathrm{opt}}_{\mathcal{A},\,\mathcal{B}} := \{\omega \in \Omega_{\sigma,\,\sigma'} : \sigma \in \mathcal{A},\ \sigma' \in \mathcal{B},\ \Phi_\omega = \Phi(\mathcal{A},\, \mathcal{B})\}.$$

For any $\sigma \in \mathcal{X}$, let $\mathcal{I}_\sigma := \{\eta \in \mathcal{X} : H(\eta) < H(\sigma)\}$ be the set of configurations with energy strictly smaller than $H(\sigma)$. Then, we define the *stability level* of σ as

$$V_\sigma := \Phi(\sigma, \mathcal{I}_\sigma) - H(\sigma). \tag{7.8}$$

If $\mathcal{I}_\sigma = \varnothing$ (i.e. if $\sigma \in \mathcal{X}^s$), we set $V_\sigma := \infty$. Finally, we define the collection of *metastable states* as

$$\mathcal{X}^m := \big\{\eta \in \mathcal{X} : V_\eta = \max_{\sigma \in \mathcal{X} \setminus \mathcal{X}^s} V_\sigma\big\}. \tag{7.9}$$

Furthermore, for any $\sigma \in \mathcal{X}$ and any $\varnothing \neq \mathcal{A} \subset \mathcal{X}$, we set

$$\Gamma(\sigma, \mathcal{A}) := \Phi(\sigma, \mathcal{A}) - H(\sigma).$$

From the definition it immediately follows that $V_\sigma = \Gamma(\sigma, \mathcal{I}_\sigma)$.

First, we investigate the stability level of configurations **2** and **3**. We define (cf. Assumption 7.0.1-**B**)

$$\ell^\star := \left\lceil \frac{2\gamma_{12} + \gamma_1}{2\gamma_1} \right\rceil \quad \text{and} \quad \Gamma^\star := f_{\gamma_1}(\gamma_{12}) = 2(K+1)\gamma_{23}. \tag{7.10}$$

By definition (7.43) we have that

$$\Gamma^\star = 4\ell^\star\Big(\gamma_{12} + \frac{\gamma_1}{2}\Big) - 2\gamma_1(\ell^{\star 2} - \ell^\star + 1) = 4\ell^\star\gamma_{12} - 2\gamma_1(\ell^{\star 2} - 2\ell^\star + 1). \tag{7.11}$$

The result below shows that the communication height between stable and metastable states is exactly $\Gamma^\star$ above the energy level of metastable configurations.

Theorem 7.1.2 (Communication height)**.** *It holds that*

$$\Gamma(\mathbf{2}, \mathbf{1}) = \Gamma(\mathbf{3}, \mathbf{1}) = \Gamma(\mathbf{2}, \mathbf{3}) = \Gamma^\star.$$

By definition, the previous theorem is equivalent to $\Phi(\mathbf{2}, \mathbf{1}) = \Phi(\mathbf{3}, \mathbf{1}) =$

$\Phi(\mathbf{2},\,\mathbf{3}) = H(\mathbf{2}) + \Gamma^\star$. This theorem is proved in Section 7.4.1.

Next, we claim that stability levels of any other configurations are significantly smaller than $\Gamma^\star$. We present a proof of the following proposition in Section 7.4.2.

Proposition 7.1.3 (Stability level of other configurations)**.** *For any configuration $\eta \in \mathcal{X} \setminus \{\mathbf{1},\,\mathbf{2},\,\mathbf{3}\}$,*

$$V_\eta \le 2(\ell^\star - 1)(\gamma_{23} + \gamma_1).$$

Remark 7.1.4. By (7.10), it holds that $\ell^\star < \dfrac{2\gamma_{12} + \gamma_1}{2\gamma_1} + 1$. Employing this inequality to the formula of $\Gamma^\star$ given in (7.11), we obtain

$$\Gamma^\star > 4\ell^\star\gamma_{12} - 2\gamma_1 \frac{2\gamma_{12} + \gamma_1}{2\gamma_1}(\ell^\star - 1) = (2\gamma_{12} - \gamma_1)\ell^\star + (2\gamma_{12} + \gamma_1).$$

Again using $\ell^\star < \dfrac{2\gamma_{12} + \gamma_1}{2\gamma_1} + 1$ on the last term, we have

$$\Gamma^\star > (2\gamma_{12} - \gamma_1)\ell^\star + 2\gamma_1(\ell^\star - 1) = 2\gamma_{12}\ell^\star + \gamma_1(\ell^\star - 2) \ge 2\gamma_{12}\ell^\star.$$

On the other hand, the upper bound appearing in Proposition 7.1.3 is estimated via Assumption 7.0.1-**C** as

$$2(\ell^\star - 1)(\gamma_{23} + \gamma_1) < 2\ell^\star \times \frac{2\gamma_{12}}{k} = \frac{4}{k}\gamma_{12}\ell^\star$$

where k is sufficiently large. Therefore, we conclude that

$$\Gamma^\star > \frac{k}{2} \times 2(\ell^\star - 1)(\gamma_{23} + \gamma_1),$$

which implies that the stability levels of configurations other than **1**, **2**, and **3** are significantly smaller than the stability level of metastable configurations **2** and **3**.

By combining Theorem 7.1.2 and Proposition 7.1.3, we now identify the set $\mathcal{X}^m$.

Theorem 7.1.5 (Identification of $\mathcal{X}^m$)**.** *We have* $V_{\mathbf{2}} = V_{\mathbf{3}} = \Gamma^\star$ *and* $\mathcal{X}^m = \{\mathbf{2}, \mathbf{3}\}$.

Proof. To prove the theorem, it suffices to demonstrate that

$$V_{\mathbf{2}} = \Gamma^\star. \tag{7.12}$$

Indeed, then by symmetry we also have $V_{\mathbf{3}} = \Gamma^\star$, and combining these with Proposition 7.1.3 we conclude that $\mathcal{X}^m = \{\mathbf{2}, \mathbf{3}\}$.

Before proving (7.12), we claim that

$$\Gamma(\eta, \mathbf{1}) < \Gamma^\star \quad \text{for all } \eta \in \mathcal{X} \setminus \{\mathbf{1}, \mathbf{2}, \mathbf{3}\}. \tag{7.13}$$

To prove the claim, we fix $\eta \in \mathcal{X} \setminus \{\mathbf{1}, \mathbf{2}, \mathbf{3}\}$. Starting from η, we find another configuration η_1 with lower energy such that an optimal path from η to η_1 realizes the stability level V_η. Repeating this algorithm, since $\mathcal{X}$ is finite and $\mathcal{X}^s = \{\mathbf{1}\}$, we can take a finite sequence $\eta = \eta_0, \eta_1, \dots, \eta_m = \mathbf{1}$ of configurations such that $H(\eta_i) > H(\eta_{i+1})$ and $V_{\eta_i} = \Gamma(\eta_i, \eta_{i+1})$ for all $0 \le i \le m-1$. Then, we estimate

$$\Gamma(\eta, \mathbf{1}) = \Phi(\eta, \mathbf{1}) - H(\eta) \le \max_{0 \le i \le m-1} \Phi(\eta_i, \eta_{i+1}) - H(\eta),$$

where the inequality holds by concatenating the $m-1$ optimal paths from η_i to η_{i+1}. By construction, the last term equals

$$\max_{0 \le i \le m-1} [V_{\eta_i} + H(\eta_i)] - H(\eta).$$

By Theorem 7.1.2 and Proposition 7.1.3, $V_\sigma \le \Gamma^\star$ for all $\sigma \ne \mathbf{1}$. Thus, the last display is bounded by

$$\Gamma^\star + H(\eta_0) - H(\eta) = \Gamma^\star.$$

This concludes the proof of (7.13).

Finally, we prove $V_{\mathbf{2}} = \Gamma^\star$. Theorem 7.1.2 readily implies that $V_{\mathbf{2}} \le \Gamma^\star$. If, on the contrary, $V_{\mathbf{2}} < \Gamma^\star$ then by definition, there exists $\sigma \in \mathcal{X}$ with $H(\sigma) < H(\mathbf{2})$ such that $\Phi(\mathbf{2},\, \sigma) < \Gamma^\star + H(\mathbf{2})$, where clearly $\sigma \neq \mathbf{1},\, \mathbf{2},\, \mathbf{3}$. Then by the claim (7.13), we have $\Phi(\sigma,\, \mathbf{1}) < \Gamma^\star + H(\sigma)$. Thus,

$$\Phi(\mathbf{2},\, \mathbf{1}) \le \max\{\Phi(\mathbf{2},\, \sigma),\, \Phi(\sigma,\, \mathbf{1})\} < \Gamma^\star + H(\mathbf{2}),$$

which contradicts Theorem 7.1.2. This conclude the proof of Theorem 7.1.5. □

We have a following another important consequence of Proposition 7.1.3, which is called the *recurrence property*. With probability tending to one in the limit $\beta \to \infty$, starting from any configuration in $\mathcal{X}$, the process visits $\mathcal{X}^s \cup \mathcal{X}^m$ within a time of order $e^{[2(\ell^\star-1)(\gamma_{23}+\gamma_1)]\beta}$ which is much smaller than the metastable timescale $e^{\Gamma^\star \beta}$.

Theorem 7.1.6 (Recurrence property)**.** *For any $\sigma \in \mathcal{X}$ and for any $\epsilon > 0$, there exists $\kappa > 0$ such that for β sufficiently large, we have*

$$\mathbb{P}\big[\tau^{\sigma}_{\{\mathbf{1},\,\mathbf{2},\,\mathbf{3}\}} > e^{\beta[2(\ell^\star-1)(\gamma_{23}+\gamma_1)+\epsilon]}\big] \le e^{-e^{\kappa\beta}}.$$

Proof. We apply [67, Theorem 3.1] for the level set with respect to $2(\ell^\star - 1)(\gamma_{23} + \gamma_1)$. This concludes the proof since $\mathcal{X}^s = \{\mathbf{1}\}$ by Proposition 7.1.1, $V_{\mathbf{2}} = V_{\mathbf{3}} = \Gamma^\star > 2(\ell^\star-1)(\gamma_{23}+\gamma_1)$ by Theorem 7.1.5 and $V_\eta \le 2(\ell^\star-1)(\gamma_{23}+\gamma_1)$ for all $\eta \in \mathcal{X} \setminus \{\mathbf{1},\, \mathbf{2},\, \mathbf{3}\}$ by Proposition 7.1.3. □

7.1.2 Transition time, mixing time, and spectral gap

Our next goal is to study the large deviation-type results. Recall the objects defined before Theorem 4.1.4.

Theorem 7.1.7 (Metastable transition time, mixing time, and spectral gap)**.** *For any* $\boldsymbol{m} \in \{\mathbf{2},\, \mathbf{3}\}$ *the following statements hold.*

(1) For every $\epsilon > 0$, $\lim_{\beta\to\infty} \mathbb{P}_{\boldsymbol{m}}(e^{\beta(\Gamma^\star-\epsilon)} < \tau_{\mathbf{1}} < e^{\beta(\Gamma^\star+\epsilon)}) = 1.$

(2) $\lim_{\beta\to\infty} \dfrac{1}{\beta} \log \mathbb{E}_{\boldsymbol{m}}[\tau_{\mathbf{1}}] = \Gamma^\star.$

(3) For every $\epsilon \in (0,\, 1)$, $\lim_{\beta\to\infty} \dfrac{1}{\beta} \log t^{\mathrm{mix}}_{\beta}(\epsilon) = \Gamma^\star$ *and there exist two constants* $0 < c_1 \le c_2 < \infty$ *independent of* β *such that for any* $\beta > 0$, $c_1 e^{-\beta\Gamma^\star} \le \lambda_\beta \le c_2 e^{-\beta\Gamma^\star}$.

Proof. Item (1) follows by [67, Theorem 4.1], while item (2) follows by [67, Theorem 4.9]. In both cases we applied the model-independent results with $\eta_0 = \boldsymbol{m}$ and $\Gamma = \Gamma^\star$. To prove item (3), by [70, Proposition 3.24], it suffices to demonstrate in our model that $\widetilde{\Gamma}(\mathcal{X} \setminus \{\mathbf{1}\}) = \Gamma^\star$ (see equation (21) in [70] for the definition of $\widetilde{\Gamma}$). Indeed, by [70, Lemma 3.6] we know that

$$\widetilde{\Gamma}(\mathcal{X} \setminus \{\mathbf{1}\}) = \max_{\eta\in\mathcal{X}\setminus\{\mathbf{1}\}} \Gamma(\eta,\, \mathbf{1}).$$

By Theorem 7.1.2, $\Gamma(\mathbf{2},\, \mathbf{1}) = \Gamma(\mathbf{3},\, \mathbf{1}) = \Gamma^\star$. Moreover, by the claim (7.13) we have that $\Gamma(\eta,\, \mathbf{1}) < \Gamma^\star$ for all $\eta \ne \mathbf{1},\, \mathbf{2},\, \mathbf{3}$. This concludes the proof. ☐

7.1.3 Minimal gates

Next we are interested in identifying the set of minimal gates for the metastable transitions. First, we need a few more model-independent definitions.

The set

$$\mathcal{S}(\mathcal{A},\, \mathcal{B}) := \big\{\xi \in \mathcal{X} : \exists \omega \in \Omega^{\mathrm{opt}}_{\mathcal{A},\mathcal{B}},\ \xi \in \mathrm{argmax}_\omega H\big\}. \tag{7.14}$$

is known as the set of *minimal saddles* between $\mathcal{A},\, \mathcal{B} \subseteq \mathcal{X}$. In particular, any $\xi \in \mathcal{S}(\mathcal{A},\, \mathcal{B})$ is called an *essential saddle* if there exists $\omega \in \Omega^{\mathrm{opt}}_{\mathcal{A},\mathcal{B}}$ such that

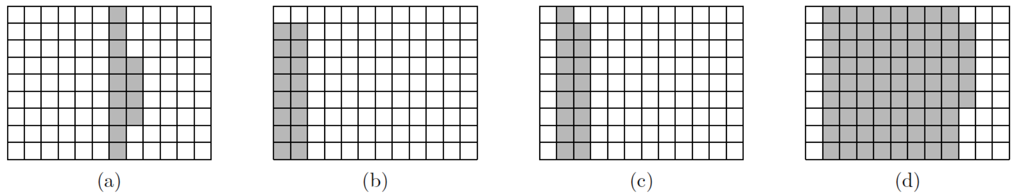


Figure 7.1: Examples of configurations on a grid graph 12×9 belonging to (a) $B^4_{1,K}(r,\, s) \subset \mathscr{H}_4(\boldsymbol{r},\, \boldsymbol{s})$, (b) $R_{2,K-1}(r,\, s) \subset \mathscr{Q}(\boldsymbol{r},\, \boldsymbol{s})$, (c) $B^{K-1}_{1,K}(r,\, s) \subset \mathscr{P}(\boldsymbol{r},\, \boldsymbol{s})$ and (d) $B^5_{8,K}(r,\, s) \subset \mathscr{W}^5_8(\boldsymbol{r},\, \boldsymbol{s})$. Spins r and s are represented by colors white and gray, respectively.

$\xi \in \mathrm{argmax}_\omega H$ and

$$\mathrm{argmax}_{\omega'} H \nsubseteq \mathrm{argmax}_\omega H \setminus \{\xi\} \quad \text{for all } \omega' \in \Omega^{\mathrm{opt}}_{\mathcal{A},\mathcal{B}} \setminus \{\omega\}.$$

A saddle $\xi \in \mathcal{S}(\mathcal{A},\, \mathcal{B})$ which does not satisfy the condition is said to be *unessential.* One can easily check that this definition coincides with the classic one [67] but is simpler.

A collection $\mathcal{W}$ of configurations is a *gate* for the transition between $\mathcal{A},\, \mathcal{B} \in \mathcal{X}$ if $\mathcal{W} \subseteq \mathcal{S}(\mathcal{A},\, \mathcal{B})$ and $\omega \cap \mathcal{W} \neq \varnothing$ for all $\omega \in \Omega^{\mathrm{opt}}_{\mathcal{A},\mathcal{B}}$. Moreover, $\mathcal{W}$ is said to be a *minimal gate* for the transition $\mathcal{A} \to \mathcal{B}$ if it is a gate and for any $\mathcal{W}' \subsetneq \mathcal{W}$ there exists $\omega' \in \Omega^{\mathrm{opt}}_{\mathcal{A},\mathcal{B}}$ such that $\omega' \cap \mathcal{W}' = \varnothing$. The set $\mathcal{G} = \mathcal{G}(\mathcal{A},\, \mathcal{B})$ denotes the union of all minimal gates for the transition $\mathcal{A} \to \mathcal{B}$.

Let us now focus on some model-dependent definitions concerning our setting. We refer to Figures 7.1 and 7.2 for illustrations.

- We say that $R \subseteq V$ is a *rectangle of shape* $a \times b$ if the sites in R form a rectangle with a columns and b rows. It is a *strip* if it wraps around Λ, i.e., if $a = L$ or $b = K$.

- For $r,\, s \in S$, we denote by $R_{a,b}(r,\, s)$ the collection of configurations in which all vertices have spins r, except for those in a rectangle $a \times b$,

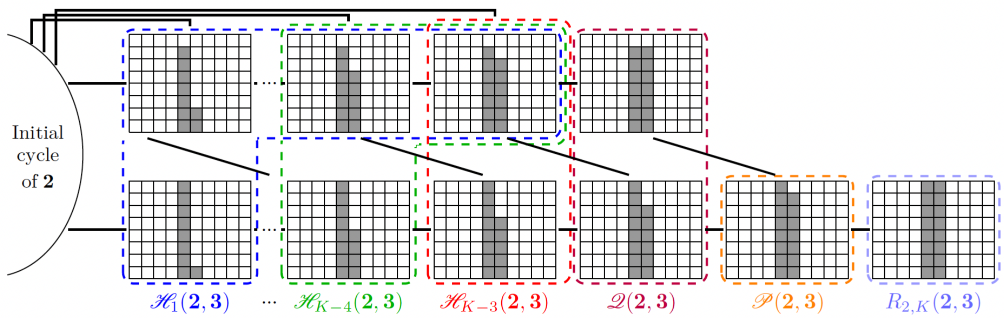


Figure 7.2: Local geometry of the configurations belonging to $\mathscr{P}(\mathbf{2},\,\mathbf{3})$, $\mathscr{Q}(\mathbf{2},\,\mathbf{3})$ and $\mathscr{H}_i(\mathbf{2},\,\mathbf{3})$, $1 \le i \le K-3$, where $K = 8$ and $L = 10$. We refer to (7.32) for the definition of initial cycles.

which have spins s. Note that $R_{a,\,b}(r,\,s) \neq R_{b,\,a}(r,\,s)$ if $a \neq b$. Moreover, we write $B^l_{a,\,b}(r,\,s)$ (resp. $\hat{B}^l_{a,\,b}(r,\,s)$) the collection of configurations in which all vertices have spins r, except for those which have spins s, in a rectangle $a \times b$ with a bar of length l adjacent to one of the sides of length b (resp. a), with $1 \le l \le b-1$ (resp. $1 \le l \le a-1$).

- We set

$$\mathscr{P}(\boldsymbol{r},\,\boldsymbol{s}) := \begin{cases} B^{K-1}_{1,K}(r,\,s), & \text{if } K < L, \\ B^{K-1}_{1,K}(r,\,s) \cup \hat{B}^{K-1}_{K,1}(r,\,s), & \text{if } K = L. \end{cases}$$

- We define

$$\mathscr{Q}(\boldsymbol{r},\,\boldsymbol{s}) := \begin{cases} R_{2,K-1}(r,\,s) \cup B^{K-2}_{1,K}(r,\,s), & K < L, \\ R_{2,K-1}(r,\,s) \cup B^{K-2}_{1,K}(r,\,s) \cup R_{K-1,2}(r,\,s) \cup \hat{B}^{K-2}_{K,1}(r,\,s), & K = L. \end{cases}$$

- For $1 \le i \le K-3$, we define $\mathscr{H}_i(\boldsymbol{r},\, \boldsymbol{s})$ as

$$\begin{cases} B^i_{1,K}(r,\, s) \cup \displaystyle\bigcup_{j=i+1}^{K-2} B^j_{1,K-1}(r,\, s), & K < L, \\ B^i_{1,K}(r,\, s) \cup \displaystyle\bigcup_{j=i+1}^{K-2} B^j_{1,K-1}(r,\, s) \cup \hat{B}^i_{K,1}(r,\, s) \cup \displaystyle\bigcup_{j=i+1}^{K-2} \hat{B}^j_{K-1,1}(r,\, s), & K = L. \end{cases}$$

- Finally, for $2 \le j \le L-3$ and $1 \le h \le K-1$ we set

$$\mathscr{W}^h_j(\boldsymbol{r},\, \boldsymbol{s}) := \begin{cases} B^h_{j,K}(r,\, s), & \text{if } K < L, \\ B^h_{j,K}(r,\, s) \cup \hat{B}^h_{K,j}(r,\, s), & \text{if } K = L. \end{cases}$$

Using the sets defined above, we now formulate all the possible minimal gates for the metastable transitions. For $m \in \{2,\, 3\}$, we write

$$\mathcal{W}(\boldsymbol{m},\, \mathbf{1}) := B^1_{\ell^\star-1,\, \ell^\star}(m,\, 1) \cup \hat{B}^1_{\ell^\star,\, \ell^\star-1}(m,\, 1). \tag{7.15}$$

Moreover, we abbreviate

$$\begin{aligned} \mathcal{W}(\mathbf{2},\, \mathbf{3}) := & \bigcup_{i=1}^{K-3} \mathscr{H}_i(\mathbf{2},\, \mathbf{3}) \cup \mathscr{Q}(\mathbf{2},\, \mathbf{3}) \cup \mathscr{P}(\mathbf{2},\, \mathbf{3}) \\ & \cup \bigcup_{j=2}^{L-3} \bigcup_{h=1}^{K-1} \mathscr{W}^h_j(\mathbf{2},\, \mathbf{3}) \cup \mathscr{P}(\mathbf{3},\, \mathbf{2}) \cup \mathscr{Q}(\mathbf{3},\, \mathbf{2}) \cup \bigcup_{i=1}^{K-3} \mathscr{H}_i(\mathbf{3},\, \mathbf{2}). \end{aligned}$$

First, we address the metastable transition from $\boldsymbol{m} \in \{\mathbf{2},\, \mathbf{3}\}$ to $\mathbf{1}$. We refer to Figure 7.3 for a viewpoint from above the energy landscape.

Theorem 7.1.8 (Minimal gates for $\mathbf{2} \to \mathbf{1}$ and $\mathbf{3} \to \mathbf{1}$)**.** *Fix $\boldsymbol{m} \in \{\mathbf{2},\, \mathbf{3}\}$ and consider the metastable transition from $\boldsymbol{m}$ to $\mathbf{1}$. Take any set $\mathscr{A}$ in*

$$\big\{\mathscr{W}^h_j(\mathbf{2},\, \mathbf{3})\big\}_{j,h} \cup \big\{\mathscr{Q}(\mathbf{2},\, \mathbf{3}),\, \mathscr{P}(\mathbf{2},\, \mathbf{3}),\, \mathscr{P}(\mathbf{3},\, \mathbf{2}),\, \mathscr{Q}(\mathbf{3},\, \mathbf{2})\big\} \cup \big\{\mathscr{H}_i(\mathbf{2},\, \mathbf{3})\big\}_i \cup \big\{\mathscr{H}_i(\mathbf{3},\, \mathbf{2})\big\}_i,$$

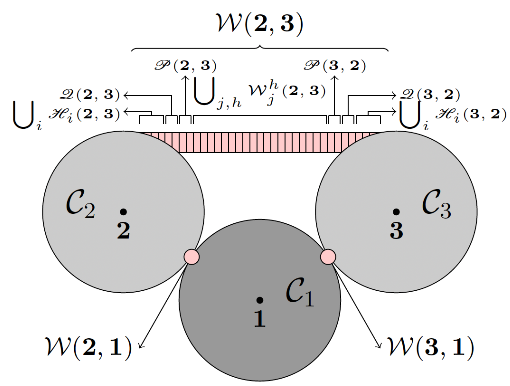


Figure 7.3: Viewpoint from above of the energy landscape cut at the energy level $\Phi(\mathbf{2},\,\mathbf{1}) = \Phi(\mathbf{3},\,\mathbf{1}) = \Phi(\mathbf{2},\,\mathbf{3}) = \Gamma^\star + H(\mathbf{2})$. Here, $\mathcal{C}_r$ denotes the initial cycle of $\boldsymbol{r}$; see (7.32) for the exact definition. The gates $\mathcal{W}(\boldsymbol{m},\,\mathbf{1})$ between $\boldsymbol{m} \in \{\mathbf{2},\,\mathbf{3}\}$ and $\mathbf{1}$ consist of singletons, whereas the gate $\mathcal{W}(\mathbf{2},\,\mathbf{3})$ between $\mathbf{2}$ and $\mathbf{3}$ is a complex union of essential saddles.

where the collections are over all $2 \le j \le L-3$, $1 \le h \le K-1$ *and* $1 \le i \le K-3$. *Then,*

(1) $\mathcal{W}(\mathbf{2},\,\mathbf{1}) \cup \mathcal{W}(\mathbf{3},\,\mathbf{1})$ *is a minimal gate;*

(2) $\mathcal{W}(\boldsymbol{m},\,\mathbf{1}) \cup \mathscr{A}$ *is a minimal gate;*

(3) moreover, these are all the minimal gates in the sense that

$$\mathcal{G}(\mathbf{2},\,\mathbf{1}) = \mathcal{G}(\mathbf{3},\,\mathbf{1}) = \mathcal{W}(\mathbf{2},\,\mathbf{1}) \cup \mathcal{W}(\mathbf{3},\,\mathbf{1}) \cup \mathcal{W}(\mathbf{2},\,\mathbf{3}).$$

Next, we state a theorem regarding the minimal gates for the transition between **2** and **3**.

Theorem 7.1.9 (Minimal gates for $\mathbf{2} \to \mathbf{3}$)**.** *Consider the transition from* **2** *to* **3**. *Take any set* $\mathscr{A}$ *in*

$$\big\{\mathscr{W}_j^h(\mathbf{2},\,\mathbf{3})\big\}_{j,h} \cup \big\{\mathscr{Q}(\mathbf{2},\,\mathbf{3}), \mathscr{P}(\mathbf{2},\,\mathbf{3}), \mathscr{P}(\mathbf{3},\,\mathbf{2}), \mathscr{Q}(\mathbf{3},\,\mathbf{2})\big\} \cup \big\{\mathscr{H}_i(\mathbf{2},\,\mathbf{3})\big\}_i \cup \big\{\mathscr{H}_i(\mathbf{3},\,\mathbf{2})\big\}_i,$$

as in Theorem 7.1.8. Then,

(1) $\mathcal{W}(\mathbf{2},\,\mathbf{1})\cup\mathscr{A}$ *is a minimal gate;*

(2) $\mathcal{W}(\mathbf{3},\,\mathbf{1})\cup\mathscr{A}$ *is a minimal gate;*

(3) these are all the minimal gates in the sense that

$$\mathcal{G}(\mathbf{2},\,\mathbf{3})=\mathcal{W}(\mathbf{2},\,\mathbf{1})\cup\mathcal{W}(\mathbf{3},\,\mathbf{1})\cup\mathcal{W}(\mathbf{2},\,\mathbf{3}).$$

We prove Theorems 7.1.8 and 7.1.9 in Section 7.4.4.

Finally, in the last result of this section we show that during the metastable transition, the process typically visits the corresponding gates identified in Theorems 7.1.8 and 7.1.9.

Corollary 7.1.10. *Take a set* $\mathscr{A}$ *in the collection*

$$\big\{\mathscr{W}_j^h(\mathbf{2},\,\mathbf{3})\big\}_{j,h}\cup\big\{\mathscr{Q}(\mathbf{2},\,\mathbf{3}),\mathscr{P}(\mathbf{2},\,\mathbf{3}),\mathscr{P}(\mathbf{3},\,\mathbf{2}),\mathscr{Q}(\mathbf{3},\,\mathbf{2})\big\}\cup\big\{\mathscr{H}_i(\mathbf{2},\,\mathbf{3})\big\}_i\cup\big\{\mathscr{H}_i(\mathbf{3},\,\mathbf{2})\big\}_i$$

as we did in Theorems 7.1.8 and 7.1.9.

(1) For the transition from $\boldsymbol{m}\in\{\mathbf{2},\,\mathbf{3}\}$ *to* $\mathbf{1}$*,*

$$\lim_{\beta\to\infty}\mathbb{P}_{\boldsymbol{m}}[\tau_{\mathcal{W}(\mathbf{2},\,\mathbf{1})\cup\mathcal{W}(\mathbf{3},\,\mathbf{1})}<\tau_{\mathbf{1}}]=1\quad\text{and}\quad\lim_{\beta\to\infty}\mathbb{P}_{\boldsymbol{m}}[\tau_{\mathcal{W}(\boldsymbol{m},\,\mathbf{1})\cup\mathscr{A}}<\tau_{\mathbf{1}}]=1.$$

(2) For the transition $\mathbf{2}\to\mathbf{3}$*,*

$$\lim_{\beta\to\infty}\mathbb{P}_{\mathbf{2}}[\tau_{\mathcal{W}(\mathbf{2},\,\mathbf{1})\cup\mathscr{A}}<\tau_{\mathbf{3}}]=1\quad\text{and}\quad\lim_{\beta\to\infty}\mathbb{P}_{\mathbf{2}}[\tau_{\mathcal{W}(\mathbf{3},\,\mathbf{1})\cup\mathscr{A}}<\tau_{\mathbf{3}}]=1.$$

Proof. By Theorems 7.1.8 and 7.1.9, the four sets in the subscripts are gates for the corresponding transitions. Thus, [67, Theorem 5.4] implies the desired equations. □

7.2 Projection operator

In this section, we introduce the notion of projection operators which act on the configuration space $\mathcal{X}$. These operators are extremely useful for analyzing the energy landscape, especially when we want to focus only on two given spin values. First, we introduce some notation which will be useful in this section and following ones. For each $\sigma \in \mathcal{X}$ and $i, j \in S$, we define the number of spins i in σ as

$$\mathfrak{N}_i(\sigma) := \big|\{v \in V : \ \sigma(v) = i\}\big|. \tag{7.16}$$

Then we define, for $n \geq 0$, the set of configurations which have exactly n spins i:

$$\mathscr{V}_n^i := \{\eta \in \mathcal{X} : \ \mathfrak{N}_i(\eta) = n\}. \tag{7.17}$$

Moreover, for an edge $e \in E$, we say that e is an *ij-edge* of σ if the corresponding two spins are i and j in σ. We write

$$\mathfrak{n}_{ij}(\sigma) := \big|\{e \in E : \ e \text{ is an } ij\text{-edge of } \sigma\}\big|. \tag{7.18}$$

Finally, for spin values r, $s \in S$, we define the *projection operator* $\mathscr{P}^{rs} : \mathcal{X} \to \mathcal{X}$ as

$$(\mathscr{P}^{rs}\sigma)(x) = \begin{cases} s, & \text{if } \sigma(x) = r, \\ \sigma(x), & \text{if } \sigma(x) \neq r. \end{cases} \tag{7.19}$$

The operator $\mathscr{P}^{rs}$ projects all spins r to s and preserves all the other spins. Intuitively, one would expect the projected configuration to have lower energy than the original configuration, since all disagreeing edges between r and s disappear. This is in fact the case, unless the spin value r is more stable than s (for example, if $r = 1$ and $s = 2$), in which case the projected configuration may still have higher energy than the original configuration.

Two projections which are important for us are $\mathscr{P}^{32}$ and $\mathscr{P}^{12}$. We begin by analyzing $\mathscr{P}^{32}$. The analysis is simpler because spins 2 and 3 have the same level of stability.

Lemma 7.2.1 (Projection $3 \to 2$)**.** *For any* $\sigma \in \mathcal{X}$*, we have*

$$H(\mathscr{P}^{32}\sigma) \le H(\sigma).$$

Moreover, equality holds if and only if $\mathfrak{n}_{23}(\sigma) = 0$*.*

Proof. By the definition of $\mathscr{P}^{32}$, it is easy to check that $\mathfrak{n}_{11}(\mathscr{P}^{32}\sigma) = \mathfrak{n}_{11}(\sigma)$, $\mathfrak{n}_{12}(\mathscr{P}^{32}\sigma) = \mathfrak{n}_{12}(\sigma) + \mathfrak{n}_{13}(\sigma)$, $\mathfrak{n}_{13}(\mathscr{P}^{32}\sigma) = 0$, $\mathfrak{n}_{22}(\mathscr{P}^{32}\sigma) = \mathfrak{n}_{22}(\sigma) + \mathfrak{n}_{23}(\sigma) + \mathfrak{n}_{33}(\sigma)$ and $\mathfrak{n}_{23}(\mathscr{P}^{32}\sigma) = \mathfrak{n}_{33}(\mathscr{P}^{32}\sigma) = 0$. Thus, using the interpretation (7.41) we may write

$$H(\mathscr{P}^{32}\sigma) = H(\mathbf{2}) - \gamma_1\mathfrak{n}_{11}(\sigma) + \gamma_{12}[\mathfrak{n}_{12}(\sigma) + \mathfrak{n}_{13}(\sigma)]$$

and

$$H(\sigma) = H(\mathbf{2}) - \gamma_1\mathfrak{n}_{11}(\sigma) + \gamma_{12}\mathfrak{n}_{12}(\sigma) + \gamma_{13}\mathfrak{n}_{13}(\sigma) + \gamma_{23}\mathfrak{n}_{23}(\sigma).$$

Recalling that $\gamma_{12} = \gamma_{13}$ from (7.2) and (7.3), we deduce

$$H(\mathscr{P}^{32}\sigma) - H(\sigma) = -\gamma_{23}\mathfrak{n}_{23}(\sigma) \le 0.$$

This proves the first statement. Moreover, from (7.3) it follows that the equality holds if and only if $\mathfrak{n}_{23}(\sigma) = 0$. This concludes the proof. $\square$

For a configuration $\sigma \in \mathcal{X}$, we say that a row (resp. column) in Λ is a *horizontal bridge* (resp. *vertical bridge*) of σ if all spins on it have the same value. If there exist both a horizontal bridge and a vertical bridge simultaneously (in which case the spin value must be the same), we call the union a *cross*.

Given a configuration $\sigma \in \mathcal{X}$ and a spin $r \in S$, we say that $A \subseteq V$ is an r*-cluster* of σ if it is a maximal connected subset of V on which all spins are r; i.e., if A is connected, $\sigma(v) = r$ for all $v \in A$ and $\sigma(v) \neq r$ for all $v \in \partial A$, where ∂A is the *outer boundary* of A:

$$\partial A := \big\{ w \in V \setminus A : \ \exists w' \in A, \ \{w, w'\} \in E \big\}. \tag{7.20}$$

Next we deal with the projection $\mathscr{P}^{12}$. In this case, as we mentioned in the beginning of this section, the statement becomes much more restrictive because spin 1 is more stable than spin 2. Indeed, the next lemma shows that the projection $\mathscr{P}^{12}$ lowers the energy of a configuration only when this has a low number of spins 1.

Lemma 7.2.2 (Projection $1 \to 2$)**.** *Suppose that $\sigma \in \mathcal{X}$ satisfies $H(\sigma) - H(\mathbf{2}) \le \Gamma^\star$ and $\mathfrak{N}_1(\sigma) \le \ell^{\star 2}$. Then, we have*

$$H(\mathscr{P}^{12}\sigma) \le H(\sigma).$$

Moreover, equality holds if and only if $\mathfrak{N}_1(\sigma) = 0$.

Proof. Abbreviate $\tilde{\sigma} := \mathscr{P}^{12}\sigma$ and $\bar{\sigma} := \mathscr{P}^{32}\sigma$. Clearly, we have $\mathfrak{N}_1(\bar{\sigma}) = \mathfrak{N}_1(\sigma)$. We divide into three cases according to the type of 1-bridges of σ.

- If σ has an 1-cross, then we can regard $\bar{\sigma}$ as a configuration of spins 2 in the sea of spins 1. Applying the well-known isoperimetric inequality (e.g. [1, Corollary 2.5]) to the 2-clusters, the perimeter is at least

  $$4\sqrt{\mathfrak{N}_2(\bar{\sigma})} = 4\sqrt{KL - \mathfrak{N}_1(\bar{\sigma})} \ge 4\sqrt{KL - \ell^{\star 2}}.$$

  Since the perimeter is exactly $\mathfrak{n}_{12}(\sigma)$, we have

  $$\mathfrak{n}_{12}(\bar{\sigma}) \ge 4\sqrt{KL - \ell^{\star 2}}.$$

  Next, since $\mathfrak{N}_1(\bar{\sigma}) \le \ell^{\star 2}$ and each vertex with spin 1 is contained in at most four 11-edges, we have that

  $$\mathfrak{n}_{11}(\bar{\sigma}) \le \frac{1}{2} \times 4 \times \mathfrak{N}_1(\bar{\sigma}) \le 2\ell^{\star 2}, \tag{7.21}$$

where the factor $\frac{1}{2}$ appears because there are two spins 1 in a single 11-edge. Therefore, by (7.41) we deduce that

$$H(\bar{\sigma}) - H(\mathbf{2}) = -\gamma_1 \mathfrak{n}_{11}(\bar{\sigma}) + \gamma_{12}\mathfrak{n}_{12}(\bar{\sigma}) \geq 4\sqrt{KL - \ell^{\star 2}}\gamma_{12} - 2\ell^{\star 2}\gamma_1.$$

This is strictly bigger than $\Gamma^\star = 4\ell^\star\gamma_{12} - (2\ell^{\star 2} - 4\ell^\star + 2)\gamma_1$ (cf. (7.11)). Indeed, we have to verify that

$$[2\sqrt{KL - \ell^{\star 2}} - 2\ell^\star]\gamma_{12} > (2\ell^\star - 1)\gamma_1.$$

This holds since by Assumption 7.0.1-**C** we have $\gamma_{12} > \gamma_1$, and since the lattice size K and L are assumed to be sufficiently larger than the critical length $\ell^\star$ we have that $2\sqrt{KL - \ell^{\star 2}} - 2\ell^\star \geq 2\ell^\star - 1$. Therefore, in this case, by Lemma 7.2.1 we always have $H(\sigma) - H(\mathbf{2}) \geq H(\bar{\sigma}) - H(\mathbf{2}) > \Gamma^\star$, which contradicts the assumption.

- If σ has an 1-bridge but no 1-cross, then there are at least K rows or L columns in $\bar{\sigma}$ which are not bridges. In each non-bridge of $\bar{\sigma}$, there are at least two 12-edges. Moreover, by the same logic as in (7.21) there are at most $2\ell^{\star 2}$ 11-edges. Therefore, we have

$$H(\bar{\sigma}) - H(\mathbf{2}) \geq 2\min\{K, L\}\gamma_{12} - 2\ell^{\star 2}\gamma_1 = 2K\gamma_{12} - 2\ell^{\star 2}\gamma_1.$$

  Similarly, this is strictly bigger than $\Gamma^\star$ due to Assumption 7.0.1-**C**, so that we get a contradiction.

- If σ does not have an 1-bridge, then all 1-clusters of σ do not wrap around the periodic lattice, and thus we may apply the isoperimetric inequality. By the projection $\sigma \mapsto \tilde{\sigma} = \mathscr{P}^{12}\sigma$, only the 11-, 12- and 13-edges of σ are affected. Thus, by (7.41) we may write

$$H(\tilde{\sigma}) - H(\sigma) = \gamma_1 \mathfrak{n}_{11}(\sigma) - \gamma_{12}\mathfrak{n}_{12}(\sigma) + (\gamma_{23} - \gamma_{13})\mathfrak{n}_{13}(\sigma).$$

Since $\gamma_{12} = \gamma_{13} > 0$ and $\gamma_{23} > 0$ by (7.3),

$$H(\tilde{\sigma}) - H(\sigma) \le \gamma_1 \mathfrak{n}_{11}(\sigma) - [\mathfrak{n}_{12}(\sigma) + \mathfrak{n}_{13}(\sigma)] \times (\gamma_{12} - \gamma_{23}).$$

By (7.42), it holds that $2\mathfrak{n}_{11}(\sigma) + \mathfrak{n}_{12}(\sigma) + \mathfrak{n}_{13}(\sigma) = 4\mathfrak{N}_1(\sigma)$. Again by the isoperimetric inequality, $\mathfrak{n}_{12}(\sigma) + \mathfrak{n}_{13}(\sigma) \ge 4\sqrt{\mathfrak{N}_1(\sigma)}$ and thus the last-displayed formula is bounded above by

$$2\big[\mathfrak{N}_1(\sigma) - \sqrt{\mathfrak{N}_1(\sigma)}\big]\gamma_1 - 4\sqrt{\mathfrak{N}_1(\sigma)}(\gamma_{12} - \gamma_{23}).$$

Thus to prove $H(\tilde{\sigma}) \le H(\sigma)$, it suffices to verify that

$$2(\gamma_{12} - \gamma_{23}) > (\sqrt{\mathfrak{N}_1(\sigma)} - 1)\gamma_1.$$

Since $\mathfrak{N}_1(\sigma) \le \ell^{\star 2}$ and $\ell^\star = \lceil \frac{2\gamma_{12} + \gamma_1}{2\gamma_1} \rceil < \frac{2\gamma_{12} + \gamma_1}{2\gamma_1} + 1$ (cf. (7.10)), we have

$$(\sqrt{\mathfrak{N}_1(\sigma)} - 1)\gamma_1 < \frac{2\gamma_{12} + \gamma_1}{2\gamma_1} \times \gamma_1 = \gamma_{12} + \frac{\gamma_1}{2} \le 2(\gamma_{12} - \gamma_{23}). \quad (7.22)$$

The last inequality follows from Assumption 7.0.1-**C**. Therefore, we conclude the proof of the first statement.

Finally, we investigate the equality condition. Carefully inspecting the proof above, the equality holds if and only if σ does not have an 1-bridge, $\mathfrak{n}_{12}(\sigma) = 0$ and $\mathfrak{N}_1(\sigma) = 0$. This is equivalent to saying that $\mathfrak{N}_1(\sigma) = 0$, in which case $\tilde{\sigma} = \sigma$ and thus the equality is obvious. □

Remark 7.2.3. The last inequality in (7.22) is where the exact condition **C** is required. Indeed,

$$\gamma_{12} + \frac{\gamma_1}{2} \le 2(\gamma_{12} - \gamma_{23}) \quad \text{if and only if} \quad 2\gamma_{12} \ge 4\gamma_{23} + \gamma_1.$$

7.3 Comparison with the original Ising path

In this section, we prove that if a path is restricted to only two spins, then it is equivalent, in the sense of communication height and gates, to the original Ising path with positive external field (if the spins are $\{1,2\}$ or $\{1,3\}$) or the original Ising path with zero external field (if the spins are $\{2,3\}$).

We say that a path ω is an *ij-path* if it involves spins i and j only, i.e., $\omega_n(v) \in \{i,j\}$ for all n and $v \in V$. According to the notation (7.44), this is equivalent to $\omega \subseteq \mathcal{X}^{ij}$.

Proposition 7.3.1 (Gate property 1)**.** *Suppose that $\omega = (\omega_n)_{n=0}^N$ is an $1r$-path from $\boldsymbol{r}$ to $\mathbf{1}$ for some $r \in \{2,3\}$.*

(1) $\Phi_\omega \geq H(\mathbf{2}) + \Gamma^\star$.

(2) If $\Phi_\omega = H(\mathbf{2}) + \Gamma^\star$, then $\omega \cap \mathcal{W}(\boldsymbol{r},\mathbf{1}) \neq \varnothing$ (cf. (7.15)).

Remark 7.3.2. Item (1) in Proposition 7.3.1, along with the reference path constructed in Section 7.5.4, corresponds to the communication height. Moreover, item (2) implies that $\mathcal{W}(\boldsymbol{r},\mathbf{1})$ works as a gate.

Proof of Proposition 7.3.1. For $\sigma \in \mathcal{X}^{1r}$, we have by (7.41) and (7.42) that

$$H(\sigma) = H(\mathbf{2}) - \gamma_1 \mathfrak{n}_{11}(\sigma) + \gamma_{1r}\mathfrak{n}_{1r}(\sigma) = H(\mathbf{2}) - 2\gamma_1 \mathfrak{N}_1(\sigma) + \Big(\frac{1}{2}\gamma_1 + \gamma_{1r}\Big)\mathfrak{n}_{1r}(\sigma).$$

Therefore, $\mathcal{X}^{1r}$ is isomorphic to the original Ising configuration space $\{+1,\,-1\}^V$ via correspondence of spins $1 \leftrightarrow +1$ and $r \leftrightarrow -1$, and moreover the Hamiltonian is the same as the original Ising Hamiltonian with coupling constant $J := \frac{1}{2}\gamma_1 + \gamma_{1r}$ and external field $h := 2\gamma_1$, translated by a fixed real number $H(\mathbf{2})$. Therefore, provided that the Glauber transitions happen inside the restricted set $\mathcal{X}^{1r}$, we may refer to the previous well-known results. Item (1) is equivalent to the lower bound of the communication height, which is provided in [71, Theorem 3]. Moreover, item (2) is equivalent to saying that the collection of critical configurations in the Ising model is a gate for the metastable transition. This is also a very classic result which was first proved in [67, Theorem 5.10]. □

Similarly, we argue that a 23-path behaves in the same way as the original Ising path with zero external field. Recall the sets defined in Section 7.1.3.

Proposition 7.3.3 (Gate property 2)**.** *Suppose that* $\omega = (\omega_n)_{n=0}^N$ *is a* 23*-path from* $\mathbf{2}$ *to* $\mathbf{3}$*.*

(1) $\Phi_\omega \geq H(\mathbf{2}) + \Gamma^\star$.

(2) Suppose that $\Phi_\omega = H(\mathbf{2}) + \Gamma^\star$*. Take* $\mathscr{A}$ *in*

$$\{\mathscr{W}_j^h(\mathbf{2},\mathbf{3})\}_{j,h} \cup \{\mathscr{Q}(\mathbf{2},\mathbf{3}), \mathscr{P}(\mathbf{2},\mathbf{3}), \mathscr{P}(\mathbf{3},\mathbf{2}), \mathscr{Q}(\mathbf{3},\mathbf{2})\} \cup \{\mathscr{H}_i(\mathbf{2},\mathbf{3})\}_i \cup \{\mathscr{H}_i(\mathbf{3},\mathbf{2})\}_i,$$

where the collections are over all $2 \leq j \leq L-3$*,* $1 \leq h \leq K-1$ *and* $1 \leq i \leq K-3$*. Then,*

$$\omega \cap \mathscr{A} \neq \varnothing.$$

Proof. We may use the same argument as in the proof of Proposition 7.3.1, with the modification that here we identify $\mathcal{X}^{23}$ with the Ising model with zero external field [11, 69]. This is possible since we have an alternative expression of energy for $\sigma \in \mathcal{X}^{23}$, which is

$$H(\sigma) = H(\mathbf{2}) + \gamma_{23}\mathfrak{n}_{23}(\sigma).$$

Thus, item (1) is equivalent to [69, Proposition 2.6] and item (2) is proved in [11, Theorem 3.3]. □

7.4 Proofs

7.4.1 Communication height

In this subsection we prove Theorem 7.1.2. We divide the proof into three propositions. Specifically, Proposition 7.4.1 establishes the upper bound $\Gamma^\star + H(\mathbf{2})$ for the communication heights, and Propositions 7.4.2 and 7.4.4 establish the matching lower bound.

Proposition 7.4.1. *It holds that* $\Gamma(\mathbf{2},\mathbf{1}) \le \Gamma^\star$, $\Gamma(\mathbf{3},\mathbf{1}) \le \Gamma^\star$ *and* $\Gamma(\mathbf{2},\mathbf{3}) \le \Gamma^\star$.

Proof. The reference paths constructed in Section 7.5.4 have height $\Gamma^\star + H(\mathbf{2})$. From this, the upper bounds immediately follow. □

Proposition 7.4.2. *We have* $\Gamma(\mathbf{2},\mathbf{1}) = \Gamma(\mathbf{3},\mathbf{1}) \ge \Gamma^\star$.

Proof. By the model symmetry between spins 2 and 3, it suffices to prove that $\Gamma(\mathbf{2},\mathbf{1}) \ge \Gamma^\star$. To this end, take an arbitrary path $\omega = (\omega_n)_{n=0}^N$ so that $\omega_0 = \mathbf{2}$ and $\omega_N = \mathbf{1}$. Then, define (cf. (7.19))

$$\bar{\omega}_n := \mathscr{P}^{32}\omega_n \quad \text{for each } 0 \le n \le N.$$

It holds automatically that $\bar{\omega}_0 = \mathbf{2}$, $\bar{\omega}_N = \mathbf{1}$ and $\bar{\omega}_n \in \mathcal{X}^{12}$ (cf. (7.44)). Since ω_n and ω_{n+1} differ in exactly one site, $\bar{\omega}_n$ and $\bar{\omega}_{n+1}$ differ in at most one site. These observations imply that $\bar{\omega} = (\bar{\omega}_n)_{n=0}^N$ is an 12-path (possibly with non-updating instances) from $\mathbf{2}$ to $\mathbf{1}$. Therefore, Proposition 7.3.1-(a) implies that

$$\Phi_{\bar{\omega}} \ge H(\mathbf{2}) + \Gamma^\star.$$

Then, Lemma 7.2.1 implies that $H(\omega_n) \ge H(\bar{\omega}_n)$ for all n and thus

$$\Phi_\omega \ge \Phi_{\bar{\omega}} \ge H(\mathbf{2}) + \Gamma^\star.$$

Since our choice of ω was arbitrary, we deduce that $\Gamma(\mathbf{2},\mathbf{1}) \ge \Gamma^\star$. □

All it remains is to provide a lower bound for $\Gamma(\mathbf{2},\mathbf{3})$. Before this, we state a lemma. Recall the notion of $\mathscr{V}_n^i$ defined in (7.17). Moreover, for $m \in \{2,3\}$ we define

$$\mathcal{W}'(\boldsymbol{m},\mathbf{1}) := \hat{B}^1_{\ell^\star-1,\ell^\star}(m,1) \cup B^1_{\ell^\star,\ell^\star-1}(m,1).$$

Intuitively, $\mathcal{W}'(\boldsymbol{m},\mathbf{1})$ is the collection of configurations that have a protuberance of spin 1 on a *wrong* side of the rectangular 1-cluster, in the sense that we cannot proceed further to reach $\mathbf{1}$ without returning to a protocritical configuration in $R_{\ell^\star-1,\ell^\star}(m,1) \cup R_{\ell^\star,\ell^\star-1}(m,1)$.

Lemma 7.4.3. *Suppose that* $\eta \in \mathscr{V}^1_{\ell^\star(\ell^\star-1)+1}$.

(1) It holds that $H(\eta) - H(\mathbf{2}) \geq \Gamma^\star$.

(2) Equality in (1) *holds if and only if* $\eta \in \bigcup_{m=2}^{3} [\mathcal{W}(\boldsymbol{m},\mathbf{1}) \cup \mathcal{W}'(\boldsymbol{m},\mathbf{1})]$.

Proof. (1) We abbreviate $\bar{\eta} := \mathscr{P}^{32}\eta \in \mathcal{X}^{12}$, where clearly $\bar{\eta} \in \mathscr{V}^1_{\ell^\star(\ell^\star-1)+1}$. We divide into three cases as we did in the proof of Lemma 7.2.2.

- If $\bar{\eta}$ has an 1-cross, then we may regard $\bar{\eta}$ as a configuration of spins 2 in the sea of spins 1. Recalling (7.16) and (7.18) and applying the isoperimetric inequality (cf. [1, Corollary 2.5]), we have

$$\mathfrak{n}_{12}(\bar{\eta}) \geq 4\sqrt{\mathfrak{N}_2(\bar{\eta})} = 4\sqrt{KL - \mathfrak{N}_1(\bar{\eta})} = 4\sqrt{KL - \ell^\star(\ell^\star-1) - 1}. \tag{7.23}$$

  Using the same argument as in (7.21), it holds that $\mathfrak{n}_{11}(\bar{\eta}) \leq 2\mathfrak{N}_1(\bar{\eta}) = 2\ell^\star(\ell^\star-1)+2$. Thus, by (7.41) we have

$$H(\bar{\eta}) - H(\mathbf{2}) = -\gamma_1\mathfrak{n}_{11}(\bar{\eta}) + \gamma_{12}\mathfrak{n}_{12}(\bar{\eta}) \geq 4\sqrt{KL - \ell^{\star 2} + \ell^\star - 1}\gamma_{12} - (2\ell^{\star 2} - 2\ell^\star + 2)\gamma_1.$$

  By Assumption 7.0.1-**C**, it can be shown that this is strictly larger than $\Gamma^\star = 4\ell^\star\gamma_{12} - (2\ell^{\star 2} - 4\ell^\star + 2)\gamma_1$ via a similar argument as in the first case in the proof of Lemma 7.2.2. Therefore, by Lemma 7.2.1 we obtain

$$H(\eta) \geq H(\bar{\eta}) > H(\mathbf{2}) + \Gamma^{\star}.$$

- If $\bar{\eta}$ has an 1-bridge but no 1-cross, then proceeding similarly to the second case in proof of Lemma 7.2.2, we obtain

$$H(\eta) - H(\mathbf{2}) \geq H(\bar{\eta}) - H(\mathbf{2}) \geq 2K\gamma_{12} - (2\ell^{\star 2} - 2\ell^{\star} + 2)\gamma_1 > \Gamma^{\star}.$$

- If $\bar{\eta}$ does not have an 1-bridge, then all 1-clusters of $\bar{\eta}$ are in the sea of spins 2. By (7.42) and since $\mathfrak{n}_{13}(\bar{\eta}) = 0$ and $\mathfrak{N}_1(\bar{\eta}) = \ell^{\star}(\ell^{\star} - 1) + 1$, we have

$$2\mathfrak{n}_{11}(\bar{\eta}) + \mathfrak{n}_{12}(\bar{\eta}) = 4\ell^{\star}(\ell^{\star} - 1) + 4.$$

  Then by (7.41),

$$H(\bar{\eta}) - H(\mathbf{2}) = \gamma_{12}\mathfrak{n}_{12}(\bar{\eta}) - \gamma_1\mathfrak{n}_{11}(\bar{\eta}) = (4\ell^{\star 2} - 4\ell^{\star} + 4)\gamma_{12} - \mathfrak{n}_{11}(\bar{\eta})(\gamma_1 + 2\gamma_{12}).$$

  Since $\mathfrak{N}_1(\bar{\eta}) = \ell^{\star}(\ell^{\star} - 1) + 1$, by the isoperimetric inequality, the perimeter of the 1-clusters is at least $4\ell^{\star}$. This is equivalent to $\mathfrak{n}_{12}(\bar{\eta}) \geq 4\ell^{\star}$ and thus equivalent to $\mathfrak{n}_{11}(\bar{\eta}) \leq 2\ell^{\star 2} - 4\ell^{\star} + 2$. Hence,

$$H(\bar{\eta}) - H(\mathbf{2}) \geq (4\ell^{\star 2} - 4\ell^{\star} + 4)\gamma_{12} - (2\ell^{\star 2} - 4\ell^{\star} + 2)(\gamma_1 + 2\gamma_{12}) = \Gamma^{\star},$$

  which concludes the proof of item (1) since, by Lemma 7.2.1, we have $H(\eta) \geq H(\bar{\eta})$.

(2) By the proof above, the equality holds if and only if $\bar{\eta}$ does not have an 1-bridge, the equality in the isoperimetric inequality holds and $H(\eta) = H(\bar{\eta})$. By Lemma 7.2.1, this is equivalent to

$$\eta = \bar{\eta} \in \bigcup_{m=2}^{3} [\mathcal{W}(\boldsymbol{m}, \mathbf{1}) \cup \mathcal{W}'(\boldsymbol{m}, \mathbf{1})],$$

which proves item (2). □

Now we are ready to prove the lower bound of $\Gamma(\mathbf{2},\mathbf{3})$.

Proposition 7.4.4. *It holds that* $\Gamma(\mathbf{2},\mathbf{3}) \geq \Gamma^\star$.

Proof. Assume by contradiction that there exists a path $(\omega_n)_{n=0}^N$ from $\mathbf{2}$ to $\mathbf{3}$ such that $H(\omega_n) - H(\mathbf{2}) < \Gamma^\star$ for all n. Recall $\mathscr{P}^{12}$ from (7.19) and define

$$\tilde{\omega}_n := \mathscr{P}^{12}\omega_n.$$

It is clear that $\tilde{\omega}_0 = \mathbf{2}$ and $\tilde{\omega}_N = \mathbf{3}$. Thus, $(\tilde{\omega}_n)_{n=0}^N$ is a 23-path (possibly with some non-updating instances) from $\mathbf{2}$ to $\mathbf{3}$. Then, Proposition 7.3.3-(a) indicates that

$$\max_{0\leq n\leq N} H(\tilde{\omega}_n) \geq H(\mathbf{2}) + \Gamma^\star.$$

To conclude the proof, it is enough to show that $\mathfrak{N}_1(\omega_n) \leq \ell^{\star 2}$ for all n. Indeed, if the claim holds then we may apply Lemma 7.2.2 to each ω_n, so that along with the last display we have

$$\max_{0\leq n\leq N} H(\omega_n) \geq \max_{0\leq n\leq N} H(\tilde{\omega}_n) \geq H(\mathbf{2}) + \Gamma^\star.$$

This contradicts the original assumption.

It remains to prove the claim. We prove that $\mathfrak{N}_1(\omega_n) \leq \ell^\star(\ell^\star - 1)$ for all n, which is clearly sufficient. If not, $\mathfrak{N}_1(\omega_M) \geq \ell^\star(\ell^\star - 1) + 1$ for some M. Since $\mathfrak{N}_1(\omega_0) = 0$ and $|\mathfrak{N}_1(\omega_{n+1}) - \mathfrak{N}_1(\omega_n)| \leq 1$ for any n, there exists n_0 such that $\mathfrak{N}_1(\omega_{n_0}) = \ell^\star(\ell^\star-1)+1$. Then by Lemma 7.4.3-(a), $H(\omega_{n_0}) \geq H(\mathbf{2})+\Gamma^\star$ which contradicts our assumption. Thus, we conclude the proof of the claim. □

Proof of Theorem 7.1.2. The statement now follows directly from Propositions 7.4.1, 7.4.2, and 7.4.4. □

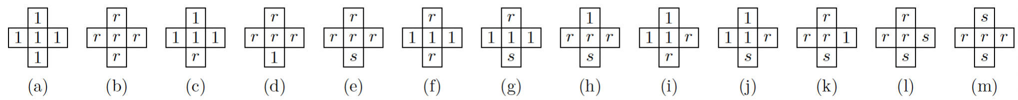


Figure 7.4: All possible stable tiles for r, $s \in \{2, 3\}$, $r \neq s$. The tiles are depicted up to rotations and reflections.

7.4.2 Stability level

In this subsection, we prove Proposition 7.1.3, i.e., we estimate the stability level of configurations other than **1**, **2** and **3**. First we introduce some notation.

- For $\sigma \in \mathcal{X}$ and $v \in V$, we denote by *tile centered at* v, or v*-tile*, the collection of five vertices consisting of v and its four nearest neighbors.
- A v-tile is *stable* for σ if any spin flip on v from $\sigma(v)$ to any other spin does not decrease the energy.
- Moreover, we say that a stable v-tile is *strictly stable* if any spin flip on v from $\sigma(v)$ to any other spin strictly increases the energy.

First, we can characterize all the stable and strictly stable tiles. Since the following lemma can be proved by simple algebra, we omit the proof.

Lemma 7.4.5 (Stable and strictly stable tiles)**.** *Let $\sigma \in \mathcal{X}$ and $v \in V$. Then, v-tile is strictly stable for σ if and only if the following statements hold.*

- *If $\sigma(v) = 1$, then v has at least two neighbors with spin 1, as in Figure 7.4-*(a)(c)(f)(g)(i)(j)*.*
- *If $\sigma(v) = r \in \{2, 3\}$, then v has either at least three neighbors with spin r, or exactly two neighbors with spin r and one neighbor with spin 1, as in Figure 7.4-*(b)(d)(e)(h)(k)*.*

Moreover, v-tile is stable but not strictly stable for σ if and only if $\sigma(v) = r \in \{2,3\}$ and v has exactly two neighbors with spin r and no neighbor with spin 1*, as in Figure 7.4-*(l)(m)*.*

Given a spin configuration σ, an edge $e = \{x,y\} \in E$ is called an *interface* of σ if $\sigma(x) \neq \sigma(y)$. Moreover, two different clusters C_1 and C_2 of σ are said to *interact with each other* if there exists $v \notin C_1 \cup C_2$ such that v is connected to both C_1 and C_2, i.e.,

$$\exists w_1 \in C_1 \text{ and } \exists w_2 \in C_2 \quad \text{such that} \quad \{v, w_1\} \in E \text{ and } \{v, w_2\} \in E. \tag{7.24}$$

Moreover, we define the set of local minima $\mathscr{M}$ as

$$\mathscr{M} := \big\{\sigma \in \mathcal{X} : \ H(\sigma) < H(\sigma') \text{ for all } \sigma' \neq \sigma \text{ with } P_\beta(\sigma, \sigma') > 0\big\}, \tag{7.25}$$

and the set of plateaux $\bar{\mathscr{M}}$ as

$$\bar{\mathscr{M}} := \bigcup_{D \text{ is a stable plateaux}} D. \tag{7.26}$$

Here, a subset $D \subset \mathcal{X}$ is a *stable plateau* if it is a maximal connected subset of equal energy, so that for any $\sigma \in D$ and $\sigma' \in \partial D$ it holds that $H(\sigma) < H(\sigma')$. It is obvious by definition that

$$\sigma \in \mathscr{M} \quad \Leftrightarrow \quad \text{every tile is strictly stable for } \sigma. \tag{7.27}$$

and

$$\sigma \in \mathscr{M} \cup \bar{\mathscr{M}} \quad \rightarrow \quad \text{every tile is stable for } \sigma. \tag{7.28}$$

First, we prove that all the 1-clusters of the configurations in $\mathscr{M} \cup \bar{\mathscr{M}}$ must be rectangles.

Lemma 7.4.6. *Suppose that $\sigma \in \mathscr{M} \cup \bar{\mathscr{M}}$. Then, each* 1*-cluster of σ is a rectangle.*

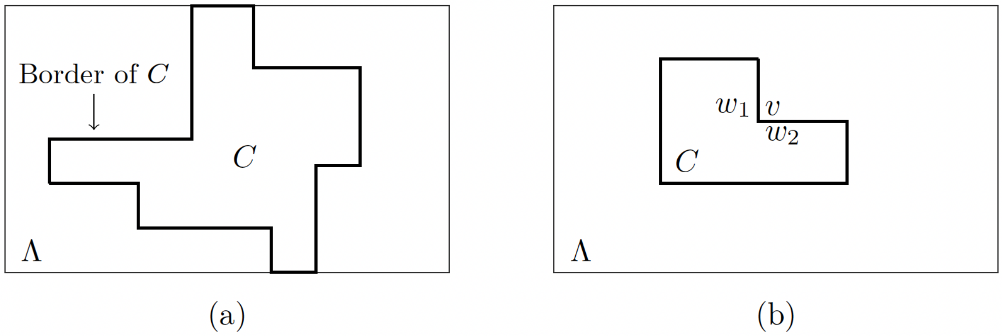


Figure 7.5: Illustrations regarding the proof of Lemma 7.4.6.

Proof. We fix $\sigma \in \mathscr{M} \cup \bar{\mathscr{M}}$ so that by (7.28), all tiles of σ must be of the form in Figure 7.4. We fix an 1-cluster C of σ. Consider the *border* of C, which is defined as

$$\big\{\{v,w\} \in E: \ v \in C \text{ and } w \in \partial C\big\}.$$

We refer to Figure 7.5-(a) for an illustration. If C is not a rectangle, then there exists at least one internal angle of $\frac{3}{2}\pi$ in the border, as one can see in Figure 7.5-(b) where $w_1, w_2 \in C$ and $v \notin C$. This implies that $\sigma(w_1) = \sigma(w_2) = 1$ whereas $\sigma(v) \neq 1$. Then by Lemma 7.4.5, v-tile is not stable for σ. This contradicts the fact that $\sigma \in \mathscr{M} \cup \bar{\mathscr{M}}$ due to (7.28). Therefore, we conclude that C is a rectangle. $\square$

Remark 7.4.7. It would possible to investigate further the equivalent conditions on the 1-clusters for a configuration to belong to $\mathscr{M} \cup \bar{\mathscr{M}}$. However, we do not pursue this further because it is not required for proving main results.

Now, we are ready to prove Proposition 7.1.3.

Proof of Proposition 7.1.3. To calculate the stability level of $\eta \in \mathcal{X} \setminus \{\mathbf{1}, \mathbf{2}, \mathbf{3}\}$, suppose first that $\eta \notin \mathscr{M} \cup \bar{\mathscr{M}}$. Then by definition (cf. (7.25) and (7.26)), there exists $\eta' \in \mathcal{X}$ such that $H(\eta') < H(\eta)$ and $P_\beta(\eta, \eta') > 0$. Thus, clearly

$V_\eta = 0$. Therefore, we may assume that $\eta \in (\mathscr{M} \cup \bar{\mathscr{M}}) \setminus \{\mathbf{1}, \mathbf{2}, \mathbf{3}\}$. It suffices to prove that

$$V_\eta \leq \max\left\{2\gamma_{12} - \gamma_1, 2(\ell^\star - 1)(\gamma_{23} + \gamma_1), 2\gamma_{23}\right\}$$

since clearly the maximum among the constants in the right-hand side is $2(\ell^\star - 1)(\gamma_{23} + \gamma_1)$. We divide into two cases.

(Case 1: η has an 1-cluster) In this case, by Lemma 7.4.6 η has an 1-cluster C which is a rectangle. Since $\eta \neq \mathbf{1}$, we have $C \subsetneq V$.

- **(If C has a side of length $\ell \geq \ell^\star$)** Since $C \subsetneq V$, we can define a path $\omega = (\omega_0, \dots, \omega_\ell)$, where $\omega_0 = \eta$ and $\omega_\ell = \bar{\eta}$, that flips consecutively those spins adjacent to a side of C of length ℓ to spin 1. Then, a simple computation shows that

  $$H(\omega_1) - H(\eta) \leq 2\gamma_{12} - \gamma_1 \quad \text{and} \quad H(\omega_i) - H(\omega_{i-1}) \leq -2\gamma_1 \text{ for any } 2 \leq i \leq \ell. \tag{7.29}$$

  Thanks to (7.29), we have that

  $$H(\bar{\eta}) - H(\eta) \leq 2\gamma_{12} - (2\ell^\star - 1)\gamma_1 < 0.$$

  The last inequality holds since $\ell^\star = \lceil \frac{2\gamma_{12} + \gamma_1}{2\gamma_1} \rceil > \frac{2\gamma_{12} + \gamma_1}{2\gamma_1}$ by Assumption 7.0.1-**A**. Moreover, the height of ω is attained by either $\omega_0 = \eta$ or ω_1, which has energy at most $H(\eta) + (2\gamma_{12} - \gamma_1)$. Therefore, we deduce in this case that $V_\eta \leq 2\gamma_{12} - \gamma_1$.

- **(If all sides of C have lengths smaller than $\ell^\star$)** Suppose that C is a rectangle $p \times q$. Since $|\partial C| = 2(p + q)$ and all spins on ∂C are either 2 or 3, $\mathfrak{N}_2(\partial C) + \mathfrak{N}_3(\partial C) = 2(p + q)$. Without loss of generality, we assume that

  $$\mathfrak{N}_2(\partial C) \geq p + q \quad \text{and} \quad \mathfrak{N}_3(\partial C) \leq p + q. \tag{7.30}$$

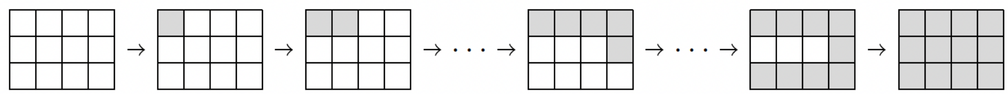


Figure 7.6: The 4×3 rectangle represents the 1-cluster whose spins are sequentially flipped to 2.

We define a path $\omega = (\omega_n)_{n=0}^{pq}$ from $\omega_0 = \eta$ to $\omega_{pq} =: \eta'$ as follows: starting from the upper-left corner of C, we update each spin 1 in C to spin 2 consecutively in a clockwise manner, until all the spins 1 in C are updated to spins 2, see Figure 7.6.

First, we calculate $H(\eta') - H(\eta)$. To this end, note that the edges contained in $V \setminus C$ are not affected by the pq spin updates. Thus,

$$H(\eta') - H(\eta) = (2pq - p - q)\gamma_1 \big[- \mathfrak{N}_2(\partial C)\gamma_{12} + \mathfrak{N}_3(\partial C)(\gamma_{23} - \gamma_{13})\big].$$

Here, $2pq - p - q$ is the number of internal edges in C. Hence, along with (7.30),

$$\begin{aligned} H(\eta') - H(\eta) &\le (2pq - p - q)\gamma_1 + (p+q)\gamma_{23} - 2(p+q)\gamma_{12} \\ &= 2pq\gamma_1 - (p+q)(2\gamma_{12} - \gamma_{23} + \gamma_1). \end{aligned}$$

Subjected to the condition $1 \le p, q < \ell^\star$, a simple algebraic computation reveals that the maximum of the last term is attained on $(p,q) = (1,1)$ or $(\ell^\star - 1, \ell^\star - 1)$. If $(p,q) = (1,1)$ then the value equals $-4\gamma_{12} + 2\gamma_{23} < 0$ by Assumption 7.0.1-**C**, whereas if $(p,q) = (\ell^\star - 1, \ell^\star - 1)$ then the value becomes

$$2(\ell^\star - 1)[(\ell^\star - 1)\gamma_1 - 2\gamma_{12} + \gamma_{23} - \gamma_1] < 2(\ell^\star - 1)\Big(- \gamma_{12} + \gamma_{23} - \frac{\gamma_1}{2}\Big) < 0,$$

where we used $\ell^\star < \dfrac{2\gamma_{12} + \gamma_1}{2\gamma_1} + 1$ in the first inequality and Assumption

7.0.1-**C** in the second inequality. Thus, we deduce that

$$H(\eta') - H(\eta) < 0.$$

Therefore, to estimate the stability level of η we may focus on the maximal energy attained along the path $\omega : \eta \to \eta'$. By (7.41), for each $1 \leq n \leq pq$ it holds that

$$H(\omega_n) - H(\eta) = -\gamma_1[\mathfrak{n}_{11}(\omega_n) - \mathfrak{n}_{11}(\eta)] + \sum_{i<j} \gamma_{ij}[\mathfrak{n}_{ij}(\omega_n) - \mathfrak{n}_{ij}(\eta)].$$

Note that the edges contained in $V \setminus C$ are unchanged along the path. Thus, we may write

$$H(\omega_n) - H(\eta) = g_1(n) + g_2(n),$$

where

$$\begin{aligned} g_1(n) :=& -\gamma_1\Big[\sum_{\{x,y\}\in E\colon \{x,y\}\cap C\neq\varnothing} \mathbb{1}_{\{\omega_n(x)=\omega_n(y)=1\}} - (2pq-p-q)\Big] \\ &+ \gamma_{12}\Big[\sum_{j=2}^{3} \sum_{\{x,y\}\in E\colon \{x,y\}\cap C\neq\varnothing} \mathbb{1}_{\{\{\omega_n(x),\omega_n(y)\}=\{1,j\}\}} - 2(p+q)\Big] \end{aligned}$$

and

$$g_2(n) := \gamma_{23} \sum_{\{x,y\}\in E\colon \{x,y\}\cap C\neq\varnothing} \mathbb{1}_{\{\{\omega_n(x),\omega_n(y)\}=\{2,3\}\}}. \tag{7.31}$$

First, note that g_1 records precisely the energy of the (reversed) reference path from **2** to a configuration with a single 1-cluster C, translated by a fixed real number which is $(2pq-p-q)\gamma_1 - 2(p+q)\gamma_{12} + H(\mathbf{2})$. Since $p, q \leq \ell^\star - 1$, it can be inferred from Definition 7.5.2 that

$$\max_{0\leq n\leq pq} g_1(n) = g_1(p-1) = 2(p-1)\gamma_1.$$

Next, note that g_2 is monotone increasing. Hence, we apply a crude bound via assumption (7.30) by

$$\max_{0\le n\le pq} g_2(n) = g_2(pq) = \gamma_{23} \times \mathfrak{N}_3(\partial C) \le (p+q)\gamma_{23}.$$

Therefore, we estimate

$$\max_n\{H(\omega_n)-H(\eta)\} \le \max_n g_1(n)+\max_n g_2(n) \le 2(p-1)\gamma_1+(p+q)\gamma_{23}.$$

Since $p, q \le \ell^\star - 1$, this is bounded above by

$$2(\ell^\star-2)\gamma_1 + 2(\ell^\star-1)\gamma_{23} < 2(\ell^\star-1)(\gamma_{23}+\gamma_1).$$

Hence, we deduce that

$$V_\eta \le \max_{0\le n\le pq}\{H(\omega_n)-H(\eta)\} < 2(\ell^\star-1)(\gamma_{23}+\gamma_1)$$

and this concludes the proof of **Case 1**.

(Case 2: η does not have an 1-cluster) In this case, $\eta \in \mathcal{X}^{23}$ (cf. (7.44)). We claim that

$$V_\eta \le 2\gamma_{23}.$$

To this end, we take a 2-cluster C' of η which is possible since $\eta \ne \mathbf{3}$. If there is an internal angle of $\frac{3}{2}\pi$ in the border of C', as in the proof of Lemma 7.4.6 we can find $w_1, w_2 \in C'$ and $v \in \partial C'$ such that $\eta(v) = 3$, $\eta(w_1) = \eta(w_2) = 2$ and $w_1 \sim v \sim w_2$. Thus, by updating the spin 3 at site v to spin 2, the energy difference is at most $2\gamma_{23} - 2\gamma_{23} = 0$, which means that the energy does not increase. Moreover, the number of spins 2 increases. If we repeat this procedure as long as there remains an internal angle of $\frac{3}{2}\pi$ in the border of some 2-cluster, we either obtain $\mathbf{2}$ (then there is nothing to prove since in this case $V_\eta = 0$), or obtain a configuration $\hat{\eta}$ where all internal angles of 2-clusters are at most π. We may assume the latter case.

Figure 7.7: Light-gray and dark-gray colors represent spins 2 and 3, respectively.

All that remains to be proved is that $V_{\hat{\eta}} \le 2\gamma_{23}$. There are two sub-cases depending on the internal angles of the 2-clusters of $\hat{\eta}$.

- **(If the internal angles are all π)** In this sub-case, all the 2-clusters are strips and in turn all the 3-clusters are also strips. Thus, taking any 3-bridge in $\hat{\eta}$ which is adjacent to a 2-cluster, we can update consecutively the spins 3 to spins 2, so that the maximal energy along the updates are $H(\hat{\eta}) + 2\gamma_{23}$, which can be attained only at the first step. Repeating this, we eventually obtain **2**. Therefore, we have proved that $V_{\hat{\eta}} \le 2\gamma_{23}$.
- **(If an internal angle is $\frac{1}{2}\pi$)** By simple inspection, there always exists a collection of spin dispositions which have the form as in Figure 7.7.

  Thus, by updating consecutively the indicated light-gray (spin 2) colors to dark-gray (spin 3) colors, the energy does not increase along the path and at the last step the energy decreases by at least $2\gamma_{23}$. Thus, we deduce that $V_{\hat{\eta}} = 0$ in this case. Therefore, we are done.

□

7.4.3 Initial cycle and restricted gate

In this subsection, we define the initial cycle for each metastable and stable configurations. Then, we prove some key lemmas regarding restricted gates, which are crucial to prove the main results in Section 7.1.3 regarding the minimal gates.

For each $r \in S$, we define the *initial cycle* of $\boldsymbol{r}$ as

$$\mathcal{C}_r := \{\sigma \in \mathcal{X} : \ \Phi(\boldsymbol{r}, \sigma) < H(\mathbf{2}) + \Gamma^\star\}. \tag{7.32}$$

By Theorem 7.1.2, **1**, **2** and **3** are mutually separated by the energy barrier $H(\mathbf{2}) + \Gamma^\star$. Therefore, it follows that $\mathcal{C}_1$, $\mathcal{C}_2$ and $\mathcal{C}_3$ are mutually disjoint.

First, we show that the domains of attraction are stable under projections.

Lemma 7.4.8. *It holds that*

(1) $\mathscr{P}^{32}\mathcal{C}_1 \subset \mathcal{C}_1$ *and* $\mathscr{P}^{32}\mathcal{C}_2 \subset \mathcal{C}_2$.

(2) $\mathscr{P}^{12}\mathcal{C}_2 \subset \mathcal{C}_2$ *and* $\mathscr{P}^{12}\mathcal{C}_3 \subset \mathcal{C}_3$.

Proof. (1) Suppose that $\sigma \in \mathcal{C}_r$ for some $r \in \{1, 2\}$. Then, there exists a path $\omega : \sigma \to \boldsymbol{r}$ whose height is strictly less than $H(\mathbf{2}) + \Gamma^\star$. Then by Lemma 7.2.1, the projected path $\mathscr{P}^{32}\omega : \mathscr{P}^{32}\sigma \to \boldsymbol{r}$ has height also strictly less than $H(\mathbf{2}) + \Gamma^\star$. This proves that $\mathscr{P}^{32}\sigma \in \mathcal{C}_r$.

(2) First, we claim that for any $\eta \in \mathcal{X}$,

$$\eta \in \mathcal{C}_2 \cup \mathcal{C}_3 \quad \text{implies} \quad \mathfrak{N}_1(\eta) \leq \ell^\star(\ell^\star - 1). \tag{7.33}$$

To this end, assume by contradiction that $\mathfrak{N}_1(\eta) > \ell^\star(\ell^\star - 1)$ and, without loss of generality, assume that $\eta \in \mathcal{C}_2$. Take a path $\omega_0 : \eta \to \mathbf{2}$ whose height is strictly less than $H(\mathbf{2}) + \Gamma^\star$. Then since $\mathfrak{N}_1(\mathbf{2}) = 0$, there exists $\zeta \in \omega_0$ such that $\mathfrak{N}_1(\zeta) = \ell^\star(\ell^\star - 1) + 1$. Then by Lemma 7.4.3, $H(\zeta) \geq H(\mathbf{2}) + \Gamma^\star$ and we obtain a contradiction.

Now, assume $\sigma \in \mathcal{C}_s$ for some $s \in \{2, 3\}$. Then, there exists a path $\omega : \sigma \to \boldsymbol{s}$ whose height is less than $H(\mathbf{2}) + \Gamma^\star$. By the claim above, the number of spins 1 of every configuration in ω does not exceed $\ell^\star(\ell^\star - 1)$. Thus by Lemma 7.2.2, the projected path $\mathscr{P}^{12}\omega : \mathscr{P}^{12}\sigma \to \boldsymbol{s}$ also has height less than $H(\mathbf{2}) + \Gamma^\star$ and we conclude that $\mathscr{P}^{12}\sigma \in \mathcal{C}_s$. $\square$

Now, the first result in this subsection analyzes the optimal paths from $\boldsymbol{m} \in \{\mathbf{2}, \mathbf{3}\}$ to $\mathbf{1}$ which do not visit $\mathcal{C}_3$. Such paths are called *restricted-paths* in [11].

Proposition 7.4.9. *Suppose that $\omega = (\omega_n)_{n=0}^N$ is an optimal path from $\boldsymbol{m}$ to $\mathbf{1}$ which does not visit $\mathcal{C}_{m'}$ where $\{m, m'\} = \{2, 3\}$. Then, we have*

$$\omega \cap \mathcal{W}(\boldsymbol{m}, \mathbf{1}) \neq \varnothing.$$

Proof. Without loss of generality, assume that $\boldsymbol{m} = \mathbf{2}$. As $\omega_0 = \mathbf{2} \notin \mathcal{C}_1$ and $\omega_N = \mathbf{1} \in \mathcal{C}_1$, we can define

$$N' := \min\{1 \leq n \leq N : \ \omega_n \in \mathcal{C}_1\}.$$

Then, $\omega_{N'} \in \mathcal{C}_1$ and

$$\omega_0, \ldots, \omega_{N'-1} \notin \mathcal{C}_1 \cup \mathcal{C}_3. \tag{7.34}$$

Define $\bar{\omega}_n := \mathscr{P}^{32}\omega_n$ for each $0 \leq n \leq N'$. Then, $\bar{\omega}_0 = \mathbf{2}$ and by Lemma 7.4.8-(a), $\bar{\omega}_{N'} \in \mathcal{C}_1$, so that $\bar{\omega} = (\bar{\omega}_n)_{n=0}^{N'}$ is an 12-path from $\mathbf{2}$ to $\mathcal{C}_1$. As the height of $(\omega_n)_{n=0}^{N'}$ is at most $H(\mathbf{2}) + \Gamma^\star$, Lemma 7.2.1 implies that the height of $\bar{\omega}$ is at most $H(\mathbf{2}) + \Gamma^\star$. Thus by Proposition 7.3.1-(a), the height of $\bar{\omega}$ must be exactly $H(\mathbf{2}) + \Gamma^\star$ and in turn by Proposition 7.3.1-(b),

$$\bar{\omega} \cap \mathcal{W}(\mathbf{2}, \mathbf{1}) \neq \varnothing.$$

Hence, there exists $0 \leq m \leq N'$ so that $\bar{\omega}_m \in \mathcal{W}(\mathbf{2}, \mathbf{1})$. It readily holds that $H(\bar{\omega}_m) = H(\mathbf{2}) + \Gamma^\star$. Moreover, by Lemma 7.2.1, $H(\omega_m) \geq H(\bar{\omega}_m)$. Thus,

$$H(\mathbf{2}) + \Gamma^\star \geq H(\omega_m) \geq H(\bar{\omega}_m) = H(\mathbf{2}) + \Gamma^\star,$$

so that equalities must hold in all places. Then, Lemma 7.2.1 again implies that

$$\omega_m \in \mathcal{W}(\mathbf{2}, \mathbf{1}) \quad \text{or} \quad \omega_m \in \mathcal{W}(\mathbf{3}, \mathbf{1}).$$

We conclude the proof of this lemma by showing that the latter is impossible. To this end, suppose on the contrary that $\omega_m \in \mathcal{W}(\mathbf{3},\mathbf{1})$. Then since $P_\beta(\omega_m, \omega_{m-1}) > 0$ and $H(\omega_m) = H(\mathbf{2}) + \Gamma^\star$, we readily deduce that

$$\omega_{m-1} \in R_{\ell^\star-1,\ell^\star}(3,1) \cup R_{\ell^\star,\ell^\star-1}(3,1) \tag{7.35}$$

or

$$\omega_{m-1} \in B^2_{\ell^\star-1,\ell^\star}(3,1) \cup \hat{B}^2_{\ell^\star,\ell^\star-1}(3,1), \tag{7.36}$$

since any other possibility implies that $H(\omega_{m-1}) > H(\omega_m) = H(\mathbf{2}) + \Gamma^\star$, which is impossible. If (7.35) holds, then a part of the reference path $\mathbf{3} \to \mathbf{1}$ with respect to ω_m guarantees that $\omega_{m-1} \in \mathcal{C}_3$ which contradicts the condition (7.34). If (7.36) holds then the other side of the reference path guarantees that $\omega_{m-1} \in \mathcal{C}_1$, and we again obtain a contradiction with (7.34). □

Next, we deal with the optimal paths from $\mathbf{2}$ to $\mathbf{3}$ which do not visit $\mathcal{C}_1$.

Proposition 7.4.10. *Suppose that $\omega = (\omega_n)_{n=0}^N$ is an optimal path from $\mathbf{2}$ to $\mathbf{3}$ which does not visit $\mathcal{C}_1$. Choose any set $\mathscr{A}$ in*

$$\big\{\mathscr{W}_j^h(\mathbf{2},\mathbf{3})\big\}_{j,h} \cup \big\{\mathscr{Q}(\mathbf{2},\mathbf{3}), \mathscr{P}(\mathbf{2},\mathbf{3}), \mathscr{P}(\mathbf{3},\mathbf{2}), \mathscr{Q}(\mathbf{3},\mathbf{2})\big\} \cup \big\{\mathscr{H}_i(\mathbf{2},\mathbf{3})\big\}_i \cup \big\{\mathscr{H}_i(\mathbf{3},\mathbf{2})\big\}_i.$$

Then, we have

$$\omega \cap \mathscr{A} \neq \varnothing.$$

Proof. First, we claim that

$$\mathfrak{N}_1(\omega_n) \le \ell^{\star 2} - 1 \quad \text{for all } 0 \le n \le N.$$

To prove the claim, suppose the contrary that there exists M such that $\mathfrak{N}_1(\omega_M) \ge \ell^{\star 2}$. Then since $\mathfrak{N}_1(\omega_0) = \mathfrak{N}_1(\mathbf{2}) = 0$, we can take the largest $n_0 \in [0, M]$ such that $\mathfrak{N}_1(\omega_{n_0}) = \ell^{\star 2} - \ell^\star + 1$. Then, $\mathfrak{N}_1(\omega_n) \ge \ell^{\star 2} - \ell^\star + 2$

for $n_0 < n \le M$. Then by Lemma 7.4.3, $H(\omega_{n_0}) = H(\mathbf{2}) + \Gamma^\star$ and

$$\omega_{n_0} \in \bigcup_{m=2}^{3} [\mathcal{W}(\boldsymbol{m}, \mathbf{1}) \cup \mathcal{W}'(\boldsymbol{m}, \mathbf{1})].$$

If $\omega_{n_0} \in \mathcal{W}(\boldsymbol{m}, \mathbf{1})$ for some $m \in \{2, 3\}$ then since $\mathfrak{N}_1(\omega_{n_0+1}) = \mathfrak{N}_1(\omega_{n_0}) + 1$, the only possible option (so that $H(\omega_{n_0+1}) \le H(\mathbf{2}) + \Gamma^\star$) is

$$\omega_{n_0+1} \in B^2_{\ell^\star-1,\ell^\star}(m, 1) \cup \hat{B}^2_{\ell^\star,\ell^\star-1}(m, 1).$$

Then, a suitable reference path from ω_{n_0+1} to $\mathbf{1}$ guarantees that $\omega_{n_0+1} \in \mathcal{C}_1$, which contradicts the assumption of the proposition. Hence, we may assume that

$$\omega_{n_0} \in \bigcup_{m=2}^{3} \mathcal{W}'(\boldsymbol{m}, \mathbf{1}).$$

We denote by R_0 the rectangle of side lengths $\ell^\star - 1$ and $\ell^\star + 1$, which is the smallest rectangle containing the 1-cluster of ω_{n_0}. We will demonstrate that

$$\{v \in V : \ \omega_n(v) = 1\} \subseteq R_0 \quad \text{for all } n_0 \le n \le M,$$

which contradicts $\mathfrak{N}_1(\omega_M) \ge \ell^{\star 2}$ and thus proves the first claim. Let us suppose the contrary. Then, there exists $m_0 \in (n_0, M]$ such that $\{v \in V : \omega_n(v) = 1\} \subseteq R_0$ for all $n_0 \le n < m_0$ and $\{v \in V : \ \omega_{m_0}(v) = 1\} \nsubseteq R_0$. As usual, we write $\bar{\omega}_n := \mathscr{P}^{32}\omega_n$.

- **(Step 1)** $H(\bar{\omega}_n) - H(\mathbf{2}) \ge 4\ell^\star\gamma_{12} - 2\gamma_1(\ell^{\star 2} - \ell^\star - 1)$ for all $n_0 \le n < m_0$.

  Since $\mathfrak{N}_1(\bar{\omega}_n) \ge \ell^{\star 2} - \ell^\star + 1$ for $n_0 \le n < m_0$, every row and column of R_0 must have at least one spin 1. Indeed, if not then we would have

  $$\mathfrak{N}_1(\bar{\omega}_n) \le \max\{(\ell^\star - 1)(\ell^\star + 1 - 1), (\ell^\star + 1)(\ell^\star - 1 - 1)\} = \ell^{\star 2} - \ell^\star,$$

  which contradicts $\mathfrak{N}_1(\bar{\omega}_n) \ge \ell^\star(\ell^\star - 1) + 1$. Thus, in each corresponding row and column there exists at least two 12-edges in $\bar{\omega}_n$, so that we have

$$\mathfrak{n}_{12}(\bar{\omega}_n) \geq 2(\ell^\star - 1) + 2(\ell^\star + 1) = 4\ell^\star. \tag{7.37}$$

Moreover, clearly the maximum of $\mathfrak{n}_{11}(\bar{\omega}_n)$ is attained when the box R_0 is full of spins 1:

$$\mathfrak{n}_{11}(\bar{\omega}_n) \leq (\ell^\star - 1)\ell^\star + (\ell^\star + 1)(\ell^\star - 2) = 2\ell^{\star 2} - 2\ell^\star - 2. \tag{7.38}$$

Thus, by (7.37), (7.38) and (7.41) we deduce

$$H(\bar{\omega}_n) - H(\mathbf{2}) = \mathfrak{n}_{12}(\bar{\omega}_n)\gamma_{12} - \mathfrak{n}_{11}(\bar{\omega}_n)\gamma_1 \geq 4\ell^\star\gamma_{12} - 2\gamma_1(\ell^{\star 2} - \ell^\star - 1).$$

- **(Step 2)** $H(\omega_{m_0}) > H(\mathbf{2}) + \Gamma^\star$, which yields a contradiction.

  Consider the spin flip from $\bar{\omega}_{m_0-1}$ to $\bar{\omega}_{m_0}$. Since this spin flip happens outside R_0, the energy difference is at least $2\gamma_{12} - \gamma_1$ and at most $4\gamma_{12}$. Therefore, by **Step 1**, we deduce that

$$\begin{aligned} H(\bar{\omega}_{m_0}) - H(\mathbf{2}) &\geq H(\bar{\omega}_{m_0-1}) - H(\mathbf{2}) + (2\gamma_{12} - \gamma_1) \\ &\geq (4\ell^\star + 2)\gamma_{12} - \gamma_1(2\ell^{\star 2} - 2\ell^\star - 1) > \Gamma^\star. \end{aligned}$$

  Indeed, the last inequality is equivalent to (cf. (7.11)) $2\gamma_{12} > (2\ell^\star - 3)\gamma_1$, which can be rearranged as

$$\frac{2\gamma_{12} + \gamma_1}{2\gamma_1} > \ell^\star - 1.$$

  This is obvious by (7.10). Hence, by Lemma 7.2.1 we have $H(\omega_{m_0}) \geq H(\bar{\omega}_{m_0})) > H(\mathbf{2}) + \Gamma^\star$.

Now, we return to the proof of Proposition 7.4.10. The idea is similar to the proof of Proposition 7.4.9. As $\omega_0 = \mathbf{2} \notin \mathcal{C}_3$ and $\omega_N = \mathbf{3} \in \mathcal{C}_3$, we may define

$$N' := \min\{1 \leq n \leq N : \ \omega_n \in \mathcal{C}_3\},$$

so that $\omega_{N'} \in \mathcal{C}_3$ and

$$\omega_0, \dots, \omega_{N'-1} \notin \mathcal{C}_1 \cup \mathcal{C}_3. \tag{7.39}$$

Define $\tilde{\omega}_n := \mathscr{P}^{12}\omega_n$ for each $0 \leq n \leq N'$. Then, $\tilde{\omega}_0 = \mathbf{2}$ and by Lemma 7.4.8-(b) $\tilde{\omega}_{N'} \in \mathcal{C}_3$, so that $\tilde{\omega} = (\tilde{\omega}_n)_{n=0}^{N'}$ is an 23-path from $\mathbf{2}$ to $\mathcal{C}_3$. As the height of $(\omega_n)_{n=0}^{N'}$ is at most $H(\mathbf{2}) + \Gamma^\star$, Lemma 7.2.2, which is applicable by the first claim, implies that the height of $\tilde{\omega}$ is also at most $H(\mathbf{2}) + \Gamma^\star$. Thus by Proposition 7.3.3-(a), the height of $\tilde{\omega}$ must be exactly $H(\mathbf{2}) + \Gamma^\star$ and thus by Proposition 7.3.3-(b),

$$\tilde{\omega} \cap \mathscr{A} \neq \varnothing.$$

Hence, there exists $0 \leq m \leq N'$ so that $\tilde{\omega}_m \in \mathscr{A}$. It holds that $H(\tilde{\omega}_m) = H(\mathbf{2}) + \Gamma^\star$. Moreover, by Lemma 7.2.2, $H(\omega_m) \geq H(\tilde{\omega}_m)$. Thus,

$$H(\mathbf{2}) + \Gamma^\star \geq H(\omega_m) \geq H(\tilde{\omega}_m) = H(\mathbf{2}) + \Gamma^\star,$$

so that equalities must hold in all places. Then Lemma 7.2.2 again implies that

$$\omega_m = \tilde{\omega}_m \in \mathscr{A},$$

which concludes the proof. □

7.4.4 Minimal gates for the metastable transition

In this final subsection, we prove the results stated in Section 7.1.3. Referring to the landscape given in Figure 7.3 shall be helpful to understand the gist of the ideas given here.

First, we focus on Theorem 7.1.8. Since the situation is totally symmetric between spins 2 and 3, we prove Theorem 7.1.8 for $\boldsymbol{m} = \mathbf{2}$.

Proof of Theorem 7.1.8-(a). We prove that $\mathcal{W}(\mathbf{2},\mathbf{1})\cup\mathcal{W}(\mathbf{3},\mathbf{1})$ is a minimal gate for the transition $\mathbf{2}\to\mathbf{1}$. First, suppose that $\omega=(\omega_n)_{n=0}^N$ is an optimal path $\mathbf{2}\to\mathbf{1}$. Consider the last visit of ω to $\mathcal{C}_2\cup\mathcal{C}_3$, which is possible because ω starts from $\mathbf{2}\in\mathcal{C}_2\cup\mathcal{C}_3$. If the last visit is to $\mathcal{C}_2$, so that after then it does not visit $\mathcal{C}_3$, then by Proposition 7.4.9 we deduce that $\omega\cap\mathcal{W}(\mathbf{2},\mathbf{1})\neq\varnothing$. If the last visit is to $\mathcal{C}_3$, then similarly by Proposition 7.4.9, we have $\omega\cap\mathcal{W}(\mathbf{3},\mathbf{1})\neq\varnothing$. This proves that $\mathcal{W}(\mathbf{2},\mathbf{1})\cup\mathcal{W}(\mathbf{3},\mathbf{1})$ is a gate.

To show that it is minimal, take any $\sigma\in\mathcal{W}(\mathbf{2},\mathbf{1})\cup\mathcal{W}(\mathbf{3},\mathbf{1})$. It suffices to show that $[\mathcal{W}(\mathbf{2},\mathbf{1})\cup\mathcal{W}(\mathbf{3},\mathbf{1})]\setminus\{\sigma\}$ is not a gate. If $\sigma\in\mathcal{W}(\mathbf{2},\mathbf{1})$, then the reference path $\mathbf{2}\to\mathbf{1}$ with respect to σ defined in Definition 7.5.2 does not visit $\mathcal{W}(\mathbf{2},\mathbf{1})\cup\mathcal{W}(\mathbf{3},\mathbf{1})$ except at σ, and thus we are done. If $\sigma\in\mathcal{W}(\mathbf{3},\mathbf{1})$, we can concatenate any reference path from $\mathbf{2}$ to $\mathbf{3}$ (given in Definition 7.5.3) and the reference path $\mathbf{3}\to\mathbf{1}$ with respect to σ (given in Definition 7.5.2) to obtain an optimal path from $\mathbf{2}$ to $\mathbf{1}$. This path does not visit $\mathcal{W}(\mathbf{2},\mathbf{1})\cup\mathcal{W}(\mathbf{3},\mathbf{1})$ except at σ. In these two cases we proved that $\mathcal{W}(\mathbf{2},\mathbf{1})\cup\mathcal{W}(\mathbf{3},\mathbf{1})$ is indeed a minimal gate. $\square$

Proof of Theorem 7.1.8-(b). As stated in the theorem, we fix a set $\mathscr{A}$ in

$$\big\{\mathscr{W}_j^h(\mathbf{2},\mathbf{3})\big\}_{j,h}\cup\big\{\mathscr{Q}(\mathbf{2},\mathbf{3}),\mathscr{P}(\mathbf{2},\mathbf{3}),\mathscr{P}(\mathbf{3},\mathbf{2}),\mathscr{Q}(\mathbf{3},\mathbf{2})\big\}\cup\big\{\mathscr{H}_i(\mathbf{2},\mathbf{3})\big\}_i\cup\big\{\mathscr{H}_i(\mathbf{3},\mathbf{2})\big\}_i.$$

We prove that $\mathcal{W}(\mathbf{2},\mathbf{1})\cup\mathscr{A}$ is a minimal gate. First, we demonstrate that it is a gate. Take an arbitrary optimal path $\omega=(\omega_n)_{n=0}^N$ from $\mathbf{2}$ to $\mathbf{1}$. As we did in the proof of part (a), we divide into two cases, but in this case we consider the first visit to $\mathcal{C}_1\cup\mathcal{C}_3$ which is possible since $\mathbf{1}\in\mathcal{C}_1\cup\mathcal{C}_3$. If the first visit to $\mathcal{C}_1\cup\mathcal{C}_3$ is to $\mathcal{C}_1$, then by Proposition 7.4.9 it holds that $\omega\cap\mathcal{W}(\mathbf{2},\mathbf{1})\neq\varnothing$. If the first visit to $\mathcal{C}_1\cup\mathcal{C}_3$ is to $\mathcal{C}_3$, then by Proposition 7.4.10 it holds that $\omega\cap\mathscr{A}\neq\varnothing$.

Finally, we prove that $\mathcal{W}(\mathbf{2},\mathbf{1})\cup\mathscr{A}$ is minimal. Take any $\sigma\in\mathcal{W}(\mathbf{2},\mathbf{1})\cup\mathscr{A}$. If $\sigma\in\mathcal{W}(\mathbf{2},\mathbf{1})$, then the reference path $\mathbf{2}\to\mathbf{1}$ with respect to σ defined in Definition 7.5.2 does not visit $\mathcal{W}(\mathbf{2},\mathbf{1})\cup\mathscr{A}$ except at σ, and thus we are done.

If $\sigma \in \mathscr{A}$, we can concatenate the reference path from $\mathbf{2}$ to $\mathbf{3}$ with respect to σ (given in Definition 7.5.3) and any reference path from $\mathbf{3}$ to $\mathbf{1}$ (given in Definition 7.5.2) to obtain an optimal path from $\mathbf{2}$ to $\mathbf{1}$. This path does not visit $\mathcal{W}(\mathbf{2},\mathbf{1}) \cup \mathscr{A}$ except at σ. Therefore, we conclude that $\mathcal{W}(\mathbf{2},\mathbf{1}) \cup \mathscr{A}$ is minimal. □

Next, we prove that there are no configurations, other than the ones characterized above, that form another minimal gate. This is exactly the content of item (c).

Proof of Theorem 7.1.8-(c). By the equivalent characterization of unessential saddles given in [67, Theorem 5.1], it suffices to prove that every $\sigma \notin \mathcal{W}(\mathbf{2},\mathbf{1}) \cup \mathcal{W}(\mathbf{3},\mathbf{1}) \cup \mathcal{W}(\mathbf{2},\mathbf{3})$ is unessential, i.e., for any $\omega \in \Omega_{\mathbf{2},\mathbf{1}}^{opt}$ with $\sigma \in \omega$, there exists another $\omega' \in \Omega_{\mathbf{2},\mathbf{1}}^{opt}$ such that $\mathrm{argmax}_{\omega'} H \subseteq \mathrm{argmax}_{\omega} H \setminus \{\sigma\}$.

The idea is nearly the same as the one presented in [11, Proof of Theorem 3.2], so we will briefly sketch the proof. We fix such σ and $\omega \in \Omega_{\mathbf{2},\mathbf{1}}^{opt}$. Then, as we demonstrated above, $\mathcal{W}(\mathbf{2},\mathbf{1}) \cup \mathcal{W}(\mathbf{3},\mathbf{1})$ is a gate for $\mathbf{2} \to \mathbf{1}$, and thus

$$\omega \cap [\mathcal{W}(\mathbf{2},\mathbf{1}) \cup \mathcal{W}(\mathbf{3},\mathbf{1})] \neq \varnothing.$$

If there exists $\zeta \in \omega \cap \mathcal{W}(\mathbf{2},\mathbf{1})$, then we may construct ω' as the reference path $\mathbf{2} \to \mathbf{1}$ with respect to ζ, so that

$$\mathrm{argmax}_{\omega'} H = \{\zeta\} \subseteq \mathrm{argmax}_{\omega} H \setminus \{\sigma\}.$$

If $\omega \cap \mathcal{W}(\mathbf{2},\mathbf{1}) = \varnothing$, then ω must visit $\mathcal{C}_3$ before $\mathcal{C}_1$; otherwise, there is a subpath of ω from $\mathbf{2}$ to $\mathcal{C}_1$ which does not visit $\mathcal{C}_3$, and then Proposition 7.4.9 implies that $\omega \cap \mathcal{W}(\mathbf{2},\mathbf{1}) \neq \varnothing$ which yields a contradiction. Thus by Proposition 7.4.10, $\omega \cap \mathscr{A} \neq \varnothing$ where $\mathscr{A}$ is any collection chosen as in Proposition 7.4.10. Therefore, we can apply the argument given in [11, Proof of Theorem 3.2], where we record the last visit to $\mathscr{H}_1(\mathbf{2},\mathbf{3})$ and then the first visit to $\mathscr{H}_1(\mathbf{3},\mathbf{2})$. Then, we can record all the gate configurations visited by ω

during this period, and then glue them together to construct a reference path ω'_1 from $\mathbf{2}$ to $\mathbf{3}$. Next, since $\omega \cap \mathcal{W}(\mathbf{2}, \mathbf{1}) = \varnothing$ it holds that $\omega \cap \mathcal{W}(\mathbf{3}, \mathbf{1}) \neq \varnothing$. Thus, there exists a reference path $\omega'_2 : \mathbf{3} \to \mathbf{1}$ which visits the configuration belonging to $\omega \cap \mathcal{W}(\mathbf{3}, \mathbf{1})$. Concatenating ω'_1 and ω'_2, we obtain a new optimal path ω' so that

$$\text{argmax}_{\omega'} H \subseteq \text{argmax}_{\omega} H.$$

Moreover, $\text{argmax}_{\omega'} H$ is clearly a subset of $\mathcal{W}(\mathbf{2}, \mathbf{3}) \cup \mathcal{W}(\mathbf{3}, \mathbf{1})$, so that $\sigma \notin \text{argmax}_{\omega'} H$. Therefore, we conclude that

$$\text{argmax}_{\omega'} H \subseteq \text{argmax}_{\omega} H \setminus \{\sigma\}.$$

This concludes the proof. For a more detailed explanation of the construction of ω'_1, we refer to [11, Proof of Theorem 3.2]. □

Proof of Theorem 7.1.9. The proof follows the same steps as the previous one; the main ingredients are Propositions 7.4.9 and 7.4.10. We omit the details of the proof to avoid unnecessary repetitions of the technical details. □

7.5 Appendix

7.5.1 Alternative form of the Hamiltonian

Recall the definition (7.1) of the Hamiltonian function $H : \mathcal{X} \to \mathbb{R}$, which is

$$H(\sigma) = -\sum_{i \in S} J_{ii} \sum_{\{v,w\} \in E} \mathbb{1}_{\{\sigma(v)=\sigma(w)=i\}} + \sum_{i,j \in S:\, i<j} J_{ij} \sum_{\{v,w\} \in E} \mathbb{1}_{\{\{\sigma(v),\sigma(w)\}=\{i,j\}\}}. \tag{7.40}$$

Recall the definitions (7.18), (7.16). Since the total number of edges is $2KL$, it is clear that

$$\sum_{i \in S} \mathfrak{n}_{ii}(\sigma) + \sum_{i<j} \mathfrak{n}_{ij}(\sigma) = 2KL.$$

Then, we may rewrite (7.40) as

$$\begin{aligned} H(\sigma) &= -\sum_{i\in S} J_{ii}\mathfrak{n}_{ii}(\sigma) + \sum_{i<j} J_{ij}\mathfrak{n}_{ij}(\sigma) \\ &= -2KLJ_{22} - \sum_{i\in S}(J_{ii}-J_{22})\mathfrak{n}_{ii}(\sigma) + \sum_{i<j}(J_{ij}+J_{22})\mathfrak{n}_{ij}(\sigma). \end{aligned}$$

Note that by (7.2), $J_{22} = J_{33}$. By (7.3) and since $H(\mathbf{2}) = -2KLJ_{22}$, we deduce that

$$H(\sigma) = H(\mathbf{2}) - \gamma_1\mathfrak{n}_{11}(\sigma) + \sum_{i<j}\gamma_{ij}\mathfrak{n}_{ij}(\sigma). \tag{7.41}$$

For a final remark, fix a configuration $\sigma \in \mathcal{X}$ and a spin $i \in S$. Consider the number of ij-edges in σ for all $j \in S$. If we count according to the fixed spin i, since each spin has exactly four neighboring spins, this is simply four times $\mathfrak{N}_i(\sigma)$. Alternatively, using the definition (7.18), this equals $2\mathfrak{n}_{ii}(\sigma) + \sum_{j\neq i}\mathfrak{n}_{ij}(\sigma)$ where the factor 2 appears in front of $\mathfrak{n}_{ii}(\sigma)$ since each ii-edge must be counted twice. Therefore, we conclude that

$$4\mathfrak{N}_i(\sigma) = 2\mathfrak{n}_{ii}(\sigma) + \sum_{j:\, j\neq i}\mathfrak{n}_{ij}(\sigma) \quad \text{for all } \sigma \in \mathcal{X} \text{ and } i \in S. \tag{7.42}$$

7.5.2 Auxiliary function

In this subsection, we provide an estimate on an auxiliary function which is used in Assumption 7.0.1. For every real number $h > 0$, we define a function $f_h : (0,\infty) \to \mathbb{R}$ by

$$f_h(x) := 4\Big(x+\frac{h}{2}\Big)\Big\lceil\frac{x+\frac{h}{2}}{h}\Big\rceil - 2h\Big(\Big\lceil\frac{x+\frac{h}{2}}{h}\Big\rceil^2 - \Big\lceil\frac{x+\frac{h}{2}}{h}\Big\rceil + 1\Big). \tag{7.43}$$

Here, $\lceil\alpha\rceil$ is the least integer not smaller than α.

Lemma 7.5.1. *The following statements hold for $h > 0$.*

(1) The function f_h is continuous, piece-wise linear and strictly increasing

on $(0, \infty)$.

(2) *We have* $f_h(\frac{h}{2}) = 2h$ *and* $\lim_{x \to \infty} f_h(x) = \infty$.

(3) *For all* $x \in (0, \infty)$,

$$0 \leq f_h(x) - \Big(\frac{2x^2}{h} + 4x - \frac{h}{2}\Big) \leq \frac{h}{2}.$$

The left (resp. right) equality holds if and only if $(x + \frac{h}{2})/h \in \mathbb{N}$ *(resp.* $x/h \in \mathbb{N}$*).*

Proof. For each integer $m \geq 0$, if $x \in ((m - \frac{1}{2})h, (m + \frac{1}{2})h]$ then $\lceil \frac{x + \frac{h}{2}}{h} \rceil = m + 1$ and thus

$$f_h(x) = 4(m+1)\Big(x + \frac{h}{2}\Big) - 2h(m^2 + m + 1) = 4(m+1)x - 2hm^2.$$

In turn, we have for each $m \geq 1$ that

$$\lim_{x \to (m - \frac{1}{2})h+} f_h(x) = 4(m+1)\Big(m - \frac{1}{2}\Big)h - 2hm^2 = f_h\Big(\Big(m - \frac{1}{2}\Big)h\Big).$$

These formulas verify both (1) and (2) of the lemma. Finally, to prove (3) notice that if $x \in ((m - \frac{1}{2})h, (m + \frac{1}{2})h]$, we have

$$f_h(x) - \Big(\frac{2x^2}{h} + 4x - \frac{h}{2}\Big) = -\frac{2}{h}(x - mh)^2 + \frac{h}{2}.$$

This concludes the proof of (3). □

7.5.3 Heuristics behind Assumption 7.0.1

Here, we provide a brief explanation which justifies each condition given in Assumption 7.0.1. We introduce a notation for convenience. For spins $i, j \in S$,

$$\mathcal{X}^{ij} := \big\{\eta \in \mathcal{X} : \ \eta(v) \in \{i, j\} \text{ for all } v \in V\big\}. \tag{7.44}$$

In other words, $\mathcal{X}^{ij}$ is the collection of configurations in which all spins are either i or j.

A. First, we focus on the (potentially metastable) transition from **2** to **1**. If $\sigma(v) \in \{1, 2\}$ for all $v \in V$, formula (7.41) can be rewritten as

$$H(\sigma) = H(\mathbf{2}) - \gamma_1 \mathfrak{n}_{11}(\sigma) + \gamma_{12} \mathfrak{n}_{12}(\sigma).$$

By (7.42) and since $\mathfrak{n}_{13}(\sigma) = 0$, we have $2\mathfrak{n}_{11}(\sigma) + \mathfrak{n}_{12}(\sigma) = 4\mathfrak{N}_1(\sigma)$. Thus,

$$H(\sigma) = H(\mathbf{2}) + \Big(\frac{1}{2}\gamma_1 + \gamma_{12}\Big)\mathfrak{n}_{12}(\sigma) - 2\gamma_1 \mathfrak{N}_1(\sigma).$$

The right-hand side is, modulo translation by a real number, equivalent to the Hamiltonian of the original Ising model (where spin 1 corresponds to +1 and spin 2 corresponds to −1), with interaction constant $J := \frac{1}{2}\gamma_1 + \gamma_{12}$ and external field $h := 2\gamma_1$. To avoid technical difficulties it is standard to assume that $\frac{2J}{h}$ is not an integer (e.g., [71, standard case]). In our context, this is equivalent to

$$\frac{2\gamma_{12} + \gamma_1}{2\gamma_1} \text{ is not an integer,}$$

which is exactly condition **A**.

B. In the original Ising metastable transition, the energy barrier is known to be $4J\lceil\frac{2J}{h}\rceil - h(\lceil\frac{2J}{h}\rceil^2 - \lceil\frac{2J}{h}\rceil + 1)$ (cf. [71]). In our context, this becomes

$$(4\gamma_{12}+2\gamma_1)\left\lceil\frac{2\gamma_{12}+\gamma_1}{2\gamma_1}\right\rceil-2\gamma_1\left(\left\lceil\frac{2\gamma_{12}+\gamma_1}{2\gamma_1}\right\rceil^2-\left\lceil\frac{2\gamma_{12}+\gamma_1}{2\gamma_1}\right\rceil+1\right)=f_{\gamma_1}(\gamma_{12}). \tag{7.45}$$

The last equality follows from the definition (7.43).

Next, we consider the (potentially metastable) transition from **2** to **3**. If $\sigma(v) \in \{2, 3\}$ for all $v \in V$, the representation (7.41) becomes

$$H(\sigma) = H(\mathbf{2}) + \gamma_{23}\mathfrak{n}_{23}(\sigma).$$

The right-hand side is, modulo translation by a real number, equivalent to the Hamiltonian of the original Ising model with interaction constant $J := \gamma_{23}$ and zero external field. The energy barrier in this setting is known to be $2J(K + 1)$ (cf. [69]). In our context, this equals

$$2(K + 1)\gamma_{23}. \tag{7.46}$$

Gathering (7.45) and (7.46), to have the same energy barrier between $\mathbf{2} \to \mathbf{1}$ and $\mathbf{2} \to \mathbf{3}$, we obtain the condition

$$f_{\gamma_1}(\gamma_{12}) = 2(K + 1)\gamma_{23},$$

which is condition **B**.

C. First, the size of the protocritical droplet $\lceil\frac{2\gamma_{12}+\gamma_1}{2\gamma_1}\rceil$ (cf. (7.45)) is assumed to be large enough:

$$\frac{\gamma_{12}}{\gamma_1} \text{ is sufficiently large.} \tag{7.47}$$

Next, we start from condition **B**. By Lemma 7.5.1-(c), we obtain that

$$2(K+1)\gamma_{23} = f_{\gamma_1}(\gamma_{12}) \le \frac{2\gamma_{12}^2}{\gamma_1} + 4\gamma_{12} < \frac{2(\gamma_{12}+\gamma_1)^2}{\gamma_1}.$$

The above display implies

$$\frac{(K+1)\gamma_1}{\gamma_{12}+\gamma_1} < \frac{\gamma_{12}+\gamma_1}{\gamma_{23}}.$$

The lattice size is large enough compared to the fixed coefficients, and thus $\frac{(K+1)\gamma_1}{\gamma_{12}+\gamma_1}$ can be assumed sufficiently large. This also implies that

$$\frac{\gamma_{12}+\gamma_1}{\gamma_{23}} \text{ is sufficiently large.} \tag{7.48}$$

Conditions (7.47) and (7.48) imply the desired condition **C**.

7.5.4 Reference paths

Reference paths in our new model are defined in the same manner as in the original Ising model. Since the reference paths for Ising/Potts models with both non-zero [12, Definition 5.1] or zero [69, Proposition 2.4] external fields are very well known, we will give our definitions in a concise manner.

Definition 7.5.2 (Reference path between $\boldsymbol{m} \in \{\mathbf{2}, \mathbf{3}\}$ and $\mathbf{1}$)**.** Recall from (7.15) that

$$\mathcal{W}(\boldsymbol{m}, \mathbf{1}) = B^1_{\ell^\star-1,\ell^\star}(m,1) \cup \hat{B}^1_{\ell^\star,\ell^\star-1}(m,1).$$

For any $\eta \in \mathcal{W}(\boldsymbol{m}, \mathbf{1})$, we construct a reference path $\omega : \boldsymbol{m} \to \mathbf{1}$ satisfying $\operatorname{argmax}_\omega H = \{\eta\}$ as follows. Denote by R_η the rectangle of side lengths $\ell^\star$ and $\ell^\star - 1$ contained in the 1-cluster of η. Starting from $\omega_0 = \boldsymbol{m}$, we consecutively update spins m in R_η to spins 1 to form $\omega_{\ell^\star(\ell^\star-1)} = \eta_0$, where

$$\eta_0(v) = \begin{cases} 1, & \text{if } v \in R_\eta, \\ m, & \text{if } v \notin R_\eta. \end{cases}$$

Next, from η_0 we create the corresponding protuberance to obtain $\omega_{\ell^\star(\ell^\star-1)+1} = \eta$. Then, we resume to enlarge the 1-cluster in the usual consecutive manner to obtain $\omega_{KL} = \mathbf{1}$. By the isomorphism argument given in Section 7.5.3-**A**, it is standard to observe that the height of ω is obtained uniquely at $\omega_{\ell^\star(\ell^\star-1)+1} = \eta$, and that the corresponding height is

$$H(\eta) = H(\mathbf{2}) + 4\ell^\star\Big(\gamma_{12} + \frac{\gamma_1}{2}\Big) - 2\gamma_1(\ell^{\star 2} - \ell^\star + 1) = H(\mathbf{2}) + \Gamma^\star.$$

Definition 7.5.3 (Reference path between **2** and **3**)**.** First, we choose an arbitrary column c. Starting from **2**, we update spins 2 in c to 3 in a consecutive manner. Then, we choose one of its neighboring column and repeat the process. Iterating this procedure, we obtain **3**. Similarly, by the isomorphism argument given in Section 7.5.3-**B**, we observe that the height of this path is obtained multiple times and that the height is

$$H(\mathbf{2}) + (2K+2)\gamma_{23} = H(\mathbf{2}) + \Gamma^\star.$$

For the reference path, we are able to select any order of columns, as long as the consecutive ones are neighboring, and also we may select any order of updates in each column, as long as the updates are consecutive. Thus, one can see that there are a huge number of possible reference paths from **2** to **3**.

Consider any selection $\mathscr{A}$ from the collection

$$\big\{\mathscr{W}_j^h(\mathbf{2},\mathbf{3})\big\}_{j,h} \cup \big\{\mathscr{Q}(\mathbf{2},\mathbf{3}), \mathscr{P}(\mathbf{2},\mathbf{3}), \mathscr{P}(\mathbf{3},\mathbf{2}), \mathscr{Q}(\mathbf{3},\mathbf{2})\big\} \cup \big\{\mathscr{H}_i(\mathbf{2},\mathbf{3})\big\}_i \cup \big\{\mathscr{H}_i(\mathbf{3},\mathbf{2})\big\}_i,$$

as in Theorem 7.1.8. By the diagram illustrated in Figure 7.2 and by the freedom to choose an arbitrary order of spin updates, it is clear that for any $\sigma \in \mathscr{A}$ we can construct a reference path $\mathbf{2} \to \mathbf{3}$ so that it visits $\mathscr{A}$ only at σ.

Finally, we remark that in the case $K = L$, we may also choose an arbitrary row and proceed as described above, which also gives the height $(2L+2)\gamma_{23} = (2K+2)\gamma_{23} = \Gamma^\star$. Thus in this case, there are exactly two times more reference paths compared to the case $K < L$. This fact is not taken into account in the qualitative analysis of metastability via pathwise approach done in this paper; however, this will be crucial in the *quantitative* analysis, when one intends to investigate the exact prefactor of the mean metastable transition time [12, 22]. This serves as a fruitful future research topic.

Part II

Inclusion process

Chapter 8

Reversible inclusion process

An interacting particle system was introduced in [35, 36] as a dual process of a certain class of energy diffusion models, known as Brownian momentum (energy) processes. In [37], this process was first named as the *(symmetric) inclusion process*, which was treated as a bosonic[1] counterpart of the well-known exclusion process. Since then, this particular random system has gathered the interest of numerous researchers. A general overview on the study of inclusion processes is provided in [25, Chapters 2 and 6].

Inclusion process

We fix a finite state space S which represents our collection of sites. Suppose that $r : S \times S \to [0, \infty)$ is a transition rate function which defines a continuous-time irreducible random walk on S. For convenience, we let $r(x, x) = 0$ for all $x \in S$.

Assumption 8.0.1. *In Chapters 8 and 9, we assume that the random walk is* reversible *with respect to a probability distribution m, namely,*

$$m(x)r(x, y) = m(y)r(y, x) \quad \textit{for all } x, y \in S.$$

[1]Bosonic particle systems represent dynamics in which particles tend to attract each other. They are mostly used to represent dynamical systems in low temperatures.

On the other hand, in Chapter 10, this reversibility assumption will be dropped and we will handle the general non-reversible situation.

In case where the underlying random walk is reversible, the sites with maximal measure deserve particular attention, as they are precisely the sites where particles condensate (cf. Proposition 8.0.5). We define

$$M_\star = \max\{m(x) : x \in S\}, \quad S_\star = \{x \in S : m(x) = M_\star\}, \quad \text{and} \quad m_\star(\cdot) = \frac{m(\cdot)}{M_\star}. \tag{8.1}$$

Notably, $m_\star(x) \le 1$ for all $x \in S$, and the equality holds if and only if $x \in S_\star$.

Based on the underlying random walk introduced above, we introduce the inclusion process on S. First, the set of configurations corresponding to the distribution of N particles on S is denoted by

$$\mathcal{H}_N = \Big\{\eta \in \mathbb{N}^S : \sum_{x \in S} \eta_x = N\Big\}.$$

Hence, η_x is regarded as the number of particles at $x \in S$ of η.

Now, we define the *inclusion process* to be a continuous-time Markov chain $\{\eta_N(t)\}_{t \ge 0}$ on $\mathcal{H}_N$ associated with generator $\mathcal{L}_N$ acting on functions $f : \mathcal{H}_N \to \mathbb{R}$ by

$$(\mathcal{L}_N f)(\eta) = \sum_{x,\, y \in S} \eta_x (d_N + \eta_y) r(x,\, y) \{f(\sigma^{x,\, y}\eta) - f(\eta)\} \quad \text{for } \eta \in \mathcal{H}_N. \tag{8.2}$$

Here, $\sigma^{x,\, y}\eta$ is the configuration obtained from η by sending a particle, if possible, from x to y. Hence, if $\eta_x = 0$, then $\sigma^{x,\, y}\eta = \eta$ and if $\eta_x \ge 1$, then $(\sigma^{x,\, y}\eta)_x = \eta_x - 1$, $(\sigma^{x,\, y}\eta)_y = \eta_y + 1$, and $(\sigma^{x,\, y}\eta)_z = \eta_z$ for $z \ne x,\, y$. Moreover, $\{d_N\}_{N \ge 1}$ is a sequence of positive real numbers converging to 0. We will further assume that d_N decays more quickly than the logarithmic scale;

$$\lim_{N \to \infty} d_N \log N = 0. \tag{8.3}$$

A typical choice for d_N in practice is the polynomial scale, $d_N = 1/N^\alpha$, $\alpha > 0$. One can readily verify that $\eta_N(\cdot)$ is irreducible. We denote the transition rate of this process by $r_N : \mathcal{H}_N \times \mathcal{H}_N \to [0, \infty)$.

We briefly explain the dynamical characteristics of the inclusion process. Given a configuration $\eta \in \mathcal{H}_N$, a particle moves from site x to site y at rate

$$r_N(\eta, \sigma^{x,y}\eta) = \eta_x(d_N + \eta_y)r(x, y) = d_N\eta_x r(x, y) + \eta_x\eta_y r(x, y).$$

Here, $d_N\eta_x r(x, y)$ denotes the *diffusive* part and $\eta_x\eta_y r(x, y)$ denotes the *inclusive* part of the dynamics. More specifically, the diffusive part represents the random walk of each particle with respect to $r(\cdot, \cdot)$, which is controlled by a parameter d_N. In contrast, the inclusive part represents the attractive behavior of particles, because the rate from x to y increases as η_y increases, and particles tend to prefer more occupied sites. As d_N decays to 0, the inclusive behavior is expected to dominate the dynamics. Consequently, particles are very likely to assemble at a single site, forming a *condensate* (cf. Proposition 8.0.5). However, the small diffusive interactions trigger a long-term evolution of this condensate among sites, which is referred to as *tunneling* or *metastable* behavior (cf. Theorem 8.0.7). Precise interpretation of these concepts is provided in the following.

Condensation of reversible inclusion process

Because the process $\eta_N(\cdot)$ is irreducible, it exhibits a unique invariant distribution. We denote the unique distribution by μ_N. The great advantage we gain by assuming reversibility of the underlying random walk is that $\eta_N(\cdot)$ likewise becomes reversible with respect to μ_N, and that μ_N admits an explicit formula. This is stated in the following proposition, whose proof is straightforward. Hereafter, $\Gamma(\cdot)$ denotes the typical Gamma function.

Proposition 8.0.2. *The inclusion process $\{\eta_N(t)\}_{t\geq 0}$ is reversible with re-*

spect to the invariant distribution μ_N, which satisfies

$$\mu_N(\eta) = \frac{1}{Z_N} \prod_{x \in S} w_N(\eta_x) m_\star(x)^{\eta_x} \quad \text{for } \eta \in \mathcal{H}_N, \tag{8.4}$$

where

$$w_N(n) = \frac{\Gamma(d_N + n)}{n!\Gamma(d_N)} \text{ for } n \in \mathbb{N}, \quad \text{and} \quad Z_N = \sum_{\eta \in \mathcal{H}_N} \prod_{x \in S} w_N(\eta_x) m_\star(x)^{\eta_x}.$$

Remark 8.0.3. The following asymptotics hold for the functions introduced in Proposition 8.0.2:

$$\begin{aligned} &1 \le \frac{(d_N + k) w_N(k)}{d_N} = \frac{(k+1) w_N(k+1)}{d_N} \le e^{d_N \log N} \quad \text{for } k \in [\![0,\, N-1]\!], \\ &\lim_{N \to \infty} \frac{N Z_N}{d_N} = |S_\star|. \end{aligned} \tag{8.5}$$

In particular, $(d_N + k) w_N(k) = (k+1) w_N(k+1) \simeq 1$ by (8.3), which is uniform in $k \in [\![0,\, N-1]\!]$. These convergence results are frequently applied in the following. The proofs are provided in [15, Lemma 3.1 and Proposition 3.2].

Next, we define the metastable valleys of the process.

Definition 8.0.4 (Metastable configurations)**.** For each $x \in S$, define

$$\mathcal{E}_N^x := \{\xi_N^x\} := \{\eta \in \mathcal{H}_N : \eta_x = N\}.$$

Hence, ξ_N^x represents the configuration where all particles are concentrated on the site x. Each $\mathcal{E}_N^x$ is referred to as a *valley* of the system. Moreover, we denote by$\mathcal{E}_N(A) = \bigcup_{x \in A} \mathcal{E}_N^x$ for $A \subseteq S$.

Valleys of further special interest are $\mathcal{E}_N^x$ for $x \in S_\star$, as explained by the following proposition. The proof of this is provided in [15, Proposition 2.1].

Proposition 8.0.5. *For each $x \in S_\star$, it holds that*

$$\lim_{N\to\infty} \mu_N(\mathcal{E}_N^x) = \frac{1}{|S_\star|}. \tag{8.6}$$

Consequently, we have $\lim_{N\to\infty} \mu_N(\mathcal{H}_N \setminus \mathcal{E}_N(S_\star)) = 0.$

Remark 8.0.6. In particular, $\mathcal{E}_N^x$, $x \in S_\star$, are referred to as *metastable valleys* of the process.

For simplicity, we write $\mathcal{E}_N^\star = \mathcal{E}_N(S_\star)$. Proposition 8.0.5 implies that the *(static) condensation* occurs on $S_\star$, i.e.,

$$\lim_{N\to\infty} \mu_N(\mathcal{E}_N^\star) = 1. \tag{8.7}$$

This fact depends heavily on the explicit formula (8.4). If the underlying random walk is non-reversible, then the right-hand side of (8.4) is not necessarily the invariant distribution of the system. In fact, we do not have a closed formula of the invariant distribution in this case. Thus, even the basic condensation result on valleys is not a simple issue for the non-reversible inclusion process. Nevertheless, condensation on $\mathcal{E}_N(S)$ *can* be demonstrated for the non-reversible system by adding a few minor conditions on d_N and $r(\cdot,\,\cdot)$. For a recent result on this topic, we refer to Theorem 10.2.14.

First time scale of the metastable behavior of reversible dynamics

The first time scale is fully characterized in [15]. Recall the trace process defined in Definition 3.1.3. Here, we trace the original process $\eta_N(\cdot)$ on $\mathcal{E}_N^\star$, where condensation occurs. For simplicity, it is denoted by

$$\eta_N^\star(\cdot) = \eta_N^{\mathcal{E}_N^\star}(\cdot). \tag{8.8}$$

As we are concerned only with the superscripts of the sets $\{\mathcal{E}_N^x : x \in S_\star\}$, we define a projection function $\Psi_{1,N} : \mathcal{E}_N^\star \to S_\star$ as

$$\Psi_{1,N}(\xi_N^x) = x \quad \text{for } x \in S_\star.$$

The symbol 1 in the subscript of $\Psi_{1,N}$ denotes the *first* time scale of metastability. Using this function, we define a process $\{X_N(t)\}_{t\geq 0}$ on $S_\star$ by

$$X_N(t) = \Psi_{1,N}(\eta_N^\star(t)) \quad \text{for } t \geq 0. \tag{8.9}$$

In general, $X_N(\cdot)$ is non-Markovian, as it is merely a process of labeling of the metastable valleys. However, in the current case, $X_N(\cdot)$ is indeed a Markov process, as $\Psi_{1,N}$ is a bijection between $\mathcal{E}_N^\star$ and $S_\star$.

Here, we can formulate the first metastable behavior in terms of the projected trace process $X_N(\cdot)$. Proof of the following theorem is provided in [15, Section 4].

Theorem 8.0.7 (First time scale of reversible inclusion process). *Fix a site $x_0 \in S_\star$ and let $\theta_{N,1} = 1/d_N$.*

(1) The law of the rescaled process $\{X_N(\theta_{N,1}t)\}_{t\geq 0}$ starting from x_0 converges (with respect to the Skorokhod topology) on the path space $D([0,\infty); S_\star)$ to the law of the Markov process $\{X_{\text{first}}(t)\}_{t\geq 0}$ on $S_\star$ starting from x_0, which is defined by the generator

$$(\mathscr{L}_1 f)(x) = \sum_{y\in S_\star} r(x,y)\{f(y) - f(x)\} \quad \textit{for } x \in S_\star \textit{ and } f : S_\star \to \mathbb{R}.$$

(2) The process spends negligible time outside the metastable valleys, i.e., for all $t > 0$,

$$\lim_{N\to\infty} \sup_{\eta\in\mathcal{E}_N^\star} \mathbb{E}_\eta\Big[\int_0^t \mathbb{1}\{\eta_N(\theta_{N,1}s) \notin \mathcal{E}_N^\star\} ds\Big] = 0.$$

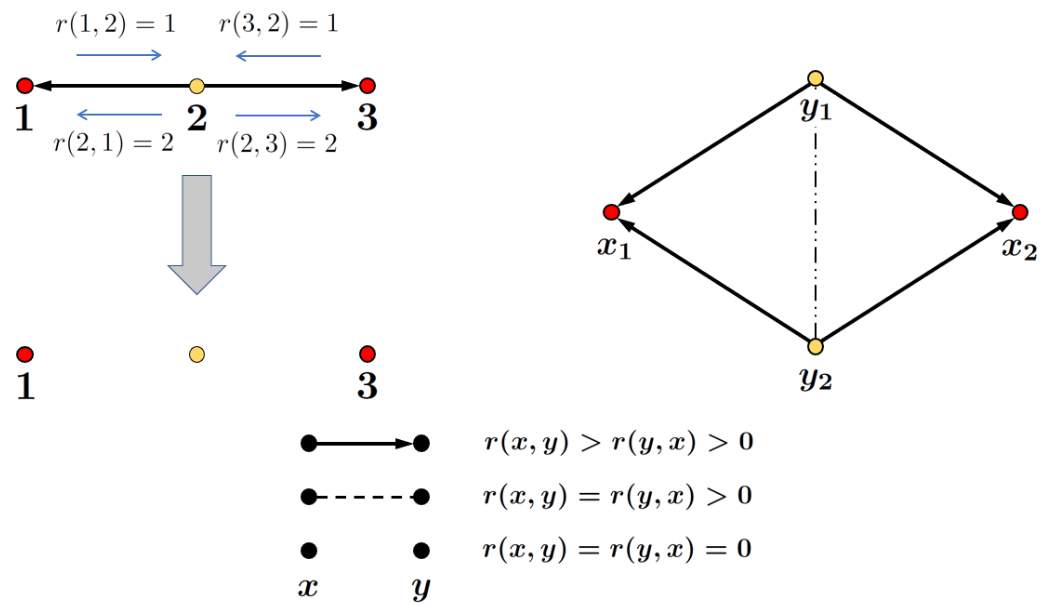


Figure 8.1: (Left) Model where the first time scale of metastability does not occur (Remark 8.0.8). Red points denote the metastable sites and yellow ones denote the rest. (Right) Simple model for the second time scale of metastability (Condition 9.1.1). The line between y_1 and y_2 implies that there is no restriction on $r(y_1, y_2)$ and $r(y_2, y_1)$.

Remark 8.0.8. In Theorem 8.0.7, the limiting dynamics $X_{\text{first}}(\cdot)$ is exactly the underlying random walk restricted to $S_\star$. Here, we must note that even though the underlying system is irreducible, $X_{\text{first}}(\cdot)$ can still not be irreducible. For example, let $S = \{1, 2, 3\}$, $r(1, 2) = r(3, 2) = 1$, and $r(2, 1) = r(2, 3) = 2$, as in the left part of Figure 8.1. Then, we have $S_\star = \{1, 3\}$; thus, $X_{\text{first}}(\cdot)$ on $S_\star$ represents the null Markov chain. This phenomenon suggests additional time scales of the metastable behavior of the reversible inclusion process.

We further remark that the *non-reversible* inclusion process exhibits a completely different scheme of metastability in the first time scale. Namely, the time scale is $1/d_N$ if the limiting Markov chain of the process (cf. $X_{\text{first}}(\cdot)$ in Theorem 8.0.7) is symmetric, and it is $1/(d_N N)$ if the limiting Markov chain is not symmetric. This is a remarkable difference in the metastability of reversible and non-reversible inclusion processes, and the details are provided in Theorems 10.2.9 and 10.2.11.

Since the scaling limit $X_{\mathrm{first}}(t)$ is not necessarily irreducible on $S_\star$, even though the original underlying random walk on the full set S is assumed to be irreducible. This implies that on the first time scale $\theta_{N,1}$, there may exist condensed states that are not transferable from one to another. This encourages us to search for the succeeding bigger time scales relevant to the metastable transitions. This is indeed the topic explained in the next chapter.

Chapter 9

Second time scale of metastability

9.1 Main results

9.1.1 Simple case

In this subsection, we present a simple case of our general main result. Namely, we assume that the following condition holds throughout this subsection.

Condition 9.1.1. $S = \{x_1, x_2, y_1, y_2\}$ *with*

$$r(y_p, x_i) > r(x_i, y_p) > 0 \quad \text{for } i, p \in [\![1, 2]\!], \tag{9.1}$$

$$r(x_1, x_2) = r(x_2, x_1) = 0, \tag{9.2}$$

$$m(x_1) = m(x_2). \tag{9.3}$$

In this setting, because the process is reversible, we have $m_\star(x_1) = m_\star(x_2) = 1$*,* $m_\star(y_1) < 1$*, and* $m_\star(y_2) < 1$*, so that* $S_\star = \{x_1, x_2\}$*. See the right part of Figure 8.1 for a visualization of this simple model.*

There are two reasons for providing a simple version of the theorem first, instead of directly addressing the general main result. The first reason is that this simple model already covers most of the mathematical essentials of the second level of metastable behavior. The second reason is that proposing the proof of the general main result in a straightforward manner would be confusing to the readers, while inspecting the proof of the simple case first is helpful.

We add the term *spl*, which denotes *simple*, in the superscripts of some quantities defined in this subsection to avoid possible confusion with the general main result in the following subsection.

By (9.2), we do not observe any movements in the first time scale by Theorem 8.0.7. Thus, it is natural to seek the following time scale, in which metastable behavior is exhibited between x_1 and x_2. Similar to the first scale, we define a projection function $\Psi^{\mathrm{spl}}_{2,\,N} : \mathcal{E}^{\star}_N \to \{1,\,2\}$ by

$$\Psi^{\mathrm{spl}}_{2,\,N}(\xi^{x_i}_N) = i \quad \text{for } i \in [\![1,\,2]\!].$$

Then, we define a process $Y^{\mathrm{spl}}_N(\cdot)$ on $\{1,\,2\}$ by (cf. (8.8))

$$Y^{\mathrm{spl}}_N(t) = \Psi^{\mathrm{spl}}_{2,\,N}(\eta^{\star}_N(t)) \quad \text{for } t \geq 0. \tag{9.4}$$

Following the notation of [15], we state that d_N *decays subexponentially*, if

$$\lim_{N\to\infty} d_N e^{\epsilon N} = \infty \quad \text{for any } \epsilon > 0. \tag{9.5}$$

Hence, (9.5) indicates that d_N decays more slowly relative to any exponential scales. Moreover, we define a positive constant $\mathfrak{R}$ by

$$\mathfrak{R} = \int_0^1 \frac{1}{\sum_{p=1}^{2} \frac{1}{(1-m_\star(y_p))(\frac{1-t}{r(x_1,\,y_p)} + \frac{t}{r(x_2,\,y_p)})}} dt. \tag{9.6}$$

Theorem 9.1.2 (Second time scale of reversible inclusion process: simple case). *Assume Condition 9.1.1. Suppose that* d_N *decays subexponentially, and that*

$$\lim_{N\to\infty} d_N N^2 (\log N)^2 = 0. \tag{9.7}$$

Define the second time scale as $\theta_{N,2} = N/d_N^2$ *and fix* $i_0 \in \{1, 2\}$*. Then, the law of the rescaled process* $\{Y_N^{\rm spl}(\theta_{N,2}t)\}_{t\ge 0}$ *starting from* i_0 *converges to the law of the Markov process on* $\{1, 2\}$*, starting from* i_0 *and jumping back and forth at rate* $1/\mathfrak{R}$*.*

Remark 9.1.3. Note that Theorem 9.1.2 slightly generalizes [15, Theorem 2.5], and there is a sole additional non-metastable site in the system. However, the approach used in [15, Section 5] fails even in this simplest case, due to two important drawbacks. First, the test function given in [15, Subsection 5.2] does not provide a direct clue of the test function we need for this generalized model, as this step requires a high-level understanding of the whole landscape of the transition rates. This is provided in Section 9.4.2. Second, it is impossible to apply the Cauchy–Schwarz inequality consecutively as in [15, Subsection 5.1]. This is because the inequalities used there do not provide a consistent equality condition; hence, this merely yields a weaker lower bound for the capacities. To overcome this, we employ Theorem 3.2.8-(2) to obtain the lower bound; see Section 9.5 for further detail.

9.1.2 General case

In this subsection, we present the main result of this article in the most general setting. To this end, we decompose $S_\star$ into *irreducible components* with respect to $X_{\rm first}(\cdot)$, which is the limiting dynamics in the first scale (see the left part of Figure 9.1):

$$S_\star = \bigcup_{i=1}^{\kappa_\star} S_i^{(2)}, \quad \text{where} \quad S_i^{(2)} = \{x_{i,1}, \ldots, x_{i,\mathfrak{n}(i)}\} \quad \text{for } 1 \le i \le \kappa_\star. \tag{9.8}$$

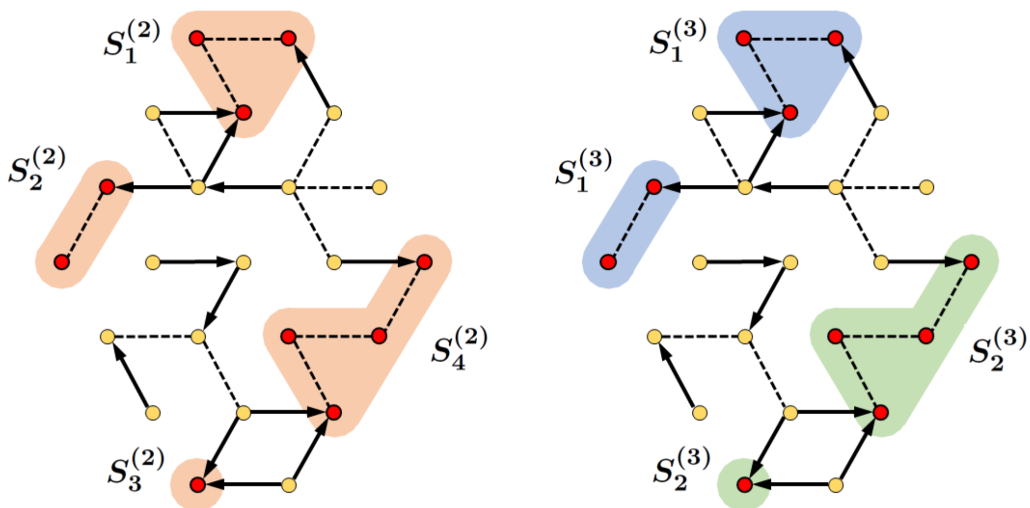


Figure 9.1: (Left) General model with four irreducible components $S_1^{(2)}$, $S_2^{(2)}$, $S_3^{(2)}$, and $S_4^{(2)}$ according to the first time scale (cf. (9.8)). (Right) Same model, in which $\{S_1^{(2)},\, S_2^{(2)}\}$ and $\{S_3^{(2)},\, S_4^{(2)}\}$ form two irreducible components $S_1^{(3)}$ and $S_2^{(3)}$, respectively, according to the second time scale (Theorem 9.1.4).

Here, we use the second label (1 to $\mathfrak{n}(i)$) in the elements of $S_i^{(2)}$ to emphasize that they belong to the same set $S_i^{(2)}$. The common superscript (2) denotes the second time scale. More specifically, the system with transition rates $r(\cdot,\, \cdot)$ restricted to $S_i^{(2)}$ is irreducible for each $i \in [\![1,\, \kappa_\star]\!]$, and $r(x_{i,\,n},\, x_{j,\,m}) = 0$ for all $i \neq j$, $1 \le n \le \mathfrak{n}(i)$, and $1 \le m \le \mathfrak{n}(j)$. By definition, we have

$$|S_\star| = \sum_{i=1}^{\kappa_\star} |S_i^{(2)}| = \sum_{i=1}^{\kappa_\star} \mathfrak{n}(i).$$

In this setting, our dynamics in the second scale $\theta_{N,\,2} = N/d_N^2$ takes place on the set of $\kappa_\star$ elements; $\{\mathcal{E}_N(S_i^{(2)}) : i \in [\![1,\, \kappa_\star]\!]\}$. All elements in $S_i^{(2)}$ that are connected in the first scale $\theta_{N,\,1}$ form a metastable group in the second scale (Theorem 9.1.4-(1)). If $\kappa_\star = 1$, we observe all possible metastable movements in the first time scale; thus, the metastable behavior is fully characterized by Theorem 8.0.7, and there is no need for an additional time scale. Hence, hereafter we assume that $\kappa_\star \ge 2$. Moreover, we write $S \setminus S_\star = \{y_1, \ldots, y_{\kappa_0}\}$, such that we have

$$S = \{x_{i,n} : i \in [\![1, \kappa_\star]\!] \text{ and } n \in [\![1, \mathfrak{n}(i)]\!]\} \cup \{y_1, \ldots, y_{\kappa_0}\}.$$

From $\kappa_\star \ge 2$ and irreducibility of the underlying random walk, it is straightforward that $\kappa_0 \ge 1$. For $A \subseteq [\![1, \kappa_\star]\!]$, we introduce the notation $\mathcal{E}_N^{(2)}(A) = \bigcup_{i\in A} \mathcal{E}_N(S_i^{(2)})$. If $A = \{a\}$, we abbreviate $\mathcal{E}_N^{(2)}(\{a\})$ as $\mathcal{E}_N^{(2)}(a)$.

As in the simple case, we define a projection function. Let $\Psi_{2,N} : \mathcal{E}_N^\star \to [\![1, \kappa_\star]\!]$ be defined by

$$\Psi_{2,N}(\xi_N^{x_{i,n}}) = i \quad \text{for } i \in [\![1, \kappa_\star]\!] \text{ and } n \in [\![1, \mathfrak{n}(i)]\!].$$

Then, we define a process $Y_N(\cdot)$ on $[\![1, \kappa_\star]\!]$ by (cf. (8.8))

$$Y_N(t) = \Psi_{2,N}(\eta_N^\star(t)) \quad \text{for } t \ge 0.$$

In contrast to $X_N(\cdot)$ defined in (8.9) (and $Y_N^{\text{spl}}(\cdot)$ defined in (9.4)), $Y_N(\cdot)$ is not necessarily Markovian, since $\Psi_{2,N}$ is generally not bijective.

We are ready to state our main theorem. We define constants $\mathfrak{R}_{i,j}$ for $i, j \in [\![1, \kappa_\star]\!]$:

$$\mathfrak{R}_{i,j} = \int_0^1 \frac{1}{\sum_{n=1}^{\mathfrak{n}(i)} \sum_{m=1}^{\mathfrak{n}(j)} \sum_{p=1}^{\kappa_0} \frac{1}{(1-m_\star(y_p))(\frac{1-t}{r(x_{i,n},\, y_p)} + \frac{t}{r(x_{j,m},\, y_p)})}} dt. \tag{9.9}$$

In (9.9), we regard the fraction in the denominator as 0 if $r(x_{i,n}, y_p) r(x_{j,m}, y_p) = 0$. In this sense, we write $\mathfrak{R}_{i,j} = \infty$ if $r(x_{i,n}, y_p) r(x_{j,m}, y_p) = 0$ for all $n \in [\![1, \mathfrak{n}(i)]\!]$, $m \in [\![1, \mathfrak{n}(j)]\!]$, and $p \in [\![1, \kappa_0]\!]$[1]. It is clear that $\mathfrak{R}_{i,j} = \mathfrak{R}_{j,i}$.

Theorem 9.1.4 (Second time scale of reversible inclusion process: general

[1] We take $1/\infty$ to be 0 in the following.

case). *Suppose that d_N decays subexponentially, and that*

$$\lim_{N\to\infty} d_N N^2 (\log N)^2 = 0. \tag{9.10}$$

Then, with $\theta_{N,2} = N/d_N^2$, the following statements hold.

(1) For each $i \in [\![1,\, \kappa_\star]\!]$, $\mathcal{E}_N(S_i^{(2)})$ thermalizes before reaching another metastable set, i.e.,

$$\lim_{N\to\infty} \inf_{\eta,\,\zeta\in\mathcal{E}_N(S_i^{(2)})} \mathbb{P}_\eta\big[\tau_{\{\zeta\}} < \tau_{\mathcal{E}_N(S_\star\setminus S_i^{(2)})}\big] = 1. \tag{9.11}$$

(2) Fix $i_0 \in [\![1,\, \kappa_\star]\!]$. Then, the law of the rescaled process $\{Y_N(\theta_{N,2}t)\}_{t\ge 0}$ starting from i_0 converges to the law of the Markov process $X_{\mathrm{second}}(\cdot)$ on $[\![1,\, \kappa_\star]\!]$ starting from i_0 and defined by the generator, acting on functions $f : [\![1,\, \kappa_\star]\!] \to \mathbb{R}$, given by

$$(\mathscr{L}_2 f)(i) = \sum_{j\in[\![1,\,\kappa_\star]\!]\setminus\{i\}} \frac{1}{|S_i^{(2)}|\mathfrak{R}_{i,\,j}} \{f(j) - f(i)\} \quad \text{for } i \in [\![1,\, \kappa_\star]\!]. \tag{9.12}$$

Consequently, $S_\star$ is decomposed into irreducible components with respect to $X_{\mathrm{second}}(\cdot)$. We denote this partition by

$$S_\star = S_1^{(3)} \cup \cdots \cup S_{\gamma_\star}^{(3)}. \tag{9.13}$$

(3) Fix $i \in [\![1,\, \kappa_\star]\!]$ and $n \in [\![1,\, \mathfrak{n}(i)]\!]$. From (9.13), there is a unique $\hat{i} \in [\![1,\, \gamma_\star]\!]$ such that $S_i^{(2)} \subseteq S_{\hat{i}}^{(3)}$ (see the right part of Figure 9.1). Then, starting from $\xi_N^{x_{i,\,n}}$, the process spends negligible time outside $\mathcal{E}_N(S_{\hat{i}}^{(3)})$, which is uniform in all choices of $(i,\, n)$, i.e., for all $t > 0$,

$$\lim_{N\to\infty} \sup_{i\in[\![1,\,\kappa_\star]\!],\, n\in[\![1,\,\mathfrak{n}(i)]\!]} \mathbb{E}_{\xi_N^{x_{i,\,n}}}\Big[\int_0^t \mathbb{1}\big\{\eta_N(\theta_{N,2}s) \notin \mathcal{E}_N(S_{\hat{i}}^{(3)})\big\}ds\Big] = 0.$$

Remark 9.1.5. We remark several issues regarding the main theorem.

(1) Note that Theorem 9.1.2 is indeed a special case of Theorem 9.1.4, where $\kappa_\star = 2$, $\mathfrak{n}(1) = \mathfrak{n}(2) = 1$, $x_{1,1} = x_1$, $x_{2,1} = x_2$, $\kappa_0 = 2$, and $r(x_{1,1}, y_p)r(x_{2,1}, y_p) > 0$ for $p = 1, 2$.

(2) Theorem 9.1.4 proves the conjecture in [15] that $\theta_{N,2} = N/d_N^2$ is indeed the *second* time scale in the metastability of reversible inclusion processes, in the sense that there are no intermediate time scales between $\theta_{N,1}$ and $\theta_{N,2}$.

(3) Remarkably, the condition (9.10) is purely technical, and it is believed that the same results hold without this minor assumption. This condition is applied in Sections 9.4.4 and 9.6.4.

(4) By (9.12), for $i, j \in [\![1, \kappa_\star]\!]$, the limit transition rate from $S_i^{(2)}$ to $S_j^{(2)}$ is $1/(|S_i^{(2)}|\mathfrak{R}_{i,j})$. This vanishes if and only if $\mathfrak{R}_{i,j} = \infty$, which is equivalent to state that the graph distance[2] between $S_i^{(2)}$ and $S_j^{(2)}$ is bigger than 2. In this sense, we cannot observe a metastable movement between $S_i^{(3)}$ and $S_j^{(3)}$, $i, j \in [\![1, \gamma_\star]\!]$, in the second time scale $\theta_{N,2} = N/d_N^2$. Because the original underlying random walk is irreducible, it is natural to suggest the existence of a third time scale, where we can detect metastable movements among $S_i^{(3)}$, $i \in [\![1, \gamma_\star]\!]$. In [15], this scale is strongly expected to be $\theta_{N,3} = N^2/d_N^3$. Moreover, even though $\theta_{N,3}$ is proved to be the longest scale possible in [15], there is a possibility that an intermediate time scale exists between $\theta_{N,2}$ and $\theta_{N,3}$. This can be considered a fruitful future research topic.

(5) According to the previous remark, we attempted to apply the methodology used in this chapter to address the third time scale of metastability

[2] For two subsets A and B of S, the *graph distance* between A and B is defined as $\min\{n \ge 0 : \exists x_0, \dots, x_n \in S$ such that $x_0 \in A$, $x_n \in B$, and $r(x_i, x_{i+1}) > 0$ for $i \in [\![0, n-1]\!]$.

of the inclusion process. The first obstacle is encountered in constructing an exquisite test function which approximates the equilibrium potential, as in Section 9.6.2. This becomes far more complicated when compared to what is done here, as the geometric property of the typical path is highly complex in the third time scale. The other obstacle is that the asymptotic value of the equilibrium potential, which is successfully determined in the second time scale in Sections 9.5.3 and 9.7.3, is unknown in the third time scale. In order to apply a similar methodology in the third scale, a precise information on the equilibrium potential of the entire typical path between metastable valleys is needed. At this point, this is a technically difficult task.

(6) Note that (9.11) is not included in the previous metastability results, i.e., Theorems 8.0.7 and 9.1.2. This is because in the setting of the previous theorems, each metastable valley is a singleton; hence, thermalization is obvious.

(7) Here, all convergence results are provided in terms of convergence of the trace process in the Skorokhod topology. In fact, there are alternatives to the stated results, represented by convergence of the original process in the soft topology [51] and convergence of finite-dimensional marginal distributions [55]. We remark that given our result, the other modes of convergence may be easily proved by verifying some additional technical conditions presented in the aforesaid studies. In Section 9.9, we prove the convergence of finite-dimensional marginal distributions using [55, Proposition 2.1]. This result is needed to prove (3) of Theorem 9.1.4.

9.2 Outline of proof of Theorems 9.1.2 and 9.1.4

In this section, we explain how to prove the main theorems, namely Theorems 9.1.2 and 9.1.4, using the general methodologies summarized in Section 3.2.

Martingale approach and outline of proof

Recall from (8.8) the trace process $\eta_N^\star(t)$, $t \ge 0$ on $\mathcal{E}_N^\star$. We denote by $r_N^\star : \mathcal{E}_N^\star \times \mathcal{E}_N^\star \to [0, \infty)$ the transition rate of the trace process $\eta_N^\star(\cdot)$, and we define the mean transition rate $\boldsymbol{r}_N^\star : [\![1, \kappa_\star]\!] \times [\![1, \kappa_\star]\!] \to [0, \infty)$ by $\boldsymbol{r}_N^\star(i, i) = 0$ and

$$\boldsymbol{r}_N^\star(i, j) = \frac{1}{\mu_N(\mathcal{E}_N(S_i^{(2)}))} \sum_{\eta \in \mathcal{E}_N(S_i^{(2)})} \mu_N(\eta) \sum_{\zeta \in \mathcal{E}_N(S_j^{(2)})} r_N^\star(\eta, \zeta) \quad \text{for } i, j \in [\![1, \kappa_\star]\!].$$

Then, for $i, j \in [\![1, \kappa_\star]\!]$, it holds that (cf. [5, Lemma 6.8] and (3.28))

$$\begin{aligned} \mu_N(\mathcal{E}_N(S_i^{(2)}))\boldsymbol{r}_N^\star(i, j) = \frac{1}{2}\Big[&\mathrm{Cap}_N(\mathcal{E}_N^{(2)}(i), \mathcal{E}_N^\star \setminus \mathcal{E}_N^{(2)}(i)) \\ &+ \mathrm{Cap}_N(\mathcal{E}_N^{(2)}(j), \mathcal{E}_N^\star \setminus \mathcal{E}_N^{(2)}(j)) \\ &- \mathrm{Cap}_N(\mathcal{E}_N^{(2)}(\{i, j\}), \mathcal{E}_N^\star \setminus \mathcal{E}_N^{(2)}(\{i, j\}))\Big]. \end{aligned} \tag{9.14}$$

The asymptotics on $\boldsymbol{r}_N^\star(\cdot, \cdot)$ is the main ingredient to describe the metastable behavior. This is explained in the following proposition, which is a consequence of the martingale approach developed in [5]. We refer to [5, Theorem 2.7] for its proof.

Proposition 9.2.1. *Suppose that there exists a sequence $\{\theta_N\}_{N \ge 1}$ of positive real numbers such that*

$$\lim_{N \to \infty} \theta_N \boldsymbol{r}_N^\star(i, j) = a(i, j) \quad \textit{for all } i, j \in [\![1, \kappa_\star]\!], \tag{9.15}$$

for some $a : [\![1, \kappa_\star]\!] \times [\![1, \kappa_\star]\!] \to [0, \infty)$. Moreover, suppose that the following *estimate holds for each $i \in [\![1,\, \kappa_\star]\!]$:*

$$\lim_{N\to\infty} \frac{\mathrm{Cap}_N(\mathcal{E}_N^{(2)}(i),\, \mathcal{E}_N^\star \setminus \mathcal{E}_N^{(2)}(i))}{\inf_{\eta,\,\zeta\in\mathcal{E}_N^{(2)}(i)} \mathrm{Cap}_N(\eta,\,\zeta)} = 0. \tag{9.16}$$

Then, for each $i \in [\![1,\, \kappa_\star]\!]$, the following statements hold.

(1) $\mathcal{E}_N^{(2)}(i)$ thermalizes before reaching another metastable set, i.e.,

$$\lim_{N\to\infty} \inf_{\eta,\,\zeta\in\mathcal{E}_N^{(2)}(i)} \mathbb{P}_\eta\big[\tau_{\{\zeta\}} < \tau_{\mathcal{E}_N^\star\setminus\mathcal{E}_N^{(2)}(i)}\big] = 1.$$

(2) For each $i \in [\![1,\, \kappa_\star]\!]$, the law of the rescaled process $\{Y_N(\theta_N t)\}_{t\ge 0}$ starting from i converges to the law of the Markov process on $[\![1,\, \kappa_\star]\!]$ starting from i with transition rates $a(\cdot,\, \cdot)$.

To prove statement (3) of Theorem 9.1.4, we also must know the mode of convergence of finite-dimensional distributions of the rescaled process $\eta_N(\theta_{N,2}\cdot)$. [55, Proposition 2.1] provides a simple approach of proving this result.

Proposition 9.2.2. *Suppose that statement (2) of Theorem 9.1.4 holds, and that the process spends negligible time outside the metastable valleys, i.e., for $t > 0$,*

$$\lim_{N\to\infty} \sup_{\eta\in\mathcal{E}_N^\star} \mathbb{E}_\eta\Big[\int_0^t \mathbb{1}\{\eta_N(\theta_{N,2}s) \notin \mathcal{E}_N^\star\}ds\Big] = 0.$$

In addition, suppose that the following holds:

$$\lim_{\delta\to 0} \limsup_{N\to\infty} \sup_{2\delta\le s\le 3\delta} \sup_{\eta\in\mathcal{E}_N^\star} \mathbb{P}_\eta\big[\eta_N(\theta_{N,2}s) \notin \mathcal{E}_N^\star\big] = 0. \tag{9.17}$$

Then, the rescaled original process $\eta_N(\theta_{N,2}\cdot)$ converges to $X_{\mathrm{second}}(\cdot)$ in the sense of finite-dimensional marginal distributions, i.e., for all $0 \le t_1 < \cdots <$

t_k, $i \in [\![1,\, \kappa_\star]\!]$, $n \in [\![1,\, \mathfrak{n}(i)]\!]$, and $A_1,\, \dots,\, A_k \subseteq [\![1,\, \kappa_\star]\!]$, it holds that

$$\begin{aligned}&\lim_{N\to\infty} \mathbb{P}_{\xi_N^{x_i,\,n}} \big[\eta_N(\theta_{N,\,2} t_1) \in \mathcal{E}_N^{(2)}(A_1),\, \dots,\, \eta_N(\theta_{N,\,2} t_k) \in \mathcal{E}_N^{(2)}(A_k)\big] \\ &\quad = \mathbf{P}_i\big[X_{\text{second}}(t_1) \in A_1,\, \dots,\, X_{\text{second}}(t_k) \in A_k\big],\end{aligned}$$

where $\mathbf{P}_i$ denotes the law of $X_{\text{second}}(\cdot)$ starting from i.

The remainder of this chapter is organized as follows. In Section 9.3, we provide some preliminaries regarding hitting times on the tubes. These are used in Sections 9.5 and 9.7. Subsequently, in Sections 9.4 and 9.5, we calculate the upper and lower bounds for the capacities, respectively, in the simple case of Theorem 9.1.2. This procedure is performed by the variational principles given in Theorems 3.2.5 and 3.2.8. In Sections 9.6 and 9.7 we provide the estimate of the capacities in the general case of Theorem 9.1.4. Then, we prove the condition (9.16) in the general case in Section 9.8. Finally, in Section 9.9, we use the estimates given in Propositions 9.2.1 and 9.2.2 to prove our main result, stated in Theorem 9.1.4. This simultaneously proves Theorem 9.1.2 as well.

9.3 Hitting times on tubes

In this section, we provide sharp estimates of hitting times on the tubes. These are used in Sections 9.5 and 9.7 to compute the asymptotic equilibrium potential (Lemmas 9.5.4 and 9.7.3). These are special (reversible) cases of more general (non-reversible) results formulated and proved in Section 10.3.2. Thus, we highlight the essential results, and refer to Section 10.3.2 for detailed proofs.

To state the results, we first define some relevant subsets of $\mathcal{H}_N$.

Definition 9.3.1.

(1) For every subset R of S, define the *R-tube* $\mathcal{A}_N^R$ as

$$\mathcal{A}_N^R = \{\eta \in \mathcal{H}_N : \eta_x = 0 \text{ for all } x \in S \setminus R\}. \tag{9.18}$$

For example, $\mathcal{A}_N^S = \mathcal{H}_N$ and $\mathcal{A}_N^{\{x\}} = \mathcal{E}_N^x$.

(2) Especially, if $R = \{x, y\}$, we write

$$\mathcal{A}_N^{x,\,y} = \mathcal{A}_N^R = \{\eta \in \mathcal{H}_N : \eta_x + \eta_y = N\}.$$

(3) For $x, y \in S$ and $i \in [\![0, N]\!]$, define the configuration $\zeta_i^{x,\,y} = \zeta_{i,\,N}^{x,\,y}$ by

$$(\zeta_i^{x,\,y})_z = \begin{cases} N - i & \text{if } z = x, \\ i & \text{if } z = y, \\ 0 & \text{otherwise,} \end{cases}$$

such that $\mathcal{A}_N^{x,\,y} = \{\zeta_0^{x,\,y}, \zeta_1^{x,\,y}, \ldots, \zeta_N^{x,\,y}\}$. Note that $\zeta_0^{x,\,y} = \xi_N^x$ and $\zeta_N^{x,\,y} = \xi_N^y$.

(4) Finally, for $x, y \in S$, define

$$\widehat{\mathcal{A}}_N^{x,\,y} = \{\eta \in \mathcal{H}_N : \eta_x + \eta_y = N \text{ and } \eta_x, \eta_y \geq 1\}.$$

Clearly, $\widehat{\mathcal{A}}_N^{x,\,y} = \{\zeta_1^{x,\,y}, \ldots, \zeta_{N-1}^{x,\,y}\}$ and $\mathcal{A}_N^{x,\,y} = \widehat{\mathcal{A}}_N^{x,\,y} \cup \{\xi_N^x, \xi_N^y\}$.

The tube $\mathcal{A}_N^R$ with $R = \{x, y\}$ has the advantage that it is an 1D bridge of typical paths between two valleys, ξ_N^x and ξ_N^y. More precisely, the following estimate holds.

Lemma 9.3.2. *Suppose that E is a subset of the path space which depends only on the hitting times of subsets of $\mathcal{H}_N \setminus \widehat{\mathcal{A}}_N^{x,\,y}$. Moreover, suppose that $x, y \in S$ satisfy $r(x, y) + r(y, x) > 0$. Then, there is a fixed constant $C > 0$*

such that

$$\left|\mathbb{P}_{\zeta_i^{x,\,y}}[E]-\frac{r(x,\,y)}{r(x,\,y)+r(y,\,x)}\mathbb{P}_{\zeta_{i+1}^{x,\,y}}[E]-\frac{r(y,\,x)}{r(x,\,y)+r(y,\,x)}\mathbb{P}_{\zeta_{i-1}^{x,\,y}}[E]\right|\le C\frac{d_N N}{i(N-i)}$$

for all $i\in[\![1,\,N-1]\!]$.

Remark 9.3.3. In the above lemma, typical examples of subsets E are the following.

$$\left\{\tau_{\mathcal{E}_N^x}<\tau_{\mathcal{E}_N^y}\right\},\quad \left\{\tau_{\mathcal{E}_N^y}=\tau_{\mathcal{E}_N(A)}\right\}\text{ for }A\subseteq S,\quad\text{and}\quad \left\{\tau_{\mathcal{E}_N^x}=\tau_{\mathcal{H}_N\setminus\widehat{\mathcal{A}}_N^{x,\,y}}\right\}.$$

Lemma 9.3.2 can be iterated to formulate $\mathbb{P}_{\zeta_i^{x,\,y}}[E]$, $i\in[\![1,\,N-1]\!]$ in terms of the boundary values $\mathbb{P}_{\xi_N^x}[E]$ and $\mathbb{P}_{\xi_N^y}[E]$. This imperatively relies on the fact that the system is approximated to be 1D.

We conclude this section with the following lemma, which estimates the equilibrium potential on one-dimensional tubes. *This lemma is the main ingredient to estimate the divergence of the test flow in Lemma 9.5.4.*

Lemma 9.3.4. *Suppose that* A *and* B *are two disjoint subsets of* S*. Further, assume that* $a\in A$*,* $b\in B$*, and* $c\in S$ *satisfy*

$$r(c,\,a)>r(a,\,c)>0\quad\text{and}\quad r(c,\,b)>r(b,\,c)>0.$$

Then, we have

$$\sup_{i\in[\![0,\,\lfloor N/2\rfloor]\!]}\left|h_{\mathcal{E}_N(A),\,\mathcal{E}_N(B)}(\zeta_i^{a,\,c})-1\right|=o(1)\tag{9.19}$$

and

$$\sup_{i\in[\![0,\,\lfloor N/2\rfloor]\!]}h_{\mathcal{E}_N(A),\,\mathcal{E}_N(B)}(\zeta_i^{b,\,c})=o(1).\tag{9.20}$$

Proof. It must be noticed that $\{\tau_{\mathcal{E}_N(A)}<\tau_{\mathcal{E}_N(B)}\}$ is a subset of the path space satisfying the assumption of Lemma 9.3.2; thus, we may apply Lemma 9.3.2 to the equilibrium potential $h_{\mathcal{E}_N(A),\,\mathcal{E}_N(B)}$.

It suffices to prove (9.19) and (9.20) for $i \in [\![1,\, \lfloor N/2 \rfloor]\!]$, as they are trivial for $i = 0$. We abbreviate $h_{\mathcal{E}_N(A),\,\mathcal{E}_N(B)}$ as h. Because $a \in A$ and $b \in B$, we have $h(\xi_N^a) = 1$ and $h(\xi_N^b) = 0$. Next, write $q = r(a,\, c)/r(c,\, a) < 1$ and

$$\alpha_i = h(\zeta_{i-1}^{a,\,c}) - h(\zeta_i^{a,\,c}) \quad \text{for } i \in [\![1,\, N]\!].$$

Then, Lemma 9.3.2 implies

$$\Big|\alpha_{i+1} - \frac{1}{q}\alpha_i\Big| \le C\frac{d_N N}{i(N-i)} \quad \text{for } i \in [\![1,\, N-1]\!]. \tag{9.21}$$

Now, fix $i \in [\![1,\, \lfloor N/2 \rfloor]\!]$. Because $h(\xi_N^a) - h(\xi_N^c) = \alpha_1 + \cdots + \alpha_N$, we may estimate,

$$\begin{aligned} &\Big|h(\xi_N^a) - h(\xi_N^c) - \frac{1-q^N}{q^{N-i}(1-q^i)}(\alpha_1 + \cdots + \alpha_i)\Big| \\ &= \frac{1-q}{q^{N-i}-q^N}\Big|\sum_{j=1}^{i}\sum_{k=i+1}^{N}(q^{N-j}\alpha_k - q^{N-k}\alpha_j)\Big|. \end{aligned} \tag{9.22}$$

Applying (9.21), the last formula is bounded by

$$\frac{1-q}{q^{N-i}-q^N}\sum_{j=1}^{i}\sum_{k=i+1}^{N} q^{N-j}\sum_{\ell=j}^{k-1}\frac{Cd_N N}{q^{\ell-j}\ell(N-\ell)}.$$

By simple double counting, this is bounded from above by

$$\frac{Cd_N N}{q^{N-i}-q^N}\Big(\sum_{\ell=1}^{i-1}\frac{q^{N-\ell}}{N-\ell} + \sum_{\ell=i}^{N-i}\frac{iq^{N-\ell}}{\ell(N-\ell)} + \sum_{\ell=N-i+1}^{N-1}\frac{q^{N-\ell}}{\ell}\Big). \tag{9.23}$$

From $\alpha_1 + \cdots + \alpha_i = h(\xi_N^a) - h(\zeta_i^{a,\,c})$, by (9.22) and (9.23), we have

$$\begin{aligned} &\Big|h(\zeta_i^{a,\,c}) - \frac{1-q^{N-i}}{1-q^N}h(\xi_N^a) - \frac{q^{N-i}-q^N}{1-q^N}h(\xi_N^c)\Big| \\ &\le 2Cd_N N\Big(\frac{q^{N-i+1}(1-q)^{-1}}{N-i+1} + \frac{2q^i(1-q)^{-1}}{N} + \frac{(1-q)^{-1}}{N-i+1}\Big) \le 16C(1-q)^{-1}d_N. \end{aligned}$$

Because $h(\xi_N^a) = 1$ and $0 \le h(\xi_N^c) \le 1$, (9.19) follows. Moreover, by a similar computation, we deduce that

$$\left| h(\zeta_i^{b,\,c}) - \frac{1-\widetilde{q}^{N-i}}{1-\widetilde{q}^N} h(\xi_N^b) - \frac{\widetilde{q}^{N-i}-\widetilde{q}^N}{1-\widetilde{q}^N} h(\xi_N^c) \right| \le 16C(1-\widetilde{q})^{-1} d_N,$$

where $\widetilde{q} = r(b,\,c)/r(c,\,b) < 1$. Because $h(\xi_N^b) = 0$ and $0 \le h(\xi_N^c) \le 1$, we have (9.20). □

9.4 Upper bound for capacities: simple case

In this section, we assume Condition 9.1.1 and establish the upper bound for $\mathrm{Cap}_N(\mathcal{E}_N^{x_1},\,\mathcal{E}_N^{x_2})$. As previously mentioned, this and the succeeding subsections have most of the mathematical essentials for proving the general main result. Notions from Section 9.1.1 are frequently employed.

Proposition 9.4.1 (Upper bound for capacities: simple case)**.** *Under the conditions of Theorem 9.1.2, the following inequality holds.*

$$\limsup_{N\to\infty} \frac{N}{d_N^2} \mathrm{Cap}_N(\mathcal{E}_N^{x_1},\,\mathcal{E}_N^{x_2}) \le \frac{1}{2\mathfrak{R}}.$$

9.4.1 Preliminary notions

Let $m_\star = \max_{p=1}^{2} m_\star(y_p) < 1$ and recall the notation (9.18). For all N, we define the following discretized version of the constant $\mathfrak{R}$ given in (9.6):

$$\mathfrak{R}^N = \sum_{t=1}^{N} \frac{1}{\sum_{p=1}^{2} \frac{1}{(1-m_\star(y_p))(\frac{N-t}{r(x_1,\,y_p)} + \frac{t-1}{r(x_2,\,y_p)})}}.$$

Clearly, we have $N^{-2}\mathfrak{R}^N \to \mathfrak{R}$ as N tends to infinity.

The constant $\mathfrak{R}^N$ has the shape of an inverse effective conductance of an electrical network consisted of conductors. In this sense, $\mathfrak{R}^N$ can be regarded as the inverse conductance of N serially connected conductors ($t \in [\![1,\,N]\!]$).

Moreover, each conductor can be decomposed into two parallelly connected conductors ($p \in \{1, 2\}$), and each of them corresponds to the motion of a particle from site x_1 to site x_2, passing through y_p, for $p = 1, 2$. In each individual conductance $(1-m_\star(y_p))^{-1}((N-t)/r(x_1, y_p)+(t-1)/r(x_2, y_p))^{-1}$, the former term corresponds to the sum of geometric series of ratio $m_\star(y_p)$, and the latter term corresponds to the serial connection of particle motions $x_1 \leftrightarrow y_p$ and $x_2 \leftrightarrow y_p$ with conductances $r(x_1, y_p)/(N-t)$ and $r(x_2, y_p)/(t-1)$, respectively. These heuristic explanations are rigorously formulated in the proof of Lemma 9.4.2.

Moreover, we define

$$\mathcal{U}_N = \bigcup_{p=1}^{2} \mathcal{A}_N^{\{x_1, y_p, x_2\}} \quad \text{and} \quad \mathcal{V}_N = \mathcal{H}_N \setminus \mathcal{U}_N. \tag{9.24}$$

9.4.2 Construction of test function f_{test}

In this subsection, we define a test function $f = f_{\text{test}}$ on $\mathcal{H}_N$, which approximates the equilibrium potential $h_{\mathcal{E}_N^{x_1}, \mathcal{E}_N^{x_2}}$. To this end, f is constructed in four steps. See Figure 9.2 for a graphical explanation of this process.

- First, we define f on $\mathcal{E}_N(S)$:

$$f(\xi_N^{x_1}) = 1 \quad \text{and} \quad f(\xi_N^{x_2}) = f(\xi_N^{y_1}) = f(\xi_N^{y_2}) = 0, \tag{9.25}$$

  so that $f \in \mathfrak{C}_{1,0}(\mathcal{E}_N^{x_1}, \mathcal{E}_N^{x_2})$ (cf. (3.33)).

- Second, we define f on $\mathcal{A}_N^{\{x_i, y_p\}}$ for $i \in \{1, 2\}$ and $p \in \{1, 2\}$ by

$$f(\eta) = f(\xi_N^{x_i}) \quad \text{if } \eta_{x_i} \in [\![1, N-1]\!]. \tag{9.26}$$

- Next, we define f on $\mathcal{U}_N$, i.e., on $\mathcal{A}_N^{\{x_1, y_p, x_2\}}$ for $p \in \{1, 2\}$. The main contribution to the Dirichlet form occurs in this part. If $\eta \in \mathcal{A}_N^{\{x_1, y_p, x_2\}}$

with $\eta_{x_1} \geq 1$ and $\eta_{x_2} \geq 1$, then

$$f(\eta) = \frac{K_p^{\eta_{x_1},\, \eta_{y_p}}}{\mathfrak{R}^N}, \tag{9.27}$$

where for $k \geq 0$ and $\ell \geq 0$,

$$\begin{aligned} K_p^{k,\,\ell} =& \sum_{t=1}^{k} \frac{\frac{N-t}{r(x_1,\, y_p)} \Big/ \big(\frac{N-t}{r(x_1,\, y_p)} + \frac{t-1}{r(x_2,\, y_p)}\big)}{\sum_{q=1}^{2} \frac{1}{(1-m_\star(y_q))(\frac{N-t}{r(x_1,\, y_q)} + \frac{t-1}{r(x_2,\, y_q)})}} \\ &+ \sum_{t=1}^{k+\ell} \frac{\frac{t-1}{r(x_2,\, y_p)} \Big/ \big(\frac{N-t}{r(x_1,\, y_p)} + \frac{t-1}{r(x_2,\, y_p)}\big)}{\sum_{q=1}^{2} \frac{1}{(1-m_\star(y_q))(\frac{N-t}{r(x_1,\, y_q)} + \frac{t-1}{r(x_2,\, y_q)})}}. \end{aligned}$$

By substituting $\eta_{y_p} = 0$, one can verify that (9.27) is well defined on $\mathcal{A}_N^{\{x_1,\, x_2\}}$.

- Finally, we define f on $\mathcal{V}_N$. Taking $\eta \in \mathcal{V}_N$,

$$f(\eta) = \begin{cases} 1 & \text{if } \eta_{x_1} > \lfloor N/2 \rfloor, \\ 0 & \text{if } \eta_{x_1} \leq \lfloor N/2 \rfloor. \end{cases} \tag{9.28}$$

- By the above construction, $0 \leq f(\eta) \leq 1$ for all $\eta \in \mathcal{H}_N$.

Here, we divide the Dirichlet form into four parts:

$$\begin{aligned} D_N(f) &= \sum_{\{\eta,\, \zeta\} \subseteq \mathcal{H}_N} \mu_N(\eta) r_N(\eta,\, \zeta) \{f(\zeta) - f(\eta)\}^2 \\ &= \Sigma_1(f) + \Sigma_2(f) + \Sigma_3(f) + \Sigma_4(f). \end{aligned}$$

The four summations are defined as follows, according to where the movement $\eta \leftrightarrow \zeta$ occurs.

- The first part $\Sigma_1(f)$ consists of movements inside $\mathcal{A}_N^{\{x_1,\, y_p,\, x_2\}}$ for $p \in \{1,\, 2\}$.

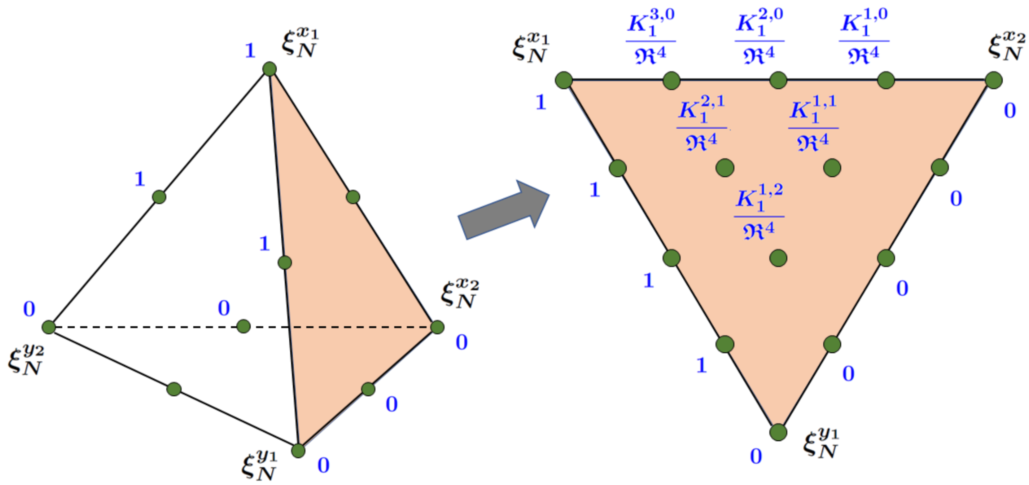


Figure 9.2: (Left) Distribution of the test function in a model satisfying Condition 9.1.1 with $N = 4$. (Right) More detailed landscape of the test function on the tube $\mathcal{A}_N^{\{x_1, y_1, x_2\}}$.

- The second part $\Sigma_2(f)$ consists of movements between the set differences of $\mathcal{A}_N^{\{x_1, y_1, x_2\}}$ and $\mathcal{A}_N^{\{x_1, y_2, x_2\}}$.
- The third part $\Sigma_3(f)$ consists of movements between $\mathcal{U}_N$ and $\mathcal{V}_N$.
- The last part $\Sigma_4(f)$ consists of movements inside $\mathcal{V}_N$.

From (9.24), the above four members are disjoint, and they characterize $D_N(f)$ completely. As shown below, $\Sigma_1(f)$ is the main contribution to $D_N(f)$, whereas the other summations vanish (compared to $\Sigma_1(f)$) as N tends to infinity.

9.4.3 Main contribution of Dirichlet form

In this subsection, we calculate the main contribution to the Dirichlet form, which is provided by $\Sigma_1(f)$. This is executed in Lemma 9.4.2.

Lemma 9.4.2. *Under the conditions of Theorem 9.1.2, it holds that*

$$\Sigma_1(f) \le \frac{d_N^2}{2N}\Big[\frac{1}{\mathfrak{R}} + O\Big(\frac{1}{N}\Big)\Big].$$

Proof. To calculate $\Sigma_1(f)$, we write down all movements inside $\mathcal{A}_N^{\{x_1,\, y_p,\, x_2\}}$ and sum it up for $p \in \{1,\, 2\}$. More precisely,

$$\Sigma_1(f) = \sum_{p=1}^{2} \sum_{\eta \in \mathcal{A}_N^{\{x_1,\, y_p,\, x_2\}}} \sum_{i=1}^{2} \mu_N(\eta) r_N(\eta,\, \sigma^{x_i,\, y_p}\eta)\{f(\sigma^{x_i,\, y_p}\eta) - f(\eta)\}^2.$$

There are no overlaps because $r(x_1,\, x_2) = r(x_2,\, x_1) = 0$. By (8.4) and (8.5), the right-hand side is asymptotically equal to

$$\begin{aligned}\frac{d_N N}{2} \sum_{p=1}^{2} \sum_{\ell=0}^{N-1} \sum_{k=0}^{N-\ell-1} m_\star(y_p)^\ell \big[w_N(k) r(x_2,\, y_p)\{f(\sigma^{x_2,\, y_p}\eta) - f(\eta)\}^2 \\ + w_N(N-\ell-k-1) r(x_1,\, y_p)\{f(\sigma^{x_1,\, y_p}\eta) - f(\eta)\}^2\big],\end{aligned} \tag{9.29}$$

where we use $\eta_{x_1} = k$, $\eta_{y_p} = \ell$, and $\eta_{x_2} = N - \ell - k$. Here, we fix $p \in \{1,\, 2\}$ and divide the range $\{\ell \in [\![0,\, N-1]\!]\}$ into $\{\ell > \lfloor N/2 \rfloor\}$ and $\{\ell \le \lfloor N/2 \rfloor\}$. First, using (8.5) and summing up the geometric series with respect to $m_\star(y_p)$, summation in the first range $\{\ell > \lfloor N/2 \rfloor\}$ is easily bounded from above by

$$C \sum_{\ell > \lfloor N/2 \rfloor} m_\star(y_p)^\ell = O(m_\star^{\frac{N}{2}}). \tag{9.30}$$

Second, we calculate summation in the range $\{\ell \le \lfloor N/2 \rfloor\}$. By (9.26), we discard the movements inside $\mathcal{A}_N^{\{x_1,\, y_p\}}$ and $\mathcal{A}_N^{\{x_2,\, y_p\}}$. Hence, we rewrite this summation as

$$\begin{aligned}\sum_{\ell=0}^{\lfloor N/2\rfloor} m_\star(y_p)^\ell \Big[&\sum_{k=1}^{N-\ell-2} w_N(N-\ell-k-1) r(x_1,\, y_p)\{f(\sigma^{x_1,\, y_p}\eta) - f(\eta)\}^2 \\ &+ \sum_{k=1}^{N-\ell-2} w_N(k) r(x_2,\, y_p)\{f(\sigma^{x_2,\, y_p}\eta) - f(\eta)\}^2 \\ &+ w_N(N-\ell-1) r(x_1,\, y_p)\{f(\sigma^{x_1,y_p}\eta) - f(\eta)\}^2 \\ &+ w_N(N-\ell-1) r(x_2,\, y_p)\{f(\sigma^{x_2,y_p}\eta) - f(\eta)\}^2 \Big],\end{aligned} \tag{9.31}$$

where, with slight abuse of notation, in the third line we set $\eta_{x_1} = 1$, $\eta_{y_p} = \ell$, and $\eta_{x_2} = N-\ell-1$, and in the fourth line we set $\eta_{x_1} = N-\ell-1$, $\eta_{y_p} = \ell$, and $\eta_{x_2} = 1$. By (8.5) and (9.27), the first line of (9.31) is given by

$$\sum_{\ell=0}^{\lfloor N/2\rfloor} m_\star(y_p)^\ell \sum_{k=1}^{N-\ell-2} w_N(N-\ell-k-1) r(x_1,\, y_p)\{f(\sigma^{x_1,\, y_p}\eta) - f(\eta)\}^2,$$

which is asymptotically equivalent to

$$\frac{d_N}{(\mathfrak{R}^N)^2} \sum_{\ell=0}^{\lfloor N/2\rfloor} m_\star(y_p)^\ell \sum_{k=1}^{N-\ell-2} \frac{r(x_1,\, y_p)}{N-\ell-k-1} \Big\{ \frac{\frac{N-k-1}{r(x_1,\, y_p)} \big/ \big(\frac{N-k-1}{r(x_1,\, y_p)} + \frac{k}{r(x_2,\, y_p)}\big)}{\sum_{q=1}^2 \frac{(1-m_\star(y_q))^{-1}}{(\frac{N-k-1}{r(x_1,\, y_q)} + \frac{k}{r(x_2,\, y_q)})}} \Big\}^2.$$

Dividing $\dfrac{1}{N-\ell-k-1} = \dfrac{1}{N-k-1} + \dfrac{\ell}{(N-\ell-k-1)(N-k-1)}$ and using $\dfrac{N-k-1}{N-\ell-k-1} \le \ell + 1$, the last line is bounded by

$$\frac{d_N}{(\mathfrak{R}^N)^2} \sum_{\ell=0}^{\lfloor N/2\rfloor} m_\star(y_p)^\ell \sum_{k=1}^{N-\ell-2} \Big[\frac{\frac{N-k-1}{r(x_1,\, y_p)} \big/ \big(\frac{N-k-1}{r(x_1,\, y_p)} + \frac{k}{r(x_2,\, y_p)}\big)^2}{\{\sum_{q=1}^2 \frac{1}{(1-m_\star(y_q))(\frac{N-k-1}{r(x_1,\, y_q)} + \frac{k}{r(x_2,\, y_q)})}\}^2} + C\ell^2 \Big].$$

By the theory of Riemann integration, this is further bounded by

$$\frac{d_N}{(\mathfrak{R}^N)^2}\sum_{\ell=0}^{\lfloor N/2\rfloor} m_\star(y_p)^\ell\Big[N^2\int_0^1 \frac{\frac{1-t}{r(x_1,\,y_p)}/(\frac{1-t}{r(x_1,\,y_p)}+\frac{t}{r(x_2,\,y_p)})^2}{\{\sum_{q=1}^2 \frac{(1-m_\star(y_q))^{-1}}{(\frac{1-t}{r(x_1,\,y_q)}+\frac{t}{r(x_2,\,y_q)})}\}^2}dt+O(N)+CN\ell^2\Big].$$

Calculating the geometric series in $\ell\in[\![0,\,\lfloor N/2\rfloor]\!]$, this asymptotically equals

$$\frac{d_N}{\mathfrak{R}^2N^2}\frac{1}{1-m_\star(y_p)}\Big[\int_0^1 \frac{\frac{1-t}{r(x_1,\,y_p)}/(\frac{1-t}{r(x_1,\,y_p)}+\frac{t}{r(x_2,\,y_p)})^2}{\{\sum_{q=1}^2 \frac{(1-m_\star(y_q))^{-1}}{(\frac{1-t}{r(x_1,\,y_q)}+\frac{t}{r(x_2,\,y_q)})}\}^2}dt+O\Big(\frac{1}{N}\Big)\Big]. \tag{9.32}$$

Similarly, the second line of (9.31) is asymptotically bounded from above by

$$\frac{d_N}{\mathfrak{R}^2N^2}\frac{1}{1-m_\star(y_p)}\Big[\int_0^1 \frac{\frac{t}{r(x_2,\,y_p)}/(\frac{1-t}{r(x_1,\,y_p)}+\frac{t}{r(x_2,\,y_p)})^2}{\{\sum_{q=1}^2 \frac{(1-m_\star(y_q))^{-1}}{(\frac{1-t}{r(x_1,\,y_q)}+\frac{t}{r(x_2,\,y_q)})}\}^2}dt+O\Big(\frac{1}{N}\Big)\Big]. \tag{9.33}$$

The remaining parts of (9.31) are asymptotically equal to

$$\begin{aligned} d_N\sum_{\ell=0}^{\lfloor N/2\rfloor} m_\star(y_p)^\ell\Big[&\frac{r(x_1,\,y_p)}{N-\ell-1}\{f(\sigma^{x_1,\,y_p}\eta)-f(\eta)\}^2\\ &+\frac{r(x_2,\,y_p)}{N-\ell-1}\{f(\sigma^{x_2,\,y_p}\eta)-f(\eta)\}^2\Big]. \end{aligned} \tag{9.34}$$

By (9.26) and (9.27), if $\eta_{x_1}=1$, $\eta_{y_p}=\ell$ and $\eta_{x_2}=N-\ell-1$, then

$$|f(\sigma^{x_1,\,y_p}\eta)-f(\eta)|=\frac{K_p^{1,\,\ell}}{\mathfrak{R}^N}\le\frac{1}{\mathfrak{R}^N}\sum_{t=1}^{\ell+1}\frac{1}{\sum_{q=1}^2\frac{1}{(1-m_\star(y_q))(\frac{N-t}{r(x_1,\,y_q)}+\frac{t-1}{r(x_2,\,y_q)})}},$$

which is of order $(\ell+1)\times O(1/N)$, and if $\eta_{x_1}=N-\ell-1$, $\eta_{y_p}=\ell$, and $\eta_{x_2}=1$, then

$$|f(\sigma^{x_2,\,y_p}\eta)-f(\eta)|=\frac{\mathfrak{R}^N-K_p^{N-\ell-1,\,\ell}}{\mathfrak{R}^N}\le\frac{1}{\mathfrak{R}^N}\sum_{t=N-\ell}^{N}\frac{1}{\sum_{q=1}^2\frac{(1-m_\star(y_q))^{-1}}{(\frac{N-t}{r(x_1,\,y_q)}+\frac{t-1}{r(x_2,\,y_q)})}},$$

which is again of order $(\ell+1)\times O(1/N)$. Hence, (9.34) is bounded from above by

$$\frac{Cd_N}{N}\sum_{\ell=0}^{\lfloor N/2\rfloor} m_\star^\ell \frac{(\ell+1)^2}{N^2} = O\Big(\frac{d_N}{N^3}\Big). \tag{9.35}$$

Therefore, by (9.32), (9.33), and (9.35), we have the following asymptotic upper bound for (9.31):

$$\frac{d_N}{\mathfrak{R}^2 N^2}\Big[\int_0^1 \frac{(1-m_\star(y_p))^{-1}(\frac{1-t}{r(x_1,y_p)}+\frac{t}{r(x_2,y_p)})^{-1}}{\{\sum_{q=1}^2 \frac{1}{(1-m_\star(y_q))(\frac{1-t}{r(x_1,y_q)}+\frac{t}{r(x_2,y_q)})}\}^2}dt + O\Big(\frac{1}{N}\Big)\Big]. \tag{9.36}$$

Collecting (9.29), (9.30), and (9.36), and the fact that d_N decays subexponentially, $\Sigma_1(f)$ has the following asymptotic upper bound:

$$\begin{aligned}&\frac{d_N^2}{2\mathfrak{R}^2 N}\Big[\int_0^1 \frac{\sum_{p=1}^2(1-m_\star(y_p))^{-1}(\frac{1-t}{r(x_1,y_p)}+\frac{t}{r(x_2,y_p)})^{-1}}{\{\sum_{q=1}^2 \frac{1}{(1-m_\star(y_q))(\frac{1-t}{r(x_1,y_q)}+\frac{t}{r(x_2,y_q)})}\}^2}dt + O\Big(\frac{1}{N}\Big)\Big]\\ &=\frac{d_N^2}{2\mathfrak{R}^2 N}\Big[\int_0^1 \frac{1}{\sum_{q=1}^2 \frac{1}{(1-m_\star(y_q))(\frac{1-t}{r(x_1,y_q)}+\frac{t}{r(x_2,y_q)})}}dt + O\Big(\frac{1}{N}\Big)\Big].\end{aligned}$$

The integral in the last line is exactly $\mathfrak{R}$. Hence, we have

$$\Sigma_1(f) \le \frac{d_N^2}{2N}\Big[\frac{1}{\mathfrak{R}} + O\Big(\frac{1}{N}\Big)\Big].$$

The last formula yields our exact expectations. □

9.4.4 Remainder of Dirichlet form

Next, we deal with the remaining terms in the Dirichlet form, $\Sigma_2(f)$, $\Sigma_3(f)$, and $\Sigma_4(f)$. Lemma 9.4.3 deals with $\Sigma_2(f)$.

Lemma 9.4.3. *Under the conditions of Theorem 9.1.2, it holds that*

$$\Sigma_2(f) = O\Big(\frac{d_N^3\log N}{N^2}\Big) = o\Big(\frac{d_N^2}{N}\Big).$$

Proof. Recall that $\Sigma_2(f)$ consists of dynamics between the set differences of $\mathcal{A}_N^{\{x_1,\,y_1,\,x_2\}}$ and $\mathcal{A}_N^{\{x_1,\,y_2,\,x_2\}}$. This happens when a sole particle moves between y_1 and y_2. Precisely,

$$\Sigma_2(f) = \sum_{k=0}^{N-1} \mu_N(\eta) d_N r(y_1,\, y_2)\{f(\sigma^{y_1,\, y_2}\eta) - f(\eta)\}^2, \tag{9.37}$$

where η in summation satisfies $\eta_{x_1} = k$, $\eta_{y_1} = 1$, and $\eta_{x_2} = N-k-1$. If $k=0$ or $N-1$, then $f(\eta) = f(\sigma^{y_1,\, y_2}\eta)$ by (9.26). If $k \in [\![1,\, N-2]\!]$, then by (9.27),

$$f(\sigma^{y_1,\, y_2}\eta) - f(\eta) = \frac{\frac{\ell}{r(x_2,\, y_2)}\Big/\big(\frac{N-\ell-1}{r(x_1,\, y_2)} + \frac{\ell}{r(x_2,\, y_2)}\big) - \frac{\ell}{r(x_2,\, y_1)}\Big/\big(\frac{N-\ell-1}{r(x_1,\, y_1)} + \frac{\ell}{r(x_2,\, y_1)}\big)}{\mathfrak{R}^N \sum_{q=1}^2 \frac{1}{(1-m_\star(y_q))(\frac{N-\ell-1}{r(x_1,\, y_q)} + \frac{\ell}{r(x_2,\, y_q)})}},$$

which is $O(1/N)$. Thus, (9.37) is bounded by

$$C\sum_{k=1}^{N-2} \frac{N d_N^3 m_\star}{k(N-k-1)} \times \frac{1}{N^2} = O\Big(\frac{d_N^3 \log N}{N^2}\Big).$$

This concludes the proof. □

Next, we consider $\Sigma_3(f)$.

Lemma 9.4.4. *Under the conditions of Theorem 9.1.2, it holds that*

$$\Sigma_3(f) = O(d_N^2 m_\star^{\frac{N}{3}} + d_N^3 N \log N) = o\Big(\frac{d_N^2}{N}\Big).$$

Proof. We can formulate

$$\Sigma_3(f) = \sum_{\eta \in \mathcal{U}_N} \sum_{\zeta \in \mathcal{V}_N} \mu_N(\eta) r_N(\eta,\, \zeta)\{f(\zeta) - f(\eta)\}^2.$$

We divide the summation into three cases, depending on which subset η belongs to.

(Case 1) $\eta \in \mathcal{A}_N^{\{x_1, x_2\}}$: In this case, there are no particle movements with $\zeta \in \mathcal{V}_N$.

(Case 2) $\eta \in \mathcal{A}_N^{\{x_i, y_p\}} \setminus \mathcal{E}_N^{x_i}$ for some $i \in \{1, 2\}$ and $p \in \{1, 2\}$: We divide again according to types of the particle movement.

- **(Case 2-1)** $\zeta = \sigma^{y_p, y_q}\eta$, where $q \in \{1, 2\} \setminus \{p\}$: The corresponding summation becomes

$$\sum_{i=1}^{2}\sum_{p=1}^{2}\sum_{\ell=1}^{N} \frac{w_N(N-\ell)w_N(\ell)}{Z_N} m_\star(y_p)^\ell \ell d_N r(y_p, y_q)\{f(\sigma^{y_p, y_q}\eta) - f(\eta)\}^2,$$

  where η in the summation is the configuration with $\eta_{x_i} = N - \ell$ and $\eta_{y_p} = \ell$. If $\ell > \lfloor N/3 \rfloor$, then as in (9.30), the summation is $O(d_N^2 m_\star^{\frac{N}{3}})$. If $\ell \in [\![1, \lfloor N/3 \rfloor]\!]$, then $f(\eta) = f(\xi_N^{x_i})$ by (9.26) and

$$f(\sigma^{y_p, y_q}\eta) = \begin{cases} 1 & \text{if } i = 1, \\ 0 & \text{if } i = 2, \end{cases}$$

  by (9.28), since $N - \ell > \lfloor N/2 \rfloor$; hence, $f(\sigma^{y_p, y_q}\eta) = f(\eta)$. Therefore, the total summation is $O(d_N^2 m_\star^{\frac{N}{3}})$ in this case.

- **(Case 2-2)** $\zeta = \sigma^{x_i, y_q}\eta$, where $q \in \{1, 2\} \setminus \{p\}$: The corresponding summation becomes

$$\sum_{i=1}^{2}\sum_{p=1}^{2}\sum_{\ell=1}^{N} \frac{w_N(N-\ell)w_N(\ell)}{Z_N} m_\star(y_p)^\ell (N-\ell) d_N r(x_i, y_q)\{f(\sigma^{x_i, y_q}\eta) - f(\eta)\}^2,$$

  where η in the summation satisfies $\eta_{x_i} = N - \ell$ and $\eta_{y_p} = \ell$. If $\ell > \lfloor N/3 \rfloor$, then as in (9.30), the summation is $O(d_N^2 m_\star^{\frac{N}{3}})$. If $\ell \in [\![1, \lfloor N/3 \rfloor]\!]$, then $f(\eta) = f(\xi_N^{x_i})$ by (9.26) and

$$f(\sigma^{x_i,\,y_q}\eta) = \begin{cases} 1 & \text{if } i = 1, \\ 0 & \text{if } i = 2, \end{cases}$$

by (9.28), since $N-\ell-1 > \lfloor N/2 \rfloor$; hence, $f(\sigma^{x_i,\,y_q}\eta) = f(\eta)$. Therefore, the total sum is $O(d_N^2 m_\star^{\frac{N}{3}})$.

Concluding, **(Case 2)** yields a contribution $O(d_N^2 m_\star^{\frac{N}{3}})$.

(Case 3) $\eta \in \mathcal{A}_N^{\{x_1,\,y_p,\,x_2\}} \setminus (\mathcal{A}_N^{\{x_1,\,x_2\}} \cup \mathcal{A}_N^{\{x_1,\,y_p\}} \cup \mathcal{A}_N^{\{x_2,\,y_p\}})$ for some $p \in \{1,\,2\}$: In this case, we can write the summation as

$$\sum_{p=1}^{2} \sum_{\ell=1}^{N-2} \sum_{k=1}^{N-\ell-1} \mu_N(\eta) \sum_{z \in \{x_1,\,y_p,\,x_2\}} \eta_z d_N r(z,\,y_q) \{f(\sigma^{z,\,y_q}\eta) - f(\eta)\}^2, \tag{9.38}$$

where in the summation, $q \in \{1,\,2\} \setminus \{p\}$ and $\eta_{x_1} = k$, $\eta_{y_p} = \ell$, and $\eta_{x_2} = N - \ell - k$. As

$$\sum_{z \in \{x_1,\,y_p,\,x_2\}} \eta_z = N,$$

(9.38) can be bounded from above by

$$C \sum_{p=1}^{2} \sum_{\ell=1}^{N-2} \sum_{k=1}^{N-\ell-1} \mu_N(\eta) N d_N.$$

From (8.5), this is bounded by

$$CN^2 d_N^3 \sum_{\ell=1}^{N-2} \sum_{k=1}^{N-\ell-1} \frac{m_\star(y_p)^\ell}{k\ell(N-\ell-k)} \le CN^2 d_N^3 \sum_{\ell=1}^{N-2} \frac{m_\star(y_p)^\ell}{\ell(N-\ell)} \log N = O(d_N^3 N \log N).$$

Collecting all cases, we conclude that $\Sigma_3(f) = O(d_N^2 m_\star^{\frac{N}{3}} + d_N^3 N \log N)$.

□

Finally, we deal with $\Sigma_4(f)$.

Lemma 9.4.5. *Under the conditions of Theorem 9.1.2, it holds that*

$$\Sigma_4(f) = O(d_N^2 N \log N m_\star^{\frac{N}{2}} + d_N^3 N(\log N)^2) = o\Big(\frac{d_N^2}{N}\Big).$$

Proof. By definition, we have

$$\Sigma_4(f) = \frac{1}{2} \sum_{\eta,\,\zeta \in \mathcal{V}_N} \mu_N(\eta) r_N(\eta,\, \zeta)\{f(\zeta) - f(\eta)\}^2.$$

By (9.28), f remains unchanged unless one of $\{\eta, \zeta\}$ has $\lfloor N/2 \rfloor + 1$ particles on x_1 and the other has $\lfloor N/2 \rfloor$ particles on x_1. Thus, we write

$$\begin{aligned} \Sigma_4(f) &= \sum_{\eta \in \mathcal{V}_N :\, \eta_{x_1} = \lfloor N/2 \rfloor + 1} \mu_N(\eta) \sum_{p=1}^{2} r_N(\eta,\, \sigma^{x_1,\, y_p}\eta) \\ &= \sum_{\eta \in \mathcal{V}_N :\, \eta_{x_1} = \lfloor N/2 \rfloor + 1} \mu_N(\eta) \Big(\Big\lfloor \frac{N}{2} \Big\rfloor + 1 \Big) \sum_{p=1}^{2} (d_N + \eta_{y_p}) r(x_1,\, y_p). \end{aligned} \tag{9.39}$$

Now, we divide the summation with respect to η in the last line by the non-empty sites. Because we already have $0 < \eta_{x_1} = \lfloor N/2 \rfloor + 1 < N$, at least 3 sites must be non-empty.

(Case 1) Non-empty sites are $\{x_1,\, y_1,\, y_2\}$: Writing $\eta_{y_1} = \ell$ and $\eta_{y_2} = \lfloor (N-1)/2 \rfloor - \ell$, this part is asymptotically equivalent to

$$\begin{aligned} &\sum_{\ell=1}^{\lfloor \frac{N-1}{2} \rfloor - 1} \frac{N d_N^2}{2} \frac{m_\star(y_1)^\ell m_\star(y_2)^{\lfloor \frac{N-1}{2} \rfloor - \ell}}{\ell(\lfloor \frac{N-1}{2} \rfloor - \ell)} \sum_{p=1}^{2} (d_N + \eta_{y_p}) r(x_1,\, y_p) \\ &\le C N^2 d_N^2 \sum_{\ell=1}^{\lfloor \frac{N}{2} \rfloor - 1} \frac{m_\star^{\frac{N}{2}}}{\ell(\lfloor \frac{N-1}{2} \rfloor - \ell)} = O(d_N^2 N \log N m_\star^{\frac{N}{2}}). \end{aligned}$$

(Case 2) Non-empty sites are $\{x_1, x_2, y_1, y_2\}$: In this case, we use

$$\sum_{p=1}^{2}(d_N + \eta_{y_p})r(x_1, y_p) \leq CN$$

to bound the summation from above by

$$CN^2 \sum_{\substack{\eta\in\mathcal{V}_N:\,\eta_{x_1}=\lfloor N/2\rfloor+1,\\ \eta \text{ has 4 non-empty sites}}} \mu_N(\eta) \leq C\frac{N^3}{d_N} \sum_{\substack{\eta\in\mathcal{H}_N:\,\eta_{x_1}=\lfloor N/2\rfloor+1,\\ \eta \text{ has 4 non-empty sites}}} \prod_{z\in S} w_N(\eta_z).$$

In the inequality above, we use $m_\star \leq 1$. Here, we divide S into $\{x_1\}$ and $\{x_2, y_1, y_2\}$; then, the last line is asymptotically equivalent to

$$C\frac{N^3}{d_N} w_N\Big(\Big\lfloor \frac{N}{2}\Big\rfloor + 1\Big) \sum_{\substack{\zeta\in\mathcal{H}_{\lfloor (N-1)/2\rfloor,\, S\setminus\{x_1\}}:\\ \zeta \text{ has 3 non-empty sites}}} \prod_{z\in S\setminus\{x_1\}:\,\zeta_z\geq 1} \frac{d_N}{\zeta_z}.$$

Here, $\mathcal{H}_{M,R}$ denotes the set of configurations on R with M particles. By (8.5) and Lemma 10.8.1, this is bounded by

$$Cd_N^3 N^2 \times \frac{(3\log(\lfloor \frac{N-1}{2}\rfloor + 1))^2}{\lfloor \frac{N-1}{2}\rfloor} = O(d_N^3 N(\log N)^2).$$

Therefore, collecting all above cases and (9.39),

$$\Sigma_4(f) = O(d_N^2 N \log N m_\star^{\frac{N}{2}} + d_N^3 N(\log N)^2).$$

This completes the proof of Lemma 9.4.5. □

9.4.5 Proof of Proposition 9.4.1

Thus, we are in the position to prove Proposition 9.4.1.

Proof of Proposition 9.4.1. By Lemmas 9.4.2, 9.4.3, 9.4.4, and 9.4.5,

$$D_N(f_{\mathrm{test}}) \le \frac{d_N^2}{2N\mathfrak{R}} + o\Big(\frac{d_N^2}{N}\Big) + O(d_N^2 m_\star^{\frac{N}{3}}) + O(d_N^3 N(\log N)^2).$$

Sending $N \to \infty$, as $\lim_{N\to\infty} d_N N^2(\log N)^2 = 0$ and d_N decays subexponentially, we have

$$\limsup_{N\to\infty} \frac{N}{d_N^2} D_N(f_{\mathrm{test}}) \le \frac{1}{2\mathfrak{R}}.$$

Therefore, by Theorem 3.2.5, we obtain the desired result. □

9.5 Lower bound for capacities: simple case

In this section, we assume Condition 9.1.1 and establish the lower bound for $\mathrm{Cap}_N(\mathcal{E}_N^{x_1}, \mathcal{E}_N^{x_2})$. Once more, we recall the notions from Section 9.1.1. The following proposition is our main objective.

Proposition 9.5.1 (Lower bound for capacities: simple case)**.** *Under the conditions of Theorem 9.1.2, the following inequality holds.*

$$\liminf_{N\to\infty} \frac{N}{d_N^2} \mathrm{Cap}_N(\mathcal{E}_N^{x_1}, \mathcal{E}_N^{x_2}) \ge \frac{1}{2\mathfrak{R}}. \tag{9.40}$$

In terms of applying Theorem 3.2.8-(2) with $g \equiv 0$, it holds that

$$\mathrm{Cap}_N(\mathcal{E}_N^{x_1}, \mathcal{E}_N^{x_2}) \ge \frac{1}{\|\psi\|^2}\Big[\sum_{\eta\in\mathcal{H}_N} h_{\mathcal{E}_N^{x_1}, \mathcal{E}_N^{x_2}}(\eta)(\mathrm{div}\,\psi)(\eta)\Big]^2. \tag{9.41}$$

Thus, the main difficulty is to find a suitable flow ψ such that

$$\sum_{\eta\in\mathcal{H}_N} h_{\mathcal{E}_N^{x_1}, \mathcal{E}_N^{x_2}}(\eta)(\mathrm{div}\,\psi)(\eta)$$

can be easily calculated. Here, the major obstacle is that the exact values of $h_{\mathcal{E}_N^{x_1}, \mathcal{E}_N^{x_2}}$ are unknown except on the 1D tubes, $\mathcal{A}_N^{a,b}$ for $a, b \in S$, as shown in

Section 9.3. Thus, the objective is to find a proper approximating flow ψ_{test} whose divergence can be neglected outside those tubes.

9.5.1 Construction of test flow ψ_{test}

In this subsection, we build the test flow $\psi = \psi_{\text{test}}$ on $\mathcal{H}_N$. As mentioned above, the key here is as follows: We must construct ψ such that

(1) the flow norm of ψ is asymptotically equal to $c\Phi_{f_{\text{test}}}$, $c \neq 0$ (cf. (3.35));

(2) the divergence of ψ can be summed up in the sense of the right-hand side of (9.41).

To overcome both issues, *we modify $\Phi_{f_{\text{test}}}$ properly, so that the divergence vanishes on $\mathcal{A}_N^{\{x_1,\,y_p,\,x_2\}} \setminus (\mathcal{A}_N^{\{x_1,\,y_p\}} \cup \mathcal{A}_N^{\{x_2,\,y_p\}})$*. It is convenient to introduce the following notation. We denote by $\zeta_{k,\,\ell}^{x_1y_px_2}$ the configuration in $\mathcal{A}_N^{\{x_1,\,y_p,\,x_2\}}$ so that $(\zeta_{k,\,\ell}^{x_1y_px_2})_{x_1} = k$, $(\zeta_{k,\,\ell}^{x_1y_px_2})_{y_p} = \ell$, and $(\zeta_{k,\,\ell}^{x_1y_px_2})_{x_2} = N - \ell - k$.

- We define, for $p \in \{1,\, 2\}$, $\ell \in [\![0,\, \lfloor N/2 \rfloor - 1]\!]$, and $k \in [\![1,\, N - \ell - 1]\!]$,

$$\psi_0(\zeta_{k,\,\ell}^{x_1y_px_2},\, \zeta_{k-1,\,\ell+1}^{x_1y_px_2}) = \frac{m_\star(y_p)^\ell / (\frac{N-\ell-k-1}{r(x_1,\,y_p)} + \frac{k+\ell}{r(x_2,\,y_p)})}{\mathfrak{R} \sum_{q=1}^{2} \frac{1}{(1-m_\star(y_q))(\frac{N-\ell-k-1}{r(x_1,\,y_q)} + \frac{k+\ell}{r(x_2,\,y_q)})}}, \tag{9.42}$$

$$\psi_0(\zeta_{k,\,\ell}^{x_1y_px_2},\, \zeta_{k,\,\ell+1}^{x_1y_px_2}) = \frac{-m_\star(y_p)^\ell / (\frac{N-\ell-k-1}{r(x_1,\,y_p)} + \frac{k+\ell}{r(x_2,\,y_p)})}{\mathfrak{R} \sum_{q=1}^{2} \frac{1}{(1-m_\star(y_q))(\frac{N-\ell-k-1}{r(x_1,\,y_q)} + \frac{k+\ell}{r(x_2,\,y_q)})}}, \tag{9.43}$$

  and 0 otherwise.

Observe that by the above construction, $(\operatorname{div} \psi_0)(\xi_N^{x_i}) = 0$ for $i \in \{1,\, 2\}$ and $(\operatorname{div} \psi_0)(\eta) = 0$ for all $\eta \in \mathcal{V}_N$.

However, it holds that $(\operatorname{div} \psi_0)(\zeta_{k,\,\ell}^{x_1y_px_2}) \neq 0$ for $\ell \in [\![1,\, \lfloor N/2 \rfloor]\!]$ and $k \in [\![0,\, N - \ell]\!]$. *We overcome this issue by adding correction flows to ψ_0 and make the divergence to be zero.*

Before the exact definition, we calculate the non-zero term $(\operatorname{div}\psi_0)(\zeta_{k,\,\ell}^{x_1y_px_2})$. We define, for $k \in [\![1,\, N-1]\!]$,

$$\mathfrak{A}(N,\,k) := \frac{1}{\mathfrak{R}}\frac{N-1}{\big(\frac{\frac{N-k}{r(x_1,\,y_2)}+\frac{k-1}{r(x_2,\,y_2)}}{1-m_\star(y_1)}+\frac{\frac{N-k}{r(x_1,\,y_1)}+\frac{k-1}{r(x_2,\,y_1)}}{1-m_\star(y_2)}\big)\big(\frac{\frac{N-k-1}{r(x_1,\,y_2)}+\frac{k}{r(x_2,\,y_2)}}{1-m_\star(y_1)}+\frac{\frac{N-k-1}{r(x_1,\,y_1)}+\frac{k}{r(x_2,\,y_1)}}{1-m_\star(y_2)}\big)}. \tag{9.44}$$

Then, by the estimate

$$\frac{N-k}{r(x_1,\,y_2)}+\frac{k-1}{r(x_2,\,y_2)} \ge \frac{N-k}{C}+\frac{k-1}{C}=\frac{N-1}{C}$$

and three additional similar bounds, it is straightforward that

$$\mathfrak{A}(N,\,k) \le \frac{C}{N}. \tag{9.45}$$

The next lemma represents $(\operatorname{div}\psi_0)(\zeta_{k,\,\ell}^{x_1y_px_2})$ in terms of $\mathfrak{A}(N,\,k+\ell)$.

Lemma 9.5.2. *For $p \in \{1,\,2\}$, $\ell \in [\![1,\, \lfloor N/2\rfloor]\!]$, and $k \in [\![1,\, N-\ell-1]\!]$, we have*

$$(\operatorname{div}\psi_0)(\zeta_{k,\,\ell}^{x_1y_px_2}) = \frac{m_\star(y_p)^{\ell-1}}{1-m_\star(y_s)}\Big[\frac{1}{r(x_1,\,y_s)r(x_2,\,y_p)}-\frac{1}{r(x_2,\,y_s)r(x_1,\,y_p)}\Big]\mathfrak{A}(N,\,k+\ell), \tag{9.46}$$

where s is the other element in $\{1,\,2\}$ so that $\{p,\,s\}=\{1,\,2\}$.

Proof. By (9.42) and (9.43), $(\operatorname{div}\psi_0)(\zeta_{k,\,\ell}^{x_1y_px_2})$ equals

$$\begin{aligned}&\psi_0(\zeta_{k,\,\ell}^{x_1y_px_2},\,\zeta_{k+1,\,\ell-1}^{x_1y_px_2})+\psi_0(\zeta_{k,\,\ell}^{x_1y_px_2},\,\zeta_{k,\,\ell-1}^{x_1y_px_2})\\ &= -\frac{m_\star(y_p)^{\ell-1}/(\frac{N-\ell-k-1}{r(x_1,\,y_p)}+\frac{k+\ell}{r(x_2,\,y_p)})}{\mathfrak{R}\sum_{q=1}^{2}\frac{1}{(1-m_\star(y_q))(\frac{N-\ell-k-1}{r(x_1,\,y_q)}+\frac{k+\ell}{r(x_2,\,y_q)})}}+\frac{m_\star(y_p)^{\ell-1}/(\frac{N-\ell-k}{r(x_1,\,y_p)}+\frac{k+\ell-1}{r(x_2,\,y_p)})}{\mathfrak{R}\sum_{q=1}^{2}\frac{1}{(1-m_\star(y_q))(\frac{N-\ell-k}{r(x_1,\,y_q)}+\frac{k+\ell-1}{r(x_2,\,y_q)})}},\end{aligned}$$

where the first line holds since the other two flow values cancel out with each other. Noting that $\{p,\,s\}=\{1,\,2\}$, we rearrange the right-hand side as

$m_\star(y_p)^{\ell-1}/\mathfrak{R}$ times

$$-\frac{\frac{N-\ell-k-1}{r(x_1,y_s)}+\frac{k+\ell}{r(x_2,y_s)}}{\frac{\frac{N-\ell-k-1}{r(x_1,y_s)}+\frac{k+\ell}{r(x_2,y_s)}}{1-m_\star(y_p)}+\frac{\frac{N-\ell-k-1}{r(x_1,y_p)}+\frac{k+\ell}{r(x_2,y_p)}}{1-m_\star(y_s)}}+\frac{\frac{N-\ell-k}{r(x_1,y_s)}+\frac{k+\ell-1}{r(x_2,y_s)}}{\frac{\frac{N-\ell-k}{r(x_1,y_s)}+\frac{k+\ell-1}{r(x_2,y_s)}}{1-m_\star(y_p)}+\frac{\frac{N-\ell-k}{r(x_1,y_p)}+\frac{k+\ell-1}{r(x_2,y_p)}}{1-m_\star(y_s)}}.$$

Reducing to a common denominator, the last display equals

$$\begin{aligned}&-\Big(\frac{N-\ell-k-1}{r(x_1,\,y_s)}+\frac{k+\ell}{r(x_2,\,y_s)}\Big)\Big(\frac{\frac{N-\ell-k}{r(x_1,y_s)}+\frac{k+\ell-1}{r(x_2,y_s)}}{1-m_\star(y_p)}+\frac{\frac{N-\ell-k}{r(x_1,y_p)}+\frac{k+\ell-1}{r(x_2,y_p)}}{1-m_\star(y_s)}\Big)\\&+\Big(\frac{N-\ell-k}{r(x_1,\,y_s)}+\frac{k+\ell-1}{r(x_2,\,y_s)}\Big)\Big(\frac{\frac{N-\ell-k-1}{r(x_1,y_s)}+\frac{k+\ell}{r(x_2,y_s)}}{1-m_\star(y_p)}+\frac{\frac{N-\ell-k-1}{r(x_1,y_p)}+\frac{k+\ell}{r(x_2,y_p)}}{1-m_\star(y_s)}\Big)\end{aligned}\tag{9.47}$$

divided by

$$\Big(\frac{\frac{N-\ell-k-1}{r(x_1,y_s)}+\frac{k+\ell}{r(x_2,y_s)}}{1-m_\star(y_p)}+\frac{\frac{N-\ell-k-1}{r(x_1,y_p)}+\frac{k+\ell}{r(x_2,y_p)}}{1-m_\star(y_s)}\Big)\Big(\frac{\frac{N-\ell-k}{r(x_1,y_s)}+\frac{k+\ell-1}{r(x_2,y_s)}}{1-m_\star(y_p)}+\frac{\frac{N-\ell-k}{r(x_1,y_p)}+\frac{k+\ell-1}{r(x_2,y_p)}}{1-m_\star(y_s)}\Big).$$

Thus, according to (9.44), it remains to prove that (9.47) equals

$$\frac{N-1}{1-m_\star(y_s)}\times\Big[\frac{1}{r(x_1,\,y_s)r(x_2,\,y_p)}-\frac{1}{r(x_2,\,y_s)r(x_1,\,y_p)}\Big].$$

In (9.47), the two terms involving $1-m_\star(y_p)$ cancel out with each other. Thus, (9.47) becomes $(1-m_\star(y_s))^{-1}$ times

$$\begin{aligned}&-\Big(\frac{N-\ell-k-1}{r(x_1,\,y_s)}+\frac{k+\ell}{r(x_2,\,y_s)}\Big)\Big(\frac{N-\ell-k}{r(x_1,\,y_p)}+\frac{k+\ell-1}{r(x_2,\,y_p)}\Big)\\&+\Big(\frac{N-\ell-k}{r(x_1,\,y_s)}+\frac{k+\ell-1}{r(x_2,\,y_s)}\Big)\Big(\frac{N-\ell-k-1}{r(x_1,\,y_p)}+\frac{k+\ell}{r(x_2,\,y_p)}\Big).\end{aligned}$$

Again, the terms cancel out with each other so that (9.47) equals

$$(1-m_\star(y_s))^{-1}\Big[\frac{N-1}{r(x_1,\,y_s)r(x_2,\,y_p)}-\frac{N-1}{r(x_2,\,y_s)r(x_1,\,y_p)}\Big],$$

as wanted. $\square$

Now, for all $p \in \{1, 2\}$ and $k \in [\![1, N-1]\!]$, we define a correction flow $\phi_{p,k}$ as follows.

- Suppose that $k \in [\![\lfloor N/2 \rfloor + 1, N-1]\!]$. Then, for $\ell \in [\![1, \lfloor N/2 \rfloor]\!]$,

$$\phi_{p,k}(\zeta_{k-\ell,\ell}^{x_1 y_p x_2}, \zeta_{k-\ell+1,\ell-1}^{x_1 y_p x_2}) := -\sum_{t=\ell}^{\lfloor N/2 \rfloor} (\operatorname{div} \psi_0)(\zeta_{k-t,t}^{x_1 y_p x_2}), \tag{9.48}$$

  and $\phi_{p,k} = 0$ on all other edges.

- Suppose that $k \in [\![1, \lfloor N/2 \rfloor]\!]$. Then, for $\ell \in [\![1, k-1]\!]$,

$$\phi_{p,k}(\zeta_{k-\ell,\ell}^{x_1 y_p x_2}, \zeta_{k-\ell+1,\ell-1}^{x_1 y_p x_2}) := -\sum_{t=\ell}^{k-1} (\operatorname{div} \psi_0)(\zeta_{k-t,t}^{x_1 y_p x_2}), \tag{9.49}$$

  and $\phi_{p,k} = 0$ on all other edges.

Finally, we define a flow

$$\psi = \psi_{\text{test}} := \psi_0 + \sum_{p=1}^{2} \sum_{k=1}^{N-1} \phi_{p,k}.$$

Then, the flows $\phi_{p,k}$ for $p \in \{1, 2\}$ and $k \in [\![1, N-1]\!]$ cancel the divergence of ψ_0 at each $\zeta_{k-\ell,\ell}^{x_1 y_p x_2} \in \mathcal{A}_N^{\{x_1, y_p, x_2\}}$. Thus, we obtain that $(\operatorname{div} \psi)(\eta) = 0$ for all η in

$$\mathcal{A}_N^{\{x_1, y_p, x_2\}} \setminus \big(\mathcal{A}_N^{\{x_1, y_p\}} \cup \mathcal{A}_N^{\{x_2, y_p\}} \cup \mathcal{A}_N^{\{x_1, x_2\}}\big) \quad \text{for } p \in \{1, 2\}.$$

9.5.2 Flow norm of ψ_{test}

In this subsection, we calculate the flow norm of the test flow ψ.

Lemma 9.5.3. *Under the conditions of Theorem 9.1.2, it holds that*

$$\|\psi\|^2 \le (1+o(1))\frac{2N}{d_N^2 \mathfrak{R}}.$$

Proof. By (9.42), (9.43), and Definition 3.2.6, we have

$$\|\psi_0\|^2 = \sum_{p=1}^{2} \sum_{\ell=0}^{\lfloor N/2\rfloor -1} \sum_{k=1}^{N-\ell-1} \Big[\frac{(\psi(\eta,\, \sigma^{x_1,\, y_p}\eta))^2}{\mu_N(\eta)k(d_N+\ell)r(x_1,\, y_p)} + \frac{(\psi(\eta,\, \sigma^{x_2,\, y_p}\eta))^2}{\mu_N(\eta)(N-\ell-k)(d_N+\ell)r(x_2,\, y_p)}\Big], \tag{9.50}$$

where $\eta_{x_1} = k$, $\eta_{y_p} = \ell$, and $\eta_{x_2} = N-\ell-k$ in the last line. By (8.5) and (9.42), the part of (9.50) including the first fraction inside bracket is asymptotically equivalent to

$$\frac{2}{d_N^2 N} \sum_{p=1}^{2} \sum_{\ell=0}^{\lfloor N/2\rfloor -1} \frac{m_\star(y_p)^\ell}{\mathfrak{R}^2} \sum_{k=1}^{N-\ell-1} \frac{\frac{N-\ell-k}{r(x_1,\, y_p)}\big/\big(\frac{N-k-\ell-1}{r(x_1,\, y_p)} + \frac{k+\ell}{r(x_2,\, y_p)}\big)^2}{\{\sum_{q=1}^2 \frac{1}{(1-m_\star(y_q))(\frac{N-k-\ell-1}{r(x_1,\, y_q)} + \frac{k+\ell}{r(x_2,\, y_q)})}\}^2}.$$

Divide $N-\ell-k = (N-k-\ell-1)+1$. Then, as in obtaining (9.32), the last formula can be bounded from above by

$$\frac{2}{d_N^2 N} \sum_{p=1}^{2} \frac{N^2\mathfrak{R}^{-2}}{1-m_\star(y_p)} \Big[\int_0^1 \frac{\frac{1-t}{r(x_1,\, y_p)}\big/\big(\frac{1-t}{r(x_1,\, y_p)} + \frac{t}{r(x_2,\, y_p)}\big)^2}{\{\sum_{q=1}^2 \frac{1}{(1-m_\star(y_q))(\frac{1-t}{r(x_1,\, y_q)} + \frac{t}{r(x_2,\, y_q)})}\}^2} dt + o(1)\Big]. \tag{9.51}$$

Similarly, the part of (9.50) including the second fraction inside bracket is asymptotically bounded from above by

$$\frac{2}{d_N^2 N} \sum_{p=1}^{2} \frac{N^2\mathfrak{R}^{-2}}{1-m_\star(y_p)} \Big[\int_0^1 \frac{\frac{t}{r(x_2,\, y_p)}\big/\big(\frac{1-t}{r(x_1,\, y_p)} + \frac{t}{r(x_2,\, y_p)}\big)^2}{\{\sum_{q=1}^2 \frac{1}{(1-m_\star(y_q))(\frac{1-t}{r(x_1,\, y_q)} + \frac{t}{r(x_2,\, y_q)})}\}^2} dt + o(1)\Big]. \tag{9.52}$$

Hence, by (9.50), (9.51), and (9.52), we have the following asymptotic upper bound for $\|\psi_0\|^2$:

$$\frac{2N}{d_N^2}\sum_{p=1}^{2}\mathfrak{R}^{-2}\int_0^1 \frac{(1-m_\star(y_p))^{-1}(\frac{1-t}{r(x_1,\,y_p)}+\frac{t}{r(x_2,\,y_p)})^{-1}}{\{\sum_{q=1}^{2}\frac{1}{(1-m_\star(y_q))(\frac{1-t}{r(x_1,\,y_q)}+\frac{t}{r(x_2,\,y_q)})}\}^2}dt=\frac{2N}{d_N^2}\times\frac{1}{\mathfrak{R}}.$$

Thus, by the triangle inequality of the flow norm, it suffices to prove that

$$\sum_{p=1}^{2}\sum_{k=1}^{N-1}\|\phi_{p,\,k}\|=o\Big(\frac{\sqrt{N}}{d_N}\Big). \tag{9.53}$$

First, we consider $k\in[\![\lfloor N/2\rfloor+1,\,N-1]\!]$. By definition, we calculate $\|\phi_{p,\,k}\|^2$ as

$$\sum_{\ell=1}^{\lfloor N/2\rfloor}\frac{(\phi_{p,\,k}(\zeta_{k-\ell,\,\ell}^{x_1y_px_2},\,\zeta_{k-\ell+1,\,\ell-1}^{x_1y_px_2}))^2}{\mu_N(\zeta_{k-\ell,\,\ell}^{x_1y_px_2})\ell(d_N+k-\ell)r(y_p,\,x_1)}.$$

By (9.48) and (8.5), this is equal to

$$(|S_\star|+o(1))\sum_{\ell=1}^{\lfloor N/2\rfloor}\frac{N-k}{Nd_N^2m_\star(y_p)^{\ell-1}r(x_1,\,y_p)}\Big[\sum_{t=\ell}^{\lfloor N/2\rfloor}(\mathrm{div}\,\psi_0)(\zeta_{k-t,\,t}^{x_1y_px_2})\Big]^2.$$

By (9.46) and the fact that $N-k\le N$, this is bounded by

$$\frac{C}{d_N^2}\sum_{\ell=1}^{\lfloor N/2\rfloor}\frac{1}{m_\star(y_p)^{\ell-1}}\Big[\sum_{t=\ell}^{\lfloor N/2\rfloor}\frac{m_\star(y_p)^{t-1}}{1-m_\star(y_s)}\Big[\frac{1}{r(x_1,\,y_s)r(x_2,\,y_p)}-\frac{1}{r(x_2,\,y_s)r(x_1,\,y_p)}\Big]\mathfrak{A}(N,\,k)\Big]^2.$$

By (9.45) and the fact that $\sum_{t=\ell}^{\infty}m_\star(y_p)^{t-1}=m_\star(y_p)^{\ell-1}/(1-m_\star(y_p))$, we further bound this by

$$\frac{C}{d_N^2}\sum_{\ell=1}^{\lfloor N/2\rfloor}\frac{1}{m_\star(y_p)^{\ell-1}}\times$$
$$\Big[\frac{m_\star(y_p)^{\ell-1}}{(1-m_\star(y_p))(1-m_\star(y_s))}\Big[\frac{1}{r(x_1,\,y_s)r(x_2,\,y_p)}-\frac{1}{r(x_2,\,y_s)r(x_1,\,y_p)}\Big]\frac{C}{N}\Big]^2.$$

Taking out the constants, we obtain that for $k \in [\![\lfloor N/2 \rfloor + 1,\, N-1]\!]$,

$$\|\phi_{p,\,k}\|^2 \le \frac{C}{d_N^2} \sum_{\ell=1}^{\lfloor N/2 \rfloor} \frac{m_\star(y_p)^{\ell-1}}{N^2} \le \frac{C}{N^2 d_N^2}. \tag{9.54}$$

We can apply the same logic for $k \in [\![1,\, \lfloor N/2 \rfloor]\!]$, which implies

$$\|\phi_{p,\,k}\|^2 \le \frac{C}{d_N^2} \sum_{\ell=1}^{k-1} \frac{m_\star(y_p)^{\ell-1}}{N^2} \le \frac{C}{N^2 d_N^2}. \tag{9.55}$$

Therefore, by (9.54) and (9.55), we conclude that for every $k \in [\![1,\, N-1]\!]$,

$$\|\phi_{p,\,k}\| \le \frac{C}{N d_N},$$

and thus

$$\sum_{p=1}^{2} \sum_{k=1}^{N-1} \|\phi_{p,\,k}\| \le 2(N-1) \times \frac{C}{N d_N} = O\Big(\frac{1}{d_N}\Big) = o\Big(\frac{\sqrt{N}}{d_N}\Big).$$

This proves (9.53) and thus concludes the proof. □

9.5.3 Remaining terms

Here, we address the remaining terms on the right-hand side of (9.41) with respect to ψ. *To this end, Lemma 9.3.4 is used to calculate the equilibrium potential near the metastable valleys.*

Lemma 9.5.4. *Under the conditions of Theorem 9.1.2, it holds that*

$$\sum_{\eta \in \mathcal{H}_N \setminus \mathcal{E}_N(S_\star)} h_{\mathcal{E}_N^{x_1},\, \mathcal{E}_N^{x_2}}(\eta)(\operatorname{div} \psi)(\eta) = \frac{1+o(1)}{\mathfrak{R}}. \tag{9.56}$$

Proof. We will abbreviate $h_{\mathcal{E}_N^{x_1},\, \mathcal{E}_N^{x_2}}$ as h. It follows from the last observation in Section 9.5.1 that we only need to sum up the configurations in $\mathcal{A}_N^{\{x_1,\, y_p\}} \setminus \mathcal{E}_N^{x_1}$,

$\mathcal{A}_N^{\{x_2, y_p\}} \setminus \mathcal{E}_N^{x_2}$, and $\mathcal{A}_N^{\{x_1, x_2\}} \setminus (\mathcal{E}_N^{x_1} \cup \mathcal{E}_N^{x_2})$. First, we claim that

$$\sum_{p=1}^{2} \Big[\sum_{\eta \in \mathcal{A}_N^{\{x_1, y_p\}} \setminus \mathcal{E}_N^{x_1}} + \sum_{\eta \in \mathcal{A}_N^{\{x_2, y_p\}} \setminus \mathcal{E}_N^{x_2}} \Big] h(\eta)(\operatorname{div} \psi_0)(\eta) = \frac{1+o(1)}{\mathfrak{R}}. \tag{9.57}$$

The left-hand side of (9.57) is

$$\sum_{p=1}^{2} \sum_{\ell=1}^{\lfloor N/2 \rfloor} h(\zeta_\ell^{x_1, y_p})(\operatorname{div} \psi_0)(\zeta_\ell^{x_1, y_p}) + \sum_{p=1}^{2} \sum_{\ell=1}^{\lfloor N/2 \rfloor} h(\zeta_\ell^{x_2, y_p})(\operatorname{div} \psi_0)(\zeta_\ell^{x_2, y_p}). \tag{9.58}$$

By Lemma 9.3.4, we have

$$\sup_{1 \le \ell \le \lfloor N/2 \rfloor} \left| h(\zeta_\ell^{x_1, y_p}) - 1 \right| = o(1), \tag{9.59}$$

and

$$\sup_{1 \le \ell \le \lfloor N/2 \rfloor} h(\zeta_\ell^{x_2, y_p}) = o(1). \tag{9.60}$$

Hence, (9.58) is equal to

$$(1+o(1)) \sum_{p=1}^{2} \sum_{\ell=1}^{\lfloor N/2 \rfloor} (\operatorname{div} \psi_0)(\zeta_\ell^{x_1, y_p}) + o(1) \sum_{p=1}^{2} \sum_{\ell=1}^{\lfloor N/2 \rfloor} (\operatorname{div} \psi_0)(\zeta_\ell^{x_2, y_p}). \tag{9.61}$$

By (9.42), the first term of (9.61) is asymptotically equivalent to

$$\frac{1}{\mathfrak{R}} \sum_{p=1}^{2} \sum_{\ell=1}^{\lfloor N/2 \rfloor} \frac{m_\star(y_p)^{\ell-1} \big/ \frac{N-1}{r(x_2, y_p)}}{\sum_{q=1}^{2} \frac{1}{(1-m_\star(y_q)) \frac{N-1}{r(x_2, y_q)}}} = \frac{1}{\mathfrak{R}} \sum_{p=1}^{2} \sum_{\ell=1}^{\lfloor N/2 \rfloor} \frac{m_\star(y_p)^{\ell-1} r(x_2,\, y_p)}{\sum_{q=1}^{2} \frac{r(x_2, y_q)}{1-m_\star(y_q)}}.$$

Summing for $\ell \in [\![1,\, \lfloor N/2 \rfloor]\!]$, the last formula equals $1/\mathfrak{R}$. Similarly, the second part of (9.61) equals $o(1)/\mathfrak{R} = o(1)$. This concludes the proof of (9.57).

Next, from the definition, note that $(\operatorname{div} \phi_{p,k})(\eta)$ vanishes unless

$$\eta \in \mathcal{A}_N^{\{x_1, y_p, x_2\}} \setminus \big(\mathcal{A}_N^{\{x_1, y_p\}} \cup \mathcal{A}_N^{\{x_2, y_p\}}\big).$$

Moreover, it is verified right after the definition of ψ that $\operatorname{div} \psi$ vanishes in

$$\mathcal{A}_N^{\{x_1, y_p, x_2\}} \setminus \big(\mathcal{A}_N^{\{x_1, y_p\}} \cup \mathcal{A}_N^{\{x_2, y_p\}} \cup \mathcal{A}_N^{\{x_1, x_2\}}\big) \quad \text{for } p \in \{1, 2\}.$$

Finally, it is straightforward that $(\operatorname{div} \psi_0)(\eta) = 0$ for $\eta \in \mathcal{A}_N^{\{x_1, x_2\}}$. Combining these observations, it remains to prove that

$$\sum_{k=1}^{N-1} \sum_{p=1}^{2} \sum_{\eta \in \mathcal{A}_N^{\{x_1, x_2\}} \setminus (\mathcal{E}_N^{x_1} \cup \mathcal{E}_N^{x_2})} h(\eta)(\operatorname{div} \phi_{p,k})(\eta) = o(1).$$

This can be rewritten as

$$\sum_{k=1}^{N-1} \sum_{p=1}^{2} h(\zeta_k^{x_1, x_2})(\operatorname{div} \phi_{p,k})(\zeta_k^{x_1, x_2}) = o(1).$$

Since $0 \le h \le 1$, it suffices to prove that

$$\sum_{k=1}^{N-1} \Big| \sum_{p=1}^{2} (\operatorname{div} \phi_{p,k})(\zeta_k^{x_1, x_2}) \Big| = o(1).$$

For $k \in [\![\lfloor N/2 \rfloor + 1,\, N-1]\!]$, by (9.48) it holds that

$$\sum_{p=1}^{2} (\operatorname{div} \phi_{p,k})(\zeta_k^{x_1, x_2}) = \sum_{p=1}^{2} \sum_{t=1}^{\lfloor N/2 \rfloor} (\operatorname{div} \psi_0)(\zeta_{k-t,\, t}^{x_1 y_p x_2}).$$

By (9.46), for fixed $p \in \{1, 2\}$, the summation in $1 \le t \le \lfloor N/2 \rfloor$ is calculated as

$$\begin{aligned}
&\sum_{t=1}^{\lfloor N/2 \rfloor} \frac{m_\star(y_p)^{t-1}}{1-m_\star(y_s)} \times \Big[\frac{1}{r(x_1,\, y_s) r(x_2,\, y_p)} - \frac{1}{r(x_2,\, y_s) r(x_1,\, y_p)}\Big] \times \mathfrak{A}(N,\, k) \\
&= \frac{\mathfrak{A}(N,\, k)}{1-m_\star(y_s)} \times \Big[\frac{1}{r(x_1,\, y_s) r(x_2,\, y_p)} - \frac{1}{r(x_2,\, y_s) r(x_1,\, y_p)}\Big] \times \Big[\frac{1}{1-m_\star(y_p)} + O(m_\star(y_p)^{\frac{N}{2}})\Big] \\
&= \frac{\mathfrak{A}(N,\, k)}{(1-m_\star(y_p))(1-m_\star(y_s))} \Big[\frac{1}{r(x_1,\, y_s) r(x_2,\, y_p)} - \frac{1}{r(x_2,\, y_s) r(x_1,\, y_p)}\Big] + O\Big(\frac{m_\star(y_p)^{\frac{N}{2}}}{N}\Big),
\end{aligned}$$

where $\{p,\, s\} = \{1,\, 2\}$, where in the first equality we used

$$\sum_{t=1}^{\lfloor N/2 \rfloor} m_\star(y_p)^{t-1} = \frac{1}{1-m_\star(y_p)} + \sum_{t > \lfloor N/2 \rfloor} m_\star(y_p)^{t-1} = \frac{1}{1-m_\star(y_p)} + O(m_\star(y_p)^{\frac{N}{2}}),$$

and where in the second equality we used (9.45). Summing up for $p \in \{1,\, 2\}$, the two terms involving the square bracket cancel out with each other. Hence, we conclude that

$$\sum_{k=\lfloor N/2 \rfloor +1}^{N-1} \Big| \sum_{p=1}^{2} (\operatorname{div} \phi_{p,\, k})(\zeta_k^{x_1,\, x_2}) \Big| \le \frac{N}{2} \times \sum_{p=1}^{2} O\Big(\frac{m_\star(y_p)^{\frac{N}{2}}}{N}\Big) = O(m_\star(y_p)^{\frac{N}{2}}) = o(1).$$

Therefore, it remains to prove that

$$\sum_{k=1}^{\lfloor N/2 \rfloor} \Big| \sum_{p=1}^{2} (\operatorname{div} \phi_{p,\, k})(\zeta_k^{x_1,\, x_2}) \Big| = o(1).$$

By a similar calculation, we obtain that the left-hand side is bounded by

$$\sum_{k=1}^{\lfloor N/2 \rfloor} \sum_{p=1}^{2} O\Big(\frac{m_\star(y_p)^{k-1}}{N}\Big) = O\Big(\frac{1}{N}\Big) = o(1).$$

Thus, we conclude the proof. □

9.5.4 Proof of Proposition 9.5.1

We are now ready to prove Proposition 9.5.1.

Proof of Proposition 9.5.1. By Lemmas 9.5.3 and 9.5.4, we have

$$\frac{1}{\|\psi_{\text{test}}\|^2}\Big[\sum_{\eta\in\mathcal{H}_N\setminus\mathcal{E}_N^\star} h_{\mathcal{E}_N^{x_1},\,\mathcal{E}_N^{x_2}}(\eta)(\operatorname{div}\psi_{\text{test}})(\eta)\Big]^2 \ge (1+o(1))\frac{d_N^2}{2N\mathfrak{R}}.$$

Therefore, we deduce from Theorem 3.2.8-(2) that

$$\operatorname{Cap}_N(\mathcal{E}_N^{x_1},\,\mathcal{E}_N^{x_2}) \ge (1+o(1))\frac{d_N^2}{2N\mathfrak{R}}.$$

This concludes the proof of Proposition 9.5.1. □

9.6 Upper bound for capacities: general case

In this section, we omit Condition 9.1.1 and extend the results of Section 9.4 to the most general setting of Theorem 9.1.4, described in Section 9.1.2. Because proofs of the assertions here are fundamentally similar to those in Section 9.4, they will be written in a brief manner.

Proposition 9.6.1 (Upper bound for capacities: general case)**.** *Assume the conditions of Theorem 9.1.4. Then, for any non-trivial partition $\{A,\,B\}$ of $[\![1,\,\kappa_\star]\!]$, the following inequality holds.*

$$\limsup_{N\to\infty}\frac{N}{d_N^2}\operatorname{Cap}_N(\mathcal{E}_N^{(2)}(A),\,\mathcal{E}_N^{(2)}(B)) \le \frac{1}{|S_\star|}\sum_{i\in A}\sum_{j\in B}\frac{1}{\mathfrak{R}_{i,\,j}}.$$

Remark 9.6.2. In Proposition 9.6.1, it is crucial to have $A\cup B=[\![1,\,\kappa_\star]\!]$; if $A\cup B\subsetneq[\![1,\,\kappa_\star]\!]$, then the equilibrium potential is significantly more complicated. Moreover, we remark that if $\mathfrak{R}_{i,\,j}=\infty$ for all $i\in A$ and $j\in B$, then

Proposition 9.6.1 asserts that

$$\mathrm{Cap}_N(\mathcal{E}_N^{(2)}(A),\, \mathcal{E}_N^{(2)}(B)) = o\Big(\frac{d_N^2}{N}\Big).$$

This equality indicates that we do not observe metastable transitions in the time scale N/d_N^2. Therefore, in this case, we expect that yet another time scale is required to observe the metastable transitions. This is conjectured to be N^2/d_N^3 in [15].

9.6.1 Preliminary notions

Once more, we define $m_\star = \max_{p=1}^{\kappa_0} m_\star(y_p) < 1$. Because there are too many subscripts in the general case, we introduce a convenient notation that helps us calculate the objects.

Notation 9.6.3. Recall (9.18); for $R \subseteq S$,

$$\mathcal{A}_N^R = \{\eta \in \mathcal{H}_N : \eta_x = 0 \text{ for all } x \in S \setminus R\}.$$

For the case $R = \{x_{i,n},\, y_p,\, x_{j,m}\}$, where $i \neq j$, $n \in [\![1,\, \mathfrak{n}(i)]\!]$, $m \in [\![1,\, \mathfrak{n}(j)]\!]$, and $p \in [\![1,\, \kappa_0]\!]$, we will simply denote $\eta \in \mathcal{A}_N^{\{x_{i,\,n},\, y_p,\, x_{j,\,m}\}}$ by $\eta = (\eta_{x_{i,\,n}},\, \eta_{y_p})_{i,\,n,\,p,\,j,\,m}$. For example, if $\eta \in \mathcal{A}_N^{\{x_{1,\,1},\, y_5,\, x_{3,\,2}\}}$ such that $\eta_{x_{1,\,1}} = N-3$, $\eta_{y_5} = 1$, and $\eta_{x_{3,\,2}} = 2$, we write $\eta = (N-3,\, 1)_{1,\,1,\,5,\,3,\,2}$.

Next, we define the following discretized version of the constant $\mathfrak{R}_{i,\,j}$ for $i,\, j \in [\![1,\, \kappa_\star]\!]$ given in (9.9):

$$\mathfrak{R}_{i,\,j}^N = \sum_{t=1}^{N} \frac{1}{\sum_{n=1}^{\mathfrak{n}(i)} \sum_{m=1}^{\mathfrak{n}(j)} \sum_{p=1}^{\kappa_0} \frac{1}{(1-m_\star(y_p))(\frac{N-t}{r(x_{i,\,n},\, y_p)} + \frac{t-1}{r(x_{j,\,m},\, y_p)})}}.$$

As in the special case in Section 9.4.1, we write $\mathfrak{R}_{i,\,j}^N = \infty$ if $r(x_{i,\,n},\, y_p) r(x_{j,\,m},\, y_p) = 0$ for all $n \in [\![1,\, \mathfrak{n}(i)]\!]$, $m \in [\![1,\, \mathfrak{n}(j)]\!]$, and $p \in [\![1,\, \kappa_0]\!]$. Clearly, we have

$N^{-2}\mathfrak{R}^N_{i,j} \to \mathfrak{R}_{i,j}$ as N tends to infinity. Moreover, define

$$I = \{(i,\, j) \in [\![1,\, \kappa_\star]\!] \times [\![1,\, \kappa_\star]\!] : i \neq j \text{ and } \mathfrak{R}_{i,j} < \infty\},$$

and for $i,\, j \in [\![1,\, \kappa_\star]\!]$ with $n \in [\![1,\, \mathfrak{n}(i)]\!]$ and $m \in [\![1,\, \mathfrak{n}(j)]\!]$,

$$P_{i,n,j,m} = \{p : r(x_{i,n},\, y_p) r(x_{j,m},\, y_p) > 0\}$$

and

$$Q_{i,n,j,m} = \{p : r(x_{i,n},\, y_p) + r(x_{j,m},\, y_p) > 0\}.$$

For example, $(i,\, j) \in I$ if and only if $r(x_{i,n},\, y_p) r(x_{j,m},\, y_p) > 0$ for some n, m, and p, which is also equivalent to

$$\bigcup_{n=1}^{\mathfrak{n}(i)} \bigcup_{m=1}^{\mathfrak{n}(j)} P_{i,n,j,m} \neq \emptyset.$$

Moreover, we have $P_{i,n,j,m} \subseteq Q_{i,n,j,m}$. Finally, we define

$$\mathcal{U}_N = \bigcup_{i,\, j \in [\![1,\, \kappa_\star]\!]} \bigcup_{n=1}^{\mathfrak{n}(i)} \bigcup_{m=1}^{\mathfrak{n}(j)} \bigcup_{p=1}^{\kappa_0} \mathcal{A}_N^{\{x_{i,n},\, y_p,\, x_{j,m}\}} \quad \text{and} \quad \mathcal{V}_N = \mathcal{H}_N \setminus \mathcal{U}_N. \tag{9.62}$$

9.6.2 Construction of test function $f^A_{\mathbf{test}}$

In this subsection, we define a test function $f = f^A_{\text{test}}$ on $\mathcal{H}_N$, which approximates the equilibrium potential $h_{\mathcal{E}_N^{(2)}(A),\, \mathcal{E}_N^{(2)}(B)}$. *This procedure is a natural extension of the definition in Section 9.4.2.*

- First, we define f on $\mathcal{E}_N(S)$:

  $$f(\xi_N^{x_{i,n}}) = 1 \text{ for } i \in A, \quad f(\xi_N^z) = 0 \text{ for } z \in S \setminus \{x_{i,n} : i \in A \text{ and } n \in [\![1,\, \mathfrak{n}(i)]\!]\}, \tag{9.63}$$

  such that we have $f\big|_{\mathcal{E}_N^{(2)}(A)} = 1$ and $f\big|_{\mathcal{E}_N^{(2)}(B)} = 0$.

- Second, we define f on $\mathcal{A}_N^{\{x_{i,n},\, y_p\}}$ for $i \in [\![1,\, \kappa_\star]\!]$, $n \in [\![1,\, \mathfrak{n}(i)]\!]$, and $p \in [\![1,\, \kappa_0]\!]$ by

$$f(\eta) = f(\xi_N^{x_{i,n}}) \quad \text{if } \eta_{x_{i,n}} \in [\![1,\, N-1]\!]. \tag{9.64}$$

- Next, we define f on $\mathcal{U}_N$, i.e., on $\mathcal{A}_N^{\{x_{i,n},\, y_p,\, x_{j,m}\}}$ for $i,\, j \in [\![1,\, \kappa_\star]\!]$, $n,\, m \geq 1$, and $p \in [\![1,\, \kappa_0]\!]$. This part is the main technical obstacle in the definition of f_{test}^A. There are four types, **(U1)** through **(U4)**.

(U1) If $(i,\, j) \in I$ and $n,\, m \geq 1$ with $p \in Q_{i,n,j,m}$, then for $\ell \in [\![0,\, N-2]\!]$ and $k \in [\![1,\, N-\ell-1]\!]$,

$$f((k,\, \ell)_{i,n,p,j,m}) = \frac{1}{\mathfrak{R}_{i,j}^N} \big[K_{i,n,p,j,m}^{k,\ell} f(\xi_N^{x_{i,n}}) + (\mathfrak{R}_{i,j}^N - K_{i,n,p,j,m}^{k,\ell}) f(\xi_N^{x_{j,m}}) \big], \tag{9.65}$$

where

$$K_{i,n,p,j,m}^{k,\ell} = \sum_{t=1}^{k} \frac{\frac{N-t}{r(x_{i,n},\, y_p)} \big/ \big(\frac{N-t}{r(x_{i,n},\, y_p)} + \frac{t-1}{r(x_{j,m},\, y_p)} \big)}{\sum_{\widetilde{n}=1}^{\mathfrak{n}(i)} \sum_{\widetilde{m}=1}^{\mathfrak{n}(j)} \sum_{q=1}^{\kappa_0} \frac{1}{(1-m_\star(y_q))(\frac{N-t}{r(x_{i,\widetilde{n}},\, y_q)} + \frac{t-1}{r(x_{j,\widetilde{m}},\, y_q)})}} + \sum_{t=1}^{k+\ell} \frac{\frac{t-1}{r(x_{j,m},\, y_p)} \big/ \big(\frac{N-t}{r(x_{i,n},\, y_p)} + \frac{t-1}{r(x_{j,m},\, y_p)} \big)}{\sum_{\widetilde{n}=1}^{\mathfrak{n}(i)} \sum_{\widetilde{m}=1}^{\mathfrak{n}(j)} \sum_{q=1}^{\kappa_0} \frac{1}{(1-m_\star(y_q))(\frac{N-t}{r(x_{i,\widetilde{n}},\, y_q)} + \frac{t-1}{r(x_{j,\widetilde{m}},\, y_q)})}}.$$

One may switch between $(i,\, n)$ and $(j,\, m)$ to verify that (9.65) is well defined. By substituting $\ell = 0$, one can verify that (9.65) is well defined on $\mathcal{A}_N^{\{x_{i,n},\, x_{j,m}\}}$. The fractions inside summations are well defined, as $(i,\, j) \in I$ implies that the common denominator is strictly positive. The numerators of the fractions must be understood naturally if $r(x_{i,n},\, y_p) r(x_{j,m},\, y_p) = 0$. Indeed, if e.g., $r(x_{i,n},\, y_p) > 0$ and $r(x_{j,m},\, y_p) = 0$, then the first one ("$0/\infty$") is 0, and the second one ("∞/∞") is 1.

(U2) If $(i,\, j) \in I$ and $n,\, m \geq 1$ with $p \notin Q_{i,n,j,m}$, then for $\ell \in [\![0,\, N-2]\!]$

and $k \le [\![1,\, N-\ell-1]\!]$,

$$f((k,\ell)_{i,n,p,j,m}) = \frac{1}{\mathfrak{R}^N_{i,j}}\big[L^{k,\ell}_{i,n,p,j,m} f(\xi_N^{x_{i,n}}) + (\mathfrak{R}^N_{i,j} - L^{k,\ell}_{i,n,p,j,m}) f(\xi_N^{x_{j,m}})\big], \tag{9.66}$$

where

$$L^{k,\ell}_{i,n,p,j,m} = \sum_{t=1}^{k} \frac{(N-t)/(N-1)}{\sum_{\widetilde{n}=1}^{\mathfrak{n}(i)} \sum_{\widetilde{m}=1}^{\mathfrak{n}(j)} \sum_{q=1}^{\kappa_0} \frac{1}{(1-m_\star(y_q))(\frac{N-t}{r(x_{i,\widetilde{n}},\, y_q)} + \frac{t-1}{r(x_{j,\widetilde{m}},\, y_q)})}} + \sum_{t=1}^{k+\ell} \frac{(t-1)/(N-1)}{\sum_{\widetilde{n}=1}^{\mathfrak{n}(i)} \sum_{\widetilde{m}=1}^{\mathfrak{n}(j)} \sum_{q=1}^{\kappa_0} \frac{1}{(1-m_\star(y_q))(\frac{N-t}{r(x_{i,\widetilde{n}},\, y_q)} + \frac{t-1}{r(x_{j,\widetilde{m}},\, y_q)})}}.$$

Note that (9.66) is well defined on $\mathcal{A}_N^{\{x_{i,n},\, x_{j,m}\}}$ and consistent with (9.65). One can substitute $\ell = 0$ to verify the equality.

(U3) If $(i,\, j) \notin I$ and $n,\, m \ge 1$ with $p \in Q_{i,n,j,m} \setminus P_{i,n,j,m}$, say $r(x_{i,n},\, y_p) > 0$ and $r(x_{j,m},\, y_p) = 0$, then for $\ell \in [\![0,\, N-2]\!]$ and $k \in [\![1,\, N-\ell-1]\!]$,

$$f((k,\, \ell)_{i,n,p,j,m}) = \frac{1}{N}\big[(k+\ell) f(\xi_N^{x_{i,n}}) + (N-\ell-k) f(\xi_N^{x_{j,m}})\big]. \tag{9.67}$$

As done previously, one can substitute $\ell = 0$ to verify that (9.67) is well defined on $\mathcal{A}_N^{\{x_{i,n},\, x_{j,m}\}}$.

(U4) If $(i,\, j) \notin I$ and $n,\, m \ge 1$ with $p \notin Q_{i,n,j,m}$, then for $\ell \in [\![0,\, N-2]\!]$ and $k \in [\![1,\, N-\ell-1]\!]$,

$$f((k,\, \ell)_{i,n,p,j,m}) = \frac{1}{N}\Big[\Big(k + \frac{\ell}{2}\Big) f(\xi_N^{x_{i,n}}) + \Big(N - k - \frac{\ell}{2}\Big) f(\xi_N^{x_{j,m}})\Big]. \tag{9.68}$$

(9.68) is well defined on $\mathcal{A}_N^{\{x_{i,n},\, x_{j,m}\}}$and consistent with (9.67); substitute $\ell = 0$.

- Finally, we define f on $\mathcal{V}_N$. Assume $\eta \in \mathcal{V}_N$. There are three types,

(V1), **(V2)**, and **(V3)** denoted by $\mathcal{V}_N^1$, $\mathcal{V}_N^2$, and $\mathcal{V}_N^3$, respectively, such that

$$\mathcal{V}_N = \mathcal{V}_N^1 \cup \mathcal{V}_N^2 \cup \mathcal{V}_N^3. \tag{9.69}$$

(V1) If $\eta \in \mathcal{A}_N^{\{x_{i,n},\, x_{i,\widetilde{n}},\, y_p\}}$ for some $i \in [\![1,\, \kappa_\star]\!]$, $n,\, \widetilde{n} \in [\![1,\, \mathfrak{n}(i)]\!]$, and $p \in [\![1,\, \kappa_0]\!]$: Because $\eta \in \mathcal{V}_N$, we necessarily have $\eta_{x_{i,n}} \ge 1$ and $\eta_{x_{i,\widetilde{n}}} \ge 1$. We define

$$f(\eta) = f(\xi_N^{x_{i,n}}) = f(\xi_N^{x_{i,\widetilde{n}}}). \tag{9.70}$$

The meaning of this definition is that we do not distinguish members of S_i for each $i \in [\![1,\, \kappa_\star]\!]$ in the second time scale $\theta_{N,2} = N/d_N^2$. Hence, configurations of this type must be defined in a same manner as in (9.64).

(V2) If $\eta \in \mathcal{A}_N^{\{x_{i,n},\, x_{i,\widetilde{n}},\, x_{j,m}\}} \setminus \mathcal{A}_N^{\{x_{i,n},\, x_{i,\widetilde{n}}\}}$ for some $i,\, j \in [\![1,\, \kappa_\star]\!]$, $n,\, \widetilde{n} \in [\![1,\, \mathfrak{n}(i)]\!]$, and $m \in [\![1,\, \mathfrak{n}(j)]\!]$: As $\eta \in \mathcal{V}_N$, we necessarily have $\eta_{x_{i,n}} \ge 1$, $\eta_{x_{i,\widetilde{n}}} \ge 1$, and $\eta_{x_{j,m}} \ge 1$. We obtain a novel configuration $\widetilde{\eta} \in \mathcal{A}_N^{\{x_{i,\, n\wedge\widetilde{n}},\, x_{j,m}\}}$ by concentrating the particles in $\{x_{i,n},\, x_{i,\widetilde{n}}\}$ to $x_{i,\, n\wedge\widetilde{n}}$. Here, $n \wedge \widetilde{n} = \min\{n,\, \widetilde{n}\}$. Then, we define

$$f(\eta) = f(\widetilde{\eta}). \tag{9.71}$$

Like **(V1)**, the meaning here is that we do not distinguish η and $\widetilde{\eta}$ in $\theta_{N,2} = N/d_N^2$.

(V3) Otherwise, we define

$$f(\eta) = \begin{cases} 1 & \text{if } \displaystyle\sum_{n=1}^{\mathfrak{n}(i)} \eta_{x_{i,n}} > \lfloor N/2 \rfloor \text{ for some } i \in A, \\ 0 & \text{if } \displaystyle\sum_{n=1}^{\mathfrak{n}(i)} \eta_{x_{i,n}} \le \lfloor N/2 \rfloor \text{ for all } i \in A. \end{cases} \tag{9.72}$$

- By construction, we have $0 \le f(\eta) \le 1$ for all $\eta \in \mathcal{H}_N$.

We divide the Dirichlet form into four parts:

$$D_N(f) = \Sigma_1(f) + \Sigma_2(f) + \Sigma_3(f) + \Sigma_4(f).$$

- The first part $\Sigma_1(f)$ consists of movements inside $\mathcal{A}_N^{\{x_{i,\,n},\, y_p,\, x_{j,\,m}\}}$ for all $i,\, j \in [\![1,\, \kappa_\star]\!]$, $n \in [\![1,\, \mathfrak{n}(i)]\!]$, $m \in [\![1,\, \mathfrak{n}(j)]\!]$, and $p \in [\![1,\, \kappa_0]\!]$.
- The second part $\Sigma_2(f)$ consists of movements between the set differences of two distinct $\mathcal{A}_N^{\{x_{i,\,n},\, y_p,\, x_{j,\,m}\}}$-type sets for same $i,\, j,\, n,\, m,\, p$.
- The third part $\Sigma_3(f)$ consists of movements between $\mathcal{U}_N$ and $\mathcal{V}_N$.
- The last part $\Sigma_4(f)$ consists of movements inside $\mathcal{V}_N$.

9.6.3 Main contribution of Dirichlet form

In this subsection, we calculate $\Sigma_1(f)$, which is the main ingredient of $D_N(f)$.

Lemma 9.6.4. *Under the conditions of Theorem 9.1.4, it holds that*

$$\Sigma_1(f) \le \frac{d_N^2}{|S_\star| N} \Big[\sum_{i \in A} \sum_{j \in B} \frac{1}{\mathfrak{R}_{i,\,j}} + o(1) \Big].$$

Proof. We write down all movements inside $\mathcal{A}_N^{\{x_{i,\,n},\, y_p,\, x_{j,\,m}\}}$ and sum it up for all $i,\, j,\, n,\, m,\, p$. Namely,

$$\Sigma_1(f) \le \frac{1}{2} \sum_{i,\, j \in [\![1,\, \kappa_\star]\!]} \sum_{n,\, m,\, p} \sum_{\eta \in \mathcal{A}_N^{\{x_{i,\,n},\, y_p,\, x_{j,\,m}\}}} \mu_N(\eta) \times$$

$$\big[r_N(\eta,\, \sigma^{x_{i,\,n},\, y_p} \eta) \{ f(\sigma^{x_{i,\,n},\, y_p} \eta) - f(\eta) \}^2 + r_N(\eta,\, \sigma^{x_{j,\,m},\, y_p} \eta) \{ f(\sigma^{x_{j,\,m},\, y_p} \eta) - f(\eta) \}^2 \big]$$

is the desired equation. The only overlapping terms on the right-hand side above are movements along $\mathcal{A}_N^{\{x_{i,\,n},\, y_p\}}$ for $i \in [\![1,\, \kappa_\star]\!]$, $n \in [\![1,\, \mathfrak{n}(i)]\!]$, and

$p \in [\![1,\, \kappa_0]\!]$. In fact, by (9.64), these terms have an exponentially small effect on the entire summation. Thus, the inequality used above is actually sharp. By (8.4) and (8.5), the right-hand side is asymptotically equal to

$$\frac{d_N N}{2|S_\star|} \sum_{i,\, j \in [\![1,\, \kappa_\star]\!]} \sum_{n,\, m} \sum_{p \in Q_{i,\, n,\, j,\, m}} \sum_{\ell=0}^{N-1} \sum_{k=0}^{N-\ell-1} m_\star(y_p)^\ell \times$$
$$\big[w_N(N-\ell-k-1) r(x_{i,\, n},\, y_p) \{ f((k,\, \ell+1)_{i,\, n,\, p,\, j,\, m}) - f((k+1,\, \ell)_{i,\, n,\, p,\, j,\, m}) \}^2$$
$$+ w_N(k) r(x_{j,\, m},\, y_p) \{ f((k,\, \ell+1)_{i,\, n,\, p,\, j,\, m}) - f((k,\, \ell)_{i,\, n,\, p,\, j,\, m}) \}^2 \big].$$

We only need to consider $p \in Q_{i,\, n,\, j,\, m}$, as otherwise $r(x_{i,\, n},\, y_p) = r(x_{j,\, m},\, y_p) = 0$. Next, if $p \in Q_{i,\, n,\, j,\, m} \setminus P_{i,\, n,\, j,\, m}$, then the terms inside the bracket vanish due to (9.65) and (9.67). If $i,\, j \in A$ or $i,\, j \in B$, then by (9.64), (9.65), and (9.67), f remains constant unless $\ell = N-1$; in which case the summation is of order $O(d_N N m_\star^N)$. Gathering the preceding observations, the last formula is asymptotically equal to

$$\frac{d_N N}{|S_\star|} \sum_{(i,\, j) \in I \cap (A \times B)} \sum_{n,\, m} \sum_{p \in P_{i,\, n,\, j,\, m}} \sum_{\ell=0}^{N-1} \sum_{k=0}^{N-\ell-1} m_\star(y_p)^\ell \times$$
$$\big[w_N(N-\ell-k-1) r(x_{i,\, n},\, y_p) \{ f((k,\, \ell+1)_{i,\, n,\, p,\, j,\, m}) - f((k+1,\, \ell)_{i,\, n,\, p,\, j,\, m}) \}^2$$
$$+ w_N(k) r(x_{j,\, m},\, y_p) \{ f((k,\, \ell+1)_{i,\, n,\, p,\, j,\, m}) - f((k,\, \ell)_{i,\, n,\, p,\, j,\, m}) \}^2 \big].$$

The rest of the proof is almost identical to that of Lemma 9.4.2; we obtain

$$\Sigma_1(f) \le \frac{d_N^2}{|S_\star| N} \Big[\sum_{(i,\, j) \in I \cap (A \times B)} \frac{1}{\mathfrak{R}_{i,\, j}} + o(1) \Big].$$

Because $\mathfrak{R}_{i,\, j} = \infty$ if $(i,\, j) \notin I$, the last formula is exactly what we expect. $\square$

9.6.4 Remainder of Dirichlet form

Here, we deal with the remaining terms in the Dirichlet form, $\Sigma_2(f)$, $\Sigma_3(f)$, and $\Sigma_4(f)$. Lemma 9.6.5 deals with $\Sigma_2(f)$.

Lemma 9.6.5. *Under the conditions of Theorem 9.1.4, it holds that*

$$\Sigma_2(f) = O\Big(\frac{d_N^3 \log N}{N^2}\Big) = o\Big(\frac{d_N^2}{N}\Big).$$

Proof. Recalling that $\Sigma_2(f)$ consists of dynamics between the set differences of two distinct $\mathcal{A}_N^{\{x_{i,n},\, y_p,\, x_{j,m}\}}$-type sets, there are two such types of movements.

(Case 1) The first case is represented when a sole particle moves between $x_{i,n}$ and $x_{i,\widetilde{n}}$. More specifically, this is written as

$$\frac{1}{2}\sum_{i,\,j\in[\![1,\,\kappa_\star]\!]}\sum_{n,\,\widetilde{n},\,m,\,p}\sum_{\ell=0}^{N-1}\mu_N((1,\,\ell)_{i,\,n,\,p,\,j,\,m})\times \\ d_N r(x_{i,\,n},\, x_{i,\,\widetilde{n}})\{f((1,\,\ell)_{i,\,\widetilde{n},\,p,\,j,\,m}) - f((1,\,\ell)_{i,\,n,\,p,\,j,\,m})\}^2. \tag{9.73}$$

If $\ell = 0$, then this vanishes by (9.65) and (9.67). If $\ell = N-1$, then this vanishes by (9.63) and (9.64). If $\ell \in [\![1,\, N-2]\!]$, then

$$f((1,\,\ell)_{i,\,\widetilde{n},\,p,\,j,\,m}) - f((1,\,\ell)_{i,\,n,\,p,\,j,\,m}) = \begin{cases} \ell \times O(1/N) & \text{if } (i,\,j) \in I, \\ 0 & \text{if } (i,\,j) \notin I, \end{cases}$$

by (9.65), (9.66), (9.67), and (9.68). Therefore, (9.73) is bounded from above by

$$C\sum_{i,\,j\in[\![1,\,\kappa_\star]\!]}\sum_{n,\,\widetilde{n},\,m,\,p}\sum_{\ell=1}^{N-2}\frac{N d_N^3 m_\star^\ell}{\ell(N-\ell-1)}\ell^2\frac{1}{N^2} = O\Big(\frac{d_N^3}{N^2}\Big). \tag{9.74}$$

(Case 2) The second case is represented when a sole particle moves between

y_p and y_q. This case is identical to Lemma 9.4.3, which is bounded by

$$C\sum_{i,\,j\in[\![1,\,\kappa_\star]\!]}\sum_{n,\,m}\sum_{p,\,q\in[\![1,\,\kappa_0]\!]}\sum_{k=1}^{N-2}\frac{Nd_N^3m_\star}{k(N-k-1)}\frac{1}{N^2}=O\Big(\frac{d_N^3\log N}{N^2}\Big). \tag{9.75}$$

Gathering the cases, we have by (9.74) and (9.75) that $\Sigma_2(f)=O(d_N^3N^{-2}\log N)$. This concludes the proof. □

Next, we consider $\Sigma_3(f)$.

Lemma 9.6.6. *Under the conditions of Theorem 9.1.4, it holds that*

$$\Sigma_3(f)=O(d_N^2m_\star^{\frac{N}{3}}+d_N^3N\log N)=o\Big(\frac{d_N^2}{N}\Big).$$

Proof. We formulate

$$\Sigma_3(f)=\sum_{\eta\in\mathcal{U}_N}\sum_{\zeta\in\mathcal{V}_N}\mu_N(\eta)r_N(\eta,\,\zeta)\{f(\zeta)-f(\eta)\}^2.$$

We divide this into several cases depending on which subset η belongs to.

(Case 1) $\eta\in\mathcal{A}_N^{\{x_{i,\,n},\,x_{j,\,m}\}}$ for some $i,\,j\in[\![1,\,\kappa_\star]\!]$ and $n,\,m\ge 1$: In this case, the movement must occur between sites in $S_i^{(2)}$ or between sites in $S_j^{(2)}$. Otherwise, $\zeta\notin\mathcal{V}_N$. Hence, f remains unchanged by (9.64) and (9.71).

(Case 2) $\eta\in\mathcal{A}_N^{\{x_{i,\,n},\,y_p\}}\setminus\mathcal{E}_N^{x_{i,\,n}}$ for some $i\in[\![1,\,\kappa_\star]\!]$ and $n,\,p\ge 1$: We divide again by types of the particle movement.

- **(Case 2-1)** Movement from y_p into $S_i^{(2)}\setminus\{x_{i,\,n}\}$: We have $\eta_{y_p}\le N-1$. Otherwise, $\zeta\notin\mathcal{V}_N$. Hence, f remains unchanged by (9.64) and (9.70).
- **(Case 2-2)** Movement from y_p into $S\setminus(S_\star\cup\{y_p\})$: This is identical to **(Case 2-1)** of Lemma 9.4.4. We obtain the upper bound $O(d_N^2m_\star^{\frac{N}{3}})$.
- **(Case 2-3)** Movement from $x_{i,\,n}$ into $S_i^{(2)}\setminus\{x_{i,\,n}\}$: f remains unchanged by (9.64) and (9.70).

- **(Case 2-4)** Movement from $x_{i,n}$ into $S \setminus (S_\star \cup \{y_p\})$: This is same with **(Case 2-2)** of Lemma 9.4.4. We obtain the upper bound $O(d_N^2 m_\star^{\frac{N}{3}})$.

In conclusion, **(Case 2)** yields $O(d_N^2 m_\star^{\frac{N}{3}})$.

(Case 3) $\eta \in \mathcal{A}_N^{\{x_{i,n}, y_p, x_{j,m}\}} \setminus (\mathcal{A}_N^{\{x_{i,n}, x_{j,m}\}} \cup \mathcal{A}_N^{\{x_{i,n}, y_p\}} \cup \mathcal{A}_N^{\{x_{j,m}, y_p\}})$ for some $i, j \in [\![1, \kappa_\star]\!]$ and $n, m, p \geq 1$: This case is identical to **(Case 3)** of Lemma 9.4.4 that we can bound by $O(d_N^3 N \log N)$.

Summarizing all cases, we conclude that $\Sigma_3(f) = O(d_N^2 m_\star^{\frac{N}{3}} + d_N^3 N \log N)$. □

Our final aim of this subsection is $\Sigma_4(f)$.

Lemma 9.6.7. *Under the conditions of Theorem 9.1.4, it holds that*

$$\Sigma_4(f) = O(d_N^2 N \log N m_\star^{\frac{N}{2}} + d_N^3 N (\log N)^2 = o\Big(\frac{d_N^2}{N}\Big).$$

Proof. By definition, we have

$$\Sigma_4(f) = \frac{1}{2} \sum_{\eta, \zeta \in \mathcal{V}_N} \mu_N(\eta) r_N(\eta, \zeta) \{f(\zeta) - f(\eta)\}^2.$$

Recalling (9.69), we divide the summation in $\eta, \zeta \in \mathcal{V}_N$ by where η and ζ belong.

(Case 1) $\eta, \zeta \in \mathcal{V}_N^1$: f remains unchanged by (9.70).

(Case 2) $\eta, \zeta \in \mathcal{V}_N^2$: Because $\{x_{i,n}, x_{i,\tilde{n}}\}$ and $\{x_{j,m}\}$ are isolated with respect to $r(\cdot, \cdot)$, only $x_{i,n} \leftrightarrow x_{i,\tilde{n}}$ is possible. Thus, f remains unchanged by (9.65), (9.67), and (9.71).

(Case 3) One of $\{\eta, \zeta\}$ is in $\mathcal{V}_N^1$ and the other is in $\mathcal{V}_N^2$: The only possible case is when a sole particle moves between y_p and $x_{j,m}$. Thus, we formulate

$$\frac{1}{2}\sum_{i,\,j\in[\![1,\,\kappa_\star]\!]}\ \sum_{n,\,\widetilde{n}\in[\![1,\,\mathfrak{n}(i)]\!]}\ \sum_{m=1}^{\mathfrak{n}(j)}\sum_{p=1}^{\kappa_0}\sum_{k=1}^{N-2}\mu_N(\eta)d_N r(y_p,\,x_{j,m})\{f(\sigma^{y_p,\,x_{j,\,m}}\eta)-f(\eta)\}^2, \tag{9.76}$$

where η satisfies $\eta_{x_{i,\,n}}=k$, $\eta_{x_{i,\,\widetilde{n}}}=N-k-1$, and $\eta_{y_p}=1$. By (9.64), (9.65), (9.67), (9.70), and (9.71), we have

$$f(\sigma^{y_p,\,x_{j,\,m}}\eta)-f(\eta)=O\Big(\frac{1}{N}\Big).$$

Therefore, with (8.5), (9.76) is bounded from above by

$$C\sum_{k=1}^{N-2}\frac{Nd_N^3}{k(N-k-1)}\times\frac{1}{N^2}=O(d_N^3N^{-2}\log N).$$

(Case 4) One of $\{\eta,\,\zeta\}$ is in $\mathcal{V}_N^1$ and the other is in $\mathcal{V}_N^3$: Let $\eta\in\mathcal{V}_N^1$ and $\zeta\in\mathcal{V}_N^3$. If $\eta\in\mathcal{A}_N^{\{x_{i,\,n},\,x_{i,\,\widetilde{n}}\}}$, then f remains unchanged by (9.63), (9.70) and (9.72). Hence, we can bound this case from above by

$$\frac{1}{2}\sum_{i=1}^{\kappa_\star}\ \sum_{n,\,\widetilde{n}\in[\![1,\,\mathfrak{n}(i)]\!]}\ \sum_{p=1}^{\kappa_0}\sum_{\ell=1}^{N-2}\sum_{k=1}^{N-\ell-1}\mu_N(\eta)\times$$
$$\sum_{z\in\{x_{i,\,n},\,x_{i,\,\widetilde{n}},\,y_p\}}\eta_z\sum_{\widetilde{z}\notin\{x_{i,\,n},\,x_{i,\,\widetilde{n}},\,y_p\}}d_N r(z,\,\widetilde{z})\{f(\sigma^{z,\,\widetilde{z}}\eta)-f(\eta)\}^2,$$

where $\eta_{x_{i,\,n}}=k$, $\eta_{x_{i,\,\widetilde{n}}}=N-\ell-k$, and $\eta_{y_p}=\ell$ in the last line. Because we have $\sum_{z\in\{x_{i,\,n},\,x_{i,\,\widetilde{n}},\,y_p\}}\eta_z=N$, we can bound this with (8.5) by

$$C\sum_{\ell=1}^{N-2}\sum_{k=1}^{N-\ell-1}\frac{Nd_N^2}{k\ell(N-\ell-k)}m_\star^\ell Nd_N=O(d_N^3N\log N).$$

(Case 5) One of $\{\eta, \zeta\}$ is in $\mathcal{V}_N^2$ and the other is in $\mathcal{V}_N^3$: We can bound from above by

$$\frac{1}{2} \sum_{i, j \in [\![1, \kappa_\star]\!]} \sum_{n, \widetilde{n} \in [\![1, \mathfrak{n}(i)]\!]} \sum_{m=1}^{\mathfrak{n}(j)} \sum_{k=1}^{N-2} \sum_{\ell=1}^{N-k-1} \mu_N(\eta) \times \sum_{z \in \{x_{i,n}, x_{i,\widetilde{n}}, x_{j,m}\}} \eta_z \sum_{\widetilde{z} \notin \{x_{i,n}, x_{i,\widetilde{n}}, x_{j,m}\}} d_N r(z, \widetilde{z}) \{f(\sigma^{z, \widetilde{z}} \eta) - f(\eta)\}^2,$$

where $\eta_{x_{i,n}} = k$, $\eta_{x_{i,\widetilde{n}}} = N - \ell - k$, and $\eta_{x_{j,m}} = \ell$ in the last line. Because we have $\sum_{z \in \{x_{i,n}, x_{i,\widetilde{n}}, x_{j,m}\}} \eta_z = N$, we can bound this with (8.5) by

$$C \sum_{k=1}^{N-2} \sum_{\ell=1}^{N-k-1} \frac{N d_N^2}{k\ell(N-\ell-k)} \times N d_N = O(d_N^3 N (\log N)^2).$$

(Case 6) $\eta, \zeta \in \mathcal{V}_N^3$: This case is similar to Lemma 9.4.5. We note (9.72) to write

$$\begin{aligned} \Sigma_4(f) &= \sum_{i \in A} \sum_{\eta \in \mathcal{V}_N^3 : \sum_{\widetilde{n}} \eta_{x_{i,\widetilde{n}}} = \lfloor N/2 \rfloor + 1} \mu_N(\eta) \sum_{n=1}^{\mathfrak{n}(i)} \sum_{p=1}^{\kappa_0} r_N(\eta, \sigma^{x_{i,n}, y_p} \eta) \\ &= \sum_{i \in A} \sum_{\eta \in \mathcal{V}_N^3 : \sum_{\widetilde{n}} \eta_{x_{i,\widetilde{n}}} = \lfloor N/2 \rfloor + 1} \mu_N(\eta) \sum_{n=1}^{\mathfrak{n}(i)} \eta_{x_{i,n}} \sum_{p=1}^{\kappa_0} (d_N + \eta_{y_p}) r(x_{i,n}, y_p). \end{aligned} \tag{9.77}$$

Now, we fix $i \in A$ and divide the summation with respect to η in the last line by the non-empty sites. As we already have $0 < \sum_{\widetilde{n}} \eta_{x_{i,\widetilde{n}}} = \lfloor N/2 \rfloor + 1 < N$, at least 3 sites must be non-empty.

- **(Case 6-1)** One is in $S_i^{(2)}$ and two are in $S \setminus S_\star$: This is identical to **(Case 1)** of Lemma 9.4.5; it is bounded by $O(d_N^2 N \log N m_\star^{\frac{N}{2}})$.
- **(Case 6-2)** Two are in $S_i^{(2)}$ and one is in $S \setminus S_\star$: There are $\lfloor (N-1)/2 \rfloor$

particles on $S \setminus S_\star$; hence, similarly to **(Case 6-1)**, the summation is of order $O(d_N^2 N \log N m_\star^{\frac{N}{2}})$.

- **(Case 6-3)** One is in $S_i^{(2)}$ and two are in $S_\star \setminus S_i^{(2)}$: Labeling the non-empty sites as $x_{i,n}$, $x_{j,m}$, and $x_{\widetilde{j},\widetilde{m}}$, it is asymptotically equivalent to

$$\sum_{j:\,j\neq i}\sum_{\widetilde{j}:\,\widetilde{j}\neq i}\sum_{n,\,m,\,\widetilde{m}}\sum_{\ell=1}^{\lfloor (N-1)/2\rfloor-1}\frac{Nd_N^2}{|S_\star|}\frac{1}{\ell(\lfloor\frac{N-1}{2}\rfloor-\ell)}\sum_{p=1}^{\kappa_0}d_N r(x_{i,n},\,y_p)$$
$$\le C\sum_{\ell=1}^{\lfloor (N-1)/2\rfloor-1}\frac{Nd_N^3}{\ell(\lfloor\frac{N-1}{2}\rfloor-\ell)}=O(d_N^3\log N).$$

- **(Case 6-4)** Two are in $S_i^{(2)}$ and one is in $S_\star \setminus S_i^{(2)}$: Labeling the non-empty sites as $x_{i,n}$, $x_{i,\widetilde{n}}$, and $x_{j,m}$, it is bounded by

$$C\sum_{j:\,j\neq i}\sum_{n,\,\widetilde{n}\in[\![1,\,\mathfrak{n}(i)]\!]}\sum_{m}\sum_{\ell=1}^{\lfloor N/2\rfloor}\frac{N}{d_N}\frac{d_N^3}{\ell(\lfloor\frac{N}{2}\rfloor+1-\ell)}\cdot d_N$$
$$=O(d_N^3)\sum_{\ell=1}^{\lfloor N/2\rfloor}\frac{N}{\ell(\lfloor\frac{N}{2}\rfloor+1-\ell)}=O(d_N^3\log N).$$

- **(Case 6-5)** At least four sites are non-empty: This case is similar to **(Case 2)** of Lemma 9.4.5. Using $\sum_{p=1}^{\kappa_0}(d_N+\eta_{y_p})r(x_{i,n},\,y_p)\le CN$, the summation is bounded by

$$CN^2\sum_{\substack{\eta\in\mathcal{V}_N^3:\,\sum_{\widetilde{n}}\eta_{x_{i,\widetilde{n}}}=\lfloor N/2\rfloor+1\\ \text{and }\eta\text{ has at least 4 non-empty sites}}}\mu_N(\eta)$$
$$\le\frac{CN^3}{d_N}\sum_{\substack{\eta\in\mathcal{V}_N^3:\,\sum_{\widetilde{n}}\eta_{x_{i,\widetilde{n}}}=\lfloor N/2\rfloor+1\\ \text{and }\eta\text{ has at least 4 non-empty sites}}}\prod_{z\in S}w_N(\eta_z).$$

In the inequality above, we employ $m_\star \le 1$. We divide S into $S_i^{(2)}$ and $S \setminus S_i^{(2)}$. Then, the last line is asymptotically equivalent to

$$C\frac{N^3}{d_N}\sum_{\substack{\alpha,\,\beta\ge1:\\ 4\le\alpha+\beta\le|S|}}\Big[\Big(\sum_{\substack{\zeta\in\mathcal{H}_{\lfloor N/2\rfloor+1,\,S_i^{(2)}}:\\ \zeta\text{ has }\alpha\text{ non-empty sites}}}\prod_{z:\,\zeta_z\ge1}\frac{d_N}{\zeta_z}\Big)\Big(\sum_{\substack{\widetilde{\zeta}\in\mathcal{H}_{\lfloor (N-1)/2\rfloor,\,S\setminus S_i^{(2)}}:\\ \widetilde{\zeta}\text{ has }\beta\text{ non-empty sites}}}\prod_{\widetilde{z}:\,\widetilde{\zeta}_{\widetilde{z}}\ge1}\frac{d_N}{\widetilde{\zeta}_{\widetilde{z}}}\Big)\Big].$$

Here, $\mathcal{H}_{M,\,R}$ denotes the set of configurations on R with M particles. By Lemma 10.8.1, and replacing $a=\alpha-1$ and $b=\beta-1$, this is bounded by

$$\begin{aligned}&Cd_NN^3\sum_{\substack{a,\,b\in\mathbb{N}:\\ 2\le a+b\le|S|-2}}d_N^{a+b}\frac{(3\log(\lfloor N/2\rfloor+2))^a}{\lfloor\frac{N}{2}\rfloor+1}\frac{(3\log(\lfloor (N-1)/2\rfloor+1))^b}{\lfloor\frac{N-1}{2}\rfloor}\\ &\le Cd_NN\sum_{a,\,b\in\mathbb{N}:\,a+b\ge2}(d_N\log N)^{a+b}.\end{aligned}$$

The last displayed term is calculated via $c=a+b$ as

$$Cd_NN\sum_{c=2}^{\infty}(c{+}1)(d_N\log N)^c = O(d_NN)\times O((d_N\log N)^2) = O(d_N^3N(\log N)^2).$$

Therefore, collecting all above cases and (9.77),

$$\Sigma_4(f) = O(d_N^2N\log N m_\star^{\frac{N}{2}} + d_N^3N(\log N)^2).$$

This completes the proof of Lemma 9.6.7. □

9.6.5 Proof of Proposition 9.6.1

Now, we are in position to prove Proposition 9.6.1.

Proof of Proposition 9.6.1. By Lemmas 9.6.4, 9.6.5, 9.6.6, and 9.6.7,

$$D_N(f_{\text{test}}^A) \le \frac{d_N^2}{|S_\star|N}\sum_{i\in A}\sum_{j\in B}\frac{1}{\mathfrak{R}_{i,\,j}} + o\Big(\frac{d_N^2}{N}\Big) + O(d_N^2 m_\star^{\frac{N}{3}}) + O(d_N^3 N(\log N)^2).$$

Sending $N \to \infty$, as $\lim_{N\to\infty} d_N N^2(\log N)^2 = 0$ and d_N decays subexponentially, we have

$$\limsup_{N\to\infty}\frac{N}{d_N^2}D_N(f_{\text{test}}^A) \le \frac{1}{|S_\star|}\sum_{i\in A}\sum_{j\in B}\frac{1}{\mathfrak{R}_{i,\,j}}.$$

Therefore, by Theorem 3.2.5, we obtain the desired result. □

9.7 Lower bound for capacities: general case

In this section, we establish the lower bound for the capacities in the most general setting given in Section 9.1.2. The following proposition explains the result. The proofs in this section will be stated concisely.

Proposition 9.7.1 (Lower bound for capacities: general case)**.** *Assume the conditions of Theorem 9.1.4. Suppose that* $\{a,\, b\}$ *is a non-trivial partition* $[\![1,\,\kappa_\star]\!]$*. Then, the following inequality holds.*

$$\liminf_{N\to\infty}\frac{N}{d_N^2}\mathrm{Cap}_N(\mathcal{E}_N^{(2)}(A),\,\mathcal{E}_N^{(2)}(B)) \ge \frac{1}{|S_\star|}\sum_{i\in A}\sum_{j\in B}\frac{1}{\mathfrak{R}_{i,\,j}}. \tag{9.78}$$

We construct a test flow, whose divergence can be handled outside the one-dimensional tubes.

9.7.1 Construction of test flow ψ_{test}^A

In this subsection, we build the test flow $\psi = \psi_{\text{test}}^A$ on $\mathcal{H}_N$. As we did in Section 9.5.1, we use the notation $\zeta_{k,\,\ell}^{x_{i,\,n}y_p x_{j,\,m}} \in \mathcal{A}_N^{\{x_{i,\,n},\,y_p,\,x_{j,\,m}\}}$ when

$$(\zeta_{k,\,\ell}^{x_{i,\,n}y_p x_{j,\,m}})_{x_{i,\,n}} = k, \quad (\zeta_{k,\,\ell}^{x_{i,\,n}y_p x_{j,\,m}})_{y_p} = \ell, \quad \text{and} \quad (\zeta_{k,\,\ell}^{x_{i,\,n},y_p,x_{j,\,m}})_{x_{j,\,m}} = N-\ell-k.$$

- We define, for $(i,\, j) \in I \cap (A \times B)$, $n,\, m \geq 1$, $p \in P_{i,n,j,m}$, $k \geq 1$, $N - \ell - k \geq 1$, and $\ell \in [\![0,\, \lfloor N/2 \rfloor - 1]\!]$,

$$\psi_0^A(\zeta_{k,\,\ell}^{x_{i,\,n} y_p x_{j,\,m}},\, \zeta_{k-1,\,\ell+1}^{x_{i,\,n} y_p x_{j,\,m}}) = \frac{m_\star(y_p)^\ell / (\frac{N-k-\ell-1}{r(x_{i,\,n},\, y_p)} + \frac{k+\ell}{r(x_{j,\,m},\, y_p)})}{\mathfrak{R}_{i,\,j} \sum_{n=1}^{\mathfrak{n}(i)} \sum_{m=1}^{\mathfrak{n}(j)} \sum_{q=1}^{\kappa_0} \frac{1}{(1-m_\star(y_q))(\frac{N-k-\ell-1}{r(x_{i,\,n},\, y_q)} + \frac{k+\ell}{r(x_{j,\,m},\, y_q)})}}, \tag{9.79}$$

$$\psi_0^A(\zeta_{k,\,\ell}^{x_{i,\,n} y_p x_{j,\,m}},\, \zeta_{k,\,\ell+1}^{x_{i,\,n} y_p x_{j,\,m}}) = \frac{-m_\star(y_p)^\ell / (\frac{N-k-\ell-1}{r(x_{i,\,n},\, y_p)} + \frac{k+\ell}{r(x_{j,\,m},\, y_p)})}{\mathfrak{R}_{i,\,j} \sum_{n=1}^{\mathfrak{n}(i)} \sum_{m=1}^{\mathfrak{n}(j)} \sum_{q=1}^{\kappa_0} \frac{1}{(1-m_\star(y_q))(\frac{N-k-\ell-1}{r(x_{i,\,n},\, y_q)} + \frac{k+\ell}{r(x_{j,\,m},\, y_q)})}}, \tag{9.80}$$

  and 0 otherwise.

- Then, for all $(i,\, j) \in I \cap (A \times B)$, $n,\, m \geq 1$, $p \in P_{i,n,j,m}$, and $k \in [\![1,\, N-1]\!]$, we define a correction flow $\phi_{i,\,j,\,p,\,k}^A$ as follows.

  - Suppose that $k \in [\![\lfloor N/2 \rfloor + 1,\, N-1]\!]$. Then, for $\ell \in [\![1,\, \lfloor N/2 \rfloor]\!]$,

  $$\phi_{i,\,j,\,p,\,k}^A(\zeta_{k-\ell,\,\ell}^{x_{i,\,n} y_p x_{j,\,m}},\, \zeta_{k-\ell+1,\,\ell-1}^{x_{i,\,n} y_p x_{j,\,m}}) := -\sum_{t=\ell}^{\lfloor N/2 \rfloor} (\mathrm{div}\, \psi_0)(\zeta_{k-t,\,t}^{x_{i,\,n} y_p x_{j,\,m}}),$$

    and $\phi_{i,\,j,\,p,\,k}^A = 0$ on all other edges.

  - Suppose that $k \in [\![1,\, \lfloor N/2 \rfloor]\!]$. Then, for $\ell \in [\![1,\, k-1]\!]$,

  $$\phi_{i,\,j,\,p,\,k}^A(\zeta_{k-\ell,\,\ell}^{x_{i,\,n} y_p x_{j,\,m}},\, \zeta_{k-\ell+1,\,\ell-1}^{x_{i,\,n} y_p x_{j,\,m}}) := -\sum_{t=\ell}^{k-1} (\mathrm{div}\, \psi_0)(\zeta_{k-t,\,t}^{x_{i,\,n} y_p x_{j,\,m}}),$$

    and $\phi_{i,\,j,\,p,\,k}^A = 0$ on all other edges.

- Finally, we define a flow

$$\psi = \psi_{\mathrm{test}}^A := \psi_0^A + \sum_{(i,\,j) \in I \cap (A \times B)} \sum_{n=1}^{\mathfrak{n}(i)} \sum_{m=1}^{\mathfrak{m}(j)} \sum_{p \in P_{i,\,n,\,j,\,m}} \sum_{k=1}^{N-1} \phi_{i,\,j,\,p,\,k}^A.$$

Then, observe that $(\operatorname{div}\psi)(\xi_N^{x_{i,n}}) = 0$ for all $i \in [\![1,\, \kappa_\star]\!]$ and $n \in [\![1,\, \mathfrak{n}(i)]\!]$. Moreover, it holds that $(\operatorname{div}\psi)(\eta) = 0$ for all η in

$$\mathcal{A}_N^{\{x_{i,n},\, y_p,\, x_{j,m}\}} \setminus (\mathcal{A}_N^{\{x_{i,n},\, y_p\}} \cup \mathcal{A}_N^{\{x_{j,m},\, y_p\}}) \quad \text{for } i \neq j \text{ and } n,\, m,\, p \geq 1.$$

9.7.2 Flow norm of $\psi_{\mathbf{test}}^{A}$

In this subsection, we calculate the flow norm of the test flow ψ.

Lemma 9.7.2. *Suppose that $I \cap (A \times B) \neq \emptyset$. Then, under the conditions of Theorem 9.1.4,*

$$\|\psi\|^2 \leq (1 + o(1)) \frac{|S_\star| N}{d_N^2} \Big(\sum_{i \in A} \sum_{j \in B} \frac{1}{\mathfrak{R}_{i,\, j}} \Big).$$

Proof. The proof is almost identical to that of Lemma 9.5.3; therefore, we omit it. □

9.7.3 Remaining terms

We estimate the remaining terms on the right-hand side of (9.41) with respect to ψ. Lemma 9.3.4 is employed once more.

Lemma 9.7.3. *Suppose that $I \cap (A \times B) \neq \emptyset$. Then, under the conditions of Theorem 9.1.4,*

$$\sum_{\eta \in \mathcal{H}_N \setminus \mathcal{E}_N^\star} h_{\mathcal{E}_N^{(2)}(A),\, \mathcal{E}_N^{(2)}(B)}(\eta) (\operatorname{div}\psi)(\eta) = (1 + o(1)) \Big(\sum_{i \in A} \sum_{j \in B} \frac{1}{\mathfrak{R}_{i,\, j}} \Big).$$

Proof. We omit the proof due to its similarity to Lemma 9.5.4. □

9.7.4 Proof of Proposition 9.7.1

We are now ready to prove Proposition 9.7.1.

Proof of Proposition 9.7.1. There remains nothing to prove if $I \cap (A \times B) = \emptyset$, as then the right-hand side of (9.78) equals 0. Thus, we may assume $I \cap (A \times B) \neq \emptyset$. Then, by Lemmas 9.7.2 and 9.7.3, we have

$$\frac{1}{\|\psi_{\text{test}}^A\|^2}\Big[\sum_{\eta \notin \mathcal{E}_N^\star} h_{\mathcal{E}_N^{(2)}(A),\, \mathcal{E}_N^{(2)}(B)}(\eta)(\operatorname{div}\psi_{\text{test}}^A)(\eta)\Big]^2 \ge (1+o(1))\frac{d_N^2}{|S_\star|N}\sum_{i\in A}\sum_{j\in B}\frac{1}{\mathfrak{R}_{i,\,j}}.$$

Therefore, we deduce from Theorem 3.2.8-(2) that

$$\mathrm{Cap}_N(\mathcal{E}_N^{(2)}(A),\, \mathcal{E}_N^{(2)}(B)) \ge (1+o(1))\frac{d_N^2}{|S_\star|N}\sum_{i\in A}\sum_{j\in B}\frac{1}{\mathfrak{R}_{i,\,j}}.$$

This concludes the proof of Proposition 9.7.1. □

9.8 Proof of condition (9.16)

In this section, we prove the condition (9.16) formulated in Proposition 9.2.1.

Proposition 9.8.1. *The condition* (9.16) *holds for every* $i \in [\![1,\, \kappa_\star]\!]$.

Proof. The numerator in (9.16) can be dealt with using Proposition 9.6.1;

$$\mathrm{Cap}_N(\mathcal{E}_N^{(2)}(i),\, \mathcal{E}_N^\star \setminus \mathcal{E}_N^{(2)}(i)) = \frac{d_N^2}{N}\cdot O(1). \tag{9.81}$$

For the denominator in (9.16), fix $\eta,\, \zeta \in \mathcal{E}_N^{(2)}(i)$ and write $\eta = \xi_N^x$ and $\zeta = \xi_N^y$ with $x,\, y \in S_i^{(2)}$. By the definition of $S_i^{(2)}$, there exist $x = x_0,\, x_1,\, \dots,\, x_t = y$ in $S_i^{(2)}$ so that $t \le |S_i^{(2)}|$ and

$$r(x_n,\, x_{n+1}) = r(x_{n+1},\, x_n) > 0$$

for all $n \in [\![0,\, t-1]\!]$. Take any $F : \mathcal{H}_N \to \mathbb{R}$ with $F(\eta) = 1$ and $F(\zeta) = 0$.

Recalling Definition 9.3.1, and by reversibility, we calculate $D_N(F)$ by

$$\frac{1}{2}\sum_{\eta\in\mathcal{H}_N}\sum_{a,\,b\in S}\mu_N(\eta)\eta_a(d_N+\eta_b)r(a,\,b)\{F(\sigma^{a,\,b}\eta)-F(\eta)\}^2$$
$$\geq\sum_{n=0}^{t-1}\sum_{j=0}^{N-1}\mu_N(\zeta_j^{x_n,\,x_{n+1}})j(d_N+N-j)r(x_n,\,x_{n+1})\{F(\zeta_{j+1}^{x_n,\,x_{n+1}})-F(\zeta_j^{x_n,\,x_{n+1}})\}^2.$$

By Proposition 8.0.2 and (8.5), the last line equals

$$(1+o(1))\sum_{n=0}^{t-1}\frac{Nd_N}{|S_\star|}r(x_n,\,x_{n+1})\sum_{j=0}^{N-1}\{F(\zeta_{j+1}^{x_n,\,x_{n+1}})-F(\zeta_j^{x_n,\,x_{n+1}})\}^2.$$

By the Cauchy–Schwarz inequality on $j\in[\![0,\,N-1]\!]$, the above is bounded from below by

$$(1+o(1))\sum_{n=0}^{t-1}\frac{d_N}{|S_\star|}r(x_n,\,x_{n+1})\{F(\xi_N^{x_{n+1}})-F(\xi_N^{x_n})\}^2.$$

Using the Cauchy–Schwarz inequality once more on $n\in[\![0,\,t-1]\!]$, we obtain the following lower bound for $D_N(F)$:

$$(1+o(1))\frac{d_N}{|S_\star|}\frac{\{F(\zeta)-F(\eta)\}^2}{\sum_{n=0}^{t-1}\frac{1}{r(x_n,\,x_{n+1})}}\geq(1+o(1))\frac{d_N}{|S_\star|}\frac{\min\{r(u,\,v)>0:u,\,v\in S_i^{(2)}\}}{|S_i^{(2)}|}.$$

As F was arbitrary, by the Dirichlet principle given in Theorem 3.2.5, we have

$$\mathrm{Cap}_N(\{\eta\},\,\{\zeta\})\geq(1+o(1))\frac{d_N}{|S_\star|}\frac{\min\{r(u,\,v)>0:u,\,v\in S_i^{(2)}\}}{|S_i^{(2)}|}.\qquad(9.82)$$

Therefore, by (9.81) and (9.82), we obtain

$$\limsup_{N\to\infty}\frac{\mathrm{Cap}_N(\mathcal{E}_N^{(2)}(i),\,\mathcal{E}_N^\star\setminus\mathcal{E}_N^{(2)}(i))}{\inf_{\eta,\,\zeta\in\mathcal{E}_N^{(2)}(i)}\mathrm{Cap}_N(\{\eta\},\,\{\zeta\})}\le C\limsup_{N\to\infty}\frac{d_N^2/N}{d_N}=C\limsup_{N\to\infty}\frac{d_N}{N}=0.$$

The last formula concludes the proof of Proposition 9.8.1. □

9.9 Proof of the main theorem

Now, we are in position to prove the main theorem given in Theorem 9.1.4. First, we provide sharp asymptotics for the transition rate of the trace process $\eta_N^\star(\cdot)$.

Proposition 9.9.1 (Transition rates of the trace process)**.** *Assume* (9.10) *and suppose that d_N decays subexponentially. Then, for $i,\,j\in[\![1,\,\kappa_\star]\!]$,*

$$\lim_{N\to\infty}\frac{N}{d_N^2}\boldsymbol{r}_N^\star(i,\,j)=\frac{1}{|S_i^{(2)}|\mathfrak{R}_{i,\,j}}.$$

Proof. By Proposition 8.0.5, $\lim_{N\to\infty}\mu_N(\mathcal{E}_N^{(2)}(i))=|S_i^{(2)}|/|S_\star|$ for each $i\in[\![1,\,\kappa_\star]\!]$. Hence, by Propositions 9.6.1, 9.7.1, and (9.14), we have

$$\begin{aligned}\frac{|S_i^{(2)}|}{|S_\star|}\boldsymbol{r}_N^\star(i,\,j)&=\frac{d_N^2}{2|S_\star|N}\Big[\sum_{k:\,k\ne i}\frac{1}{\mathfrak{R}_{i,\,k}}+\sum_{k:\,k\ne j}\frac{1}{\mathfrak{R}_{j,\,k}}-\sum_{k:\,k\ne i,\,j}\Big(\frac{1}{\mathfrak{R}_{i,\,k}}+\frac{1}{\mathfrak{R}_{j,\,k}}\Big)+o(1)\Big]\\&=\frac{d_N^2}{2|S_\star|N}\Big[\frac{2}{\mathfrak{R}_{i,\,j}}+o(1)\Big]=\frac{d_N^2}{|S_\star|N}\Big[\frac{1}{\mathfrak{R}_{i,\,j}}+o(1)\Big].\end{aligned}$$

Multiplying $(|S_\star|N)/(|S_i^{(2)}|d_N^2)$ on both sides, we obtain the desired result. □

Finally, we provide the proof of Theorem 9.1.4.

Proof of Theorem 9.1.4. By Propositions 9.8.1 and 9.9.1, the conditions (9.15) and (9.16) are verified for

$$a(i,\, j) = \frac{1}{|S_i^{(2)}|\mathfrak{R}_{i,\, j}} \text{ for } i,\, j \in [\![1,\, \kappa_\star]\!] \quad \text{and} \quad \theta_N = \theta_{N,\, 2} = \frac{d_N^2}{N}.$$

Therefore, Proposition 9.2.1 establishes the thermalization result stated in (1) and the convergence result stated in (2).

For the last statement in (3), we first show that

$$\lim_{N\to\infty} \sup_{i\in[\![1,\, \kappa_\star]\!],\, n\in[\![1,\, \mathfrak{n}(i)]\!]} \mathbb{E}_{\xi_N^{x_{i,\, n}}} \Big[\int_0^t \mathbb{1}\{\eta_N(\theta_{N,\, 2}s) \notin \mathcal{E}_N^\star\} ds \Big] = 0. \tag{9.83}$$

To this end, fix i and n. Note that

$$\mathbb{P}_{\xi_N^{x_{i,\, n}}} \big[\eta_N(\theta_{N,\, 2}s) \notin \mathcal{E}_N^\star\big] \le \frac{1}{\mu_N(\mathcal{E}_N^{x_{i,\, n}})} \mathbb{P}_{\mu_N} \big[\eta_N(\theta_{N,\, 2}s) \notin \mathcal{E}_N^\star\big] = \frac{\mu_N(\mathcal{H}_N \setminus \mathcal{E}_N^\star)}{\mu_N(\mathcal{E}_N^{x_{i,\, n}})}. \tag{9.84}$$

Here, $\mathbb{P}_{\mu_N}$ is the law of the process whose initial distribution is μ_N. The identity holds, as μ_N is the invariant distribution. Therefore,

$$\begin{aligned} \mathbb{E}_{\xi_N^{x_{i,\, n}}} \Big[\int_0^t \mathbb{1}\{\eta_N(\theta_{N,\, 2}s) \notin \mathcal{E}_N^\star\} ds \Big] &= \int_0^t \mathbb{P}_{\xi_N^{x_{i,\, n}}} \big[\eta_N(\theta_{N,\, 2}s) \notin \mathcal{E}_N^\star\big] ds \\ &\le \int_0^t \frac{\mu_N(\mathcal{H}_N \setminus \mathcal{E}_N^\star)}{\mu_N(\mathcal{E}_N^{x_{i,\, n}})} ds = t \cdot \frac{\mu_N(\mathcal{H}_N \setminus \mathcal{E}_N^\star)}{\mu_N(\mathcal{E}_N^{x_{i,\, n}})}, \end{aligned}$$

which vanishes uniformly in the limit $N \to \infty$ by Proposition 8.0.5. This proves (9.83).

It remains to show that

$$\lim_{N\to\infty} \sup_{i\in[\![1,\, \kappa_\star]\!],\, n\in[\![1,\, \mathfrak{n}(i)]\!]} \mathbb{E}_{\xi_N^{x_{i,\, n}}} \Big[\int_0^t \mathbb{1}\{\eta_N(\theta_{N,\, 2}s) \in \mathcal{E}_N^\star \setminus \mathcal{E}_N(S_{\hat{i}}^{(3)})\} ds \Big] = 0. \tag{9.85}$$

We apply Proposition 9.2.2. Because the first two conditions are already proved, it suffices to prove (9.17). This is clear from (9.84). Hence, we have the convergence of finite-dimensional marginal distributions. Therefore, for each pair $(i,\, n)$ and $s \in [0,\, t]$,

$$\lim_{N\to\infty} \mathbb{P}_{\xi_N^{x_i,\, n}} \big[\eta_N(\theta_{N,\,2} s) \in \mathcal{E}_N^\star \setminus \mathcal{E}_N(S_{\hat{i}}^{(3)})\big] = \mathbf{P}_i \big[X_{\rm second}(s) \in S_\star \setminus S_{\hat{i}}^{(3)}\big] = 0.$$

The last equality holds, as starting from i, $X_{\rm second}(\cdot)$ never visits $S_\star \setminus S_{\hat{i}}^{(3)}$ by (9.13). Because $S_\star$ is finite, we have (9.85). Finally, (9.83) and (9.85) conclude the proof of Theorem 9.1.4. □

Chapter 10

Non-reversible inclusion process

In this chapter, we turn our attention to the general *non-reversible* inclusion process. Namely, we drop the reversibility assumption of the underlying random walk as explained in Assumption 8.0.1.

10.1 Condensation of non-reversible inclusion process

In this section, we explain the condensation phenomenon in the general non-reversible context.

Condensation on metastable sets

Recall the metastable valleys defined in Definition 8.0.4. Moreover, define

$$\mathcal{E}_N := \mathcal{E}_N(S) = \bigcup_{x \in S} \mathcal{E}_N^x.$$

In the non-reversible context, we need to formulate the condensation in a more abstract manner.

Definition 10.1.1 (Condensation)**.** The inclusion process exhibits *condensation* if

$$\lim_{N\to\infty} \mu_N(\mathcal{E}_N) = 1;$$

and to exhibit condensation on $R \subseteq S$ if

$$\lim_{N\to\infty} \mu_N(\mathcal{E}_N(R)) = 1.$$

If the condensation occurs, we define the *maximal condensing set* $S_\star$ (which is redefined from the one given in (8.1)) as

$$S_\star = \left\{x \in S : \liminf_{N\to\infty} \mu_N(\mathcal{E}_N^x) > 0\right\} \neq \emptyset. \tag{10.1}$$

Hence, $S_\star$ denotes the smallest set on which the condensation occurs. Finally, we write the remainder set as

$$\Delta_N = \mathcal{H}_N \setminus \mathcal{E}_N(S_\star).$$

Formula for invariant measure: two special conditions

Now, we introduce two special conditions for the underlying random walk $r(\cdot,\, \cdot)$ that enable us to write the invariant measure in an explicit form.

- **(Rev)** The underlying random walk is *reversible* with respect to its invariant measure, i.e.,

  $$m(x)r(x,\, y) = m(y)r(y,\, x) \quad \text{for all } x,\, y \in S, \tag{10.2}$$

  such that the inclusion process is also reversible with respect to its invariant measure $\mu_N(\cdot)$; see Proposition 8.0.2.

- **(UI)** The invariant measure $m(\cdot)$ for the underlying random walk is the *uniform measure* on S.

To explain the invariant measure for these cases, we define several notations. On the basis of the invariant measure $m(\cdot)$ for the underlying random walk, we introduce the following notations:

$$M_\star = \max\{m(x) : x \in S\} \quad \text{and} \quad S_{\max} = \{x \in S : m(x) = M_*\}. \tag{10.3}$$

Finally, we recall the auxiliary function $w_N : \mathbb{N} \to (0, \infty)$ from Proposition 8.0.2.

Then, we deduce the following formula under **(Rev)** or **(UI)**.

Proposition 10.1.2. *Under the condition* **(Rev)** *or* **(UI)**, *the invariant distribution $\mu_N(\cdot)$ can be written as*

$$\mu_N(\eta) = \frac{1}{Z_N} \prod_{x\in S} \Big(\frac{m(x)}{M_\star}\Big)^{\eta_x} w_N(\eta_x) \quad \textit{for all } \eta \in \mathcal{H}_N, \tag{10.4}$$

where the partition function Z_N is given by

$$Z_N = \sum_{\eta\in\mathcal{H}_N} \prod_{x\in S} \Big(\frac{m(x)}{M_\star}\Big)^{\eta_x} w_N(\eta_x).$$

We remark that $m(x) = M_\star$ for all $x \in S$ under the condition **(UI)**. The proof for the case **(Rev)** is straightforward, as the following detailed balance condition holds:

$$\mu_N(\eta) r_N(\eta, \eta') = \mu_N(\eta') r_N(\eta', \eta).$$

This implies that the inclusion process is also reversible with respect to $\mu_N(\cdot)$. For the case **(UI)**, the proof is presented in [39, Theorem 2.1(a)]; nevertheless, we provide a short proof in Section 10.4 for completeness. Based on the explicit formula (10.4), the following result is established in [15, Proposition 2.1].

Proposition 10.1.3. *Suppose that* $\mu_N(\cdot)$ *admits the formula* (10.4) *and* $\lim_{N\to\infty} d_N \log N = 0$. *Then, it holds that*

$$\lim_{N\to\infty} \mu_N(\mathcal{E}_N^x) = \frac{1}{|S_{\max}|} \quad \text{for all } x \in S_{\max}.$$

In other words, the inclusion process exhibits the condensation on $S_{\max}$*; moreover,* $S_\star = S_{\max}$. *In particular, for the case* **(UI)**, *we have* $S_\star = S$.

Here, we emphasize that the proof of this proposition is based entirely on the formula (10.4). Without this expression, proving the condensation phenomenon becomes a completely non-trivial task; we confront this difficulty in the remainder of this chapter.

10.2 Main results

In this section, we explain the main results obtained in this chapter. Our primary concern is the metastable behavior of the condensate of the inclusion process in the following unexplored settings:

(1) inclusion process satisfying **(UI)** (cf. Section 10.2.2),

(2) inclusion process for which jump rate $r(\cdot, \cdot)$ is uniformly positive (cf. Section 10.2.3),

(3) inclusion process in the thermodynamic limit regime for which the underlying graph (d-dimensional discrete torus) grows together with the number of particles (cf. Section 10.2.4).

For these cases, the inclusion process can be non-reversible. In particular, for case (2), even the invariant distribution cannot be written in an explicit form; hence, the existence of the condensation is unknown. We shall establish this existence of the condensation in Theorem 10.2.14.

10.2.1 Description of metastable behavior

Description of movements of condensate

Using the trace process formulated in Definition 3.1.3, we are now ready to rigorously formulate the metastable behavior of the inclusion process. Denote simply by

$$\eta_N^\star(\cdot) = \eta_N^{\mathcal{E}_N(S_\star)}(\cdot)$$

the trace process on the metastable set $\mathcal{E}_N(S_\star) = \{\xi_N^x : x \in S_\star\}$. For the sake of simplicity, define an identification function $\Psi : \mathcal{E}_N(S_\star) \to S_\star$ as

$$\Psi(\xi_N^x) = x \quad \text{for } x \in S_\star.$$

Using this function, we define a process $\{Y_N(t)\}_{t\geq 0}$ on $S_\star$ by

$$Y_N(t) = \Psi(\eta_N^\star(t)). \tag{10.5}$$

Thus, the process $Y_N(\cdot)$ is obtained by taking the label of the metastable set at which the process $\eta_N^\star(\cdot)$ is staying.

The long-time movement of the condensate can be characterized by proving the convergence of the process $Y_N(\cdot)$ with a proper acceleration factor θ_N to a certain limiting Markov chain on $S_\star$. Let $\{Y(t)\}_{t\geq 0}$ denote a continuous-time Markov chain on $S_\star$, which is the candidate for the limiting Markov chain.

Definition 10.2.1 (Description of metastable behavior)**.** Suppose that the inclusion process exhibits condensation in the sense of Definition 10.1.1. Then, the dynamical movement of the condensate of an inclusion process is said to be d*escribed by a Markov chain* $\{Y(t)\}_{t\geq 0}$ *on* $S_\star$ *with scale* θ_N (which may not diverge to infinity) if the law of the process $Y_N(\theta_N\cdot)$ starting from ξ_N^x converges to that of $Y(\cdot)$ starting from x for all $x \in S_\star$, and if

$$\lim_{N\to\infty} \sup_{\eta\in\mathcal{E}_N(S_\star)} \mathbb{E}_\eta\Big[\int_0^T \mathbb{1}\{\eta_N(\theta_N s) \notin \mathcal{E}_N(S_\star)\}ds\Big] = 0 \quad \text{for all } T > 0. \quad (10.6)$$

Remark. Note that the condition (10.6) implies that the inclusion process does not spend too much time outside the metastable sets and hence guarantees that there exist only fast transitions between the metastable sets. In general models, proving (10.6) is not a trivial issue; however, in the inclusion process case, it directly follows from the definition of condensation (Definition 10.1.1), as one can see from Proposition 10.3.1.

The main objective is to prove the requirements of Definition 10.2.1 for a wide class of non-reversible inclusion processes.

Movements of condensate: reversible and non-reversible cases

Now, we explain the known result and the conjectures for the limiting chain $Y(\cdot)$ and the factor θ_N appearing in Definition 10.2.1.

First, we define a Markov chain $Y^{\mathrm{rv}}(t)$ on $S_\star$ (cf. Proposition 10.1.3) with rate

$$a^{\mathrm{rv}}(x,\, y) = r(x,\, y) \quad \text{for all } x,\, y \in S_\star. \quad (10.7)$$

Note that $r(\cdot,\, \cdot)$ is the jump rate of the original underlying random walk; thus, $Y^{\mathrm{rv}}(\cdot)$ can be regarded as the underlying random walk restricted on $S_\star$. We also remark that $Y^{\mathrm{rv}}(\cdot)$ is not necessarily an irreducible chain. Further, we define

$$\theta_N^{\mathrm{rv}} = \frac{1}{d_N}.$$

Then, in the terminology of Definition 10.2.1, the following result is equivalent to Theorem 8.0.7.

Theorem 10.2.2. *Suppose that the underlying random walk is reversible with respect to its invariant measure* $m(\cdot)$ *and that* $\lim d_N \log N = 0$*. Then,* *the movement of the condensate is described by a Markov chain* $Y^{\mathrm{rv}}(\cdot)$ *on* $S_\star = S_{\max}$ *(cf.* (10.3)*) with scale* θ_N^{rv}.

For the non-reversible case, we expect a completely different result compared to the reversible case. Suppose that we have characterized the set $S_\star$. Define $Y^{\mathrm{nrv}}(\cdot)$ as a Markov chain on $S_\star$ with rate

$$a^{\mathrm{nrv}}(x,\, y) = [r(x,\, y) - r(y,\, x)]\mathbb{1}\{r(x,\, y) > r(y,\, x)\} \quad \text{for } x,\, y \in S_\star; \tag{10.8}$$

and define the time scale as

$$\theta_N^{\mathrm{nrv}} = \frac{1}{N d_N}. \tag{10.9}$$

Conjecture 10.2.3. *Suppose that* $\lim d_N \log N = 0$. *Then, the movement of the condensate is described by the Markov chain* $Y^{\mathrm{nrv}}(\cdot)$ *with scale* θ_N^{nrv}.

We try to directly estimate the so-called mean-jump rate by exploiting several model-dependent features of the inclusion process. This is mainly because we wish to tackle the general case without the formula (10.4) on μ_N. Indeed, one of the main difficulties in the study of the non-reversible case is the lack of such an explicit formula for μ_N; in this case, it is even unclear what $S_\star$ is. Specifying $S_\star$ itself seems to be an extremely difficult problem.

Remark 10.2.4. In general, it is anticipated that the metastable transition of non-reversible dynamics occurs faster than that of its reversible counterpart. For instance, such a phenomenon has been verified for the stochastic discrete gradient descent [60], small random perturbation of dynamical systems [58], and zero-range processes [6, 50, 78]. These results show that the non-reversible dynamics is faster than the reversible one by a constant (i.e., $\Theta(1)$) factor, while Conjecture 10.2.3 indicates that the non-reversible dynamics of the inclusion process is expected to be $\Theta(N)$ times faster than the reversible one. This observation is supported by [23, Section 4.3] which performed heuristic computations for the inclusion process on one-dimensional tori in the thermodynamic limit.

Finally, suppose that the relation $r(x, y) = r(y, x)$ holds for all $x, y \in S_\star$. In this case, we have $a^{\text{nrv}}(x, y) = 0$ for all $x, y \in S_\star$; hence, Conjecture 10.2.3 implies that the scale $\theta_N^{\text{nrv}} = 1/(Nd_N)$ is too short to observe the transitions. We expect that the correct scale for this case is $\theta_N^{\text{rv}} = 1/d_N$.

Conjecture 10.2.5. *Suppose that $r(x, y) = r(y, x)$ for all $x, y \in S_\star$ and $\lim d_N \log N = 0$. Then, the movement of the condensate is described by the Markov chain $Y^{\text{rv}}(\cdot)$ on $S_\star$ with scale θ_N^{rv}.*

Here, we emphasize that Theorem 10.2.2 is a special case of this conjecture. To see this, observe that $S_\star = S_{\max}$ for the reversible case; thus, we have

$$r(x, y) = \frac{m(y)}{m(x)} r(y, x) = \frac{M_\star}{M_\star} r(y, x) = r(y, x) \quad \text{for all } x, y \in S_\star.$$

This implies that, if the previous conjecture is true, the scale θ_N^{rv} and the limiting Markov chain $Y^{\text{rv}}(\cdot)$ appear in the reversible case because $r(\cdot, \cdot)$ is symmetric on $S_\star = S_{\max}$, and the reversibility is not a fundamental reason.

We verify the validity of Conjectures 10.2.3 and 10.2.5 for wide-class of non-reversible inclusion processes.

Comments on convergence of finite-dimensional distributions

Before proceeding to the main results of this article, we remark on the mode of convergence regarding Definition 10.2.1. Although the convergence of the trace process is natural in the study of metastability, an alternative description has been presented [55], which does not need to recall the trace process in the description and is hence more intuitive to understand. To see this, fix a cemetery state $\mathfrak{o}$ and define a map $\widehat{\Psi} : \mathcal{H}_N \to S_\star \cup \{\mathfrak{o}\}$ as

$$\widehat{\Psi}(\eta) = \begin{cases} x & \text{if } \eta = \xi_N^x \text{ with } x \in S_\star, \\ \mathfrak{o} & \text{otherwise.} \end{cases}$$

Then, define a process $\{\widehat{Y}_N(t)\}_{t\geq 0}$ on $S_\star \cup \{\mathfrak{o}\}$ by

$$\widehat{Y}_N(t) = \widehat{\Psi}(\eta_N(t)).$$

In other words, we trace each metastable configuration to its label and all the other configurations to the cemetery state $\mathfrak{o}$.

Definition 10.2.6. The dynamical movement of the condensate of an inclusion process is said to be *described by a Markov chain* $\{Y(t)\}_{t\geq 0}$ *on* $S_\star$ *with scale* θ_N *in the finite-dimensional marginal sense* if, for all $k \geq 1$, we have

$$\lim_{N\to\infty} \mathbb{P}_{\xi_N^x}\big[\widehat{Y}_N(\theta_N t_1) \in A_1,\, \dots,\, \widehat{Y}_N(\theta_N t_k) \in A_k\big] = \mathbf{P}_x\big[Y(t_1) \in A_1,\, \dots,\, Y(t_k) \in A_k\big]$$

for all $0 \leq t_1 < \cdots < t_k$ and $A_1, \dots, A_k \subseteq S_\star$, where $\mathbf{P}_x$ denotes the law of the process $Y(\cdot)$ starting from x.

To establish this convergence of marginal distributions from that of the trace process defined in Definition 10.2.1, it is known from [55, Proposition 2.1] that the verification of the following technical condition is sufficient:

$$\lim_{\delta\to 0} \limsup_{N\to\infty} \sup_{2\delta\leq s\leq 3\delta} \sup_{\eta\in\mathcal{E}_N(S_\star)} \mathbb{P}_\eta\big[\eta_N(\theta_N s) \notin \mathcal{E}_N(S_\star)\big] = 0. \tag{10.10}$$

For the inclusion process, this condition is straightforward to check (cf. Proposition 10.3.1); thus, the convergence of the trace process immediately implies the convergence of the finite-dimensional distributions.

10.2.2 Main result 1: under condition (UI)

In this subsection, we explain our result of the analysis of the metastable behavior of the inclusion process under the condition **(UI)**. For this case, as mentioned in Proposition 10.1.2, the invariant measure admits the expression (10.4); therefore condensation occurs owing to Proposition 10.1.3. Moreover, as the invariant measure for the underlying random walk is uniform, we have $S_\star = S_{\max} = S$, i.e., condensation occurs on the entire state set S.

The metastable behavior of the inclusion process for this case was known only when $r(\cdot,\,\cdot)$ is completely symmetric (as in case (1) of the theorem below). The following theorem extends this result for the general case under **(UI)**.

Theorem 10.2.7. *Suppose that the underlying random walk satisfies the condition* **(UI)** *and that* $\lim_{N\to\infty} d_N \log N = 0$.

(1) Suppose that $r(x,\,y) = r(y,\,x)$ *for all* $x,\,y \in S$. *Then, Conjecture 10.2.5 holds.*

(2) Suppose that $r(x,\,y) \neq r(y,\,x)$ *for some* $x,\,y \in S$. *Then, Conjecture 10.2.3 holds.*

We remark that, for case (1), the underlying random walk is reversible; hence, this result is a consequence of [15] (i.e., Theorem 10.2.2). Our new result focuses on case (2), which is essentially the first rigorous analysis of the metastable behavior of the non-reversible inclusion process. The proof of this result relies on careful analysis of the mean-jump rates established in Section 10.3. We explain the proof in Section 10.4.

Inclusion process on torus

An interesting example satisfying condition **(UI)** is the simple random walk on the discrete torus. Suppose that the underlying random walk is a simple random walk on the torus $\mathbb{T}_L = \mathbb{Z}/(L\mathbb{Z})$ with jump rate

$$r(x,\,y) = \begin{cases} p & \text{if } y = x+1 \pmod L, \\ 1-p & \text{if } y = x-1 \pmod L, \\ 0 & \text{otherwise.} \end{cases}$$

As the uniform measure on $\mathbb{T}_L$ is the invariant measure for this random walk, the condition **(UI)** is valid. We can prove that the dynamical transition of the condensate can be described as follows. For simplicity we may assume that $p \geq 1/2$ since the case $p \leq 1/2$ can be treated in the same manner.

Corollary 10.2.8. *Suppose that* $\lim_{N\to\infty} d_N \log N = 0$*. Then, the dynamical movement of the condensate for the inclusion process on* $\mathbb{T}_L$ *defined above is described by the following limiting Markov chain and the time scale:*

(1) for $p = 1/2$*, a Markov chain* $\{Y^{\mathrm{sym}}(t)\}_{t\geq 0}$ *with jump rate*

$$a^{\mathrm{sym}}(x,\, y) = \begin{cases} 1/2 & \textit{if } |y-x| = 1, \\ 0 & \textit{otherwise}, \end{cases}$$

and scale $\theta_N^{\mathrm{rv}} = 1/d_N$*.*

(2) for $p > 1/2$*, a Markov chain* $\{Y^{\mathrm{asym}}(t)\}_{t\geq 0}$ *with jump rate*

$$a^{\mathrm{asym}}(x,\, y) = \begin{cases} 2p-1 & \textit{if } y = x+1, \\ 0 & \textit{otherwise}, \end{cases}$$

and scale $\theta_N^{\mathrm{nrv}} = 1/(Nd_N)$*.*

We note that the transition scale for the asymmetric case is $1/(Nd_N)$, and it is $\Theta(N)$ times faster than that of the symmetric case, i.e., $1/d_N$. This observation verifies the statement in Remark 10.2.4. Furthermore, it is interesting that the limiting dynamics for the partially asymmetric case (i.e., $p \in (1/2,\, 1)$) is totally asymmetric.

10.2.3 Main result 2: uniformly positive rates

As mentioned earlier, condensation of the inclusion process without condition **(Rev)** or **(UI)** is unknown. For instance, whether condensation occurs on S, i.e., $\lim_{N\to\infty} \mu_N(\mathcal{E}_N) = 1$, is an open question. This is mainly because of the lack of the explicit formula of μ_N. Under suitable assumptions, we now describe both static and dynamical analyses of condensation in such general cases.

Metastable behavior for general non-reversible inclusion processes

We assume first that the occurrence of the condensation has been verified, and then focus on the analysis of the metastable behavior. We will return to the condensation issue later in this subsection.

To prove Conjecture 10.2.3, we should first characterize $S_\star$. To this end, let us consider an auxiliary Markov chain $\{Z_1(t)\}_{t\ge 0}$ on S with jump rate

$$b(x,\, y) = [r(x,\, y) - r(y,\, x)]\mathbb{1}\{r(x,\, y) > r(y,\, x)\} \quad \text{for all } x,\, y \in S, \tag{10.11}$$

which is an extension of $a^{\text{nrv}}(\cdot,\, \cdot)$ defined in (10.8) to the set S. Let S_0 denote the set of recurrent states (including absorbing states; refer to Figure 10.1) of the Markov chain $Z_1(\cdot)$. We say that S_0 *has only one irreducible component* if the Markov chain $Z_1(\cdot)$ restricted to S_0 is irreducible, i.e., for any $x,\, y \in S_0$, there exists some $k \ge 1$ such that

$$\sum_{z_1,\, \dots,\, z_{k-1} \in S_0} b(x,\, z_1)b(z_1,\, z_2)\cdots b(z_{k-1},\, y) > 0.$$

This assumption is equivalent to the uniqueness of the invariant measure for $Z_1(\cdot)$, and for such a case S_0 is the support of the invariant measure. Then, the following result describes the metastable behavior of the inclusion process when S_0 has only one irreducible component.

Theorem 10.2.9. *Suppose that condensation occurs and that S_0 defined above has only one irreducible component. Then, $S_\star = S_0$ and Conjecture 10.2.3 holds.*

Now, we turn to Conjecture 10.2.5. To this end, we assume that $r(x,\, y) = r(y,\, x)$ for all $x,\, y \in S_0$. Then, consider another auxiliary Markov chain

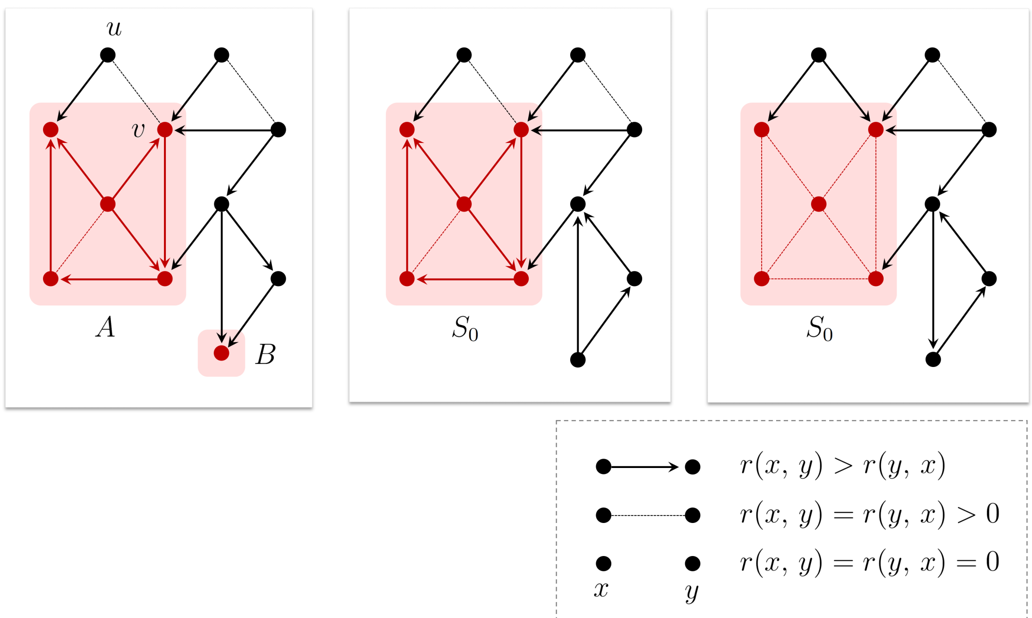


Figure 10.1: (Left) The set S_0 is given by $S_0 = A \cup B$. In this case, $Z_1(\cdot)$ restricted to S_0 has two irreducible components A and B; thus, it does not satisfy the condition of Theorem 10.2.9. The set A is semi-attracting since $r(u, v) = r(v, u)$. (Middle) The set S_0 satisfies the condition of Theorem 10.2.9, since S_0 has only one irreducible component with respect to $Z_1(\cdot)$. (Right) The set S_0 is attracting; hence S_0 satisfies all the conditions of Theorem 10.2.11.

$\{Z_2(t)\}_{t\geq 0}$ on S_0 whose rate between $x \in S_0$ and $y \in S_0$ is just $r(x, y)$. We need to introduce additional simple concepts to state our result.

Notation 10.2.10. The set $A \subseteq S$ is called *attracting* if it holds that $r(x, y) < r(y, x)$ for all $x \in A$ and $y \in A^c$ with $r(x, y) + r(y, x) > 0$. Moreover, A is called *semi-attracting* if it holds that $r(x, y) \leq r(y, x)$ for all $x \in A$ and $y \in A^c$ with $r(x, y) + r(y, x) > 0$. We refer to Figure 10.1 for the illustration.

Note that attracting sets are semi-attracting as well. For the symmetric case, we obtain the following result.

Theorem 10.2.11. *Suppose that condensation occurs and that the Markov chain $\{Z_2(t)\}_{t\geq 0}$ on S_0 defined above is irreducible. Further, assume that S_0 is attracting. Then, $S_\star = S_0$ and Conjecture 10.2.5 holds.*

Remark. Since $S_\star = S_0$ in this case, the Markov chain $Z_2(\cdot)$ is indeed $Y^{\mathrm{rv}}(\cdot)$. The condition that S_0 is attracting is required to guarantee that S_0 is the set of states at which the transition occurs.

As a consequence of Theorems 10.2.9 and 10.2.11, we can provide the following non-trivial asymptotic limit of $\mu_N(\xi_N^x)$ for $x \in S_\star = S_0$.

Theorem 10.2.12. *Under the conditions of Theorem 10.2.9 (resp. Theorem 10.2.11), it holds that*

$$\lim_{N\to\infty} \mu_N(\xi_N^x) = \nu(x) \quad \textit{for all } x \in S_\star,$$

where $\nu(\cdot)$ is the unique invariant measure of the irreducible Markov chain $Y^{\mathrm{nrv}}(\cdot)$ (resp. $Y^{\mathrm{rv}}(\cdot)$).

Remark 10.2.13. Several remarks regarding the irreducibility of $Z_1(\cdot)$ and $Z_2(\cdot)$ on S_0 are stated below.

(1) When there exist multiple irreducible components of $Z_1(\cdot)$ on S_0, a certain linear combination of the invariant measure on each component

is expected to equal the limit of μ_N on $\mathcal{E}_N$. However, at this moment, it is unclear as to which linear combination is the correct one. Moreover, characterizing $S_\star$ is not possible at this moment. The sites in $S \setminus S_0$ will be discarded in the long-time limit; however, it is unclear as to which sites of S_0 will survive, partially or completely, in the accelerated process.

(2) The reversible case in which there exist multiple irreducible components of $Z_2(\cdot)$ on S_0 has been investigated in Chapter 9. In these longer scaling limits, each irreducible component is expected to act as a single element in the limiting dynamics, and the long-time movement will occur among these component-wise elements. If the graph distance between these components is exactly 2, then the transition occurs in the second scale N/d_N^2. If the distance is greater than 2, then the transition occurs in the third scale N^2/d_N^3. However, such generality has not been analyzed even for the reversible inclusion process on general graphs, and it is currently being handled in ongoing work.

Condensation

Previously, we analyzed the metastable behavior of the inclusion process by assuming that the condensation occurs. However, without the closed-form expression for the invariant measure, the verification of the condensation is not a simple task. Here, we prove the existence of condensation under the following assumption:

- **(UP)** The jump rate of the underlying random walk is *uniformly positive* in the sense that

$$r(x, y) > 0 \quad \text{for all } x, y \in S. \tag{10.12}$$

With this assumption, we can establish the existence of condensation for inclusion process. We emphasize that this is the first verification of the condensation for the inclusion process without explicit formula (10.4) for μ_N.

Theorem 10.2.14. *Suppose that the assumption* **(UP)** *holds and*

$$\lim_{N\to\infty} d_N N^{|S|+2}(\log N)^{|S|-3} = 0. \tag{10.13}$$

Then, the condensation occurs for the inclusion process, i.e.,

$$\lim_{N\to\infty} \mu_N(\mathcal{E}_N) = 1. \tag{10.14}$$

Remark 10.2.15. We remark that the stringent condition (10.13) appeared because the estimates used in Section 10.6 are partially sub-optimal. We conjecture that Theorem 10.2.14 still holds when (10.13) is substituted by the standard condition $\lim_{N\to\infty} d_N \log N = 0$ without changing the current setting. We expect that refining the arguments carried out in Section 10.6 regarding the analysis of the inner core (cf. Notation 10.6.1) of the configuration space is crucial to get an optimal result. We believe that a totally different idea is required to get such an optimal result.

The following corollary is now immediate.

Corollary 10.2.16. *Theorems 10.2.9, 10.2.11, and 10.2.12 hold under the conditions* **(UP)** *and* (10.13).

The proof of Theorem 10.2.14 is given in Section 10.6 and relies on the results on mean-jump rates established in Section 10.3 along with a weak result on the nucleation of condensation stated below in Theorem 10.2.17.

In general, the nucleation regime explains the typical behavior of particles, starting from an arbitrary distribution among sites to condensation at a sole site. The only rigorous result regarding the nucleation was obtained in [40], where it was proved that the nucleation procedure of the inclusion process satisfying both **(Rev)** and **(UI)** can be explained by a Wright–Fisher-type slow-fast diffusion. We refer to [40] for further information on nucleation;

although our nucleation result explained hereafter is much weaker, it is the first quantitative result in the study of nucleation of non-reversible inclusion processes. Let $\delta > 0$ be an arbitrary fixed number and define

$$\mathcal{U}_N = \{\eta \in \mathcal{H}_N : \eta_x \leq \delta \log N \text{ for some } x \in S\}.$$

Then, the nucleation result can be formulated as follows.

Theorem 10.2.17. *Suppose that the assumption* **(UP)** *holds and* $\lim_{N\to\infty} d_N N^2/(\log N)^2 = 0$*. Then, there exists a constant* $C = C(\delta) > 0$ *such that*

$$\sup_{\eta\in\mathcal{H}_N} \mathbb{E}_\eta[\tau_{\mathcal{U}_N}] \leq CN.$$

Suppose that the inclusion process starts from a configuration containing $\Theta(N)$ particles at all sites. Then, the first stage of the nucleation of condensation is to empty a site, which can be deduced by studying the typical path to the set $\{\eta \in \mathcal{H}_N : \eta_x = 0 \text{ for some } x \in S\}$ and examining the mean of the hitting time. The theorem above provides a weak form of such a result, and its proof will be given in Section 10.6.4. It is strongly expected that the actual scale of the nucleation of particles is $\Theta(\log N)$, which serves as an important topic of future research.

10.2.4 Main result 3: thermodynamic limit regime

In the previous models, we fixed the state space S. In this subsection, we consider a slightly different model for which the space given by the multi-dimensional discrete torus grows together with the number of particles. Then, a suitable time-space rescaling of the movements of the condensate converges to a *continuous process* on a multi-dimensional torus; this type of result is referred to as the *thermodynamic limit of condensation* (cf. [2]).

The thermodynamic limit of condensation has been thoroughly studied for zero-range processes in [2]. In [2], the thermodynamic limit of condensation of the symmetric zero-range process on the torus has been investigated by the martingale approach. For the simple inclusion process, the thermodynamic limit of the inclusion process whose underlying random walk is either a symmetric or totally asymmetric random walk on the one-dimensional torus has been investigated in [23]. The authors used exquisitely constructed heuristic simulations to derive various time scales related to the nucleation regime of the process, which is divided into four parts: nucleation, coarsening, saturation, and stationary. Readers may refer to [23] for further details.

Our contribution to the study of condensation in the thermodynamic limit regime is *to establish the scaling limit of the movement of condensation, and we find three different time scales according to the level of asymmetry.* We explain these results in the remainder of this subsection.

Model

We start by introducing our model, which is distinguished from previous models by the characteristic that the underlying state space is growing. Recall that $\mathbb{T}_L = \mathbb{Z}/(L\mathbb{Z})$ denotes a discrete torus of length L. Now, we consider the inclusion process consisting of N interacting particles that move according to a random walk on the multi-dimensional torus $\mathbb{T}_L^d$ where L and N grow together such that

$$L \to \infty, \quad N = N_L \to \infty, \quad \text{and} \quad \frac{N}{L^d} \to \rho \text{ for some } \rho > 0. \tag{10.15}$$

Henceforth, we assume that $\rho > 0$ is fixed and regard N as a variable that is dependent on L; hence, the only control variable is L. With this convention, the condition (10.15) implies that the total density is maintained to be close to ρ as $L \to \infty$.

To get a scaling limit, we will assume that the underlying system is a translation-invariant random walk on $\mathbb{T}_L^d$, i.e., the jump rate of the underlying random walk on $\mathbb{T}_L^d$ is given by

$$r(x,\, y) = h(y - x) \tag{10.16}$$

for some nonnegative function $h : \mathbb{Z}^d \to [0,\, \infty)$ with compact support, i.e., there exists $M > 0$ such that $h(x) = 0$ if $|x| > M$. We assume that this random walk is irreducible, i.e., the support of h spans $\mathbb{Z}^d$.

Remark 10.2.18. Now, we state several remarks on this model:

(1) It should be emphasized that the simple nearest-neighbor random walk on $\mathbb{T}_L^d$ is an example of a translation-invariant random walk.

(2) By the translation invariance, it can immediately be verified that the random walk satisfies the condition **(UI)**, i.e., the invariant measure m of the underlying random walk is the uniform measure on $\mathbb{T}_L^d$. Moreover, this random walk is reversible with respect to this invariant measure only when the function h is *symmetric*, i.e., $h(x) = h(-x)$ for each $x \in \mathbb{Z}^d$.

(3) Throughout the remainder of this subsection, we shall implicitly assume $L > 2M$ so that the state space $\mathbb{T}_L^d$ is much larger than the support of h.

The inclusion process $\{\eta_L(t)\}_{t\geq 0}$ on $\mathbb{T}_L^d$ consisting of N particles where N and L satisfy (10.15) is defined as a continuous-time Markov chain on the configuration space given by

$$\mathcal{H}_L = \Big\{\eta \in \mathbb{N}^{\mathbb{T}_L^d} : \sum_{x\in\mathbb{T}_L^d} \eta_x = N\Big\}.$$

If the inclusion process consists of the translation-invariant underlying random walks described above, then the generator corresponding to the inclusion process is defined, for $f : \mathcal{H}_L \to \mathbb{R}$, by

$$(\mathscr{L}_L f)(\eta) = \sum_{x,\, y \in \mathbb{T}_L^d} \eta_x (d_L + \eta_y) r(x,\, y) \{ f(\sigma^{x,\, y}\eta) - f(\eta) \} \quad \text{for } \eta \in \mathcal{H}_L,$$

where $\{d_L\}_{L=1}^{\infty}$ is a sequence of positive real numbers converging to 0.

Condensation

We are primarily interested in the limiting behavior of the condensate of the model explained above as L tends to infinity. As before, define the metastable set corresponding to the condensation of the inclusion process as

$$\mathcal{E}_L^x = \{\xi_L^x\} \quad \text{for each } x \in \mathbb{T}_L^d,$$

where ξ_L^x denotes the configuration containing all the particles at site $x \in \mathbb{T}_L^d$. Write

$$\mathcal{E}_L = \bigcup_{x \in \mathbb{T}_L^d} \mathcal{E}_L^x. \tag{10.17}$$

Let $\mu_L(\cdot)$ denote the invariant distribution for this model. As this model satisfies the condition **(UI)** as mentioned in Remark 10.2.18-(2), we can use Proposition 10.1.2 to write the invariant distribution as

$$\mu_L(\eta) = \frac{1}{Z_L} \prod_{x \in \mathbb{T}_L^d} w_L(\eta_x) \quad \text{for } \eta \in \mathcal{H}_L, \tag{10.18}$$

where

$$w_L(n) = \frac{\Gamma(n + d_L)}{n!\Gamma(d_L)}, \quad n \in \mathbb{N}, \quad \text{and} \quad Z_L = \sum_{\eta \in \mathcal{H}_L} \prod_{x \in \mathbb{T}_L^d} w_L(\eta_x).$$

Owing to this expression, we can prove the occurrence of condensation provided that d_L converges to 0 sufficiently fast.

Theorem 10.2.19. *Suppose that* $\lim_{L\to\infty} d_L L^d \log L = 0$*. Then, we have*

$$\lim_{L\to\infty} \mu_L(\mathcal{E}_L) = 1.$$

Consequently, by the symmetry of the invariant measure (10.18)*, we have*

$$\mu_L(\mathcal{E}_L^x) = (1+o(1))\frac{1}{L^d} \quad \textit{for all } x \in \mathbb{T}_L^d.$$

We remark that this result has been proved in [42, Proposition 2] using the technique of size-biased sampling. However, we propose an alternative proof of this theorem in Section 10.7.1 for completeness.

Description of metastable behavior

Now, we turn to the dynamics of the condensate. In this model, we rescale the state space so that we can identify $x \in \mathbb{T}_L^d$ as a point $L^{-1}x \in \mathbb{T}^d$. By rescaling the time appropriately, we expect the dynamics of the condensate to converge to a process on $\mathbb{T}^d$ as $L \to \infty$. Our result presented below verifies that three different time scales appear according to the level of asymmetry of the underlying random walk. To rigorously formulate this result, we start by defining a map $\Theta_L : \mathcal{E}_L \to \mathbb{T}^d$ by

$$\Theta_L(\xi_L^x) = \frac{x}{L} \quad \text{for } x \in \mathbb{T}_L^d.$$

Define a process $\{Y_L(t)\}_{t\ge 0}$ on $\mathbb{T}^d$ by

$$Y_L(t) = \Theta_L(\eta_L^{\mathcal{E}_L}(t)),$$

where $\eta_L^{\mathcal{E}_L}(\cdot)$ is the trace process of $\eta_L(\cdot)$ on the set $\mathcal{E}_L$. The following is a variant of Definition 10.2.1.

Definition 10.2.20. The movement of the condensate of the inclusion process on $\mathbb{T}_L^d$ defined above is said to be *described by a process* $\{Y(t)\}_{t\ge 0}$ *on* $\mathbb{T}^d$

with scale θ_L if the following conditions hold simultaneously.

(1) For each sequence $(x_L)_{L=1}^{\infty}$ such that $x_L \in \mathbb{T}_L^d$ for all $L \geq 1$ and $\lim_{L\to\infty}(x_L/L) = u$, the law of the rescaled trace process $Y_L(\theta_L \cdot)$ starting from $\xi_L^{x_L}$ converges to that of the process $Y(\cdot) + u$ on $\mathbb{T}^d$.

(2) The excursions outside $\mathcal{E}_L$ are negligible at the scale θ_L in the sense that

$$\lim_{L\to\infty} \sup_{\eta\in\mathcal{E}_L} \mathbb{E}_\eta\Big[\int_0^T \mathbb{1}\{\eta_L(\theta_L s) \notin \mathcal{E}_L\} ds\Big] = 0 \quad \text{for all } T > 0. \qquad (10.19)$$

Main results for thermodynamic limit of metastable behavior

Let v denote the mean displacement (hence, the velocity) of the underlying random walk:

$$v = \sum_{y\in\mathbb{Z}^d} h(y)y.$$

We decompose the model into three cases as follows:

(1) If $v \neq 0$, the model is referred to as *totally asymmetric*.

(2) If $v = 0$ and h is not symmetric, then the model is referred to as *mean-zero asymmetric*.

(3) If $v = 0$ and h is symmetric, then the model is referred to as *symmetric*.

Then, the relevant time scales for these three cases are different, as we will see below. The following is the first main result.

Theorem 10.2.21 (First time scale for the totally asymmetric case)**.** *Suppose that* $v \neq 0$ *and assume that* $\lim d_L L^{d+1} \log L = 0$. *Then, the movement of the condensate of the inclusion process on* $\mathbb{T}_L^d$ *is described by the deterministic motion* $V(t) = \rho v t$ *with scale* $\theta_L = 1/(d_L L^{d-1})$.

Note that the limiting dynamics $V(t)$ obtained in the last theorem is non-degenerate only when the dynamics is totally asymmetric, i.e., $v \neq 0$. Hence, if $v = 0$, we have to wait for more time to observe the transitions of the condensation. Now, we formulate this result in a rigorous form. For each $y \in \mathbb{R}^d$, let $y \otimes y$ denote the outer product, i.e., $y \otimes y = yy^{\dagger}$[1]. Hence, $y \otimes y$ is a $d \times d$ matrix. Consider a non-negative symmetric matrix $\mathbb{S}_1$ given by

$$\mathbb{S}_1 = \rho \sum_{y \in \mathbb{Z}^d :\, h(y) > h(-y)} (h(y) - h(-y)) y \otimes y,$$

and let Σ_1 denote its square root[2].

Theorem 10.2.22 (Second time scale for the mean-zero asymmetric case)**.** *Suppose that $v = 0$ and assume that $\lim d_L L^{d+2} \log L = 0$. Then, the movement of the condensate of the inclusion process on $\mathbb{T}_L^d$ is described by the Brownian motion with diffusion matrix Σ_1 and scale $\theta_L = 1/(d_L L^{d-2})$.*

This theorem explains the diffusive behavior of condensation when the underlying random walk is mean-zero such that the local drift at the time scale $1/(d_L L^{d-1})$ is canceled out. However, note that the matrix $\mathbb{S}_1$, and hence Σ_1 is a zero matrix when the underlying random walk is symmetric. This indicates that we still have to wait for more time to observe the macroscopic movements of the condensate for the symmetric case. Indeed, we should wait for much longer to observe these movements. To formulate this, define a positive definite matrix $\mathbb{S}_2$ by

$$\mathbb{S}_2 = \sum_{y \in \mathbb{Z}^d} h(y) y \otimes y,$$

and let Σ_2 denote its square root.

---

[1] Given a matrix A, let $A^{\dagger}$ denote the transpose of A.

[2] Let $U^{\dagger} \Lambda U$ denote the diagonalization of the symmetric matrix $\mathbb{S}_1$, where $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_d)$. Define $\Lambda^{1/2} = \mathrm{diag}(\lambda_1^{1/2}, \ldots, \lambda_d^{1/2})$ which is well defined since $\mathbb{S}_1$ is non-negative definite. Then, Σ_1 is defined by $U^{\dagger} \Lambda^{1/2} U$. Note that $\Sigma_1 \Sigma_1 = \mathbb{S}_1$.

Theorem 10.2.23 (Third time scale for the symmetric case)**.** *Suppose that* $h(x) = h(-x)$ *for all* $x \in \mathbb{Z}^d$ *and assume that* $\lim d_L L^{2d+2} \log L = 0$. *Then, the movement of the condensate of the inclusion process on* $\mathbb{T}_L^d$ *is described by the Brownian motion with diffusion matrix* Σ_2 *and scale* $\theta_L = L^2/d_L$.

The proofs of Theorems 10.2.21, 10.2.22, and 10.2.23 are given in Section 10.7. We conclude this section with several remarks on these theorems regarding the metastable behavior of the inclusion process in thermodynamic limit regime.

Remark 10.2.24. Few remarks are in order.

(1) It should be noted that the limiting particle density ρ affects the limiting dynamics of the asymmetric cases. This is mainly because the higher density facilitates the first escape of one particle from a condensate. Subsequently, the movement of the remaining particles occurs instantaneously because of the asymmetry of the system. However, for the symmetric case, this acceleration of the first jump by the higher ρ is canceled out by the fact that we have to move more particles to the adjacent site for the higher ρ. These two effects are exactly matched for the symmetric case; consequently, the limiting dynamics becomes independent of ρ.

(2) Our conditions on d_L appeared in Theorems 10.2.21, 10.2.22, and 10.2.23 are sub-optimal for technical reasons. We believe that all the results must hold under the condition $\lim d_L L^d \log L = 0$ as in Theorem 10.2.19.

(3) Condensation of the zero-range process in the thermodynamic regime exhibits phase transition in terms of ρ (e.g., see [2]). More precisely, there exists $\rho_c > 0$ such that condensation occurs if and only if $\rho > \rho_c$. However, in the inclusion process, we do not observe such a phenomenon. We refer to [42, Proposition 1] for further details.

10.3 Movements of condensate: general results

The results obtained in this section directly imply Theorem 10.2.7 regarding the metastable behavior of the inclusion process under **(UI)**, as we are aware of the appearance of condensation for this case. We explain this in Section 10.4. However, for the general case, considerable effort is required to prove the existence of condensation to apply the results obtained in this section. This will be done under the condition **(UP)** in Sections 10.6 and 10.5. We also discuss the thermodynamic limit in Section 10.7 on the basis of the results obtained in this section.

10.3.1 Applications of the martingale approach

Here, we explain the application of the martingale approach for the inclusion setting.

Preliminary: negligibility of excursions on Δ_N

As a preliminary step, we first verify the two conditions given by (10.6) and (10.10) for the inclusion process under static condensation.

Proposition 10.3.1. *Suppose that the inclusion process exhibits condensation and let $S_\star$ be the maximal condensing set defined in* (10.1)*. Then, for any sequence $(\alpha_N)_{N=1}^{\infty}$ of positive real numbers, we have*

$$\lim_{N\to\infty} \sup_{\eta\in\mathcal{E}_N(S_\star)} \mathbb{E}_\eta\Big[\int_0^T \mathbb{1}\{\eta_N(\alpha_N s)\in\Delta_N\}ds\Big] = 0 \quad \text{for all } T>0, \tag{10.20}$$

$$\lim_{\delta\to 0}\limsup_{N\to\infty} \sup_{2\delta\le s\le 3\delta} \sup_{\eta\in\mathcal{E}_N(S_\star)} \mathbb{P}_\eta\big[\eta_N(\alpha_N s)\in\Delta_N\big] = 0, \tag{10.21}$$

where $\Delta_N = \mathcal{E}_N(S_\star)^c$. In other words, the two conditions given by (10.6) *and* (10.10) *hold.*

Proof. For $x \in S_\star$, we have

$$\mathbb{P}_{\xi_N^x}\big[\eta_N(\alpha_N s) \in \Delta_N\big] \le \frac{1}{\mu_N(\mathcal{E}_N^x)}\mathbb{P}_{\mu_N}\big[\eta_N(\alpha_N s) \in \Delta_N\big] = \frac{\mu_N(\Delta_N)}{\mu_N(\mathcal{E}_N^x)} = o(1),$$

where the last identity follows from $\mu_N(\Delta_N) = o(1)$ and (10.1). Now, (10.20) directly follows from the Fubini theorem, as does (10.21). □

Estimation of the mean-jump rate

For $A \subseteq S$, we consider the trace process $\eta_N^{\mathcal{E}_N(A)}(\cdot)$ as defined in Definition 3.1.3, which is a Markov chain on $\mathcal{E}_N(A)$. Denote the jump rate of this Markov chain by $\mathbf{r}_N^A(\cdot,\,\cdot) : \mathcal{E}_N(A) \times \mathcal{E}_N(A) \to [0,\,\infty)$. In view of the theory summarized in Section 3.2.2, the analysis of the metastable behavior of the inclusion process is reduced to finding a suitable scaling limit for the mean-jump rates. Such a scaling limit stated as Proposition 10.3.2 below is the main result of this section. Write

$$\ell_N = d_N \log N + q^N,$$

where $q \in (0,\,1)$ is a fixed constant that will be specified later in (10.27).

Proposition 10.3.2. *Suppose that* $\lim_{N\to\infty} d_N \log N = 0$. *Fix a non-empty set* $A \subseteq S$ *and define*

$$r_N^A(x,\,y) = \frac{1}{d_N N}\mathbf{r}_N^A(\xi_N^x,\,\xi_N^y) \quad \text{for } x,\,y \in A.$$

(1) If A is a semi-attracting set, we have

$$r_N^A(x,\,y) = \begin{cases} (1 + O(N^{-1} + \ell_N))(r(x,\,y) - r(y,\,x)) & \text{if } r(x,\,y) > r(y,\,x), \\ O(N^{-1} + \ell_N) & \text{if } r(x,\,y) < r(y,\,x), \\ N^{-1} r(x,\,y) + O(N^{-1} + \ell_N) & \text{if } r(x,\,y) = r(y,\,x). \end{cases} \tag{10.22}$$

(2) If A is an attracting set, we have

$$r_N^A(x,\,y) = \begin{cases} (1+O(\ell_N))(r(x,\,y)-r(y,\,x)) & \text{if } r(x,\,y) > r(y,\,x), \\ O(\ell_N) & \text{if } r(x,\,y) < r(y,\,x), \\ N^{-1} r(x,\,y) + O(\ell_N) & \text{if } r(x,\,y) = r(y,\,x). \end{cases} \tag{10.23}$$

It should be noted that the only difference between (10.22) and (10.23) is the appearance of the additional $\Theta(1/N)$-order error term. Note that the error term $\Theta(1/N)$ can be ignored when we consider the time scale $\theta_N^{\mathrm{nrv}} = 1/(Nd_N)$. Hence, in view of the following lemma, part (1) of the previous theorem provides sufficient control regarding the proof of Theorem 10.2.9.

Lemma 10.3.3. *The set S_0 defined right after* (10.11) *is a semi-attracting set.*

Proof. By contrast, suppose that some $x \in S_0$ and $y \in S_0^c$ satisfy $r(x,\,y) > r(y,\,x)$. Pick an invariant measure π of $Z_1(\cdot)$ such that $\pi(x) > 0$ and $\pi(y) = 0$. Then, we have

$$0 = \sum_{z\in S} \pi(y) b(y,\,z) = \sum_{z \in S} \pi(z) b(z,\,y) \geq \pi(x) b(x,\,y) = \pi(x)(r(x,\,y) - r(y,\,x)) > 0,$$

which is a contradiction. ☐

Meanwhile, we cannot afford this error when we consider the time scale $\theta_N^{\mathrm{rv}} = 1/d_N$. Hence, we need to assume the attractiveness of A in Theorem 10.2.11 to eliminate this error in (10.23).

The remainder of this section is devoted to proving Proposition 10.3.2. We establish several preliminary estimates in Section 10.3.2, and the proof of Proposition 10.3.2 is then given in Section 10.3.3.

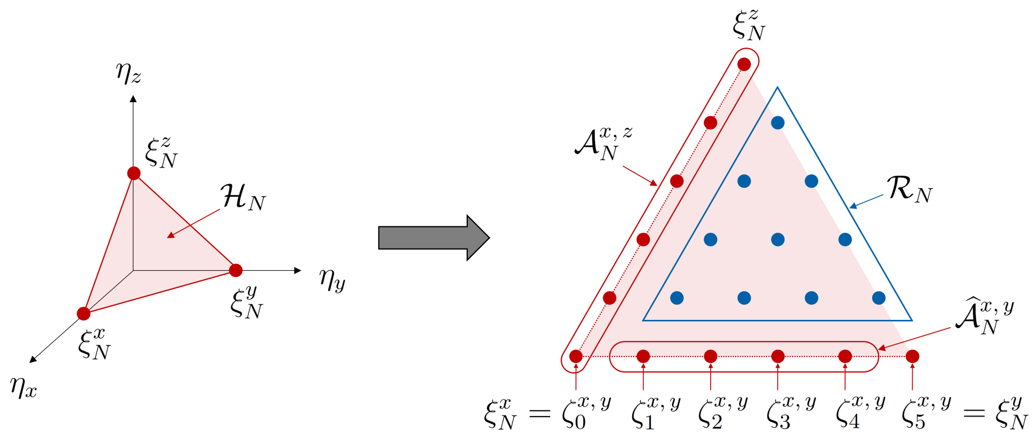


Figure 10.2: Visualization of the objects introduced in Notation 10.3.4 when $S = \{x,\, y,\, z\}$ and $r(y,\, z) = r(z,\, y) = 0$.

10.3.2 Hitting times on the tubes

A set playing a significant role in the estimate of $\mathbf{r}_N^A(\xi_N^x,\, \xi_N^y)$ for $x,\, y \in A$ is the *tube* $\mathcal{A}_N^{x,\,y}$ between ξ_N^x and ξ_N^y, defined in Definition 9.3.1, as the transition from ξ_N^x to ξ_N^y takes place only along this tube with dominating probability.

Notation 10.3.4 (Tube between metastable sets)**.** Here, we gather all the relevant notation related to the tube that will be frequently used in the remainder of this chapter. We refer to Figure 10.2 for the illustration of the notation introduced here.

Recall the notions of tubes defined in Definition 9.3.1.

If $x,\, y \in S$ satisfy $r(x,\, y) + r(y,\, x) > 0$, then we write $x \sim y$. With this notation, we write

$$\mathcal{A}_N = \bigcup_{x,\, y \in S\,:\, x \sim y} \mathcal{A}_N^{x,\,y} \quad \text{and} \quad \widehat{\mathcal{A}}_N = \bigcup_{x,\, y \in S\,:\, x \sim y} \widehat{\mathcal{A}}_N^{x,\,y}. \tag{10.24}$$

Note that $\mathcal{A}_N = \widehat{\mathcal{A}}_N \cup \mathcal{E}_N$. The remainder set is denoted by $\mathcal{R}_N$:

$$\mathcal{R}_N = \mathcal{H}_N \setminus \mathcal{A}_N.$$

Finally, we define several constants for convenience:

$$\begin{aligned} R_1 &= \min\{r(x,\, y) : x,\, y \in S \text{ such that } r(x,\, y) > 0\} > 0, \\ R_2 &= \max\{r(x,\, y) : x,\, y \in S\}, \\ \Lambda &= \max\{\lambda(x) : x \in S\}, \end{aligned} \tag{10.25}$$

where $\lambda(x) = \sum_{y \in S} r(x,\, y)$ denotes the holding rate of the underlying random walk. For $x,\, y \in S$ satisfying $x \sim y$, we write

$$q_{x,\, y} = \frac{\min\{r(x,\, y),\, r(y,\, x)\}}{\max\{r(x,\, y),\, r(y,\, x)\}} \in [0,\, 1]. \tag{10.26}$$

Then, we define

$$q = \max\{q_{x,\, y} : x,\, y \in S,\ x \sim y \text{ and } r(x,\, y) \neq r(y,\, x)\} < 1. \tag{10.27}$$

In the remainder of this section, we fix $A \subseteq S$ and $x,\, y \in A$. Then, we define an event $E_0 = E_0^{y,\, A}$ by

$$E_0 = \{\tau_{\mathcal{E}_N^y} = \tau_{\mathcal{E}_N(A)}\}.$$

Now, we provide a sequence of lemmas regarding the probability of the event E_0. We remark that these lemmas are also valid for a wide class of events that depend only on the hitting times of subsets of $(\widehat{\mathcal{A}}_N^{x,\, y})^c$ such as $\{\tau_{\mathcal{E}_N^x} < \tau_{\mathcal{E}_N^y}\}$.

The first lemma asserts that, provided d_N is sufficiently small, the inclusion process on $\widehat{\mathcal{A}}_N^{x,\, y}$ behaves as a nearest-neighbor random walk whose jump rate from ζ_i^{xy} to ζ_{i+1}^{xy} is $r(x,\, y)$ and from ζ_{i+1}^{xy} to ζ_i^{xy} is $r(y,\, x)$, especially when we are only concerned with the event E_0.

Lemma 10.3.5. *Suppose that $x,\, y \in S$ satisfy $x \sim y$. Then, there exists*

$C > 0$ such that

$$\Big|\mathbb{P}_{\zeta_i^{xy}}[E_0] - \frac{r(x,\, y)}{r(x,\, y) + r(y,\, x)}\mathbb{P}_{\zeta_{i+1}^{xy}}[E_0] - \frac{r(y,\, x)}{r(x,\, y) + r(y,\, x)}\mathbb{P}_{\zeta_{i-1}^{xy}}[E_0]\Big| \le C\frac{d_N N}{i(N-i)}$$

for all $i \in [\![1,\, N-1]\!]$.

Proof. Denote by $\lambda_N(\cdot)$ and $\mathbf{p}_N(\cdot,\, \cdot)$ the holding rate and the transition probability of the inclusion process:

$$\lambda_N(\eta) := \sum_{\zeta \in \mathcal{H}_N} r_N(\eta,\, \zeta) \quad \text{and} \quad \mathbf{p}_N(\eta,\, \zeta) := \frac{r_N(\eta,\, \zeta)}{\lambda_N(\eta)}.$$

Then, we can write

$$r_N(\zeta_i^{xy},\, \zeta_{i+1}^{xy}) = (N-i)(d_N + i)r(x,\, y), \tag{10.28}$$

$$r_N(\zeta_i^{xy},\, \zeta_{i-1}^{xy}) = i(d_N + N - i)r(y,\, x), \tag{10.29}$$

$$r_N(\zeta_i^{xy},\, \sigma^{x,\,z}\zeta_i^{xy}) = (N-i)d_N r(x,\, z) \text{ for } z \ne x,\, y,$$

$$r_N(\zeta_i^{xy},\, \sigma^{y,\,z}\zeta_i^{xy}) = i d_N r(y,\, z) \text{ for } z \ne x,\, y.$$

Thus, the holding rate at ζ_i^{xy} is given by

$$\lambda_N(\zeta_i^{xy}) = i(N-i)\{r(x,\, y) + r(y,\, x)\} + d_N\{(N-i)\lambda(x) + i\lambda(y)\}. \tag{10.30}$$

Hence, by (10.28) and (10.30),

$$\begin{aligned}
&\Big|\mathbf{p}_N(\zeta_i^{xy},\, \zeta_{i+1}^{xy}) - \frac{r(x,\, y)}{r(x,\, y) + r(y,\, x)}\Big| \\
&= \frac{d_N r(x,\, y) \cdot |(N-i)\{r(x,\, y) + r(y,\, x)\} - \{(N-i)\lambda(x) + i\lambda(y)\}|}{[i(N-i)\{r(x,\, y) + r(y,\, x)\} + d_N\{(N-i)\lambda(x) + i\lambda(y)\}]\{r(x,\, y) + r(y,\, x)\}} \\
&\le \frac{2R_2\Lambda}{R_1^2} d_N \frac{N}{i(N-i)},
\end{aligned} \tag{10.31}$$

where the last line follows from the definition (10.25). Similarly, by (10.29) and (10.30),

$$\left|\mathbf{p}_N(\zeta_i^{xy},\, \zeta_{i-1}^{xy}) - \frac{r(y,\, x)}{r(x,\, y) + r(y,\, x)}\right| \le \frac{2R_2\Lambda}{R_1^2} d_N \frac{N}{i(N-i)}. \tag{10.32}$$

The last two bounds imply that

$$\sum_{z:\, z\neq x,\, y} \mathbf{p}_N(\zeta_i^{xy},\, \sigma^{x,\, z}\zeta_i^{xy}) + \sum_{z:\, z\neq x,\, y} \mathbf{p}_N(\zeta_i^{xy},\, \sigma^{y,\, z}\zeta_i^{xy}) \le \frac{4R_2\Lambda}{R_1^2} d_N \frac{N}{i(N-i)}. \tag{10.33}$$

By the Markov property, we have

$$\begin{aligned}\mathbb{P}_{\zeta_i^{xy}}[E_0] =& \mathbf{p}_N(\zeta_i^{xy},\, \zeta_{i+1}^{xy})\mathbb{P}_{\zeta_{i+1}^{xy}}[E_0] + \mathbf{p}_N(\zeta_i^{xy},\, \zeta_{i-1}^{xy})\mathbb{P}_{\zeta_{i-1}^{xy}}[E_0] \\ &+ \sum_{z:\, z\neq x,\, y} \mathbf{p}_N(\zeta_i^{xy},\, \sigma^{x,\, z}\zeta_i^{xy})\mathbb{P}_{\sigma^{x,\, z}\zeta_i^{xy}}[E_0] \\ &+ \sum_{z:\, z\neq x,\, y} \mathbf{p}_N(\zeta_i^{xy},\, \sigma^{y,\, z}\zeta_i^{xy})\mathbb{P}_{\sigma^{y,\, z}\zeta_i^{xy}}[E_0].\end{aligned}$$

Finally, inserting the estimates (10.31), (10.32), and (10.33) into the last identity completes the proof. □

On the basis of the previous estimate, we can estimate the probabilities $\mathbb{P}_{\zeta_1^{xy}}[E_0]$ and $\mathbb{P}_{\zeta_{N-1}^{xy}}[E_0]$ in terms of $\mathbb{P}_{\xi_N^x}[E_0]$ and $\mathbb{P}_{\xi_N^y}[E_0]$. We divide this estimate into three cases according to the relation between $r(x,\, y)$ and $r(y,\, x)$ as follows.

Lemma 10.3.6. *Suppose that $x,\, y \in S$ satisfy $r(x,\, y) > r(y,\, x) > 0$. Then, it holds that*

$$\left|\mathbb{P}_{\zeta_1^{xy}}[E_0] - \frac{q_{x,\, y} - q_{x,\, y}^N}{1 - q_{x,\, y}^N}\mathbb{P}_{\xi_N^x}[E_0] - \frac{1 - q_{x,\, y}}{1 - q_{x,\, y}^N}\mathbb{P}_{\xi_N^y}[E_0]\right| = O(d_N \log N),$$

$$\left|\mathbb{P}_{\zeta_{N-1}^{xy}}[E_0] - \frac{q_{x,\, y}^{N-1} - q_{x,\, y}^N}{1 - q_{x,\, y}^N}\mathbb{P}_{\xi_N^x}[E_0] - \frac{1 - q_{x,\, y}^{N-1}}{1 - q_{x,\, y}^N}\mathbb{P}_{\xi_N^y}[E_0]\right| = O(d_N \log N).$$

Proof. Following (10.26) and Lemma 10.3.5, it holds for $i \in [\![1,\ N-1]\!]$ that

$$\left|\mathbb{P}_{\zeta_i^{xy}}[E_0] - \frac{1}{1+q_{x,y}}\mathbb{P}_{\zeta_{i+1}^{xy}}[E_0] - \frac{q_{x,y}}{1+q_{x,y}}\mathbb{P}_{\zeta_{i-1}^{xy}}[E_0]\right| \le C\frac{d_N N}{i(N-i)}. \quad (10.34)$$

Write

$$b_i = \mathbb{P}_{\zeta_{i-1}^{xy}}[E_0] - \mathbb{P}_{\zeta_i^{xy}}[E_0] \quad \text{for } i \in [\![1,\ N]\!];$$

so that we can rewrite (10.34) as

$$|b_{i+1} - q_{x,y}b_i| \le C\frac{d_N N}{i(N-i)}(1+q_{x,y}),$$

and therefore, for $i \in [\![1,\ N]\!]$,

$$|b_i - q_{x,y}^{i-1}b_1| \le Cd_N N(1+q_{x,y})\sum_{j=1}^{i-1}\frac{q_{x,y}^{i-1-j}}{j(N-j)}.$$

Since $\mathbb{P}_{\xi_N^x}[E_0] - \mathbb{P}_{\xi_N^y}[E_0] = b_1 + \cdots + b_N$, the previous bound implies that

$$\begin{aligned}
\left|\mathbb{P}_{\xi_N^x}[E_0] - \mathbb{P}_{\xi_N^y}[E_0] - \sum_{i=1}^{N} q_{x,y}^{i-1}b_1\right| &\le Cd_N N(1+q_{x,y})\sum_{i=1}^{N}\sum_{j=1}^{i-1}\frac{q_{x,y}^{i-1-j}}{j(N-j)} \\
&= Cd_N N(1+q_{x,y})\sum_{j=1}^{N-1}\frac{1}{j(N-j)}\sum_{i=j+1}^{N} q_{x,y}^{i-1-j} \\
&\le Cd_N\sum_{j=1}^{N-1}\left[\frac{1}{j}+\frac{1}{N-j}\right]\frac{1+q_{x,y}}{1-q_{x,y}} \le Cd_N\log N.
\end{aligned}$$

From this computation, we can deduce that

$$\left|b_1 - \frac{1-q_{x,y}}{1-q_{x,y}^N}\left(\mathbb{P}_{\xi_N^x}[E_0] - \mathbb{P}_{\xi_N^y}[E_0]\right)\right| \le Cd_N\log N.$$

By inserting $b_1 = \mathbb{P}_{\xi_N^x}[E_0] - \mathbb{P}_{\zeta_1^{xy}}[E_0]$, we obtain the first estimate of the lemma. The second one can be proved similarly. □

Now, we consider the second case in which the jump from y to x is excluded.

Lemma 10.3.7. *Suppose that $x,\, y \in S$ satisfy $r(x,\, y) > r(y,\, x) = 0$. Then, it holds that*

$$\left|\mathbb{P}_{\zeta_1^{xy}}[E_0] - \mathbb{P}_{\xi_N^y}[E_0]\right| = O(d_N \log N) \quad \textit{and} \quad \left|\mathbb{P}_{\zeta_{N-1}^{xy}}[E_0] - \mathbb{P}_{\xi_N^y}[E_0]\right| = O(d_N).$$

Proof. By Lemma 10.3.5, it holds that

$$\left|\mathbb{P}_{\zeta_i^{xy}}[E_0] - \mathbb{P}_{\zeta_{i+1}^{xy}}[E_0]\right| \le C\frac{d_N N}{i(N-i)} \quad \text{for all } i \in [\![1,\, N-1]\!].$$

By inserting $i = N-1$, we immediately obtain the second estimate. For the first estimate, it suffices to apply the triangle inequality such that

$$\left|\mathbb{P}_{\zeta_1^{xy}}[E_0] - \mathbb{P}_{\xi_N^y}[E_0]\right| \le \sum_{i=1}^{N-1} C\frac{d_N N}{i(N-i)} = O(d_N \log N).$$

This completes the proof of the first estimate. □

Now, we consider the last case, i.e., the symmetric case.

Lemma 10.3.8. *Suppose that $x,\, y \in S$ satisfy $r(x,\, y) = r(y,\, x) > 0$. Then, it holds that*

$$\left|\mathbb{P}_{\zeta_1^{xy}}[E_0] - \frac{N-1}{N}\mathbb{P}_{\xi_N^x}[E_0] - \frac{1}{N}\mathbb{P}_{\xi_N^y}[E_0]\right| = O(d_N \log N). \tag{10.35}$$

Proof. For $i \in [\![1,\, N-1]\!]$, write

$$c_i = \mathbb{P}_{\zeta_{i-1}^{xy}}[E_0] - \mathbb{P}_{\zeta_i^{xy}}[E_0] - \frac{1}{N}(\mathbb{P}_{\xi_N^x}[E_0] - \mathbb{P}_{\xi_N^y}[E_0]). \tag{10.36}$$

Then, we can observe that

$$c_1 + \cdots + c_N = 0, \tag{10.37}$$

and that the left-hand side of (10.35) is $|c_1|$. Thus, it suffices to show that $|c_1| = O(d_N \log N)$.

By Lemma 10.3.5, it holds that

$$\left|\mathbb{P}_{\zeta_i^{xy}}[E_0] - \frac{1}{2}\mathbb{P}_{\zeta_{i+1}^{xy}}[E_0] - \frac{1}{2}\mathbb{P}_{\zeta_{i-1}^{xy}}[E_0]\right| \le C\frac{d_N N}{i(N-i)} \quad \text{for all } i \in [\![1,\, N-1]\!].$$

By (10.36) , this inequality can be written as

$$|c_i - c_{i+1}| \le C\frac{d_N N}{i(N-i)}.$$

Therefore, by the triangle inequality, we obtain

$$|c_1 - c_i| \le \sum_{j=1}^{i-1} |c_j - c_{j+1}| \le C d_N \sum_{j=1}^{i-1} \frac{N}{j(N-j)} \le C d_N \log N.$$

Hence, by (10.37),

$$|Nc_1| = |Nc_1 - (c_1 + \cdots + c_N)| \le \sum_{i=2}^{N} |c_1 - c_i| \le C d_N N \log N.$$

This completes the proof of $|c_1| = O(d_N \log N)$. □

10.3.3 Proof of Proposition 10.3.2

Proof of Proposition 10.3.2. Fix $A \subseteq S$ and fix $x, y \in A$. By [5, Corollary 6.2], we can write the jump rate $\mathbf{r}_N^A(\xi_N^x, \xi_N^y)$ as

$$\begin{aligned}\mathbf{r}_N^A(\xi_N^x, \xi_N^y) =& r_N(\xi_N^x, \xi_N^y) + \sum_{\eta \in \mathcal{H}_N \setminus \mathcal{E}_N(A)} r_N(\xi_N^x, \eta)\mathbb{P}_\eta[\tau_{\mathcal{E}_N^y} = \tau_{\mathcal{E}_N(A)}] \\ =& \sum_{z:\, z \neq x} N d_N r(x, z)\mathbb{P}_{\zeta_1^{xz}}[E_0].\end{aligned} \tag{10.38}$$

Hence, it suffices to estimate $\mathbb{P}_{\zeta_1^{xz}}[E_0]$ for $z \neq x$ with $r(x, z) > 0$ to estimate $\mathbf{r}_N^A(\xi_N^x, \xi_N^y)$.

Suppose first that $z \neq y$. Then, we divide the estimate of $\mathbb{P}_{\zeta_1^{xz}}[E_0]$ into two cases:

(Case 1: $z \in A$**)** Since $\mathbb{P}_{\xi_N^z}[E_0] = 0$, we deduce from Lemmas 10.3.6, 10.3.7, and 10.3.8 that

$$\mathbb{P}_{\zeta_1^{xz}}[E_0] = O(d_N \log N). \tag{10.39}$$

(Case 2: $z \notin A$**)** We divide this case into two as following:

- If A is attracting, we have $r(x, z) < r(z, x)$. Thus by Lemma 10.3.6 we obtain

$$\mathbb{P}_{\zeta_1^{xz}}[E_0] = O(q^N)\mathbb{P}_{\xi_N^z}[E_0] + O(d_N \log N) = O(\ell_N). \tag{10.40}$$

- If A is semi-attracting, we only have $r(x, z) \leq r(z, x)$. Thus by Lemmas 10.3.6 and 10.3.8 we obtain

$$\mathbb{P}_{\zeta_1^{xz}}[E_0] = O\Big(\frac{1}{N} + q^N\Big) \cdot \mathbb{P}_{\xi_N^z}[E_0] + O(d_N \log N) = O\Big(\frac{1}{N} + \ell_N\Big). \tag{10.41}$$

Now it remains to estimate $\mathbb{P}_{\zeta_1^{xy}}[E_0]$ when $r(x, y) \neq 0$ to estimate (10.38). To this end, we consider four cases separately:

(1) $r(x,\, y) > r(y,\, x) > 0$: By Lemma 10.3.6 and the fact that

$$\mathbb{P}_{\xi_N^x}[E_0] = 0 \quad \text{and} \quad \mathbb{P}_{\xi_N^y}[E_0] = 1, \tag{10.42}$$

we have that

$$\left|\mathbb{P}_{\zeta_1^{xy}}[E_0] - \frac{q_{x,\,y} - q_{x,\,y}^N}{1 - q_{x,\,y}^N} \cdot 0 - \frac{1 - q_{x,\,y}}{1 - q_{x,\,y}^N} \cdot 1\right| = O(d_N \log N).$$

Thus, we have that

$$\mathbb{P}_{\zeta_1^{xy}}[E_0] = \frac{1 - q_{x,\,y}}{1 - q_{x,\,y}^N} + O(d_N \log N) = (1 + O(\ell_N))(1 - q_{x,\,y}). \tag{10.43}$$

(2) $r(y,\, x) > r(x,\, y) > 0$: By Lemma 10.3.6 and (10.42),

$$\left|\mathbb{P}_{\zeta_1^{xy}}[E_0] - \frac{1 - q_{x,\,y}^{N-1}}{1 - q_{x,\,y}^N} \cdot 0 - \frac{q_{x,\,y}^{N-1} - q_{x,\,y}^N}{1 - q_{x,\,y}^N} \cdot 1\right| = O(d_N \log N).$$

Therefore, we obtain that

$$\mathbb{P}_{\zeta_1^{xy}}[E_0] = \frac{q_{x,\,y}^{N-1} - q_{x,\,y}^N}{1 - q_{x,\,y}^N} + O(d_N \log N) = O(\ell_N). \tag{10.44}$$

(3) $r(x,\, y) > r(y,\, x) = 0$: By Lemma 10.3.7 and (10.42),

$$\mathbb{P}_{\zeta_1^{xy}}[E_0] = 1 + O(d_N \log N). \tag{10.45}$$

(4) $r(x,\, y) = r(y,\, x) > 0$: By Lemma 10.3.8 and (10.42),

$$\left|\mathbb{P}_{\zeta_1^{xy}}[E_0] - \frac{N-1}{N} \cdot 0 - \frac{1}{N} \cdot 1\right| = O(d_N \log N).$$

Hence, we can conclude that

$$\mathbb{P}_{\zeta_1^{xy}}[E_0] = \frac{1}{N} + O(d_N \log N). \tag{10.46}$$

Finally, we can combine (10.39)-(10.46) along with the identity (10.38) to complete the proof of the proposition. □

10.4 Metastable behavior of inclusion process under condition (UI)

In this section, we investigate the metastable behavior of the inclusion process under the condition **(UI)**. We first show that the invariant measure $\mu_N(\cdot)$ admits the expression (10.4).

Proof of Proposition 10.1.2 for case ***(UI)****.* It suffices to prove that, for $\eta \in \mathcal{H}_N$,

$$\sum_{x,\,y\in S:\,\eta_y\geq 1} \mu_N(\sigma^{y,\,x}\eta)(\sigma^{y,\,x}\eta)_x(d_N+(\sigma^{y,\,x}\eta)_y)r(x,\,y) = \mu_N(\eta)\sum_{x,\,y\in S}\eta_y(d_N+\eta_x)r(y,\,x). \tag{10.47}$$

Calculating the left-hand side of (10.47), it holds that

$$\begin{aligned}
&\sum_{x,\,y\in S:\,\eta_y\geq 1} \mu_N(\sigma^{y,\,x}\eta)(\sigma^{y,\,x}\eta)_x(d_N+(\sigma^{y,\,x}\eta)_y)r(x,\,y)\\
&= \sum_{y\in S:\,\eta_y\geq 1}\sum_{x\in S}\mu_N(\sigma^{y,\,x}\eta)(\eta_x+1)(d_N+\eta_y-1)r(x,\,y)\\
&= \mu_N(\eta)\sum_{y:\,\eta_y\geq 1}\sum_{x\in S}\eta_y(d_N+\eta_x)r(x,\,y) = \mu_N(\eta)\sum_{x,\,y\in S}(\eta_x\eta_y+d_N\eta_y)r(x,\,y).
\end{aligned}$$

Comparing to the right-hand side of (10.47), it suffices to show that

$$\sum_{x,\,y\in S}\eta_y r(x,\,y) = \sum_{x,\,y\in S}\eta_y r(y,\,x).$$

This identity holds since

$$\sum_{x,\,y\in S}\eta_y r(x,\,y)=\sum_{y\in S}\eta_y\sum_{x\in S}r(x,\,y)\overset{\textbf{(UI)}}{=}\sum_{y\in S}\eta_y\sum_{x\in S}r(y,\,x)=\sum_{x,\,y\in S}\eta_y r(y,\,x).$$

□

Now, we can prove Theorem 10.2.7 by gathering the results obtained so far.

Proof of Theorem 10.2.7. As we mentioned before, part (1) follows from the investigation of the reversible case. Hence, we shall only concentrate on part (2). By Propositions 10.1.2 and 10.1.3, we know that condensation occurs on the entire set S, i.e., $S=S_\star$. Then, the condition **(H0)** (of the form (3.26)) follows from Proposition 10.3.2 with $A=S$, with $\theta_N=\dfrac{1}{Nd_N}$ and

$$a(x,\,y)=[r(x,\,y)-r(y,\,x)]\mathbb{1}\{r(x,\,y)>r(y,\,x)\}\quad\text{for all }x,\,y\in S.$$

These scale and limiting chain correspond to (10.8) and (10.9) of Conjecture 10.2.3, and the proof is completed. □

10.5 Metastable behavior of inclusion process with condensation

In this section, we are concerning on the metastable behavior of the condensate of non-reversible inclusion processes under the condition that the condensation occurs, namely Theorems 10.2.9, 10.2.11 and 10.2.12. By assuming several irreducibility conditions on the limiting Markov chain, we derive the followings in this section based on the results obtained in Section 10.3:

- characterization of the maximal condensing set $S_\star\subseteq S$,

- asymptotic limit of $\mu_N(\xi_N^x)$ for $x \in S_\star$ as $N \to \infty$,
- limiting Markov chain on $S_\star$ describing the movement of condensate.

We prove these main results in Section 10.5.2 based on a lemma introduced in 10.5.1.

10.5.1 A preliminary lemma

In this short subsection, we introduce an elementary lemma. We believe that this result is not new, but we include the full proof since we were not able to find an exact reference that states the exact result that we need.

Lemma 10.5.1. *Let $(Z_N(\cdot))_{N=1}^\infty$ be a sequence of continuous-time Markov chains on a finite set $\mathfrak{S}$. Denote the jump rate of $Z_N(\cdot)$ by $a_N(\cdot,\, \cdot)$ and fix an invariant measure $\pi_N(\cdot)$ of $Z_N(\cdot)$ for each N. Suppose in addition that*

$$\lim_{N\to\infty} a_N(x,\, y) = a(x,\, y) \quad \textit{for all } x,\, y \in \mathfrak{S}. \tag{10.48}$$

Then each limit point of $\{\pi_N\}$ becomes an invariant measure for the Markov chain $Z(\cdot)$ with jump rate $a(\cdot,\, \cdot)$. Moreover, if $Z(\cdot)$ admits the unique invariant measure π, then we have that

$$\lim_{N\to\infty} \pi_N(x) = \pi(x) \quad \textit{for all } x,\, y \in \mathfrak{S}. \tag{10.49}$$

Remark. In the second statement above, note that we did not assume the irreducibility of $Z(\cdot)$. However, the uniqueness of the invariant measure for $Z(\cdot)$ is a crucial condition for this statement.

Proof of Lemma 10.5.1. Suppose that a subsequence $(\pi_{N_k})_{k=1}^\infty$ converges to π_0. Note that π_0 must be a probability measure on $\mathfrak{S}$ as well. Since π_{N_k} is an invariant measure for the chain Z_{N_k}, we have

$$\sum_{y\in\mathfrak{S}} \pi_{N_k}(x) a_{N_k}(x,\, y) = \sum_{y\in\mathfrak{S}} \pi_{N_k}(y) a_{N_k}(y,\, x) \quad \text{for all } x,\, y \in \mathfrak{S}.$$

By letting $k \to \infty$ at the last identity, we obtain that

$$\sum_{y \in \mathfrak{S}} \pi_0(x) a(x,\, y) = \sum_{y \in \mathfrak{S}} \pi_0(y) a(y,\, x) \quad \text{for all } x,\, y \in \mathfrak{S}.$$

Therefore, π_0 is an invariant measure of $Z(\cdot)$. This concludes the first statement.

Next we consider the second statement. Since $\{\pi_N : N \geq 1\}$ is a bounded subset of $\mathbb{R}^{\mathfrak{S}}$, we know that this set is precompact. Moreover, we have shown above that every convergent subsequence converges to an invariant measure of $Z(\cdot)$, which should be π by the uniqueness assumption for this case. This completes the proof. □

10.5.2 Proof of main results

Now, we are ready to prove Theorems 10.2.9, 10.2.11, and 10.2.12. We consider the asymmetric case and the symmetric case separately. Recall two Markov chains $\{Z_1(t)\}_{t \geq 0}$ and $\{Z_2(t)\}_{t \geq 0}$ and the set $S_0 \subseteq S$ from Section 10.2.3. We start with the asymmetric case.

Proof of Theorem 10.2.9 and the asymmetric case of Theorem 10.2.12. To start the proof, we first prove Theorem 10.2.9 by using Proposition 10.3.2. It suffices to verify condition **(H0)** (convergence of the jump rate of the trace process, as in (3.26)) and the fact that $S_\star = S_0$. We recall the invariant measure ν of $Y^{\mathrm{nrv}}(\cdot)$ on S_0 (cf. Theorem 10.2.12), and the rate $b(\cdot,\, \cdot) : S \times S \to [0,\, \infty)$ defined in (10.11). Recalling the remark after Notation 10.2.10, the set S_0 is semi-attracting. Thus, by Proposition 10.3.2, we know that

$$\lim_{N \to \infty} \theta_N^{\mathrm{nrv}} \mathbf{r}_N^S(\xi_N^x,\, \xi_N^y) = b(x,\, y) \quad \text{for all } x,\, y \in S,$$

where $\theta_N^{\mathrm{nrv}} = 1/(N d_N)$. We assumed that the Markov chain $Z_1(\cdot)$ with jump kernel b has the only irreducible component S_0, and this guarantees the uniqueness of the invariant measure of $Z_1(\cdot)$, which will be denoted by π.

Since the invariant measure of the trace process $\eta_N^{\mathcal{E}_N}(\theta_N^{\mathrm{nrv}}\cdot)$ is the conditioned measure $\mu_N(\cdot|\mathcal{E}_N) = \mu_N(\cdot)/\mu_N(\mathcal{E}_N)$ on $\mathcal{E}_N$, we can deduce from Lemma 10.5.1 that

$$\lim_{N\to\infty} \frac{\mu_N(\xi_N^x)}{\mu_N(\mathcal{E}_N)} = \pi(x) \quad \text{for all } x \in S.$$

Since condensation occurs, i.e., $\lim_{N\to\infty} \mu_N(\mathcal{E}_N) = 1$, we obtain that

$$\lim_{N\to\infty} \mu_N(\xi_N^x) = \pi(x). \tag{10.50}$$

Since S_0 is the unique irreducible component of the chain $Z_1(\cdot)$, we know that $\pi(x) = 0$ for $x \in S \setminus S_0$, and that $\pi(x) > 0$ for $x \in S_0$. From this and (10.50), we can conclude that $S_\star = S_0$. Next, using Proposition 10.3.2 with $A = S_0$, we obtain

$$\lim_{N\to\infty} \theta_N^{\mathrm{nrv}} \mathbf{r}_N^{S_0}(\xi_N^x,\, \xi_N^y) = b(x,\, y) \quad \text{for all } x,\, y \in S_0,$$

Hence, the jump rate of the speeded-up trace process $\eta_N^{\mathcal{E}_N(S_0)}(\theta_N^{\mathrm{nrv}}\cdot)$ converges to $b(\cdot,\, \cdot)$, by identifying ξ_N^x with x. This concludes Theorem 10.2.9.

Finally, note that π conditioned on the irreducible component S_0 is the invariant measure of the Markov chain $Z_1(\cdot)$ conditioned on S_0, which is indeed the Markov chain $Y^{\mathrm{nrv}}(\cdot)$ defined in the paragraph preceding (10.8). Thus, we can conclude that $\pi(x) = \nu(x)$ for $x \in S_0$ as well. This and (10.50) finish the proof of the asymmetric case of Theorem 10.2.12. $\square$

Now, we consider the symmetric case, for which the time scale is now $1/d_N$ instead of $1/(Nd_N)$.

Proof for Theorem 10.2.11 and the symmetric case of Theorem 10.2.12. As in the previous proof, we prove condition **(H0)** and the fact that $S_\star = S_0$.

We first prove that condensation occurs on S_0. By Proposition 10.3.2, we know that

$$\lim_{N\to\infty} \frac{1}{Nd_N} \mathbf{r}_N^S(\xi_N^x,\, \xi_N^y) = b(x,\, y) \quad \text{for all } x,\, y \in S.$$

Here, the Markov chain $Z_1(\cdot)$ does not necessarily admit a unique invariant measure. Nevertheless, all the invariant measures of $Z_1(\cdot)$ do share the characteristic that they should vanish on $S \setminus S_0$, which is clear from the definition of S_0. Hence, it follows from the first statement of Lemma 10.5.1 that

$$\lim_{N\to\infty} \frac{\mu_N(\xi_N^x)}{\mu_N(\mathcal{E}_N)} = 0 \quad \text{for all } x \in S \setminus S_0.$$

By the above and the assumption of condensation on S, we have $\lim_{N\to\infty} \mu_N(\mathcal{E}_N(S_0)) = 1$, so that condensation occurs on S_0.

Next, using part (1) of Proposition 10.3.2 with $A = S_0$, which is possible since S_0 is assumed to be attracting, we obtain that

$$\lim_{N\to\infty} \theta_N^{\mathrm{rv}} \mathbf{r}_N^{S_0}(\xi_N^x,\, \xi_N^y) = r(x,\, y) \quad \text{for all } x,\, y \in S_0,$$

which establishes the convergence of the jump rate of the trace process.

Since the Markov chain $Z_2(\cdot)$ on S_0 with jump kernel b is irreducible by the condition of the theorem, it admits the unique invariant measure ν on S_0. Hence, Lemma 10.5.1 implies that

$$\lim_{N\to\infty} \frac{\mu_N(\xi_N^x)}{\mu_N(\mathcal{E}_N(S_0))} = \nu(x) \quad \text{for all } x \in S_0.$$

Since condensation occurs on S_0, this implies that $\lim_{N\to\infty} \mu_N(\xi_N^x) = \nu(x)$; thus, $S_\star = S_0$. Therefore, Theorem 10.2.12 is proved for the symmetric case. Finally, Theorem 10.2.11 is concluded via Proposition 10.3.2. $\square$

10.6 Condensation under condition (UP)

In this section, we establish condensation of the inclusion process under the condition **(UP)**, i.e., prove Theorem 10.2.14. With this result on the occurrence of condensation, the analysis of the metastable behavior, as well as the characterization of $S_\star$ and asymptotic mass of the invariant measure, follows immediately from the results obtained in Section 10.5. We mention that we do not have an explicit formula of the invariant measure μ_N for this case as well, and hence all the proof should follow the ways that have never been explored before.

We assume the condition **(UP)** throughout this section, i.e., $r(x,\, y) > 0$ for all $x,\, y \in S$. We start by summarizing several sets that are repeatedly used in the proof of the main result of this section. We refer to Figure 10.3 for the illustration of these sets. Some of the notions overlap with the ones in Definition 9.3.1.

Notation 10.6.1. Let R be a non-empty subset of S.

Define the *R-tube* as

$$\mathcal{A}_N^R = \{\eta \in \mathcal{H}_N : \eta_x = 0 \text{ for all } x \in S \setminus R\}.$$

For example, $\mathcal{A}_N^S = \mathcal{H}_N$, $\mathcal{A}_N^{\{x\}} = \mathcal{E}_N^x$, and $\mathcal{A}_N^{\{x,\, y\}} = \mathcal{A}_N^{x,\, y}$ for all $x,\, y \in S$.

We decompose each R-tube $\mathcal{A}_N^R$ into its boundary $\partial\mathcal{A}_N^R$ and the core $\mathcal{R}_N^R$ where

$$\begin{aligned}\partial\mathcal{A}_N^R =& \{\eta \in \mathcal{A}_N^R : \eta_x = 0 \text{ for some } x \in R\},\\ \mathcal{R}_N^R =& \{\eta \in \mathcal{A}_N^R : \eta_x > 0 \text{ for all } x \in R\}.\end{aligned}$$

For example, we have $\partial\mathcal{A}_N^{\{x,\, y\}} = \mathcal{E}_N^x \cup \mathcal{E}_N^y$ and $\mathcal{R}_N^{\{x,\, y\}} = \widehat{\mathcal{A}}_N^{x,\, y}$.

We further decompose the core $\mathcal{R}_N^R$ into the inner core $\mathcal{I}_N^R$ and the outer core $\mathcal{O}_N^R$ where

$$\mathcal{I}_N^R = \{\eta \in \mathcal{R}_N^R : \eta_x > \epsilon \log N \text{ for all } x \in R\},$$
$$\mathcal{O}_N^R = \{\eta \in \mathcal{R}_N^R : \eta_x \le \epsilon \log N \text{ for some } x \in R\},$$

where ϵ is a small enough number that will be specified later (cf. (10.69)). We stress that ϵ does not depend on N. For the convenience of notation, we assume in this and the next subsections that $\epsilon \log N$ is an integer. (For general case, it suffices to replace all $\epsilon \log N$ below with $\lfloor \epsilon \log N \rfloor$.) For instance, a configuration η belonging to $\mathcal{I}_N^R$ does not have particles at $S \setminus R$ while have more than $\epsilon \log N$ particles at each site of R. Summing up, we decompose each R-tube $\mathcal{A}_N^R$ into the following disjoint union:

$$\mathcal{A}_N^R = \partial \mathcal{A}_N^R \cup \mathcal{O}_N^R \cup \mathcal{I}_N^R. \tag{10.51}$$

Write $|S| = \kappa$. For $k \in [\![1,\, \kappa]\!]$, we define

$$\mathcal{B}_N^k = \bigcup_{R \subseteq S,\, |R| = k} \mathcal{A}_N^R.$$

Namely, $\mathcal{B}_N^k$ is a collection of configurations that have at most k sites with at least one particle. For instance, $\mathcal{B}_N^1 = \mathcal{E}_N$, $\mathcal{B}_N^2 = \mathcal{A}_N$ (by the assumption **(UP)**), and $\mathcal{B}_N^\kappa = \mathcal{H}_N$.

In this section, we are mainly focusing on the following proposition.

Proposition 10.6.2. *Suppose that* (10.13) *holds. Then, for all* $\ell \in [\![2,\, \kappa]\!]$*, we have that*

$$\lim_{N \to \infty} \frac{\mu_N(\mathcal{B}_N^\ell)}{\mu_N(\mathcal{B}_N^{\ell-1})} = 1. \tag{10.52}$$

Proof. We explain the proof based on the results that will be proved in the remaining part of this section. We prove this proposition by means of the backward induction on ℓ from κ to 2. We note that the initial case $\ell = \kappa$

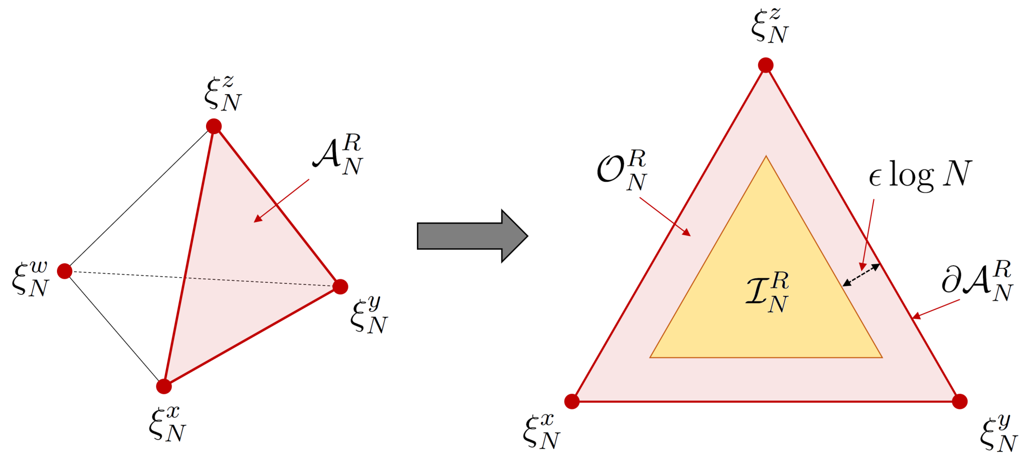


Figure 10.3: Visualization of the notation introduced in Notation 10.6.1 when $S = \{x,\, y,\, z,\, w\}$ and $R = \{x,\, y,\, z\}$.

is proved by Propositions 10.6.3 and 10.6.7 (cf. discussion between (10.54) and (10.55)). Then, by the induction step proved in Proposition 10.6.15, the assertion of the proposition holds for all $\ell \in [\![2,\, \kappa]\!]$. □

With this proposition, Theorem 10.2.14 is immediate.

Proof of Theorem 10.2.14. Since $\mathcal{B}_N^1 = \mathcal{E}_N$ and $\mathcal{B}_N^\kappa = \mathcal{H}_N$, it suffices to check that

$$\lim_{N\to\infty} \frac{\mu_N(\mathcal{B}_N^\kappa)}{\mu_N(\mathcal{B}_N^1)} = 1. \tag{10.53}$$

This is immediate from (10.52) and we are done. □

Now, we explain our plan to prove the detailed ingredients appeared in the proof of Proposition 10.6.2. The initial step $\ell = \kappa$ for the backward induction is proved in Sections 10.6.1 and 10.6.2, and the induction step is established in Section 10.6.3. For the proof of these steps, an auxiliary Markov chain introduced in Definition 10.6.9 of Section 10.6.2 is crucially used. As a by-product of our investigation of the hitting time of this Markov chain carried out in Lemma 10.6.11, we prove the nucleation result presented as Theorem 10.2.17 in Section 10.6.4 as well.

10.6.1 Initial step (1): negligibility of the outer core

Now, we prove the case $\ell = \kappa$ for Proposition 10.6.2. Since $\mathcal{B}_N^{\kappa} = \mathcal{A}_N^S (= \mathcal{H}_N)$ and $\mathcal{B}_N^{\kappa-1} = \partial\mathcal{A}_N^S$ by the definition of the boundary, it suffices to prove

$$\lim_{N\to\infty} \frac{\mu_N(\mathcal{A}_N^S)}{\mu_N(\partial\mathcal{A}_N^S)} = 1. \tag{10.54}$$

Since $\mu_N(\mathcal{A}_N^S) = \mu_N(\partial\mathcal{A}_N^S) + \mu_N(\mathcal{O}_N^S) + \mu_N(\mathcal{I}_N^S)$ by (10.51), it suffices to prove that

$$\lim_{N\to\infty} \frac{\mu_N(\mathcal{O}_N^S)}{\mu_N(\partial\mathcal{A}_N^S)} = 0 \quad \text{and} \quad \lim_{N\to\infty} \frac{\mu_N(\mathcal{I}_N^S)}{\mu_N(\partial\mathcal{A}_N^S)} = 0. \tag{10.55}$$

The proof of The latter one is considered in the next subsection, and we focus only on the former one in the current subsection. Thus, the main object now is to prove the following proposition.

Proposition 10.6.3. *Suppose that* $\lim_{N\to\infty} d_N N = 0$*. Then, for sufficiently small* $\epsilon > 0$*, we have that*

$$\lim_{N\to\infty} \frac{\mu_N(\mathcal{O}_N^S)}{\mu_N(\partial\mathcal{A}_N^S)} = 0.$$

To prove this, we decompose the outer core $\mathcal{O}_N^S$ into more refined objects, and estimate each of them carefully.

Decomposition of outer core

For $x \in R \subseteq S$ and $k \in [\![1,\, N]\!]$, we define

$$\mathcal{C}_N^R(x,\, k) = \{\eta \in \mathcal{A}_N^R : \eta_x = k\}.$$

For instance, we have

$$\mathcal{C}_N^R(x,\,N) = \mathcal{E}_N^x \quad \text{and} \quad \mathcal{C}_N^R(x,\,0) = \mathcal{A}_N^{R\setminus\{x\}}. \tag{10.56}$$

Then, it holds that

$$\mathcal{O}_N^R \subseteq \bigcup_{x\in R} \bigcup_{k=1}^{\epsilon \log N} \mathcal{C}_N^R(x,\,k); \tag{10.57}$$

thus,

$$\mu_N(\mathcal{O}_N^S) \le \sum_{x\in S} \sum_{k=1}^{\epsilon \log N} \mu_N(\mathcal{C}_N^S(x,\,k)). \tag{10.58}$$

Hence, it suffices to estimate $\mu_N(\mathcal{C}_N^S(x,\,k))$ for $k \in [\![1,\,\epsilon \log N]\!]$ and $x \in S$.

Estimation of $\mu_N(\mathcal{C}_N^S(x,\,k))$

For $k \in [\![0,\,N-1]\!]$ and $x \in R \subseteq S$, we define

$$\begin{aligned}\mathbf{F}_N^R(x;\,k \to k+1) &= \sum_{\eta\in\mathcal{C}_N^R(x,\,k),\,\zeta\in\mathcal{C}_N^R(x,\,k+1)} \mu_N(\eta) r_N(\eta,\,\zeta),\\ \mathbf{F}_N^R(x;\,k+1 \to k) &= \sum_{\eta\in\mathcal{C}_N^R(x,\,k+1),\,\zeta\in\mathcal{C}_N^R(x,\,k),} \mu_N(\eta) r_N(\eta,\,\zeta).\end{aligned}$$

Lemma 10.6.4. *For all $k \in [\![0,\,N-1]\!]$ and $x \in S$, it holds that*

$$\mathbf{F}_N^S(x;\,k \to k+1) = \mathbf{F}_N^S(x;\,k+1 \to k).$$

Proof. Since μ_N is the invariant measure for the inclusion process, we have that,

$$\sum_{x,\,y\in S} \mu_N(\eta) r_N(\eta,\,\sigma^{x,\,y}\eta) = \sum_{x,\,y\in S} \mu_N(\sigma^{x,\,y}\eta) r_N(\sigma^{x,\,y}\eta,\,\eta) \quad \text{for all } \eta \in \mathcal{H}_N. \tag{10.59}$$

Here, we use the convention that $r_N(\eta,\,\eta) = 0$ for $\eta \in \mathcal{H}_N$. By summing

(10.59) over $\eta \in \mathcal{C}_N^S(x,\, k)$,

$$\begin{aligned}
&\sum_{\eta\in\mathcal{C}_N^S(x,\,k)}\sum_{y,\,z\in S\setminus\{x\}}\mu_N(\eta)r_N(\eta,\,\sigma^{y,\,z}\eta)+\sum_{\eta\in\mathcal{C}_N^S(x,\,k)}\sum_{y\in S\setminus\{x\}}\mu_N(\eta)r_N(\eta,\,\sigma^{y,\,x}\eta)\\
&+\sum_{\eta\in\mathcal{C}_N^S(x,\,k)}\sum_{y\in S\setminus\{x\}}\mu_N(\eta)r_N(\eta,\,\sigma^{x,\,y}\eta)\\
&=\sum_{\eta\in\mathcal{C}_N^S(x,\,k)}\sum_{y,\,z\in S\setminus\{x\}}\mu_N(\sigma^{y,\,z}\eta)r_N(\sigma^{y,\,z}\eta,\,\eta)+\sum_{\eta\in\mathcal{C}_N^S(x,\,k)}\sum_{y\in S\setminus\{x\}}\mu_N(\sigma^{y,\,x}\eta)r_N(\sigma^{y,\,x}\eta,\,\eta)\\
&\quad+\sum_{\eta\in\mathcal{C}_N^S(x,\,k)}\sum_{y\in S\setminus\{x\}}\mu_N(\sigma^{x,\,y}\eta)r_N(\sigma^{x,\,y}\eta,\,\eta).
\end{aligned} \tag{10.60}$$

Note that the first summations in the respective sides of (10.60) are canceled out with each other. Therefore, (10.60) can be simply rewritten as

$$\mathbf{F}_N^S(x;\,k\to k+1)+\mathbf{F}_N^S(x;\,k\to k-1)=\mathbf{F}_N^S(x;\,k\to k+1)+\mathbf{F}_N^S(x;\,k-1\to k), \tag{10.61}$$

where $\mathbf{F}_N^S(x;\,-1\to 0)$ and $\mathbf{F}_N^S(x;\,0\to -1)$ are defined to be 0. Inserting $k=0$ to (10.61) implies

$$\mathbf{F}_N^S(x;\,0\to 1)=\mathbf{F}_N^S(x;\,1\to 0). \tag{10.62}$$

Therefore, (10.61) and (10.62) along with induction on k finish the proof. □

Lemma 10.6.5. *For $k\in[\![0,\,N-1]\!]$ and $x\in S$, we have that*

$$\mu_N(\mathcal{C}_N^S(x,\,k+1))\le\frac{R_2(k+d_N)(N-k)}{R_1(k+1)(N-k-1+d_N)}\mu_N(\mathcal{C}_N^S(x,\,k)),$$

where the constants R_1 and R_2 are introduced in (10.25)*.*

Proof. Looking at $\mathbf{F}_N^S(x;\,k\to k+1)$ more carefully, we get the following bound:

$$\begin{aligned}\mathbf{F}_N^S(x;\,k\to k+1) &= \sum_{\eta\in\mathcal{C}_N^S(x,\,k),\,\zeta\in\mathcal{C}_N^S(x,\,k+1)} \mu_N(\eta)r_N(\eta,\,\zeta)\\ &= \sum_{\eta\in\mathcal{C}_N^S(x,\,k)}\sum_{y\in S\setminus\{x\}} \mu_N(\eta)r_N(\eta,\,\sigma^{y,\,x}\eta)\\ &= \sum_{\eta\in\mathcal{C}_N^S(x,\,k)}\Big[\mu_N(\eta)\sum_{y\in S\setminus\{x\}}\eta_y(d_N+\eta_x)r(y,\,x)\Big] \qquad (10.63)\\ &= (k+d_N)\sum_{\eta\in\mathcal{C}_N^S(x,\,k)}\mu_N(\eta)\sum_{y\in S\setminus\{x\}}r(y,\,x)\eta_y\\ &\le R_2(k+d_N)(N-k)\mu_N(\mathcal{C}_N^S(x,\,k)).\end{aligned}$$

Similarly, we can get

$$\begin{aligned}\mathbf{F}_N^S(x;\,k+1\to k) &= \sum_{\eta\in\mathcal{C}_N^S(x,\,k+1)}\sum_{y\in S\setminus\{x\}} \mu_N(\eta)r_N(\eta,\,\sigma^{x,\,y}\eta)\\ &= \sum_{\eta\in\mathcal{C}_N^S(x,\,k+1)}\Big[\mu_N(\eta)\sum_{y\in S\setminus\{x\}}\eta_x(d_N+\eta_y)r(x,\,y)\Big] \qquad (10.64)\\ &\ge R_1(k+1)(N-k-1+d_N)\mu_N(\mathcal{C}_N^S(x,\,k+1)).\end{aligned}$$

Combining (10.63), (10.64) with Lemma 10.6.4, we can complete the proof of the lemma. □

In the proof above, it is crucial to have $r(x,\,y)>0$ for all $x,\,y\in S$ to deduce (10.64). Hence, the condition **(UP)** is critically used.

Lemma 10.6.6. *For sufficiently small $\epsilon>0$, we have that*

$$\sum_{k=1}^{\epsilon\log N}\mu_N(\mathcal{C}_N^S(x,\,k))\le O(Nd_N)\mu_N(\mathcal{A}_N^{S\setminus\{x\}}).$$

Proof. Inserting $k=0$ to Lemma 10.6.5 yields that, for some constant $C_1>$

0,

$$\mu_N(\mathcal{C}_N^S(x,\,1)) \le C_1 d_N \mu_N(\mathcal{C}_N^S(x,\,0)), \tag{10.65}$$

while inserting $k \in [\![1,\, N-2]\!]$ provides us that for some constant $C_2 > 0$,

$$\mu_N(\mathcal{C}_N^S(x,\,k+1)) \le C_2 \mu_N(\mathcal{C}_N^S(x,\,k)). \tag{10.66}$$

Let $C_0 = \max\{C_1,\, C_2\}$. Then, (10.65) and (10.66) imply that

$$\mu_N(\mathcal{C}_N^S(x,\,k)) \le C_0^k d_N \mu_N(\mathcal{C}_N^S(x,\,0)) \quad \text{for } k \in [\![1,\, N-1]\!]. \tag{10.67}$$

Summing this up for $k = 1,\, 2,\, \dots,\, \epsilon \log N$, we get

$$\sum_{k=1}^{\epsilon \log N} \mu_N(\mathcal{C}_N^S(x,\,k)) \le \frac{C_0^{(\epsilon \log N)+1} - C_0}{C_0 - 1} d_N \mu_N(\mathcal{C}_N^S(x,\,0)). \tag{10.68}$$

Take ϵ small enough so that

$$\frac{C_0^{(\epsilon \log N)+1} - C_0}{C_0 - 1} = O(N). \tag{10.69}$$

The proof is completed since $\mathcal{C}_N^S(x,\,0) = \mathcal{A}_N^{S\setminus\{x\}}$ by (10.56). □

Now, we are ready to prove the main goal of this subsection.

Proof of Proposition 10.6.3. By (10.57) and the previous lemma, we get

$$\mu_N(\mathcal{O}_N^S) \le \sum_{x\in S} \sum_{k=1}^{\epsilon \log N} \mu_N(\mathcal{C}_N^S(x,\,k)) \le C d_N N \sum_{x\in S} \mu_N(\mathcal{A}_N^{S\setminus\{x\}}).$$

The proof is completed since

$$\sum_{x\in S} \mu_N(\mathcal{A}_N^{S\setminus\{x\}}) = \mu_N(\partial \mathcal{A}_N^S),$$

and since $\lim_{N\to\infty} d_N N = 0$ by the assumption of the proposition. □

10.6.2 Initial step (2): negligibility of the inner core

In this subsection, we prove the negligibility of the inner core $\mathcal{I}_N^S$ via the following proposition.

Proposition 10.6.7. *Suppose that* $\lim_{N\to\infty} d_N N^{\kappa+2}(\log N)^{\kappa-3} = 0$. *Then, we have that*

$$\lim_{N\to\infty} \frac{\mu_N(\mathcal{I}_N^S)}{\mu_N(\partial\mathcal{A}_N^S)} = 0.$$

The proof of this part is more demanding than that of the outer core, and we have to introduce a sequence of new concepts.

Define the closure and the (outer) boundary of $\mathcal{I}_N^R$ for $R \subseteq S$ as

$$\begin{aligned}
\overline{\mathcal{I}}_N^R &= \{\eta \in \mathcal{A}_N^R : r_N(\zeta,\, \eta) > 0 \text{ for some } \zeta \in \mathcal{I}_N^R\},\\
\partial\mathcal{I}_N^R &= \overline{\mathcal{I}}_N^R \setminus \mathcal{I}_N^R.
\end{aligned}$$

Thus, $\overline{\mathcal{I}}_N^S$ consists of configurations η such that $\eta_x \ge \epsilon \log N$ for all x and there exists *at most* one $x \in S$ with $\eta_x = \epsilon \log N$, while $\partial\mathcal{I}_N^S$ consists of configurations η such that $\eta_x \ge \epsilon\log N$ for all x and there exist *exactly* one $x \in S$ with $\eta_x = \epsilon \log N$. Therefore, we have the following decomposition for $\partial\mathcal{I}_N^S$

$$\partial\mathcal{I}_N^S \subseteq \bigcup_{x\in S} \mathcal{C}_N^S(x,\, \epsilon\log N).$$

Therefore, by (10.67) and (10.69), we have that

$$\mu_N(\partial\mathcal{I}_N^S) \le \sum_{x\in S} \mu_N(\mathcal{C}_N^S(x,\, \epsilon\log N)) \le CNd_N \sum_{x\in S} \mu_N(\mathcal{C}_N^S(x,\, 0)) = O(Nd_N)\mu_N(\partial\mathcal{A}_N^S). \tag{10.70}$$

Hence, Proposition 10.6.7 is the consequence of the following proposition.

Proposition 10.6.8. *Suppose that* $\lim_{N\to\infty} d_N N^{\kappa+2}(\log N)^{\kappa-3} = 0$. *Then, we have that*

$$\mu_N(\mathcal{I}_N^S) = O(N^{\kappa-2}(\log N)^{\kappa})\mu_N(\partial\mathcal{I}_N^S). \tag{10.71}$$

Proof of Proposition 10.6.7. By (10.70) and (10.71), we get that

$$\mu_N(\mathcal{I}_N^S) = O(N^{\kappa-2}(\log N)^{\kappa})\mu_N(\partial\mathcal{I}_N^S) = O(N^{\kappa-1}(\log N)^{\kappa}d_N)\mu_N(\partial\mathcal{A}_N^S).$$

By the condition $d_N N^{\kappa+2}(\log N)^{\kappa-3} = o(1)$, we are done. □

The remaining part of this subsection is devoted to prove Proposition 10.6.8.

Auxiliary Markov chain $\widehat{\eta}_N^R(\cdot)$ and its hitting time estimate

The crucial ingredient in the proof of Proposition 10.6.8 is an auxiliary discrete time Markov chain on $\overline{\mathcal{I}}_N^S = \mathcal{I}_N^S \cup \partial\mathcal{I}_N^S$ and the estimate of the hitting time of the set $\partial\mathcal{I}_N^S$ when the chain starts from $\mathcal{I}_N^S$. To use these results at the induction step in Section 10.6.3, we will work on $\overline{\mathcal{I}}_N^R$ for $R \subseteq S$.

Definition 10.6.9. For $R \subseteq S$, let $(\widehat{\eta}_N^R(t))_{t\in\mathbb{N}}$ denote the discrete-time Markov chain on $\overline{\mathcal{I}}_N^R$ whose transition probability $\widehat{\mathbf{p}}_N^R$ is given by

$$\widehat{\mathbf{p}}_N^R(\eta,\, \sigma^{x,\,y}\eta) = \frac{\eta_y(d_N+\eta_x)r(y,\,x)}{\sum_{a,\,b\in R}\eta_a(d_N+\eta_b)r(a,\,b)} \quad \text{for } \eta,\, \sigma^{x,\,y}\eta \in \overline{\mathcal{I}}_N^R, \tag{10.72}$$

and set

$$\widehat{\mathbf{p}}_N^R(\eta,\, \eta) = 1 - \sum_{\zeta:\,\zeta\neq\eta} \widehat{\mathbf{p}}_N^R(\eta,\, \zeta) \quad \text{for } \eta \in \partial\mathcal{I}_N^R.$$

In other words, $\widehat{\eta}_N^R(\cdot)$ is attained from the discrete version of the inclusion process by changing the jump rate $\eta_x(d_N+\eta_y)r(x,\,y)$ to $\eta_y(d_N+\eta_x)r(y,\,x)$ and then restricting to $\overline{\mathcal{I}}_N^R$. This chain is well defined since $\eta_x,\, \eta_y > 0$ for $\eta \in \overline{\mathcal{I}}_N^R$.

Let $\widehat{\mathbf{L}}_N^R$ denote the corresponding generator and by $\widehat{\mathbb{E}}_\eta^R$ the expectation with respect to the chain $\widehat{\eta}_N^R(\cdot)$ starting from $\eta \in \overline{\mathcal{I}}_N^R$. Finally, let $\sigma_R := \tau_{\partial \mathcal{I}_N^R}$ be the hitting time the set $\partial \mathcal{I}_N^R$ by the chain $\widehat{\eta}_N^R(\cdot)$. *Then, the primary purpose is to estimate* $\widehat{\mathbb{E}}_\eta^R[\sigma_R]$ *for* $\eta \in \mathcal{I}_N^R$. The crucial step for this estimate is the following construction of a test function, which based on the so-called Gordan's lemma.

Lemma 10.6.10. *Suppose that* $R \subseteq S$ *and* $\lim_{N\to\infty} d_N N^2/(\log N)^2 = 0$. *Then, there exist a constant* $C = C(\epsilon) > 0$ *and a test function* $\mathbf{f}_0 = \mathbf{f}_0^R : \overline{\mathcal{I}}_N^R \to \mathbb{R}$ *such that*

$$\max_{\overline{\mathcal{I}}_N^R} \mathbf{f}_0 - \min_{\overline{\mathcal{I}}_N^R} \mathbf{f}_0 \le C \log N, \tag{10.73}$$

$$(\widehat{\mathbf{L}}_N^R \mathbf{f}_0)(\eta) \ge \frac{\log N}{CN^3} \quad \text{for all } \eta \in \mathcal{I}_N^R. \tag{10.74}$$

Proof. Fix $R \subseteq S$ and consider a $|R| \times |R|$ skew-symmetric matrix $\boldsymbol{Q}$ defined by

$$\boldsymbol{Q}_{x,\,y} = r(x,\,y) - r(y,\,x), \quad x \in R \text{ and } y \in R.$$

By Gordan's lemma stated in Lemma 10.8.2 at the appendix, we have that

$$\exists \boldsymbol{\alpha} = (\alpha_x)_{x\in R} \in \mathbb{R}^{|R|} \text{ such that } (\boldsymbol{Q\alpha})_1,\,\dots,\,(\boldsymbol{Q\alpha})_{|R|} < 0, \tag{10.75}$$

or

$$\exists \boldsymbol{\beta}(\neq \mathbf{0}) = (\beta_x)_{x\in R} \in \mathbb{R}^{|R|} \text{ so that } \beta_1,\,\dots,\,\beta_{|R|} \le 0 \text{ and } \boldsymbol{Q\beta} = 0. \tag{10.76}$$

We consider these two cases separately.

(Case 1: (10.75)**)** In this case, define $\mathbf{f}_0 : \overline{\mathcal{I}}_N^R \to \mathbb{R}$ as

$$\mathbf{f}_0(\eta) = \sum_{x\in R} \alpha_x \Big(1 + \frac{1}{2} + \cdots + \frac{1}{\eta_x}\Big).$$

Then, for each $\eta \in \overline{\mathcal{I}}_N^R$,

$$|\mathbf{f}_0(\eta)| \le C \sum_{x \in R} |\alpha_x| \log \eta_x \le C' \log N;$$

hence, the condition (10.73) follows immediately. To check the condition (10.74), we define

$$\mathbf{w}(\eta) = \sum_{a,\, b \in R} \eta_a (d_N + \eta_b) r(a,\, b),$$

so that

$$\begin{aligned}
(\widehat{\mathbf{L}}_N^R \mathbf{f}_0)(\eta) =& \frac{1}{\mathbf{w}(\eta)} \sum_{x,\, y \in R} \eta_y (d_N + \eta_x) r(y,\, x) \Big(\frac{\alpha_y}{\eta_y + 1} - \frac{\alpha_x}{\eta_x} \Big) \\
=& \frac{1}{\mathbf{w}(\eta)} \Big\{ \sum_{x,\, y \in R} r(y,\, x) \eta_x \eta_y \Big(\frac{\alpha_y}{\eta_y + 1} - \frac{\alpha_x}{\eta_x} \Big) + O\Big(d_N \frac{N}{\log N} \Big) \Big\} \\
=& \frac{1}{\mathbf{w}(\eta)} \Big\{ \sum_{x,\, y \in R} r(y,\, x) \eta_x \eta_y \Big(\frac{\alpha_y}{\eta_y} - \frac{\alpha_x}{\eta_x} \Big) + O\Big(\frac{N}{\log N} \Big) + O\Big(d_N \frac{N}{\log N} \Big) \Big\}.
\end{aligned} \tag{10.77}$$

The seemingly not so serious last identity is indeed the main reason that we introduced the inner core $\mathcal{I}_N^R$. The error coming from this identity is not able to control if η_y is close to 0. In this case the bound $\eta_y \ge \epsilon \log N$ provides us the small error term of $O(N/\log N)$.

Now the last summation can be computed as

$$\begin{aligned}
\sum_{x,\, y \in R} r(y,\, x)(\alpha_y \eta_x - \alpha_x \eta_y) =& \sum_{x \in R} \Big[\eta_x \sum_{y \in R} \alpha_y \{ r(y,\, x) - r(x\,, y) \} \Big] \\
=& \sum_{x \in R} \Big[\eta_x \sum_{y \in R} -\boldsymbol{Q}_{x,\, y} \alpha_y \Big] = \sum_{x \in R} \eta_x (-\boldsymbol{Q}\boldsymbol{\alpha})_x \ge \frac{N}{C}.
\end{aligned}$$

where the last inequality is due to (10.75). Since $\mathbf{w}(\eta) = O(N^2)$, applying the last inequality to (10.77) verifies the condition (10.74) because clearly $1/N \ge 1/N^3$.

(Case 2: (10.76)**)** Define $\mathbf{f}_0 : \overline{\mathcal{I}}_N^R \to \mathbb{R}$ by

$$\mathbf{f}_0(\eta) = \sum_{x\in R} \beta_x \Big(1 + \frac{1}{2} + \cdots + \frac{1}{\eta_x}\Big).$$

Then, the condition (10.73) follows similarly as **(Case 1)**. By a similar calculation, for $\eta \in \mathcal{I}_N^R$,

$$\begin{aligned}
&(\widehat{\mathbf{L}}_N^R \mathbf{f}_0)(\eta) \\
&= \frac{1}{\mathbf{w}(\eta)} \cdot \sum_{x,\, y\in R} \eta_y (d_N + \eta_x) r(y,\, x) \Big(\frac{\beta_y}{\eta_y + 1} - \frac{\beta_x}{\eta_x}\Big) \\
&= \frac{1}{\mathbf{w}(\eta)} \cdot \Big[\sum_{x,\, y\in R} r(y,\, x) \eta_x \eta_y \Big(\frac{\beta_y}{\eta_y} - \frac{\beta_x}{\eta_x}\Big) + \sum_{x,\, y\in R} r(y,\, x) \frac{-\beta_y \eta_x}{\eta_y + 1} + O\Big(d_N \frac{N}{\log N}\Big)\Big] \\
&= \frac{1}{\mathbf{w}(\eta)} \cdot \Big[\sum_{x\in R} \eta_x (-\boldsymbol{Q}\boldsymbol{\beta})_x + \sum_{x,\, y\in R} r(y,\, x) \frac{\eta_x}{\eta_y + 1} (-\beta_y) + O\Big(d_N \frac{N}{\log N}\Big)\Big].
\end{aligned}$$

The first summation in the last line vanishes since $\boldsymbol{Q}\boldsymbol{\beta} = 0$. Hence by (10.76),

$$(\widehat{\mathbf{L}}_N^R \mathbf{f}_0)(\eta) \ge \frac{1}{\mathbf{w}(\eta)} \Big[\frac{1}{C} \sum_{x,\, y\in R} \frac{\eta_x}{\eta_y + 1} (-\beta_y) + O\Big(d_N \frac{N}{\log N}\Big)\Big] \ge \frac{1}{C'} N^{-3} \log N, \tag{10.78}$$

where the last inequality holds because $\mathbf{w}(\eta) = O(N^2)$, and $\lim_{N\to\infty} d_N N^2/(\log N)^2 = 0$ along with $\eta \in \mathcal{I}_N^R$ imply that the first term inside the bracket dominates the second term. □

We remark that, at the first inequality of (10.78), the condition **(UP)** is strongly used again. Now, we estimate the expectation of the hitting time σ_R of the outer boundary $\partial\mathcal{I}_N^R$.

Lemma 10.6.11. *Suppose that $R \subseteq S$ and that $\lim_{N\to\infty} d_N N^2/(\log N)^2 = 0$. Then, there exists $C = C(\epsilon) > 0$ such that*

$$\sup_{\eta\in\mathcal{I}_N^R} \widehat{\mathbb{E}}_\eta^R [\sigma_R] \le CN^3.$$

Proof. For $\mathbf{f} : \overline{\mathcal{I}}_N^R \to \mathbb{R}$, we know that

$$\mathscr{M}(n) = \mathbf{f}(\widehat{\eta}_N^R(n)) - \mathbf{f}(\widehat{\eta}_N^R(0)) - \sum_{k=0}^{n-1} (\widehat{\mathbf{L}}_N^R \mathbf{f})(\widehat{\eta}_N^R(k)) \quad \text{for } n \in \mathbb{N}$$

is a discrete-time martingale with initial value 0. Therefore, by the optional stopping theorem, we have for all $\eta \in \mathcal{I}_N^R$ and $n \geq 0$ that

$$\widehat{\mathbb{E}}_\eta^R[\mathbf{f}(\widehat{\eta}_N^R(\sigma_R \wedge n))] = \mathbf{f}(\eta) + \widehat{\mathbb{E}}_\eta^R\Big[\sum_{k=0}^{(\sigma_R \wedge n)-1} (\widehat{\mathbf{L}}_N^R \mathbf{f})(\widehat{\eta}_N^R(k)) \Big]. \tag{10.79}$$

Now, we insert $\mathbf{f} = \mathbf{f}_0$ where $\mathbf{f}_0$ is the test function obtained in Lemma 10.6.10. Using the bounds in (10.73) and (10.74), it holds for all $n \geq 0$ that

$$\begin{aligned} C \log N \geq & \widehat{\mathbb{E}}_\eta^R[\mathbf{f}_0(\widehat{\eta}_N^R(\sigma_R \wedge n))] - \mathbf{f}_0(\eta) \\ = & \widehat{\mathbb{E}}_\eta^R\Big[\sum_{k=0}^{(\sigma_R \wedge n)-1} (\widehat{\mathbf{L}}_N^R \mathbf{f}_0)(\widehat{\eta}_N^R(k)) \Big] \geq \frac{\log N}{CN^3} \widehat{\mathbb{E}}_\eta^R[\sigma_R \wedge n]. \end{aligned}$$

Thus, the proof is completed by letting $n \to \infty$. □

Remark 10.6.12. A careful reading of the proofs shows that Lemmas 10.6.10 and 10.6.11 holds for any $\epsilon > 0$.

Lemma 10.6.13. *Fix a set $R \subseteq S$ and a constant $\delta \geq 0$. Suppose that $\lim_{N\to\infty} d_N N^2/(\log N)^2 = 0$, and that a function $\mathbf{f} : \overline{\mathcal{I}}_N^R \to \mathbb{R}$ satisfies*

$$\mathbf{f}(\eta) \leq \sum_{\zeta \in \overline{\mathcal{I}}_N^R} \widehat{\mathbf{p}}_N^R(\eta, \zeta) \mathbf{f}(\zeta) + \delta \quad \text{for all } \eta \in \mathcal{I}_N^R. \tag{10.80}$$

Then, for each $\eta \in \overline{\mathcal{I}}_N^R$, we have that

$$\mathbf{f}(\eta) \leq \max_{\partial \mathcal{I}_N^R} \mathbf{f} + CN^3 \delta.$$

Proof. Define $\mathbf{g} : \overline{\mathcal{I}}_N^R \to \mathbb{R}$ by

$$\mathbf{g}(\eta) = \widehat{\mathbb{E}}_\eta^R[\mathbf{f}(\widehat{\eta}_N^R(\sigma_R)) + \delta\sigma_R].$$

For $\eta \in \mathcal{I}_N^R$, the Markov property gives us that

$$\begin{aligned}\mathbf{g}(\eta) &= \sum_{\zeta\in\overline{\mathcal{I}}_N^R} \widehat{\mathbf{p}}_N^R(\eta,\, \zeta)\mathbb{E}_\zeta[\mathbf{f}(\widehat{\eta}_N^R(\sigma_R)) + \delta(\sigma_R + 1)] \\ &= \sum_{\zeta\in\overline{\mathcal{I}}_N^R} \widehat{\mathbf{p}}_N^R(\eta,\, \zeta)\mathbf{g}(\zeta) + \delta.\end{aligned} \tag{10.81}$$

Let $\mathbf{h} = \mathbf{f} - \mathbf{g}$. Then, by (10.80) and (10.81), we have that

$$\mathbf{h}(\eta) \le \sum_{\zeta\in\overline{\mathcal{I}}_N^R} \widehat{\mathbf{p}}_N^R(\eta,\, \zeta)\mathbf{h}(\zeta) \quad \text{for all } \eta \in \mathcal{I}_N^R.$$

On the other hand, we have $\mathbf{h} \equiv 0$ on $\partial\mathcal{I}_N^R$ since $\sigma_R = 0$ on $\partial\mathcal{I}_N^R$. Therefore, since $\widehat{\eta}_N^R(\cdot)$ is irreducible, the maximum principle implies that $\mathbf{h} \le 0$, i.e., $\mathbf{f} \le \mathbf{g}$ on $\overline{\mathcal{I}}_N^R$. Since $\mathbf{g}(\eta) \le \max_{\partial\mathcal{I}_N^R} \mathbf{f} + \delta\widehat{\mathbb{E}}_\eta^R[\sigma_R]$ by the definition of $\mathbf{g}$, the proof is completed by Lemma 10.6.11. □

Now, we define $\mathbf{m} : \mathcal{H}_N \to \mathbb{R}$ by

$$\mathbf{m}(\eta) = \mu_N(\eta) \prod_{x\in S} \eta_x. \tag{10.82}$$

Then we can obtain the following estimate on $\mathbf{m}$ based on the maximum principle given in Lemma 10.6.13.

Lemma 10.6.14. *There exists $C = C(\epsilon)$ such that for each $\eta \in \mathcal{I}_N^S$,*

$$\mathbf{m}(\eta) \le \max_{\partial\mathcal{I}_N^S} \mathbf{m} + C\frac{d_N N^3}{(\log N)^2} \max_{\overline{\mathcal{I}}_N^S} \mathbf{m}.$$

Proof. We can deduce from (10.59) that, for each $\eta \in \mathcal{I}_N^S$,

$$\sum_{x,\,y\in S} \mu_N(\eta)\eta_x(d_N+\eta_y)r(x,\,y) = \sum_{x,\,y\in S} \mu_N(\sigma^{y,\,x}\eta)(\eta_x+1)(d_N+\eta_y-1)r(x,\,y).$$

Inserting $\mu_N(\eta) = \mathbf{m}(\eta)(\prod_{x\in S}\eta_x)^{-1}$ and rearranging it yield that

$$\mathbf{m}(\eta) = \sum_{x,\,y\in S} \frac{\eta_x(d_N+\eta_y)r(x,\,y)\frac{\eta_y(d_N+\eta_y-1)}{(d_N+\eta_y)(\eta_y-1)}}{\sum_{a,\,b\in S}\eta_a(d_N+\eta_b)r(a,\,b)}\mathbf{m}(\sigma^{y,\,x}\eta).$$

By recalling the definition of $\widehat{\mathbf{p}}_N^S$ (cf. (10.72)), we can rewrite the last identity as

$$\mathbf{m}(\eta) = \sum_{x,\,y\in S}\Big[1+\frac{d_N}{(d_N+\eta_y)(\eta_y-1)}\Big]\widehat{\mathbf{p}}_N^S(\eta,\,\sigma^{y,\,x}\eta)\mathbf{m}(\sigma^{y,\,x}\eta). \tag{10.83}$$

For $\eta \in \mathcal{I}_N^S$, we have

$$\sum_{x,\,y\in S}\frac{d_N}{(d_N+\eta_y)(\eta_y-1)}\widehat{\mathbf{p}}_N^S(\eta,\,\sigma^{y,\,x}\eta)\mathbf{m}(\sigma^{y,\,x}\eta) \le \frac{Cd_N}{(\log N)^2}\max_{\overline{\mathcal{I}}_N^S}\mathbf{m} \tag{10.84}$$

since $\eta_x \ge \epsilon\log N$ for all $x \in S$. By (10.83) and (10.84), $\mathbf{m}$ satisfies

$$\mathbf{m}(\eta) \le \sum_{\zeta\in\overline{\mathcal{I}}_N^S}\widehat{\mathbf{p}}_N^S(\eta,\,\zeta)\mathbf{m}(\zeta) + \frac{Cd_N}{(\log N)^2}\max_{\overline{\mathcal{I}}_N^S}\mathbf{m}. \tag{10.85}$$

Hence, the proof is completed by Lemma 10.6.13 with $R = S$ and $\mathbf{f} = \mathbf{m}$. $\square$

Now, we are ready to prove Proposition 10.6.8 by combining results obtained in Lemmas 10.6.10-10.6.14.

Proof of Proposition 10.6.8. By Lemma 10.6.14,

$$\begin{aligned}\mu_N(\mathcal{I}_N^S) &= \sum_{\eta\in\mathcal{I}_N^S}\mu_N(\eta) = \sum_{\eta\in\mathcal{I}_N^S}\frac{\mathbf{m}(\eta)}{\prod_{x\in S}\eta_x}\\ &\le \sum_{\eta\in\mathcal{I}_N^S}\frac{1}{\prod_{x\in S}\eta_x}\Big\{\max_{\partial\mathcal{I}_N^S}\mathbf{m} + \frac{d_N}{(\log N)^2}CN^3\max_{\overline{\mathcal{I}}_N^S}\mathbf{m}\Big\} \qquad (10.86)\\ &\le CN^{-1}(\log N)^{\kappa-1}\Big\{\max_{\partial\mathcal{I}_N^S}\mathbf{m} + \frac{d_N}{(\log N)^2}CN^3\max_{\overline{\mathcal{I}}_N^S}\mathbf{m}\Big\},\end{aligned}$$

where the last line follows from Lemma 10.8.1 (note that $\kappa = |S|$). Recall the definition of $\mathbf{m}$ from (10.82) and note that

$$\prod_{x\in S}\eta_x = \begin{cases} O(N^{\kappa-1}\log N) & \text{for } \eta\in\partial\mathcal{I}_N^S,\\ O(N^\kappa) & \text{for } \eta\in\overline{\mathcal{I}}_N^S.\end{cases}$$

Based on this, we can further deduce from (10.86) that

$$\begin{aligned}\mu_N(\mathcal{I}_N^S) &\le CN^{\kappa-2}(\log N)^\kappa\max_{\partial\mathcal{I}_N^S}\mu_N + Cd_N N^{\kappa+2}(\log N)^{\kappa-3}\max_{\overline{\mathcal{I}}_N^S}\mu_N\\ &\le CN^{\kappa-2}(\log N)^\kappa\mu_N(\partial\mathcal{I}_N^S) + Cd_N N^{\kappa+2}(\log N)^{\kappa-3}\mu_N(\overline{\mathcal{I}}_N^S).\end{aligned}$$

By the condition on d_N given at the statement of the proposition, we complete the proof. □

10.6.3 Induction step

Next, we consider the induction step. We shall prove the following two statements together by the backward induction: there exists $C > 0$ such that, for all $i \in [\![2,\,\kappa]\!]$,

$$\lim_{N\to\infty}\frac{\mu_N(\mathcal{B}_N^i)}{\mu_N(\mathcal{B}_N^{i-1})} = 1, \qquad (10.87)$$

and for all $R \subseteq S$ with $|R| = i$, and for all $z \in R$,

$$\mu_N(\mathcal{C}_N^R(z,\,1)) \le C d_N \mu_N(\mathcal{B}_N^{i-1}). \tag{10.88}$$

Note that the initial case $i = \kappa$ for (10.87) is proved in Propositions 10.6.3, 10.6.7, and for (10.88) is proved in Lemma 10.6.5.

Now, we will assume the following condition throughout this subsection:

$$\lim_{N\to\infty} d_N N^{\kappa+2} (\log N)^{\kappa-3} = 0. \tag{10.89}$$

Proposition 10.6.15. *Suppose that the induction hypotheses* (10.87) *and* (10.88) *hold for* $i = \ell + 1$*. Then,* (10.87) *and* (10.88) *hold for* $i = \ell$ *as well.*

The overall outline of the proof is similar to the initial step, but several additional technical difficulties arise in the course of the proof. As before, we investigate the outer core and inner core separately in Lemmas 10.6.16 and 10.6.19, respectively.

Estimation of the outer core

For the outer core $\mathcal{O}_N^R$ with $R \subseteq S$, we will prove the following bound.

Lemma 10.6.16. *For all* $R \subseteq S$*, it holds that*

$$\mu_N(\mathcal{O}_N^R) = o(1)[\mu_N(\partial \mathcal{A}_N^R) + \mu_N(\mathcal{A}_N^R)].$$

We first prove two preliminary lemmas before proving this lemma. Recall the notions introduced after Proposition 10.6.7.

Lemma 10.6.17. *For all* $R \subseteq S$*,* $x \in R$*, and* $j \in [\![0,\, N-1]\!]$*, it holds that*

$$\mathbf{F}_N^R(x;\, j+1 \to j) - \mathbf{F}_N^R(x;\, j \to j+1) \le C d_N N \mu_N(\mathcal{A}_N^R). \tag{10.90}$$

Proof. By summing (10.59) over $\eta \in \mathcal{C}_N^R(x,\, k)$,

$$\begin{aligned}
&\sum_{\eta\in\mathcal{C}_N^R(x,\,k)}\sum_{y,\,z\in R\setminus\{x\}}\mu_N(\eta)r_N(\eta,\,\sigma^{y,\,z}\eta)+\sum_{\eta\in\mathcal{C}_N^R(x,\,k)}\sum_{y\in R\setminus\{x\}}\mu_N(\eta)r_N(\eta,\,\sigma^{y,\,x}\eta)\\
&+\sum_{\eta\in\mathcal{C}_N^R(x,\,k)}\sum_{y\in R\setminus\{x\}}\mu_N(\eta)r_N(\eta,\,\sigma^{x,\,y}\eta)+\sum_{\eta\in\mathcal{C}_N^R(x,\,k)}\sum_{y\in R,\,z\in R^c}\mu_N(\eta)r_N(\eta,\,\sigma^{y,\,z}\eta)\\
&=\sum_{\eta\in\mathcal{C}_N^R(x,\,k)}\sum_{y,\,z\in R\setminus\{x\}}\mu_N(\sigma^{y,\,z}\eta)r_N(\sigma^{y,\,z}\eta,\,\eta)+\sum_{\eta\in\mathcal{C}_N^R(x,\,k)}\sum_{y\in R\setminus\{x\}}\mu_N(\sigma^{y,\,x}\eta)r_N(\sigma^{y,\,x}\eta,\,\eta)\\
&\quad+\sum_{\eta\in\mathcal{C}_N^R(x,\,k)}\sum_{y\in R\setminus\{x\}}\mu_N(\sigma^{x,\,y}\eta)r_N(\sigma^{x,\,y}\eta,\,\eta)+\sum_{\eta\in\mathcal{C}_N^R(x,\,k)}\sum_{y\in R,\,z\in R^c}\mu_N(\sigma^{y,\,z}\eta)r_N(\sigma^{y,\,z}\eta,\,\eta).
\end{aligned}\tag{10.91}$$

Compared to the corresponding computations in Lemma 10.6.4, the last terms in both sides of (10.91) should be handled in addition. The term in the left-hand side is bounded above by

$$\begin{aligned}
\sum_{\eta\in\mathcal{C}_N^R(x,\,k)}\sum_{y\in R,\,z\in R^c}\mu_N(\eta)r_N(\eta,\,\eta^{y,\,z}) &= O(d_N N)\sum_{\eta\in\mathcal{C}_N^R(x,\,k)}\mu_N(\eta)\\
&= O(d_N N)\mu_N(\mathcal{C}_N^R(x,\,k)).
\end{aligned}$$

The term in the right-hand side of (10.91) is bounded below by 0. Hence, we can obtain from (10.91) that

$$\begin{aligned}
&[\mathbf{F}_N^R(x;\,k+1\to k)-\mathbf{F}_N^R(x;\,k\to k+1)]-[\mathbf{F}_N^R(x;\,k\to k-1)-\mathbf{F}_N^R(x;\,k-1\to k)]\\
&\le C d_N N\mu_N(\mathcal{C}_N^R(x,\,k)).
\end{aligned}$$

By summing the bound over $k = 0,\, 1,\, \dots,\, j$, we obtain (10.90). □

Lemma 10.6.18. *There exists $C > 0$ such that for all $R \subseteq S$, $x \in R$, and*

$k \in [\![0,\, N-1]\!]$, *we have*

$$\mu_N(\mathcal{C}_N^R(x,\, k+1)) \leq C\frac{(k+d_N)(N-k)}{(k+1)(N-k-1+d_N)}\mu_N(\mathcal{C}_N^R(x,\, k)) + C\frac{d_N N}{(k+1)(N-k-1+d_N)}\mu_N(\mathcal{A}_N^R).$$

Proof. The proof is identical to Lemma 10.6.5 if we replace the role of Lemma 10.6.4 with that of Lemma 10.6.17. □

Now, we prove Lemma 10.6.16 based on Lemmas 10.6.17 and 10.6.18.

Proof of Lemma 10.6.16. Fix $x \in R$. Inserting $k = 0$ in Lemma 10.6.18 implies that there exists a constant $C_1 > 1$ such that

$$\mu_N(\mathcal{C}_N^R(x,\, 1)) \leq C_1 d_N \mu_N(\mathcal{C}_N^R(x,\, 0)) + C_1 d_N \mu_N(\mathcal{A}_N^R). \tag{10.92}$$

On the other hand, inserting $k \in [\![1,\, N-1]\!]$ to Lemma 10.6.18 implies that there exists a constant $C_2 > 1$ such that

$$\mu_N(\mathcal{C}_N^R(x,\, k+1)) \leq C_2 \mu_N(\mathcal{C}_N^R(x,\, k)) + C_2 d_N \mu_N(\mathcal{A}_N^R). \tag{10.93}$$

Let $C_0 = \max\{C_1,\, C_2\}$. Then, by (10.92) and (10.93), we obtain that

$$\mu_N(\mathcal{C}_N^R(x,\, k)) \leq C_0^k d_N \mu_N(\mathcal{C}_N^R(x,\, 0)) + \frac{C_0^{k+1} - C_0}{C_0 - 1} d_N \mu_N(\mathcal{A}_N^R) \quad \text{for } k \in [\![1,\, N-1]\!]. \tag{10.94}$$

Summing this up for for $k \in [\![1,\, \epsilon \log N]\!]$, it holds that

$$\sum_{k=1}^{\epsilon \log N} \mu_N(\mathcal{C}_N^R(x,\, k)) \leq C \times C_0^{\epsilon \log N} d_N [\mu_N(\mathcal{C}_N^R(x,\, 0)) + \mu_N(\mathcal{A}_N^R)].$$

Take ϵ small enough so that

$$C_0^{\epsilon \log N} \ll N. \tag{10.95}$$

Therefore, by (10.57),

$$\begin{aligned}\mu_N(\mathcal{O}_N^R) &\le \sum_{x\in R}\sum_{k=1}^{\epsilon\log N}\mu_N(\mathcal{C}_N^R(x,\,k)) \le Cd_N N\sum_{x\in R}\{\mu_N(\mathcal{A}_N^{R\setminus\{x\}})+\mu_N(\mathcal{A}_N^R)\}\\ &= O(d_N N)[\mu_N(\partial\mathcal{A}_N^R)+\mu_N(\mathcal{A}_N^R)].\end{aligned}$$

This finishes the proof. □

Estimation of the inner core

Next, we control the inner core $\mathcal{I}_N^R$. The proof of the following lemma also relies on Lemma 10.6.11 regarding the estimate of the hitting time.

Lemma 10.6.19. *Suppose that* (10.88) *holds for* $i=\ell+1$. *Then, for all* $R\subseteq S$ *with* $|R|=\ell$, *we have that*

$$\mu_N(\mathcal{I}_N^R)=o(1)[\mu_N(\partial\mathcal{A}_N^R)+\mu_N(\mathcal{B}_N^\ell)].$$

Proof. Fix $R\subseteq S$ and define $\mathbf{m}^R:\mathcal{H}_N\to\mathbb{R}$ by

$$\mathbf{m}^R(\eta)=\mu_N(\eta)\prod_{x\in R}\eta_x. \tag{10.96}$$

Similarly to Lemma 10.6.14, for $\eta\in\mathcal{I}_N^R$, we get

$$\mu_N(\eta)=\sum_{y\in R,\,x\in S\setminus\{y\}}\frac{(\eta_x+1)(d_N+\eta_y-1)r(x,\,y)}{\sum_{a\in R,\,b\in S\setminus\{a\}}\eta_a(d_N+\eta_b)r(a,\,b)}\mu_N(\sigma^{y,\,x}\eta).$$

In the denominator of the right-hand side, we discard the transitions escaping

R to get the following upper bound for $\mu_N(\eta)$:

$$\begin{aligned}\mu_N(\eta) \le \sum_{x,\, y\in R} \frac{(\eta_x+1)(d_N+\eta_y-1)r(x,\, y)}{\sum_{a,\, b\in R}\eta_a(d_N+\eta_b)r(a,\, b)}\mu_N(\sigma^{y,\, x}\eta) \\ + \sum_{y\in R,\, x\in S\setminus R} \frac{(d_N+\eta_y-1)r(x,\, y)}{\sum_{a,\, b\in R}\eta_a(d_N+\eta_b)r(a,\, b)}\mu_N(\sigma^{y,\, x}\eta).\end{aligned} \tag{10.97}$$

By the assumption that (10.88) holds for $i=\ell+1$, the last term is bounded by

$$\sum_{x\in S\setminus R} \frac{C}{\log N}\mu_N(\mathcal{C}_N^{R\cup\{x\}}(x,\, 1)) \le \frac{Cd_N}{\log N}\mu_N(\mathcal{B}_N^\ell).$$

Inserting this to (10.97) and using the formula (10.96) of $\mathbf{m}^R$, we can deduce that

$$\mathbf{m}^R(\eta) \le \sum_{x,\, y\in R} \frac{\eta_x(d_N+\eta_y)r(x,\, y)\frac{\eta_y(d_N+\eta_y-1)}{(d_N+\eta_y)(\eta_y-1)}}{\sum_{a,\, b\in R}\eta_a(d_N+\eta_b)r(a,\, b)}\mathbf{m}^R(\sigma^{y,\, x}\eta) + \frac{Cd_N N^\ell}{\log N}\mu_N(\mathcal{B}_N^\ell). \tag{10.98}$$

Now, as in the proof of Lemma 10.6.14 (cf. (10.83), (10.84), and (10.85)), we can obtain from the previous inequality that

$$\mathbf{m}^R(\eta) \le \sum_{x,\, y\in R} \mathbf{p}_N^R(\eta,\, \sigma^{y,\, x}\eta)\mathbf{m}^R(\sigma^{y,\, x}\eta) + \frac{2d_N}{(\log N)^2}\max_{\overline{\mathcal{I}}_N^R}\mathbf{m}^R + \frac{Cd_N N^\ell}{\log N}\mu_N(\mathcal{B}_N^\ell).$$

Therefore, Lemma 10.6.13 with $\mathbf{f}=\mathbf{m}^R$ and Lemma 10.6.11 give that,

$$\mathbf{m}^R(\eta) \le \max_{\partial\mathcal{I}_N^R}\mathbf{m}^R + \max_{\overline{\mathcal{I}}_N^R}\mathbf{m}^R\frac{Cd_N N^3}{(\log N)^2} + \frac{Cd_N N^{\ell+3}}{\log N}\mu_N(\mathcal{B}_N^\ell) \tag{10.99}$$

for all $\eta\in\mathcal{I}_N^R$. Now recalling the definition (10.96) and applying Lemma

10.8.1,

$$
\begin{aligned}
\mu_N(\mathcal{I}_N^R) \le & \sum_{\eta \in \mathcal{I}_N^R} \frac{1}{\prod_{x\in R}\eta_x} \Big\{ \max_{\partial \mathcal{I}_N^R} \mathbf{m}^R + \max_{\overline{\mathcal{I}}_N^R} \mathbf{m}^R \frac{Cd_N N^3}{(\log N)^2} + \frac{Cd_N N^{\ell+3}}{\log N} \mu_N(\mathcal{B}_N^\ell) \Big\} \\
\le & \frac{C(\log N)^{\ell-1}}{N} \Big\{ N^{\ell-1} \log N \max_{\partial \mathcal{I}_N^R} \mu_N + d_N \frac{N^{\ell+3}}{(\log N)^2} \max_{\overline{\mathcal{I}}_N^R} \mu_N + d_N \frac{N^{\ell+3}}{\log N} \mu_N(\mathcal{B}_N^\ell) \Big\} \\
= & CN^{\ell-2}(\log N)^\ell \mu_N(\partial \mathcal{I}_N^R) + Cd_N N^{\ell+2}(\log N)^{\ell-3} \mu_N(\overline{\mathcal{I}}_N^R) \\
& + Cd_N N^{\ell+2} (\log N)^{\ell-2} \mu_N(\mathcal{B}_N^\ell).
\end{aligned}
$$

By (10.89), we can finally deduce that

$$
\mu_N(\mathcal{I}_N^R) = O(N^{\ell-2}(\log N)^\ell)\mu_N(\partial \mathcal{I}_N^R) + O(d_N N^{\ell+2}(\log N)^{\ell-2})\mu_N(\mathcal{B}_N^\ell). \tag{10.100}
$$

Recall the notation defined after Proposition 10.6.3 to see that

$$
\partial \mathcal{I}_N^R \subseteq \bigcup_{x\in R} \mathcal{C}_N^R(x,\, \epsilon \log N).
$$

Therefore by (10.94),

$$
\mu_N(\partial \mathcal{I}_N^R) \le \sum_{x \in R} \mu_N(\mathcal{C}_N^R(x,\, \epsilon \log N)) = O(d_N N)[\mu_N(\partial \mathcal{A}_N^R) + \mu_N(\mathcal{A}_N^R)]. \tag{10.101}
$$

(10.100) and (10.101) give

$$
\mu_N(\mathcal{I}_N^R) = O(d_N N^{\ell-1}(\log N)^\ell)\mu_N(\partial \mathcal{A}_N^R) + O(d_N N^{\ell+2}(\log N)^{\ell-2})\mu_N(\mathcal{B}_N^\ell).
$$

By (10.89), we finish the proof. □

Proof of Proposition 10.6.15. Take $R \subseteq S$ with $|R| = \ell$. Since $\mathcal{R}_N^R$ is decomposed into $\mathcal{O}_N^R$ and $\mathcal{I}_N^R$, and since $\partial \mathcal{A}_N^R \subseteq \mathcal{B}_N^{\ell-1}$, we can derive from

Propositions 10.6.16 and 10.6.19 that

$$\mu_N(\mathcal{R}_N^R) = o(1)[\mu_N(\partial \mathcal{A}_N^R) + \mu_N(\mathcal{B}_N^\ell)] \le o(1)[\mu_N(\mathcal{B}_N^{\ell-1}) + \mu_N(\mathcal{B}_N^\ell)].$$

Summing the last bound over all $R \subseteq S$ with $|R| = \ell$ yields that

$$\mu_N(\mathcal{B}_N^\ell \setminus \mathcal{B}_N^{\ell-1}) = o(1)[\mu_N(\mathcal{B}_N^{\ell-1}) + \mu_N(\mathcal{B}_N^\ell)].$$

We can deduce (10.87) with $i = \ell$ from here. On the other hand, we can verify (10.88) with $i = \ell$ from (10.87) and (10.94). To be more specific, for $x \in R$, inserting $k = 1$ in (10.94) gives us

$$\mu_N(\mathcal{C}_N^R(x,\, 1)) \le Cd_N \mu_N(\mathcal{C}_N^R(x,\, 0)) + Cd_N \mu_N(\mathcal{A}_N^R).$$

Since $\mathcal{C}_N^R(x,\, 0) \subseteq \mathcal{B}_N^{\ell-1}$ and $\mu_N(\mathcal{A}_N^R) \le \mu_N(\mathcal{B}_N^\ell) = (1 + o(1))\mu_N(\mathcal{B}_N^{\ell-1})$ by (10.87), we conclude that $\mu_N(\mathcal{C}_N^R(x,\, 1)) \le Cd_N \mu_N(\mathcal{B}_N^{\ell-1})$ and thus conclude the proof of Proposition 10.6.15. □

Remark 10.6.20. We remark that the final step in (10.52), i.e., $\ell = 2$, can be proved in a completely independent way without assumption **(UP)**, and with a much weaker assumption on d_N. To be more specific, we can prove the following result:

Theorem. Suppose that $\lim_{N\to\infty} d_N N \log N = 0$. *Then, we have*

$$\lim_{N\to\infty} \frac{\mu_N(\mathcal{E}_N)}{\mu_N(\mathcal{A}_N)} = 1.$$

Note that under condition **(UP)**, this is exactly the case $\ell = 2$ in (10.52). We omit the proof of this statement, and only remark that it can be proved by tracing the original process on $\mathcal{A}_N$ and calculating the transition rates of the trace process, as done in Section 10.3.3.

10.6.4 Proof of Theorem 10.2.17

Now, we explain the proof of Theorem 10.2.17 whose main idea of proof is nearly identical to that of Lemma 10.6.11. Slight difference is that here we are dealing with the original continuous-time chain $\eta_N(\cdot)$, instead of the reversed discrete-time chain $\hat{\eta}_N^R(\cdot)$.

Proof of Theorem 10.2.17. We recall the definition of $\mathcal{U}_N$ from the display before Theorem 10.2.17. Let us identify ϵ in the definition of $\mathcal{I}_N^S$ with δ in the definition of $\mathcal{U}_N$. Then, in the terminology introduced in this section, we have $\mathcal{U}_N = (\mathcal{I}_N^S)^c$ and thus $\tau_{\mathcal{U}_N} = \tau_{\partial\mathcal{I}_N^S}$ provided that the chain starts in $\mathcal{U}_N^c$. Thus a deduction similar to that in Lemma 10.6.10 guarantees the existence of test function $\mathbf{g}_0 : \overline{\mathcal{I}}_N^S \to \mathbb{R}$ such that

$$\max_{\overline{\mathcal{I}}_N^S} \mathbf{g}_0 - \min_{\overline{\mathcal{I}}_N^S} \mathbf{g}_0 \le C \log N \quad \text{and} \quad (\mathcal{L}_N \mathbf{g}_0)(\eta) \ge \frac{\log N}{CN} \text{ for all } \eta \in \mathcal{I}_N^S.$$

Here, the denominator of the lower bound of $(\mathcal{L}_N \mathbf{g}_0)(\eta)$ is CN instead of CN^3, since there is no $\mathbf{w}(\eta)$ term as in Lemma 10.6.10 in the calculation of the continuous-time generator $\mathcal{L}_N$. Let us consider an arbitrary extension of $\mathbf{g}_0$ to a function on $\mathcal{H}_N$ and then consider the continuous-time martingale

$$M_{\mathbf{g}_0}(t) := \mathbf{g}_0(\eta_N(t)) - \mathbf{g}_0(\eta_N(0)) - \int_0^t (\mathcal{L}_N \mathbf{g}_0)(\eta_N(s))ds, \quad t \ge 0.$$

Then, proceeding as in Lemma 10.6.11, we can conclude that $\mathbb{E}_\eta[\tau_{\mathcal{U}_N}] \le CN$. □

10.7 Inclusion process in thermodynamic limit regime

In this section, we consider the inclusion process in the thermodynamic limit regime and prove the condensation (Theorem 10.2.19) and the metastable behavior (Theorems 10.2.21-10.2.23).

Organization of the section

In Section 10.7.1, we prove the existence of the condensation (Theorem 10.2.19), which is indeed not very far from that of the fixed L case under **(UI)**. On the other hand, the metastable behavior is more delicate than the fixed L case, mainly because the limiting dynamic is now a continuous process on $\mathbb{T}^d$, while the trace process is a jump process on $\mathbb{T}_L^d$. The proof of this convergence is based on two ingredients: the convergence of the generator (Proposition 10.7.1) and the tightness (Proposition 10.7.3). These ingredients are obtained in Sections 10.7.2 and 10.7.3, respectively. Finally, we prove Theorems 10.2.21-10.2.23 in Section 10.7.4.

10.7.1 Condensation

We first establish condensation by proving Theorem 10.2.19. This should be distinguished from the former cases by the fact that the graph grows along with the number of particles. Although the proof is given in [42, Proposition 2], we present a proof here for the completeness of the article.

Proof of Theorem 10.2.19. Recall $\mathcal{E}_L$ from (10.17). Then, it suffices to show that

$$\lim_{L\to\infty} \frac{\mu_L(\mathcal{H}_L \setminus \mathcal{E}_L)}{\mu_L(\mathcal{E}_L)} = 0. \tag{10.102}$$

Since the inclusion process that we consider here satisfies the condition **(UI)**, thanks to Proposition 10.1.2, the invariant measure of the process denoted by μ_L can be expressed explicitly by

$$\mu_L(\eta) = \frac{1}{Z_L} \prod_{x\in\mathbb{T}_L^d} w_L(\eta_x), \quad \eta \in \mathcal{H}_L, \tag{10.103}$$

where

$$w_L(n) = \frac{\Gamma(n+d_L)}{n!\Gamma(d_L)} \text{ for } n \in \mathbb{N} \quad \text{and} \quad Z_L = \sum_{\eta \in \mathcal{H}_L} \prod_{x \in \mathbb{T}_L^d} w_L(\eta_x).$$

Recall the inequality from (8.5). Since we assumed that $\lim_{L\to\infty} d_L L^d \log L = 0$, it implies that

$$w_L(k) = (1+o(1))\frac{d_L}{k} \quad \text{uniformly for } k \in [\![1,\, L]\!]. \tag{10.104}$$

Decompose

$$\mathcal{H}_L \setminus \mathcal{E}_L = \bigcup_{i=2}^{L} \Delta_i \tag{10.105}$$

where, for each $i \in [\![2,\, L]\!]$,

$$\Delta_i = \{\eta \in \mathcal{H}_L : \text{exactly } i \text{ coordinates of } \eta = (\eta_x)_{x\in\mathbb{T}_L} \text{ are non-zero}\}.$$

By (10.104) and the definition of $S_{n,\,k}$ in Lemma 10.8.1, for large enough L,

$$\mu_L(\Delta_i) \le \frac{1}{Z_L}(2d_L)^i S_{N,\,i} \times \binom{L^d}{i},$$

where the last term appears since there are $\binom{L}{i}$ ways to select i coordinates that are non-zero. By Lemma 10.8.1, it holds for all large enough L that

$$\begin{aligned} \mu_L(\Delta_i) \le& \frac{1}{Z_L}\frac{1}{3N\log(N+1)}(6d_L\log(N+1))^i\binom{L^d}{i} \\ \le& \frac{1}{Z_L}\frac{1}{N\log N}(7d_L\log L^d)^i\binom{L^d}{i}. \end{aligned} \tag{10.106}$$

For convenience, write $u_L = 7d_L \log L^d$. Then, by combining (10.105) and

(10.106), we obtain for all large enough L that

$$\begin{aligned}\mu_L(\mathcal{H}_L \setminus \mathcal{E}_L) = \sum_{i=2}^{L} \mu_L(\Delta_i) &\le \frac{1}{Z_L}\frac{1}{N\log N}\{(1+u_L)^{L^d} - 1 - L^d u_L\} \\ &\le \frac{1}{Z_L}\frac{1}{N\log N}\{e^{L^d u_L} - 1 - L^d u_L\} \\ &\le \frac{1}{Z_L}\frac{1}{N\log N}(L^d u_L)^2,\end{aligned}$$

where the last inequality follows because $\lim L^d u_L = 0$. Thus,

$$\mu_L(\mathcal{H}_L \setminus \mathcal{E}_L) \le \frac{C}{Z_L} d_L^2 L^d \log L. \tag{10.107}$$

On the other hand, by the explicit formula (10.103) and the asymptotic (10.15), we have that

$$\mu_L(\mathcal{E}_L) = L^d \times \frac{1}{Z_L} w_L(N) w_L(0)^{L^d-1} = (1+o(1)) L^d \times \frac{1}{Z_L}\frac{d_L}{N} = (1+o(1))\frac{1}{\rho Z_L} d_L. \tag{10.108}$$

Now, (10.102) is straightforward from (10.107) and (10.108). □

10.7.2 Convergence of the generator

Now, we consider the metastable behavior associated with the condensation proved above. The generator $\mathcal{L}^{\mathbb{T}^d}$ associated with the limiting object presented in Theorems 10.2.21-10.2.23 can be written as, for all sufficiently smooth $f : \mathbb{T}^d \to \mathbb{R}$,

$$(\mathscr{L}^{\mathbb{T}^d} f)(x) = \begin{cases} \rho(\sum_{y\in\mathbb{Z}^d} h(y)y) \cdot \nabla f(x) & \text{for totally asym. case,} \\ \frac{\rho}{2} \sum_{y\in\mathbb{Z}^d:\, h(y)>h(-y)} (h(y) - h(-y))y^\dagger[\nabla^2 f(x)]y & \text{for mean-zero asym. case,} \\ \frac{1}{2}\sum_{y\in\mathbb{Z}^d} h(y)y^\dagger[\nabla^2 f(x)]y & \text{for symmetric case,} \end{cases} \tag{10.109}$$

where $(\nabla^2 f)(x)$ denotes the Hessian of f at x. The main objective of this subsection is to prove the convergence of the generator of the trace process to the generator $\mathscr{L}^{\mathbb{T}^d}$ in an appropriate sense as $L \to \infty$ (cf. Proposition 10.7.2). The proof of this result again relies on the asymptotics of the mean-jump rate.

Asymptotics of mean-jump rate

We start by introducing several notations related to the mean-jump rate. Recall that $\eta_L^{\mathcal{E}_L}(\cdot)$ denotes the trace process of $\eta_L(\cdot)$ on the set $\mathcal{E}_L$. We let $\boldsymbol{r}_L^{\mathcal{E}_L}(\cdot,\, \cdot)$, $\mathscr{L}_L^{\mathcal{E}_L}$, and $\mu_L^{\mathcal{E}_L}$ denote the jump rate, the infinitesimal generator and the invariant measure of the trace process $\eta_L^{\mathcal{E}_L}(\cdot)$, respectively. For $x,\, y \in \mathbb{T}_L^d$, we write

$$\mathbf{b}_L(x,\, y) = \boldsymbol{r}_L^{\mathcal{E}_L}(\xi_L^x,\, \xi_L^y). \tag{10.110}$$

With these notation, we summarize the asymptotic relations for $\mathbf{b}_L(\cdot,\, \cdot)$ which are immediate from Proposition 10.3.2.

Proposition 10.7.1. *The followings hold for the inclusion process on $\mathbb{T}_L^d$ with $N \simeq \rho L^d$ particles:*

(1) for (either totally or mean-zero) asymmetric case, we have that

$$\mathbf{b}_L(x,\, x{+}y) = \begin{cases} (1+O(d_L\log L+q^N))d_LN(h(y)-h(-y)) & \textit{if } h(y)>h(-y), \\ O(d_L\log L+q^N)d_LN & \textit{otherwise}; \end{cases} \tag{10.111}$$

(2) for symmetric case, we have that

$$\mathbf{b}_L(x,\, x{+}y) = \begin{cases} (h(y)+O(d_LL^d\log L+L^dq^N))d_L & \textit{if } h(y)=h(-y)>0, \\ O(d_LL^d\log L+L^dq^N)d_L & \textit{otherwise.} \end{cases} \tag{10.112}$$

Convergence of generator of speeded-up trace process

Now, we are ready to proceed to the main result regarding the convergence of the generator. We are primarily interested in the convergence of the speeded-up (Markov) process defined by

$$W_L(t) = Y_L(\theta_L t), \tag{10.113}$$

where

$$\theta_L = \begin{cases} 1/(d_LL^{d-1}) & \text{for totally asymmetric case,} \\ 1/(d_LL^{d-2}) & \text{for mean-zero asymmetric case,} \\ L^2/d_L & \text{for symmetric case.} \end{cases}$$

Let $\mathcal{L}^{W_L}$ denote the infinitesimal generator associated with the continuous-time Markov chain $W_L(\cdot)$. Then, we can write this generator as, for all $F:\mathbb{T}^d\to\mathbb{R}$,

$$\begin{aligned} (\mathcal{L}^{W_L}F)\Big(\frac{x}{L}\Big) &= \theta_L\mathcal{L}_L^{\mathcal{E}_L}(F\circ\Theta_L)(\xi_L^x) \\ &= \theta_L\sum_{y\in\mathbb{T}_L^d}\mathbf{b}_L(x,\, x+y)\Big\{F\Big(\frac{x+y}{L}\Big)-F\Big(\frac{x}{L}\Big)\Big\}. \end{aligned} \tag{10.114}$$

The following is the main result of the current subsection.

Proposition 10.7.2. *Under the conditions of Theorems 10.2.21-10.2.23, it holds for all* $f \in C^3(\mathbb{T}^d)$ *that*

$$\lim_{L\to\infty} \sup_{x\in\mathbb{T}_L^d} \left|(\mathcal{L}^{W_L} f)\Big(\frac{x}{L}\Big) - (\mathcal{L}^{\mathbb{T}^d} f)\Big(\frac{x}{L}\Big)\right| = 0.$$

Proof. We fix $f \in C^3(\mathbb{T}^d)$ and consider three cases separately.

(Case 1: Totally asymmetric case) For this case, $\theta_L = 1/(d_L L^{d-1})$. Hence, by (10.114) and by part (1) of Proposition 10.7.1, we can deduce that

$$\begin{aligned}
&(\mathcal{L}^{W_L} f)(\xi_L^x) - (\mathcal{L}^{\mathbb{T}^d} f)\Big(\frac{x}{L}\Big) \\
&= \frac{1}{d_L L^{d-1}} \sum_{y\in\mathbb{T}_L^d} \mathbf{b}_L(x,\, x+y)\Big\{f\Big(\frac{x+y}{L}\Big) - f\Big(\frac{x}{L}\Big)\Big\} - \rho \sum_{y\in\mathbb{Z}^d} h(y) y \cdot \nabla f\Big(\frac{x}{L}\Big) \\
&= \sum_{y\in\mathbb{Z}^d:\, h(y)>h(-y)} \frac{N}{L^d}(h(y)-h(-y)) y\cdot\nabla f\Big(\frac{x}{L}\Big) + o(1) - \rho \sum_{y\in\mathbb{T}_L^d} h(y) y\cdot\nabla f\Big(\frac{x}{L}\Big).
\end{aligned}$$

The second equality holds by the first-order Taylor expansion and the condition $\lim_{L\to\infty} d_L L^{d+1}\log L = 0$. Since $N/L^d \to \rho$, the last line converges to 0 as $L\to\infty$ and we are done.

(Case 2: Mean-zero asymmetric case) For this case, $\theta_L = 1/(d_L L^{d-2})$; thus, by (10.114) and part (1) of Proposition 10.7.1, we obtain that

$$\begin{aligned}
&(\mathcal{L}^{W_L} f)(\xi_L^x) - (\mathcal{L}^{\mathbb{T}^d} f)\Big(\frac{x}{L}\Big) \\
&= \frac{1}{d_L L^{d-2}} \sum_{y\in\mathbb{T}_L^d} \mathbf{b}_L(x,\, x+y)\Big[f\Big(\frac{x+y}{L}\Big) - f\Big(\frac{x}{L}\Big)\Big] - (\mathcal{L}^{\mathbb{T}^d} f)\Big(\frac{x}{L}\Big) \\
&= \frac{1}{d_L L^{d-2}} \sum_{y\in\mathbb{Z}^d:\, h(y)>h(-y)} d_L N(h(y)-h(-y))\Big[f\Big(\frac{x+y}{L}\Big) - f\Big(\frac{x}{L}\Big)\Big] \\
&\quad + o(1) - (\mathcal{L}^{\mathbb{T}^d} f)\Big(\frac{x}{L}\Big).
\end{aligned}$$

In this case, unlike in **(Case 1)**, the first-order terms at the Taylor expansion cancel out each other. Thus, we apply the second-order Taylor expansion to get

$$\frac{N}{2L^d}\sum_{y\in\mathbb{Z}^d:\,h(y)>h(-y)}(h(y)-h(-y))y^\dagger\nabla^2 f\Big(\frac{x}{L}\Big)y-(\mathcal{L}^{\mathbb{T}^d}f)\Big(\frac{x}{L}\Big)+o(1).$$

This concludes the proof for this case since $N/L^d\to\rho$.

(Case 3: Symmetric case) For this case, $\theta_L=L^2/d_L$. Thus by (10.114) and by part (2) of Proposition 10.7.1, we obtain

$$\begin{aligned}&(\mathcal{L}^{W_L}f)(\xi_L^x)-(\mathcal{L}^{\mathbb{T}^d}f)\Big(\frac{x}{L}\Big)\\&=\frac{L^2}{d_L}\sum_{y\in\mathbb{T}_L^d}\mathbf{b}_L(x,\,x+y)\Big[f\Big(\frac{x+y}{L}\Big)-f\Big(\frac{x}{L}\Big)\Big]-(\mathcal{L}^{\mathbb{T}^d}f)\Big(\frac{x}{L}\Big)\\&=\frac{L^2}{2d_L}\sum_{y\in\mathbb{Z}^d}d_Lh(y)\Big[f\Big(\frac{x+y}{L}\Big)+f\Big(\frac{x-y}{L}\Big)-2f\Big(\frac{x}{L}\Big)\Big]-(\mathcal{L}^{\mathbb{T}^d}f)\Big(\frac{x}{L}\Big)+o(1).\end{aligned}$$

Note that the last error term is $o(1)$, since $\lim_{L\to\infty}d_LL^{2d+2}\log L=0$. Hence, we apply the second-order Taylor expansion to deduce that the last expression is equal to

$$\frac{1}{2}\sum_{y\in\mathbb{Z}^d}h(y)y^\dagger\nabla f^2\Big(\frac{x}{L}\Big)y-(\mathcal{L}^{\mathbb{T}^d}f)\Big(\frac{x}{L}\Big)+o(1).$$

This finishes the proof the definition of $\mathcal{L}^{\mathbb{T}^d}$. □

10.7.3 Tightness

The last ingredient for the proof of the convergence stated in part (1) of Definition 10.2.20 is the tightness of the process $W_L(t)=Y_L(\theta_Lt)$. Let $\mathbb{Q}_\eta^L$, $\eta\in\mathcal{E}_L$ denote the law of the process $W_L(\cdot)$ on the path space $D([0,\,\infty),\,\mathbb{T}^d)$ when the inclusion process starts from η, i.e., associated with the law $\mathbb{P}_\eta^L$.

Proposition 10.7.3. *Let $(x_L)_{L=1}^{\infty}$ be a sequence such that $x_L \in \mathbb{T}_L^d$ for all $L \geq 1$. Then, under the conditions of Theorems 10.2.21-10.2.23, the sequence $\{\mathbb{Q}^L_{\xi_L^{x_L}}\}_{L\geq 1}$ of path measures is tight in $D([0,\infty),\, \mathbb{T}^d)$.*

The natural way of proving this proposition is to use the Aldous criterion. Of course, we found a proof of the tightness based on this criterion, but controlling errors coming from the non-regularity of distance function $d(x,\, 0) = |x|$ around 0 requires complicated computations based on the large-deviation principle and the local central limit theorem for the random walk on the discrete torus. Instead, we realized that the criterion presented as Proposition 10.8.3 is more adequate to apply, in that it only considers smooth functions F, which guarantees sufficiently small error terms via Taylor expansion.

Proof of Proposition 10.7.3. The condition (1) of Proposition 10.8.3 is straightforward, since $\mathbb{T}^d$ is compact. Now let us check the condition (2). To this end, fix $f \in C_c^\infty(\mathbb{T}^d)$ and $\delta > 0$. Then, by the martingale problem associated with the Markov chain $W_L(\cdot)$, we know that the process given by

$$M_f^L(t) = f(W_L(t)) - f(W_L(0)) - \int_0^t (\mathcal{L}^{W_L} f)(W_L(s))ds \tag{10.115}$$

is a $\mathbb{Q}^L_{\xi_L^{x_L}}$-martingale. Let $(\mathscr{F}_t^L)_{t\geq 0}$ denote the canonical filtration associated with the process $W_L(\cdot)$ and by $\mathbf{E}^L_\eta$ the expectation associated with $\mathbb{Q}^L_\eta$. Then, the previous observation implies that, for all $t \geq 0$ and $0 \leq u \leq \delta$, we have that

$$\mathbf{E}^L_{\xi_L^{x_L}}\big[f(W_L(t+u)) - f(W_L(t))\big|\mathscr{F}_t^L\big] = \mathbf{E}^L_{\xi_L^{x_L}}\Big[\int_t^{t+u} (\mathcal{L}^{W_L} f)(W_L(s))ds\Big|\mathscr{F}_t^L\Big].$$

Hence, in view of Proposition 10.8.3, it suffices to check

$$\lim_{\delta\to 0}\limsup_{L\to\infty} \mathbf{E}^L_{\xi_L^{x_L}} \sup_{0\leq u\leq \delta}\Big|\int_t^{t+u} (\mathcal{L}^{W_L} f)(W_L(s))ds\Big| = 0. \tag{10.116}$$

By Proposition 10.7.2, it suffices to prove that

$$\lim_{\delta\to 0}\limsup_{L\to\infty}\mathbf{E}^L_{\xi_L^{x_L}}\sup_{0\le u\le\delta}\Big|\int_t^{t+u}(\mathcal{L}^{\mathbb{T}^d}f)(W_L(s))ds\Big| = 0.$$

This is obvious since $\mathcal{L}^{\mathbb{T}^d}f$ is a bounded function on $\mathbb{T}^d$. □

10.7.4 Proof of the main results

Proof of Theorems 10.2.21-10.2.23. Fix a sequence $(x_L)_{L=1}^\infty$ that satisfies $x_L \in \mathbb{T}^d_L$ for all $L \ge 1$ and $\lim_{L\to\infty}(x_L/L) = u$, as in part (1) of Definition 10.2.20. For simplicity, we write $\mathbb{Q}^L = \mathbb{Q}^L_{\xi_L^{x_L}}$ and $\mathbf{E}^L = \mathbf{E}^L_{\xi_L^{x_L}}$.

Let us first identify the limit points of the sequence $\{\mathbb{Q}^L\}_{L\ge 1}$. Let $\mathbb{Q}$ denote an arbitrary limit point of $\{\mathbb{Q}^L\}_{L\ge 1}$. Fix $f \in C^3(\mathbb{T}^d)$ and consider

$$M_f(t) = f(\omega(t)) - f(\omega(0)) - \int_0^t(\mathcal{L}^{\mathbb{T}^d}f)(\omega(s))ds, \quad t\ge 0,$$

where $\omega(t)$ is the canonical coordinate process on $D([0,\,\infty),\,\mathbb{T}^d)$. Then, we claim that $\{M_f(t)\}_{t\ge 0}$ is a $\mathbb{Q}$-martingale, i.e.,

$$\mathbb{E}^{\mathbb{Q}}\big[g((\omega(u): 0\le u\le s))(M_f(t) - M_f(s))\big] = 0 \tag{10.117}$$

for all $0 \le s \le t$ and for all bounded, continuous function g on $D([0,\,s],\,\mathbb{T}^d)$. To prove (10.117), we recall the $\mathbb{Q}^L$-martingale $M_f^L(t)$ defined in (10.115) so that we have

$$\mathbf{E}^L\big[g((\omega(u): 0\le u\le s))(M_f^L(t) - M_f^L(s))\big] = 0. \tag{10.118}$$

By Proposition 10.7.2, we have

$$\lim_{L\to\infty}\Big|M_f^L(t) - \Big[f(W_L(t)) - f(W_L(0)) - \int_0^t(\mathcal{L}^{\mathbb{T}^d}f)(W_L(s))ds\Big]\Big| = 0 \tag{10.119}$$

for all $t \geq 0$, and hence by (10.118) and (10.119), we obtain that

$$\lim_{L\to\infty} \mathbf{E}^L\big[g((\omega(u) : 0 \leq u \leq s))(M_f(t) - M_f(s))\big] = 0. \tag{10.120}$$

Therefore, the proof of (10.117) is completed if we can establish the following limit:

$$\begin{aligned}&\mathbf{E}^L\big[g((\omega(u) : 0 \leq u \leq s))(M_f(t) - M_f(s))\big] \\ &\quad \to \mathbb{E}^{\mathbb{Q}}\big[g((\omega(u) : 0 \leq u \leq s))(M_f(t) - M_f(s))\big] \quad \text{as } L \to \infty.\end{aligned} \tag{10.121}$$

This is not trivial since the map $H : \omega \mapsto g((\omega(u) : 0 \leq u \leq s))(M_f(t) - M_f(s))$ is not continuous on $D([0, \infty), \mathbb{T}^d)$. However, in [2, Proposition 3.2], this limiting procedure has been robustly confirmed and can be applied to our situation as well. Thus, the claim is proved. It completes the identification of limit points since the solution of the martingale problem is unique and since $C^3(\mathbb{T}^d)$ consists the core of the generator $\mathcal{L}^{\mathbb{T}^d}$ given in (10.109) because $\mathbb{T}^d$ is compact. Finally, along with the tightness established in Proposition 10.7.3, we can conclude the convergence of the process $W_L(\cdot)$ to $Y(\cdot)+u$ where $Y(\cdot)$ is the process generated by $\mathcal{L}_{\mathbb{T}^d}$ and starting from 0. This finally completes the verification of part (1) of Definition 10.2.20.

Now, we turn to part (2) of Definition 10.2.20, i.e., we prove

$$\lim_{L\to\infty} \sup_{\eta\in\mathcal{E}_L} \mathbb{E}^L_\eta\Big[\int_0^t \mathbb{1}_{\mathcal{H}_L\setminus\mathcal{E}_L}(\eta_L(\theta_L s))ds\Big] = 0 \quad \text{for all } t > 0. \tag{10.122}$$

To this end, let us first fix $x \in \mathbb{T}^d_L$ and $t > 0$. Then, by the translation invariance of the model, we have

$$\mathbb{E}^L_{\xi^x_L}\Big[\int_0^t \mathbb{1}_{\mathcal{H}_L\setminus\mathcal{E}_L}(\eta_L(\theta_L s))ds\Big] = \mathbb{E}^L_{\mu^{\mathcal{E}_L}_L}\Big[\int_0^t \mathbb{1}_{\mathcal{H}_L\setminus\mathcal{E}_L}(\eta_L(\theta_L s))ds\Big]$$

since the invariant measure $\mu^{\mathcal{E}_L}_L(\cdot)$ of the trace process is a uniform measure on $\mathcal{E}_L = \{\xi_L^x : x \in \mathbb{T}_L^d\}$. Now, we can deduce from Fubini theorem that

$$\begin{aligned}\mathbb{E}^L_{\mu_L^{\mathcal{E}_L}}\Big[\int_0^t \mathbb{1}_{\mathcal{H}_L\setminus\mathcal{E}_L}(\eta_L(\theta_L s))ds\Big] &\le \frac{1}{\mu_L(\mathcal{E}_L)}\mathbb{E}^L_{\mu_L}\Big[\int_0^t \mathbb{1}_{\mathcal{H}_L\setminus\mathcal{E}_L}(\eta_L(\theta_L s))ds\Big] \\ &= \frac{1}{\mu_L(\mathcal{E}_L)}\cdot t\cdot \mu_L(\mathcal{H}_L\setminus\mathcal{E}_L).\end{aligned}$$

Thus, (10.122) follows from static condensation established in Theorem 10.2.19.

□

10.8 Appendix

In the appendix, we collect several known results for the completeness of the article.

10.8.1 A lemma on the sum of reciprocals

The following elementary lemma is repeatedly used throughout the article.

Lemma 10.8.1. *For integers $n \ge k \ge 1$, define*

$$A_{n,\,k} = \Big\{(a_1,\,\dots,\,a_k) \in \mathbb{N}^k : a_1,\,\dots,\,a_k \ge 1 \text{ and } \sum_{i=1}^k a_i = n\Big\},$$

and define

$$S_{n,\,k} = \sum_{(a_1,\,\dots,\,a_k)\in A_{n,\,k}} \prod_{i=1}^k \frac{1}{a_i}.$$

Then, it holds that

$$S_{n,\,k} \le \frac{(3\log(n+1))^{k-1}}{n} \quad \text{for all } n \ge k \ge 1. \tag{10.123}$$

Proof. We proceed by the mathematical induction on k. Note that the inequality (10.123) is trivial for the initial case $k = 1$. Now, we fix $k \ge 2$ and assume that (10.123) holds for $S_{n,\ell}$ with $\ell = k-1$ and $n \geq \ell$. Then, look at the inequality for $S_{n,k}$ for some fixed n.

Since a_k can take values from 1 to $n-(k-1)$, we can write

$$S_{n,k} = \sum_{m=1}^{n-(k-1)} \sum_{(a_1,\dots,a_{k-1}) \in A_{n-m,k-1}} \frac{1}{m} \prod_{i=1}^{k} \frac{1}{a_i} = \sum_{m=1}^{n-(k-1)} \frac{1}{m} S_{n-m,k-1}.$$

Thus, by the induction hypothesis, we get that

$$S_{n,k} \leq \sum_{m=1}^{n-(k-1)} \frac{1}{m} \frac{(3\log(n-m+1))^{k-2}}{n-m} \leq (3\log(n+1))^{k-2} \sum_{m=1}^{n-(k-1)} \frac{1}{m(n-m)}. \tag{10.124}$$

The proof of the inequality (10.123) is completed since the last summation can be estimated by

$$\sum_{m=1}^{n-(k-1)} \frac{1}{m(n-m)} = \frac{1}{n} \sum_{m=1}^{n-(k-1)} \left(\frac{1}{m} + \frac{1}{n-m} \right) \leq \frac{3}{n} \log(n+1). \tag{10.125}$$

Inserting (10.125) to (10.124) finishes the proof of the induction step, and thus concludes the proof. □

10.8.2 Gordan's lemma

The following elementary lemma is used in the proof of Lemma 10.6.10. This lemma has many equivalent statements, which include the one known as Farkas' lemma.

Lemma 10.8.2 (Gordan's lemma)**.** *Let $\boldsymbol{A}$ be an $m \times n$ matrix for integers m, $n \geq 1$. Then, exactly one of the following statements holds.*

- *There exists a vector $\boldsymbol{\alpha} \in \mathbb{R}^m$ such that all the components of $\boldsymbol{A}^\dagger \boldsymbol{\alpha}$ are positive.*

- *There exists a vector* $\mathbf{0} \neq \boldsymbol{\beta} \in \mathbb{R}^n$ *such that all the components of* $\boldsymbol{\beta}$ *are non-positive and such that* $\boldsymbol{A}\boldsymbol{\beta} = 0$*.*

Proof. We refer to e.g., [30, Section 3]. □

10.8.3 A criterion for the tightness

We introduce a criterion for the tightness of the random process which is used in the proof of tightness of the speeded-up trace process in the thermodynamic limit case in Section 10.7. This criterion is thoroughly explained in [81], and is also used in [40] to prove the metastable behavior of symmetric inclusion processes.

Proposition 10.8.3. *For each* $N \geq 1$*, let* $X_\cdot^N$ *be a continuous-time Markov chain on* $\Omega = \mathbb{R}^d$ *or* $\mathbb{T}^d$*, and let* $\mathcal{F}_t^N$*,* $t \geq 0$ *be its natural filtration. Fix* $\{x_N\}_{N\geq 1} \subseteq \Omega$ *and let* $\mathbb{P}_{x_N}$ *and* $\mathbb{E}_{x_N}$ *denote the law and expectation of* $X_\cdot^N$ *starting from* x_N*, respectively. Then, the collection of laws* $\{\mathbb{P}_{x_N}\}_{N\geq 1}$ *is tight in the path space* $D([0,\, \infty);\, \Omega)$ *provided that both of the following conditions hold.*

(1) The sequence $\{X_\cdot^N\}_{N\geq 1}$ *is stochastically bounded in* $D([0,\, \infty);\, \Omega)$*.*

(2) For all $F \in C_c^\infty(\Omega)$*, there exists a family of non-negative random variables* $Z_N(\delta,\, F)$*,* $\delta > 0$*, such that, for all* $t \geq 0$ *and* $0 \leq u \leq \delta$*,*

$$\left|\mathbb{E}_{x_N}[F(X_{t+u}^N) - F(X_t^N)|\mathcal{F}_t^N]\right| \leq \mathbb{E}_{x_N}\left[Z_N(\delta,\, F)|\mathcal{F}_t^N\right] \quad \mathbb{P}_{x_N}\text{-a.s.,} \tag{10.126}$$

and

$$\lim_{\delta\to 0+} \limsup_{N\to\infty} \mathbb{E}_{x_N} Z_N(\delta,\, F) = 0. \tag{10.127}$$

Proof. See [81, Lemma 3.11] for the proof for the Euclidean case, i.e., $\Omega = \mathbb{R}^d$. The proof for the case $\Omega = \mathbb{T}^d$ is obviously the same with that of the Euclidean space. □

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국문초록

이 박사학위논문에서는 복잡한 확률시스템, 특히 강자기성 스핀시스템 또는 상호작용입자계에서 일어나는 메타안정성 현상의 정량적 분석을 다룬다. 추가로, 메타안정성을 분석하는 새로운 방법론인 H^1-근사이론을 소개한다. 이 방법론은 특히 비가역적 시스템을 분석할 때 유용하다. 정량적 분석으로 크게 두 가지를 다루는데, 하나는 메타안정 전이시간의 기댓값을 정확히 추산하는 Eyring–Kramers 공식이며, 다른 하나는 연이은 메타안정 전이들을 마르코프 체인으로 묘사하는 이론이다. 결과는 크게 두 범주로 나누어 기술되어 있는데, 첫 번째로 저온에서의 강자성 이징/포츠 모델과 관련된 모델들에 대해 다루고, 두 번째로 응축하는 포함 과정이 가역적일 때와 비가역적일 때 어떻게 다른 양태를 나타내는지 분석한다.

주요어휘: 메타안정성, H^1-근사, 이징 모델, 포츠 모델, 포함 과정

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