Critical configurations and tube of typical trajectories for the Potts and Ising models with zero external field

Gianmarco Bet 1,a , Anna Gallo 2,a,† , and Francesca R. Nardi 3,a,b

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Abstract

We consider the ferromagnetic q-state Potts model with zero external field in a finite volume evolving according to Glauber-type dynamics described by the Metropolis algorithm in the low temperature asymptotic limit. Our analysis concerns the multispin system that has q stable equilibria. Focusing on grid graphs with periodic boundary conditions, we study the tunneling between two stable states and from one stable state to the set of all other stable states. In both cases we identify the set of gates for the transition and prove that this set has to be crossed with high probability during the transition. Moreover, we identify the tube of typical paths and prove that the probability to deviate from it during the transition is exponentially small.

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^a Università degli Studi di Firenze, ^b Eindhoven University of Technology

 $^{^1}$ gianmarco.bet@unifi.it, 2 anna.gallo1@stud.unifi.it, 3 francescaromana.nardi@unifi.it

[†] Corresponding author

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1 Introduction

Metastability is a phenomenon that occurs when a physical system is close to a first order phase transition. More precisely, the phenomenon of metastability occurs when a system is trapped for a long time in a state different from the stable state, the so-called metastable state. After a long (random) time or due to random fluctuations the system makes a sudden transition from the metastable state to the stable state. When this happens, the system is said to display metastable behavior. Another class of transitions that has been studied is the tunneling behavior, i.e., the transition between two stable states, that occurs when the parameters of the system are the ones corresponding to the phase coexistence line. Since metastability occurs in several physical situations, such as supercooled liquids and supersaturated gases, many models for metastable behavior have been formulated throughout the years. Broadly speaking, in each case, the following three main issues are investigated. The first is the study of the first hitting time at which the process starting from a metastable state visits a stable state. The second issue is the study of the so-called set of critical configurations, i.e., the set of those configurations that are crossed by the process during the transition from the metastable state to the stable state. The final issue is the study of the typical trajectories that the system follows during the transition from the metastable state to the stable state. This is the so-called tube of typical paths.

In this paper we focus on the dynamics of the q-state Potts model on a two-dimensional discrete torus. At each site i of the lattice lies a spin with value $\sigma(i) \in \{1, \ldots, q\}$. In particular, the q-state Potts model is an extension of the classical Ising model from q = 2 to an arbitrary number of spins states. We study the q-state ferromagnetic Potts model with zero external magnetic field (h = 0) in the limit of large inverse temperature $\beta \to \infty$. When the external magnetic field is zero, the system lies on a coexistence line. The stochastic evolution is described by a Glauber-type dynamics, that consists of a single-spin flip Markov chain on a finite state space \mathcal{X} with transition probabilities given by the Metropolis algorithm and with stationary distribution given by the Gibbs measure μ_{β} , see (2.3). We consider the setting where there is no external magnetic field, and so to each configuration $\sigma \in \mathcal{X}$ we associate an energy $H(\sigma)$ that only depends on the local interactions between nearest-neighbor spins.

In the low-temperature regime $\beta \to \infty$ there are q stable states, corresponding to the configurations where all spins are equal. In this setting, the metastable states are not interesting since they do not have a clear physical interpretation, hence we focus our attention on the tunneling behavior between stable configurations.

The goal of this paper is to investigate the second and third issues introduced above for the tunneling behavior of the system. Indeed, given the set of stable states \mathcal{X}^s , we describe the set of minimal gates, which have the physical meaning of "critical configurations", and the tube of typical paths for three different types of transitions. More precisely, we study the transition from any $\mathbf{r} \in \mathcal{X}^s$ to (a) some fixed $\mathbf{s} \in \mathcal{X}^s \setminus \{\mathbf{r}\}$ under the constraint that the path followed does not intersect $\mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}$, to (b) the set $\mathcal{X}^s \setminus \{\mathbf{r}\}$, and to (c) some fixed $\mathbf{s} \in \mathcal{X}^s \setminus \{\mathbf{r}\}$.

In Section 3.1.1 we introduce the notion of *minimal restricted-gates* to denote the minimal gates for the transition (a). For the same reason, in Section 4.1.1 we introduce the notion of *restricted-tube of typical paths* to denote the tube of typical paths that are followed during the transition (a).

Let us now to briefly describe the strategy that we adopt. First we focus on the study of the energy landscape between two stable configurations. Roughly speaking, we prove that the set of minimal-restricted gates for any transition introduced in (a) contains those configurations in which all the spins are r except those, which have spins s, in a rectangle $a \times K$ with a bar $1 \times h$ attached on one of the two longest sides with $1 \le a \le L - 1$ and $1 \le h \le K - 1$. Later we exploit this result for describing the set of the minimal gates for the transitions (b) and (c). Next we describe the tube of typical trajectories for the three transitions above. The analysis is based on the notions of cycle, plateaux and extended-cycle, see Section 3.1.1 for the formal definitions. Once again we first describe the restricted case, i.e., the restricted-tube of typical paths between two stable configurations, and then we use this result to complete the description of the tube of typical paths for the transitions (b) and (c). Moreover, at the end of Section 3 and Section 4 we state two main results on the minimal gates and on the tube of typical paths for the Ising model with zero external magnetic field, which has exactly two stable configurations denoted by $\mathcal{X}^s = \{-1, +1\}$.

In [38] the authors study the asymptotic behavior of the first hitting time associated with the transitions (b) and (c) above. They obtain convergence results in probability, in expectation and in distribution. They also investigate the *mixing time*, which describes the rate of convergence of the Markov chain $\{X_t^{\beta}\}_{t\in\mathbb{N}}$ to its stationary distribution μ_{β} . They further show that the mixing time grows as $e^{c\ell\beta}$, where c>0 is some constant constant factor and ℓ is the smallest side length of Λ .

In this paper we use the so-called pathwise approach, that was initiated in 1984 [14] and it was developed in [42, 43, 44, 15]. The pathwise approach relies on a detailed knowledge of the energy landscape and on ad hoc large deviations estimates to give a quantitative answer to the three issues of metastability. This approach was further developed in [35, 18, 19, 39, 28, 29] to distinguish the study of transition time and gates from the one of typical paths. Furthermore, this method has been applied to study metastability in statistical mechanics lattice models. In particular, in [44, 35] the pathwise approach has been developed with the aim of finding answers valid with maximal generality and of reducing as much as possible the number of model dependent inputs necessary to study the metastable behaviour of a system. This method was applied in [3, 16, 23, 34, 37, 40, 41, 44] to find an answer to the three issues for Ising-like models with Glauber dynamics. Moreover, it was used in [32, 25, 31, 2, 39, 46] to find the transition time and the gates for Ising-like and hard-core models with Kawasaki and Glauber dynamics. Moreover, the pathwise approach was applied to probabilistic cellular automata (parallel dynamics) in [17, 20, 21, 45, 24].

The potential-theoretical approach exploits the Dirichlet form and spectral properties of

the transition matrix to characterize the study of the hitting time using. One of the advantages of this method is that it provides an estimate of the expected value of the transition time including the pre-factor, by exploiting a detailed knowledge of the critical configurations and on the configurations connected with them by one step of the the dynamics, see [11, 12, 9, 22]. This method was applied to find the pre-factor for Ising-like and hard-core model in [4, 13, 22, 10, 26, 33, 27] for Glauber and Kawasaki dynamics and in [36, 7] for parallel dynamics.

Recently, other approaches are developed in [5, 6, 30] and in [8]. These approaches are particularly well-suited to find the pre-factor when dealing with the tunnelling between two or more stable states like we do.

The outline of the paper is as follows. At the beginning of Section 2, we define the model. In Section 3 we give a list of definitions in order to state our main results on the set of minimal restricted-gates and on the set of minimal gates. In Section 3.2.1 we give the main results for the minimal restricted-gates for the transition (a). In Section 3.2.2 and Section 3.2.3 we state our main results for the minimal gates for the transitions (b) and (c), respectively. Next, at the beginning of Section 4 we expand the list of definitions in order to state the main results on the restricted-tube and on the tube of typical paths. More precisely, see Section 4.2.1 for the main results on the restricted-tube of typical paths. See Sections 4.2.2 and 4.2.3 for the main results on the tube of typical paths for the transitions (b) and (c), respectively. In Section 5 we prove some useful lemmas that allows us to complete the proof of the main results stated in Section 3.2.1. In Section 6 we are able to carry out the proof of the main results introduced in Section 3.2.2 and Section 3.2.3. Finally, in Section 7 we describe the typical paths between two Potts stable states and we prove the main results given in Section 4.2.

2 Model description

The q-state Potts model is represented by a finite two-dimensional rectangular lattice $\Lambda = (V, E)$, where $V = \{0, ..., K-1\} \times \{0, ..., L-1\}$ is the vertex set and E is the edge set, namely the set of the pairs of vertices whose spins interact with each other.

Let $S = \{1, ..., q\}$ be the set of spin values. We define $\mathcal{X} := S^V$ as the configuration set of the grid Λ ; in particular, to each vertex $v \in V$ is associated a spin value $\sigma(v) \in S$. Given $s \in \{1, ..., q\}$, let

$$N_s(\sigma) := |\{v \in V : \ \sigma(v) = s\}|$$
 (2.1)

be the number of vertices with spin s in the configuration σ and let $\mathbf{1}, \dots, \mathbf{q} \in \mathcal{X}$ be the configurations in which all the vertices have spin value $1, \dots, q$, respectively.

To each configuration $\sigma \in \mathcal{X}$ we associate the energy $H(\sigma)$ given by

$$H(\sigma) := -J_c \sum_{(v,w)\in E} \mathbb{1}_{\{\sigma(v)=\sigma(w)\}}, \quad \sigma \in \mathcal{X}, \tag{2.2}$$

where J_c is the coupling or interation constant. The function $H: \mathcal{X} \to \mathbb{R}$ is called Hamiltonian or energy function $H: \mathcal{X} \to \mathbb{R}$. In particular, there is no external magnetic field and H describes the local interactions between nearest-neighbor spins. When $J_c > 0$, the Potts model is said to be ferromagnetic, otherwise it is said to be antiferromagnetic. In this paper we focus on the ferromagnetic Potts model and, without loss of generality, we set $J_c = 1$, since in absence of a magnetic field it amounts to rescaling the temperature.

The Gibbs measure for the q-state Potts model on Λ is the probability distribution on \mathcal{X} given by

$$\mu_{\beta}(\sigma) := \frac{e^{-\beta H(\sigma)}}{\sum_{\sigma' \in \mathcal{X}} e^{-\beta H(\sigma')}},\tag{2.3}$$

where $\beta > 0$ is the inverse temperature. In particular, when $J_c > 0$ in the low-temperature regime $\beta \to \infty$ the Gibbs measure μ_{β} concentrates around the configurations $\mathbf{1}, \dots, \mathbf{q}$, which are the global minima of the Hamiltonian H.

The spin system evolves according to a Glauber-type dynamics. This is described by a single-spin update Markov chain $\{X_t^\beta\}_{t\in\mathbb{N}}$ on the state space \mathcal{X} with the following transition probabilities: for $\sigma, \sigma' \in \mathcal{X}$,

$$P_{\beta}(\sigma, \sigma') := \begin{cases} Q(\sigma, \sigma') e^{-\beta [H(\sigma') - H(\sigma)]^{+}}, & \text{if } \sigma \neq \sigma', \\ 1 - \sum_{\eta \neq \sigma} P_{\beta}(\sigma, \eta), & \text{if } \sigma = \sigma', \end{cases}$$
(2.4)

where $[n]^+ := \max\{0, n\}$ is the positive part of n and Q is the *connectivity matrix* defined by

$$Q(\sigma, \sigma') := \begin{cases} \frac{1}{q|V|}, & \text{if } |\{v \in V : \sigma(v) \neq \sigma'(v)\}| = 1, \\ 0, & \text{if } |\{v \in V : \sigma(v) \neq \sigma'(v)\}| > 1, \end{cases}$$
 (2.5)

for any $\sigma, \sigma' \in \mathcal{X}$. The matrix Q is symmetric and irreducible, i.e., for all $\sigma, \sigma' \in \mathcal{X}$, there exists a finite sequence of configurations $\omega_1, \ldots, \omega_n \in \mathcal{X}$ such that $\omega_1 = \sigma, \omega_n = \sigma'$ and $Q(\omega_i, \omega_{i+1}) > 0$ for $i = 1, \ldots, n-1$. Hence, the resulting stochastic dynamics defined by (2.4) is reversible with respect to the Gibbs measure (2.3). We shall refer to the triplet (\mathcal{X}, H, Q) as the energy landscape.

The dynamics defined above belongs to the class of a Metropolis dynamics. More precisely, given a configuration $\sigma \in \mathcal{X}$, at each step

- 1. a vertex $v \in V$ and a spin value $s \in S$ are selected independently and uniformly at random;
- 2. the spin at v is updated to spin s with probability

$$\begin{cases}
1, & \text{if } H(\sigma^{v,s}) - H(\sigma) \le 0, \\
e^{-\beta[H(\sigma^{v,s}) - H(\sigma)]}, & \text{if } H(\sigma^{v,s}) - H(\sigma) > 0,
\end{cases}$$
(2.6)

where $\sigma^{v,s}$ is the configuration obtained from σ by updating the spin in the vertex v to s, i.e.,

$$\sigma^{v,s}(w) := \begin{cases} \sigma(w) & \text{if } w \neq v, \\ s & \text{if } w = v. \end{cases}$$
 (2.7)

We say that $\sigma \in \mathcal{X}$ communicates with another configuration $\bar{\sigma} \in \mathcal{X}$ if there exist a vertex $v \in V$ and a spin value $s \in \{1, \ldots, q\}$, such that $\sigma(v) \neq s$ and $\bar{\sigma} = \sigma^{v,s}$. Hence, at each step the update of vertex v depends on the neighboring spins of v and on the energy difference

$$H(\sigma^{v,s}) - H(\sigma) = \sum_{w \sim v} (\mathbb{1}_{\{\sigma(v) = \sigma(w)\}} - \mathbb{1}_{\{\sigma(w) = s\}}). \tag{2.8}$$

3 Minimal restricted-gates and minimal gates

In this section we introduce our main results on the set of minimal restricted-gates and the one of minimal gates for the transition either from a Potts stable configurations to the other Potts stable states or from a Potts stable state to another Potts stable configuration. In order to state these main results, we need to give some notations and definitions which are used throughout the next sections.

3.1 Definitions and notations

The spatial structure is modeled by a $K \times L$ grid graph Λ with periodic boundary conditions, i.e., we consider the grid graph Λ and identify two by two the sides of the rectangle so that it corresponds to the bidimensional torus. Using this representation, two vertices $v, w \in V$ are said to be nearest-neighbors when they share an edge of Λ . Without loss of generality, we assume $K \leq L$ and $L \geq 3$.

We will denote the edge that links the vertices v and w as $(v, w) \in E$. Each $v \in V$ is naturally identified by its coordinates (i, j), where i and j denote respectively the row and the column where v lies. Moreover, the collection of vertices with first coordinate equal to $i = 0, \ldots, K - 1$ is denoted as r_i , which is the i-th row of Λ . The collection of those vertices with second coordinate equal to $j = 0, \ldots, L - 1$ is denoted as c_j , which is the j-th column of Λ .

3.1.1 Model-independent definitions and notations

We now give a list of model-independent definitions and notations that will be useful in formulating the main results concerning the set of minimal restricted-gates and the one of minimal gates for the transition either from a Potts stable configurations to the other Potts stable states or from a Potts stable state to another Potts stable configuration.

- We call path a finite sequence ω of configurations $\omega_0, \ldots, \omega_n \in \mathcal{X}$, $n \in \mathbb{N}$, such that $Q(\omega_i, \omega_{i+1}) > 0$ for $i = 0, \ldots, n-1$. Given $\sigma, \sigma' \in \mathcal{X}$, if $\omega_1 = \sigma$ and $\omega_n = \sigma'$, we denote a path from σ to σ' as $\omega : \sigma \to \sigma'$. Finally, $\Omega(\sigma, \sigma')$ denotes the set of all paths between σ and σ' .
- Given a path $\omega = (\omega_0, \dots, \omega_n)$, we define the *height* of ω as

$$\Phi_{\omega} := \max_{i=0,\dots,n} H(\omega_i). \tag{3.1}$$

- We say that a path $\omega: \sigma \to \sigma'$ is the *concatenation* of the L paths

$$\omega^{(i)} = (\omega_0^{(i)}, \dots, \omega_{m_i}^{(i)}), \text{ for some } m_i \in \mathbb{N}, i = 1, \dots, L$$

if

$$\omega = (\omega_0^{(1)} = \sigma, \dots, \omega_{m_1}^{(1)}, \omega_0^{(2)}, \dots, \omega_{m_2}^{(2)}, \dots, \omega_0^{(L)}, \dots, \omega_{m_L}^{(L)} = \sigma').$$

- For any pair $\sigma, \sigma' \in \mathcal{X}$, the communication height $\Phi(\sigma, \sigma')$ between σ and σ' is the minimal energy across all paths $\omega : \sigma \to \sigma'$. Formally,

$$\Phi(\sigma, \sigma') := \min_{\omega: \sigma \to \sigma'} \Phi_{\omega} = \min_{\omega: \sigma \to \sigma'} \max_{\eta \in \omega} H(\eta).$$
(3.2)

More generally, the communication energy between any pair of non-empty disjoint subsets $\mathcal{A}, \mathcal{B} \subset \mathcal{X}$ is

$$\Phi(\mathcal{A}, \mathcal{B}) := \min_{\sigma \in \mathcal{A}, \ \sigma' \in \mathcal{B}} \Phi(\sigma, \sigma'). \tag{3.3}$$

- The bottom $\mathscr{F}(\mathcal{A})$ of a non-empty set $\mathcal{A} \subset \mathcal{X}$ is the set of global minima of H in \mathcal{A} , i.e.,

$$\mathscr{F}(\mathcal{A}) := \{ \eta \in \mathcal{A} : H(\eta) = \min_{\sigma \in \mathcal{A}} H(\sigma) \}. \tag{3.4}$$

In particular,

$$\mathcal{X}^s := \mathscr{F}(\mathcal{X}) \tag{3.5}$$

is the set of the stable states.

- The set of optimal paths between $\sigma, \sigma' \in \mathcal{X}$ is defined as

$$(\sigma \to \sigma')_{opt} := \{ \omega \in \Omega(\sigma, \sigma') : \max_{\eta \in \omega} H(\eta) = \Phi(\sigma, \sigma') \}. \tag{3.6}$$

In other words, the optimal paths are those that realize the min-max in (3.2) between σ and σ' .

- The set of minimal saddles between $\sigma, \sigma' \in \mathcal{X}$ is defined as

$$S(\sigma, \sigma') := \{ \xi \in \mathcal{X} : \exists \omega \in (\sigma \to \sigma')_{opt}, \ \xi \in \omega : \max_{\eta \in \omega} H(\eta) = H(\xi) \}.$$
 (3.7)

- We say that $\eta \in \mathcal{S}(\sigma, \sigma')$ is an essential saddle if either
 - there exists $\omega \in (\sigma \to \sigma')_{opt}$ such that $\{\operatorname{argmax}_{\omega} H\} = \{\eta\}$ or
 - there exists $\omega \in (\sigma \to \sigma')_{opt}$ such that $\{\operatorname{argmax}_{\omega} H\} \supset \{\eta\}$ and $\{\operatorname{argmax}_{\omega'} H\} \not\subseteq \{\operatorname{argmax}_{\omega} H\} \setminus \{\eta\}$ for all $\omega' \in (\sigma \to \sigma')_{opt}$.

A saddle $\eta \in \mathcal{S}(\sigma, \sigma')$ that is not essential is said to be unessential.

- Given $\sigma, \sigma' \in \mathcal{X}$, we say that $\mathcal{W}(\sigma, \sigma')$ is a gate for the transition from σ to σ' if $\mathcal{W}(\sigma, \sigma') \subseteq \mathcal{S}(\sigma, \sigma')$ and $\omega \cap \mathcal{W}(\sigma, \sigma') \neq \emptyset$ for all $\omega \in (\sigma \to \sigma')_{opt}$.
- We say that $\mathcal{W}(\sigma, \sigma')$ is a minimal gate for the transition from σ to σ' if it is a minimal (by inclusion) subset of $\mathcal{S}(\sigma, \sigma')$ that is visited by all optimal paths, namely, it is a gate and for any $\mathcal{W}' \subset \mathcal{W}(\sigma, \sigma')$ there exists $\omega' \in (\sigma \to \sigma')_{opt}$ such that $\omega' \cap \mathcal{W}' = \emptyset$. We denote by $\mathcal{G} = \mathcal{G}(\sigma, \sigma')$ the union of all minimal gates for the transition from σ to σ' .
- Given $|\mathcal{X}^s| > 2$ and $\sigma, \sigma' \in \mathcal{X}^s, \sigma \neq \sigma'$, we define restricted-gate for the transition from σ to σ' a subset $\mathcal{W}_{\text{RES}}(\sigma, \sigma') \subset \mathcal{S}(\sigma, \sigma')$ which is intersected by all $\omega \in (\sigma \to \sigma')_{opt}$ such that $\omega \cap \mathcal{X}^s \setminus \{\sigma, \sigma'\} = \emptyset$.

We say that a restricted-gate $W_{\text{RES}}(\sigma, \sigma')$ for the transition from σ to σ' is a minimal restricted-gate if for any $W' \subset W_{\text{RES}}(\sigma, \sigma')$ there exists $\omega' \in (\sigma \to \sigma')_{opt}$ such that $\omega' \cap W' = \emptyset$. We denote by $\mathcal{F}(\sigma, \sigma')$ the union of all minimal restricted-gates for the transition from σ to σ' .

- Given a non-empty subset $\mathcal{A} \subset \mathcal{X}$ and a configuration $\sigma \in \mathcal{X}$, we define

$$\tau_{\mathcal{A}}^{\sigma} := \inf\{t > 0: \ X_t^{\beta} \in \mathcal{A}\} \tag{3.8}$$

as the first hitting time of the subset \mathcal{A} for the Markov chain $\{X_t^{\beta}\}_{t\in\mathbb{N}}$ starting from σ at time t=0. The hitting time is called tunnelling time when both the starting and the target configurations are stable configurations.

3.1.2 Model-dependent definitions and notations

Given $\sigma \in \mathcal{X}$ a q-Potts configuration and two different spin values $r, s \in \{1, \dots, q\}$, in order to state our main theorems, we also need to give some further model-dependent notations

- We define the set $C^s(\sigma) \subseteq \mathbb{R}^2$ as the union of unit closed squares centered at the vertices $v \in V$ such that $\sigma(v) = s$. We define s-clusters the maximal connected components C_1^s, \ldots, C_m^s , $m \in \mathbb{N}$, of $C^s(\sigma)$ and we consider separately two s-clusters which share only one unit square. In particular, two clusters C_1^s, C_2^s of spins are said to be interacting if either C_1^s and C_2^s intersect or are disjoint but there exists a site $x \notin C_1^s \cup C_2^s$ such that $\sigma(x) \neq s$ with two distinct nearest-neighbor sites y, z lying inside C_1^s, C_2^s respectively. In particular, we say that a q-Potts configuration has s-interacting clusters when all its s-clusters are interacting.

Note that the boundary of the clusters of a Potts configuration corresponds to the Peierls contour, which live on the dual lattice $\Lambda + (\frac{1}{2}, \frac{1}{2})$.

- We set $R(C^s(\sigma))$ as the smallest surrounding rectangle to the union of the clusters of spins s in σ .
- $\bar{R}_{a,b}(r,s)$ denotes the set of those configurations in which all the vertices have spins equal to r, except those, which have spins s, in a rectangle $a \times b$, see Figure 1(a);
- $\bar{B}_{a,b}^h(r,s)$ denotes the set of those configurations in which all the vertices have spins r, except those, which have spins s, in a rectangle $a \times b$ with a bar $1 \times h$ adjacent to one of the sides of length b, with $1 \le h \le b-1$, see Figure 1(b).
- Analogously, we set $\tilde{R}_{a,b}(r,s)$ and $\tilde{B}_{a,b}^h(r,s)$ interchanging the role of spins r and s, see Figure 1(c).

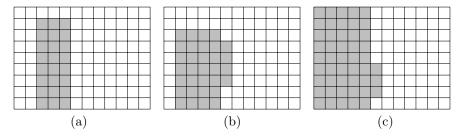


Figure 1: Examples of configurations which belong to $\bar{R}_{3,8}(r,s)$ (a), $\bar{B}_{4,7}^4(r,s)$ (b) and $\tilde{\mathcal{B}}_{6,9}^6(r,s)$ (c). For semplicity we color white the vertices whose spin is r and we color gray the vertices whose spin is s.

Note that

$$\bar{R}_{a,K}(r,s) \equiv \tilde{R}_{L-a,K}(r,s) \text{ and } \bar{B}_{a,K}^h(r,s) \equiv \tilde{B}_{L-a-1,K}^{K-h}(r,s).$$
 (3.9)

- We set

$$\overline{\mathscr{P}}(\mathbf{r}, \mathbf{s}) := \bar{B}_{1,K}^{K-1}(r, s), \qquad \widetilde{\mathscr{P}}(\mathbf{r}, \mathbf{s}) := \tilde{B}_{1,K}^{K-1}(r, s). \tag{3.10}$$

- We define

$$\overline{\mathcal{Q}}(\mathbf{r}, \mathbf{s}) := \overline{R}_{2,K-1}(r, s) \cup \bigcup_{h=2}^{K-2} \overline{B}_{1,K}^{h}(r, s),$$

$$\widetilde{\mathcal{Q}}(\mathbf{r}, \mathbf{s}) := \widetilde{R}_{2,K-1}(r, s) \cup \bigcup_{h=2}^{K-2} \widetilde{B}_{1,K}^{h}(r, s).$$
(3.11)

- We define

$$\overline{\mathcal{H}}(\mathbf{r}, \mathbf{s}) := \overline{B}_{1,K}^{1}(r, s) \cup \bigcup_{h=2}^{K-2} \overline{B}_{1,K-1}^{h}(r, s)$$

$$\widetilde{\mathcal{H}}(\mathbf{r}, \mathbf{s}) := \widetilde{B}_{1,K}^{1}(r, s) \cup \bigcup_{h=2}^{K-2} \widetilde{B}_{1,K-1}^{h}(r, s).$$
(3.12)

- We set

$$W_j^{(h)}(\mathbf{r}, \mathbf{s}) := \bar{B}_{j,K}^h(r, s) = \tilde{B}_{L-j-1,K}^{K-h}(r, s) \text{ for } j = 2, \dots, L-3,$$
 (3.13)

and

$$\mathcal{W}_{j}(\mathbf{r}, \mathbf{s}) := \bigcup_{h=1}^{K-1} \mathcal{W}_{j}^{(h)}(\mathbf{r}, \mathbf{s}). \tag{3.14}$$

We refer the reader to Section 5 for some illustrations of the sets above.

3.2 Main results

We are now ready to state the main results on minimal restricted-gates between two stable configurations and on minimal gates for the transition between a stable configuration and the other stable states and between a stable configuration and another one.

3.2.1 Minimal restricted-gates between two Potts stable configurations

In Section 5 we study the energy landscape between two given stable configurations $\mathbf{r}, \mathbf{s} \in \mathcal{X}^s$, $\mathbf{s} \neq \mathbf{r}$ and describe the set of all minimal restricted-gates for the transition between them. We recall that these gates are said to be "restricted" because they are gates for the transition from \mathbf{r} to \mathbf{s} following an optimal path $\omega \in (\mathbf{r} \to \mathbf{s})_{opt}$ such that $\omega \cap (\mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}) = \emptyset$. More precisely, we shall prove the following results.

Theorem 3.1. Consider the q-state Potts model on a $K \times L$ grid Λ with max $\{K, L\} \geq 3$ and with periodic boundary conditions. For every $\mathbf{r}, \mathbf{s} \in \mathcal{X}^s$, $\mathbf{s} \neq \mathbf{r}$, the following sets are minimal restricted-gates for the transition $\mathbf{r} \to \mathbf{s}$:

- (a) $\overline{\mathscr{P}}(\mathbf{r}, \mathbf{s})$ and $\widetilde{\mathscr{P}}(\mathbf{r}, \mathbf{s})$;
- (b) $\overline{\mathcal{Q}}(\mathbf{r}, \mathbf{s})$ and $\widetilde{\mathcal{Q}}(\mathbf{r}, \mathbf{s})$;
- (c) $\overline{\mathscr{H}}(\mathbf{r}, \mathbf{s})$ and $\widetilde{\mathscr{H}}(\mathbf{r}, \mathbf{s})$;
- (d) $W_i^{(h)}(\mathbf{r}, \mathbf{s})$ for any j = 2, ..., L-3 and any h = 1, ..., K-1.

Theorem 3.2. Consider the q-state Potts model on a $K \times L$ grid Λ with max $\{K, L\} \geq 3$ and with periodic boundary conditions. For every $\mathbf{r}, \mathbf{s} \in \mathcal{X}^s$, $\mathbf{s} \neq \mathbf{r}$, the set of all minimal restricted-gates for the transition $\mathbf{r} \to \mathbf{s}$ is given by

$$\mathcal{F}(\mathbf{r}, \mathbf{s}) = \bigcup_{j=2}^{L-3} \mathcal{W}_j(\mathbf{r}, \mathbf{s}) \cup \overline{\mathcal{H}}(\mathbf{r}, \mathbf{s}) \cup \widetilde{\mathcal{H}}(\mathbf{r}, \mathbf{s}) \cup \overline{\mathcal{Q}}(\mathbf{r}, \mathbf{s}) \cup \widetilde{\mathcal{Q}}(\mathbf{r}, \mathbf{s}) \cup \overline{\mathcal{P}}(\mathbf{r}, \mathbf{s}) \cup \widetilde{\mathcal{P}}(\mathbf{r}, \mathbf{s}). \quad (3.15)$$

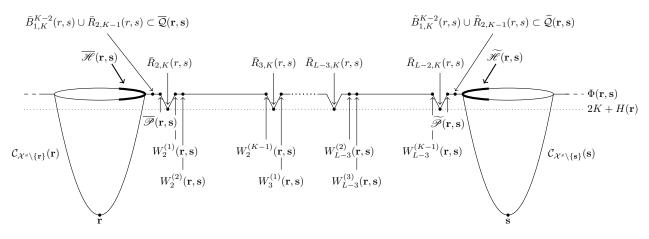


Figure 2: Focus on the energy landscape between \mathbf{r} and \mathbf{s} and example of some essential saddles for the transition $\mathbf{r} \to \mathbf{s}$ following an optimal path which does not pass through other stable states.

Corollary 3.1. Consider the q-state Potts model on a $K \times L$ grid Λ with $\max\{K, L\} \geq 3$ and with periodic boundary conditions. Consider any $\mathbf{r}, \mathbf{s} \in \mathcal{X}^s$ and the transition from \mathbf{r} to \mathbf{s} . Then, the following properties hold:

(a)
$$\lim_{\beta \to \infty} \mathbb{P}_{\mathbf{r}}(\tau_{\overline{\mathscr{P}}(\mathbf{r},\mathbf{s})} < \tau_{\mathcal{X}^s \setminus \{\mathbf{r}\}} | \tau_{\mathbf{s}} < \tau_{\mathcal{X}^s \setminus \{\mathbf{r},\mathbf{s}\}})$$

= $\lim_{\beta \to \infty} \mathbb{P}_{\mathbf{r}}(\tau_{\widetilde{\mathscr{P}}(\mathbf{r},\mathbf{s})} < \tau_{\mathcal{X}^s \setminus \{\mathbf{r}\}} | \tau_{\mathbf{s}} < \tau_{\mathcal{X}^s \setminus \{\mathbf{r},\mathbf{s}\}}) = 1;$

(b)
$$\lim_{\beta \to \infty} \mathbb{P}_{\mathbf{r}}(\tau_{\overline{Q}(\mathbf{r},\mathbf{s})} < \tau_{\mathcal{X}^s \setminus \{\mathbf{r}\}} | \tau_{\mathbf{s}} < \tau_{\mathcal{X}^s \setminus \{\mathbf{r},\mathbf{s}\}})$$

= $\lim_{\beta \to \infty} \mathbb{P}_{\mathbf{r}}(\tau_{\widetilde{Q}(\mathbf{r},\mathbf{s})} < \tau_{\mathcal{X}^s \setminus \{\mathbf{r}\}} | \tau_{\mathbf{s}} < \tau_{\mathcal{X}^s \setminus \{\mathbf{r},\mathbf{s}\}}) = 1;$

(c)
$$\lim_{\beta \to \infty} \mathbb{P}_{\mathbf{r}}(\tau_{\widetilde{\mathscr{H}}(\mathbf{r},\mathbf{s})} < \tau_{\mathcal{X}^s \setminus \{\mathbf{r}\}} | \tau_{\mathbf{s}} < \tau_{\mathcal{X}^s \setminus \{\mathbf{r},\mathbf{s}\}})$$

= $\lim_{\beta \to \infty} \mathbb{P}_{\mathbf{r}}(\tau_{\widetilde{\mathscr{H}}(\mathbf{r},\mathbf{s})} < \tau_{\mathcal{X}^s \setminus \{\mathbf{r}\}} | \tau_{\mathbf{s}} < \tau_{\mathcal{X}^s \setminus \{\mathbf{r},\mathbf{s}\}}) = 1;$

(d)
$$\lim_{\beta \to \infty} \mathbb{P}_{\mathbf{r}}(\tau_{\mathcal{W}_{j}^{(h)}(\mathbf{r},\mathbf{s})} < \tau_{\mathcal{X}^{s} \setminus \{\mathbf{r}\}} | \tau_{\mathbf{s}} < \tau_{\mathcal{X}^{s} \setminus \{\mathbf{r},\mathbf{s}\}}) = 1 \text{ for any } j = 2, \ldots, L-3, h = 1, \ldots, K-1.$$

3.2.2 Minimal gates for the transition from a stable state to the other stable states

Using the results about the minimal restricted-gates, we will prove the following results concerning the set of minimal gates for the transition from a stable configuration to the other stable states. We assume q > 2, otherwise when q = 2 the Hamiltonian has only two global minima, $|\mathcal{X}^s| = 2$, and the results on the minimal gates between a stable configuration to the other unique stable state is given by Theorem 3.1 and Theorem 3.2.

Theorem 3.3. Consider the q-state Potts model on a $K \times L$ grid Λ with max $\{K, L\} \geq 3$ and with periodic boundary conditions. Consider $\mathbf{r} \in \mathcal{X}^s$. Then, the following sets are minimal gates for the transition $\mathbf{r} \to \mathcal{X}^s \setminus \{\mathbf{r}\}$:

(a)
$$\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathscr{P}}(\mathbf{r}, \mathbf{t})$$
 and $\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \widetilde{\mathscr{P}}(\mathbf{r}, \mathbf{t})$

(b)
$$\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathcal{Q}}(\mathbf{r}, \mathbf{t}) \text{ and } \bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \widetilde{\mathcal{Q}}(\mathbf{r}, \mathbf{t});$$

(c)
$$\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathscr{H}}(\mathbf{r}, \mathbf{t}) \text{ and } \bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \widetilde{\mathscr{H}}(\mathbf{r}, \mathbf{t});$$

(d)
$$\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \mathcal{W}_j^{(h)}(\mathbf{r}, \mathbf{t})$$
 for any $j = 2, \dots, L-3$ and any $h = 1, \dots, K-1$.

Theorem 3.4. Consider the q-state Potts model on a $K \times L$ grid Λ with $\max\{K, L\} \geq 3$ and with periodic boundary conditions. Given $\mathbf{r} \in \mathcal{X}^s$, the set of all minimal gates for the transition $\mathbf{r} \to \mathcal{X}^s \setminus \{\mathbf{r}\}$ is given by

$$\mathcal{G}(\mathbf{r}, \mathcal{X}^s \setminus \{\mathbf{r}\}) = \bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \mathcal{F}(\mathbf{r}, \mathbf{t}), \tag{3.16}$$

where

$$\mathcal{F}(\mathbf{r}, \mathbf{t}) = \bigcup_{j=2}^{L-3} \mathcal{W}_j(\mathbf{r}, \mathbf{t}) \cup \overline{\mathcal{H}}(\mathbf{r}, \mathbf{t}) \cup \widetilde{\mathcal{H}}(\mathbf{r}, \mathbf{t}) \cup \overline{\mathcal{Q}}(\mathbf{r}, \mathbf{t}) \cup \widetilde{\mathcal{Q}}(\mathbf{r}, \mathbf{t}) \cup \overline{\mathcal{P}}(\mathbf{r}, \mathbf{t}) \cup \widetilde{\mathcal{P}}(\mathbf{r}, \mathbf{t}). \quad (3.17)$$

Corollary 3.2. Consider the q-state Potts model on a $K \times L$ grid Λ with $\max\{K, L\} \geq 3$ and with periodic boundary conditions. Consider any $\mathbf{r} \in \mathcal{X}^s$ and the transition from \mathbf{r} to $\mathcal{X}^s \setminus \{\mathbf{r}\}$. Then, the following properties hold:

(a)
$$\lim_{\beta \to \infty} \mathbb{P}_{\mathbf{r}}(\tau_{\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}}} \overline{\mathscr{P}}(\mathbf{r}, \mathbf{t}) < \tau_{\mathcal{X}^s \setminus \{\mathbf{r}\}})$$

= $\lim_{\beta \to \infty} \mathbb{P}_{\mathbf{r}}(\tau_{\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}}} \widetilde{\mathscr{P}}(\mathbf{r}, \mathbf{t}) < \tau_{\mathcal{X}^s \setminus \{\mathbf{r}\}}) = 1;$

(b)
$$\lim_{\beta \to \infty} \mathbb{P}_{\mathbf{r}}(\tau_{\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}}} \overline{\mathcal{Q}}(\mathbf{r}, \mathbf{t}) < \tau_{\mathcal{X}^s \setminus \{\mathbf{r}\}})$$

= $\lim_{\beta \to \infty} \mathbb{P}_{\mathbf{r}}(\tau_{\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}}} \widetilde{\mathcal{Q}}(\mathbf{r}, \mathbf{t}) < \tau_{\mathcal{X}^s \setminus \{\mathbf{r}\}}) = 1;$

(c)
$$\lim_{\beta \to \infty} \mathbb{P}_{\mathbf{r}}(\tau_{\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}}} \overline{\mathscr{H}}(\mathbf{r}, \mathbf{t}) < \tau_{\mathcal{X}^s \setminus \{\mathbf{r}\}})$$

= $\lim_{\beta \to \infty} \mathbb{P}_{\mathbf{r}}(\tau_{\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}}} \widetilde{\mathscr{H}}(\mathbf{r}, \mathbf{t}) < \tau_{\mathcal{X}^s \setminus \{\mathbf{r}\}}) = 1;$

(d)
$$\lim_{\beta \to \infty} \mathbb{P}_{\mathbf{r}}(\tau_{\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \mathcal{W}_j^{(h)}(\mathbf{r}, \mathbf{t})} < \tau_{\mathcal{X}^s \setminus \{\mathbf{r}\}}) = 1 \text{ for any } j = 2, \dots, L-3, h = 1, \dots, K-1.$$

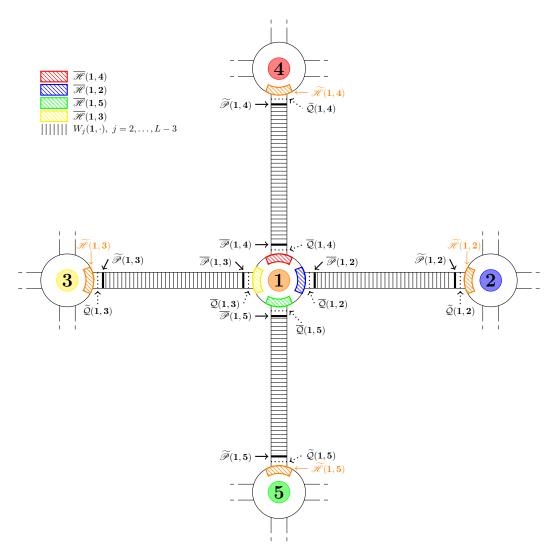


Figure 3: Example of 5-Potts model with $S = \{1, 2, 3, 4, 5\}$. Viewpoint from above on the set of minimal gates around the stable configuration $\mathbf{1}$ at energy $2K + 2 + H(\mathbf{1})$. For any $\mathbf{s} \in \{\mathbf{2}, \mathbf{3}, \mathbf{4}, \mathbf{5}\}$, starting from $\mathbf{1}$, the process hits $\mathcal{X}^s \setminus \{\mathbf{1}\}$ for the first time in \mathbf{s} with probability $\frac{1}{q-1} = \frac{1}{4}$.

3.2.3 Minimal gates for the transition from a stable state to another stable state

Finally, using the results concerning the minimal gates between a stable state and the other stable configurations, we will describe the set of minimal gates for the transition from a stable configuration to another stable state. Starting from $\mathbf{r} \in \mathcal{X}^s$, before hitting for the first time $\mathbf{s} \in \mathcal{X}^s \setminus \{\mathbf{r}\}$ the process could pass through some stable configurations different from the target \mathbf{s} . Therefore, we describe the set of all minimal gates for the transition $\mathbf{r} \to \mathbf{s}$ in terms of a sequence of transitions between two stable states such that the path followed by the process does not intersect other stable configurations. In particular, for these transitions the main results about minimal restricted-gates hold. It follows that in order to prove the next results, Theorem 3.1 and Theorem 3.2 will be crucial. We assume q > 2, otherwise when q = 2 the Hamiltonian has only two global minima and the results on the minimal gates coincide with Theorem 3.1 and Theorem 3.2.

Theorem 3.5. Consider the q-state Potts model on a $K \times L$ grid Λ with $\max\{K, L\} \geq 3$ and with periodic boundary conditions. Consider $\mathbf{r}, \mathbf{s} \in \mathcal{X}^s, \mathbf{r} \neq \mathbf{s}$. Then, the following sets

are minimal gates for the transition $\mathbf{r} \to \mathbf{s}$:

(a)
$$\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathscr{P}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \overline{\mathscr{P}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \overline{\mathscr{P}}(\mathbf{t}', \mathbf{s}) \text{ and }$$

 $\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \widetilde{\mathscr{P}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \widetilde{\mathscr{P}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \widetilde{\mathscr{P}}(\mathbf{t}', \mathbf{s});$

$$\begin{array}{l} \text{(b)} \;\; \bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \; \overline{\mathcal{Q}}(\mathbf{r},\mathbf{t}) \cup \bigcup_{\mathbf{t},\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\},\mathbf{t} \neq \mathbf{t}'} \; \overline{\mathcal{Q}}(\mathbf{t},\mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r},\mathbf{s}\}} \; \overline{\mathcal{Q}}(\mathbf{t}',\mathbf{s}) \; \textit{and} \\ \bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \; \widetilde{\mathcal{Q}}(\mathbf{r},\mathbf{t}) \cup \bigcup_{\mathbf{t},\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\},\mathbf{t} \neq \mathbf{t}'} \; \widetilde{\mathcal{Q}}(\mathbf{t},\mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r},\mathbf{s}\}} \; \widetilde{\mathcal{Q}}(\mathbf{t}',\mathbf{s}); \end{array}$$

(c)
$$\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathscr{H}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \overline{\mathscr{H}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \overline{\mathscr{H}}(\mathbf{t}', \mathbf{s}) \text{ and }$$

 $\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \widetilde{\mathscr{H}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \widetilde{\mathscr{H}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \widetilde{\mathscr{H}}(\mathbf{t}', \mathbf{s});$

(d)
$$\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \mathcal{W}_j^{(h)}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \mathcal{W}_j^{(h)}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \mathcal{W}_j^{(h)}(\mathbf{t}', \mathbf{s})$$
 for any $j = 2, ..., L - 3$ and any $h = 1, ..., K - 1$.

Theorem 3.6. Consider the q-state Potts model on a $K \times L$ grid Λ with $\max\{K, L\} \geq 3$ and with periodic boundary conditions. Consider $\mathbf{r}, \mathbf{s} \in \mathcal{X}^s$, $\mathbf{r} \neq \mathbf{s}$. Then, the set of all minimal gates for the transition $\mathbf{r} \to \mathbf{s}$ is given by

$$\mathcal{G}(\mathbf{r}, \mathbf{s}) = \bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \mathcal{F}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \mathcal{F}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \mathcal{F}(\mathbf{t}', \mathbf{s}), \tag{3.18}$$

where

$$\mathcal{F}(\mathbf{t}, \mathbf{t}') = \bigcup_{j=2}^{L-3} \mathcal{W}_j(\mathbf{t}, \mathbf{t}') \cup \overline{\mathscr{H}}(\mathbf{t}, \mathbf{t}') \cup \widetilde{\mathscr{H}}(\mathbf{t}, \mathbf{t}') \cup \overline{\mathscr{Q}}(\mathbf{t}, \mathbf{t}') \cup \widetilde{\mathscr{Q}}(\mathbf{t}, \mathbf{t}') \cup \overline{\mathscr{P}}(\mathbf{t}, \mathbf{t}') \cup \widetilde{\mathscr{P}}(\mathbf{t}, \mathbf{t}'),$$
(3.19)

for any $\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s$, $\mathbf{t} \neq \mathbf{t}'$.

Corollary 3.3. Consider the q-state Potts model on a $K \times L$ grid Λ with max $\{K, L\} \geq 3$ and with periodic boundary conditions. Consider any $\mathbf{r}, \mathbf{s} \in \mathcal{X}^s$, with $\mathbf{r} \neq \mathbf{s}$, and the transition from \mathbf{r} to \mathbf{s} . Then, the following properties hold:

(a)
$$\lim_{\beta \to \infty} \mathbb{P}_{\mathbf{r}}(\tau_{\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}}} \overline{\mathscr{P}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \overline{\mathscr{P}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \overline{\mathscr{P}}(\mathbf{t}', \mathbf{s})} < \tau_{\mathbf{s}}) = \lim_{\beta \to \infty} \mathbb{P}_{\mathbf{r}}(\tau_{\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \widetilde{\mathscr{P}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \widetilde{\mathscr{P}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \widetilde{\mathscr{P}}(\mathbf{t}', \mathbf{s})} < \tau_{\mathbf{s}}) = 1;$$

$$\begin{split} \text{(b) } &\lim_{\beta \to \infty} \mathbb{P}_{\mathbf{r}} \big(\tau_{\bigcup_{\mathbf{t} \in \mathcal{X}^s \backslash \{\mathbf{r}\}}} \, \overline{\mathcal{Q}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \backslash \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \, \overline{\mathcal{Q}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \backslash \{\mathbf{r}, \mathbf{s}\}} \, \overline{\mathcal{Q}}(\mathbf{t}', \mathbf{s}) < \tau_{\mathbf{s}} \big) = \\ &\lim_{\beta \to \infty} \mathbb{P}_{\mathbf{r}} \big(\tau_{\bigcup_{\mathbf{t} \in \mathcal{X}^s \backslash \{\mathbf{r}\}}} \, \widetilde{\mathcal{Q}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \backslash \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \, \widetilde{\mathcal{Q}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \backslash \{\mathbf{r}, \mathbf{s}\}} \, \widetilde{\mathcal{Q}}(\mathbf{t}', \mathbf{s}) < \tau_{\mathbf{s}} \big) = 1; \end{split}$$

(c)
$$\lim_{\beta \to \infty} \mathbb{P}_{\mathbf{r}}(\tau_{\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}}} \overline{\mathscr{H}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \overline{\mathscr{H}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \overline{\mathscr{H}}(\mathbf{t}', \mathbf{s}) < \tau_{\mathbf{s}}) = \lim_{\beta \to \infty} \mathbb{P}_{\mathbf{r}}(\tau_{\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \widetilde{\mathscr{H}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \widetilde{\mathscr{H}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \widetilde{\mathscr{H}}(\mathbf{t}', \mathbf{s}) < \tau_{\mathbf{s}}) = 1;$$

(d)
$$\lim_{\beta \to \infty} \mathbb{P}_{\mathbf{r}}(\tau_{\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \mathcal{W}_j^{(h)}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \mathcal{W}_j^{(h)}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \mathcal{W}_j^{(h)}(\mathbf{t}', \mathbf{s})} < \tau_{\mathbf{s}}) = 1$$
 for any $j = 2, \dots, L - 3, h = 1, \dots, K - 1$.

3.2.4 Minimal gates of the Ising model with zero external magnetic field

When q = 2, the Potts model corresponds to the Ising model with no external magnetic field, in which $S = \{-1, +1\}$ and $\mathcal{X}^s = \{-1, +1\}$. In this scenario, starting from -1, the target is necessarily +1 and the following corollary holds.

Corollary 3.4. Consider the Ising model on a $K \times L$ grid Λ with $\max\{K, L\} \geq 3$ and with periodic boundary conditions. Then, the following sets are minimal gates for the transition $-1 \rightarrow +1$:

- (a) $\overline{\mathscr{P}}(-1,+1)$ and $\widetilde{\mathscr{P}}(-1,+1)$;
- (b) $\overline{\mathcal{Q}}(-1,+1)$ and $\widetilde{\mathcal{Q}}(-1,+1)$;
- (c) $\overline{\mathscr{H}}(-1,+1)$ and $\widetilde{\mathscr{H}}(-1,+1)$;
- (d) $W_i^{(h)}(-1,+1)$ for any $j=2,\ldots,L-3$ and any $h=1,\ldots,K-1$.

Moreover

$$\mathcal{G}(-\mathbf{1}, +\mathbf{1}) = \bigcup_{j=2}^{L-3} \mathcal{W}_j(-\mathbf{1}, +\mathbf{1}) \cup \overline{\mathcal{H}}(-\mathbf{1}, +\mathbf{1}) \cup \widetilde{\mathcal{H}}(-\mathbf{1}, +\mathbf{1}) \cup \overline{\mathcal{Q}}(-\mathbf{1}, +\mathbf{1})$$
$$\cup \widetilde{\mathcal{Q}}(-\mathbf{1}, +\mathbf{1}) \cup \overline{\mathcal{P}}(-\mathbf{1}, +\mathbf{1}) \cup \widetilde{\mathcal{P}}(-\mathbf{1}, +\mathbf{1}). \tag{3.20}$$

4 Restricted-tube of typical paths and tube of typical paths

At the ending of this section we state our main results on the restricted-tube of typical paths and on the tube of typical paths for the transition from a Potts stable state to the other stable configurations and from a stable state to another one.

4.1 Definitions and notations

In order to describe the tube of typical trajectories performing the transition between two Potts stable configurations, we recall the definitions given in Section 3.1 and we add some new ones.

4.1.1 Model-independent definitions and notations

In addition to the list of Section 3.1.1, we give also the following model-independent definitions. In particular, these definitions are taken from [39], [19] and [44].

- Given a non-empty subset $A \subseteq \mathcal{X}$, it is said to be *connected* if for any $\sigma, \eta \in A$ there exists a path $\omega : \sigma \to \eta$ totally contained in A. Moreover, we define ∂A as the *external boundary* of A, i.e., the set

$$\partial \mathcal{A} := \{ \eta \notin \mathcal{A} : P(\sigma, \eta) > 0 \text{ for some } \sigma \in \mathcal{A} \}.$$
 (4.1)

- A maximal connected set of equal energy states is called a plateau.
- A non-empty subset $\mathcal{C} \subset \mathcal{X}$ is called *cycle* if it is either a singleton or a connected set such that

$$\max_{\sigma \in \mathcal{C}} H(\sigma) < H(\mathscr{F}(\partial \mathcal{C})). \tag{4.2}$$

When C is a singleton, it is said to be a *trivial cycle*.

We define *extended cycle* a collection of connected equielevated cycles, i.e., cycles of equal energy which belong to the same plateau. It is easy to see that an example of extended cycle is a plateau that may be depicted as union of equielevated trivial cycles.

Let $\mathscr{C}(\mathcal{X})$ be the set of cycles and extended cycles of \mathcal{X} .

- For any $C \in \mathcal{C}(\mathcal{X})$, we define external boundary of C by (4.1), i.e., as the set can be reached from C in one step of the dynamics.

- For any $\mathcal{C} \in \mathscr{C}(\mathcal{X})$, we define

$$\mathcal{B}(\mathcal{C}) := \begin{cases} \mathscr{F}(\partial \mathcal{C}) & \text{if } \mathcal{C} \text{ is a non-trivial cycle,} \\ \{\eta \in \partial \mathcal{C} : H(\eta) < H(\sigma)\} & \text{if } \mathcal{C} = \{\sigma\} \text{ is a trivial cycle,} \\ \{\eta \in \partial \mathcal{C} : \exists \{\sigma\} \in \mathcal{C} \text{ s.t. } H(\eta) < H(\sigma)\} & \text{if } \mathcal{C} \text{ is an extended cycle,} \end{cases}$$

as the principal boundary of \mathcal{C} . Furthermore, let $\partial^{np}\mathcal{C}$ be the non-principal boundary of \mathcal{C} , i.e., $\partial^{np}\mathcal{C} := \partial \mathcal{C} \setminus \mathcal{B}(\mathcal{C})$.

- Given a non-empty set \mathcal{A} and $\sigma \in \mathcal{X}$, we define the *initial cycle* $\mathcal{C}_{\mathcal{A}}(\sigma)$ by

$$C_{\mathcal{A}}(\sigma) := \{\sigma\} \cup \{\eta \in \mathcal{X} : \Phi(\sigma, \eta) < \Phi(\sigma, \mathcal{A})\}. \tag{4.4}$$

If $\sigma \in \mathcal{A}$, then $\mathcal{C}_{\mathcal{A}}(\sigma) = \{\sigma\}$ and thus is a trivial cycle. Otherwise, $\mathcal{C}_{\mathcal{A}}(\sigma)$ is either a trivial cycle (when $\Phi(\sigma, \mathcal{A}) = H(\sigma)$) or a non-trivial cycle containing σ , if $\Phi(\sigma, \mathcal{A}) > H(\sigma)$. In any case, if $\sigma \notin \mathcal{A}$, then $C_{\mathcal{A}}(\sigma) \cap \mathcal{A} = \emptyset$.

- We define the relevant cycle $\mathcal{C}_{\mathcal{A}}^+(\sigma)$ by

$$\mathcal{C}_{A}^{+}(\sigma) := \{ \eta \in \mathcal{X} : \ \Phi(\sigma, \eta) < \Phi(\sigma, \mathcal{A}) + \epsilon \}, \tag{4.5}$$

for any $\epsilon > 0$.

- Given a non-empty set $A \subset \mathcal{X}$, we denote by $\mathcal{M}(A)$ the collection of maximal cycles and extended cycles that partitions A, i.e.,

$$\mathcal{M}(\mathcal{A}) := \{ \mathcal{C} \in \mathscr{C}(\mathcal{X}) | \mathcal{C} \text{ maximal by inclusion under constraint } \mathcal{C} \subseteq \mathcal{A} \}.$$

- We call *cycle-path* a finite sequence (C_1, \ldots, C_m) of trivial, non-trivial and extended cycles $C_1, \ldots, C_m \in \mathcal{C}(\mathcal{X})$, such that

$$C_i \cap C_{i+1} = \emptyset$$
 and $\partial C_i \cap C_{i+1} \neq \emptyset$, for every $i = 1, ..., m-1$.

We denote the set of cycle-paths that lead from σ to \mathcal{A} and consist of maximal cycles in $\mathcal{X} \setminus \mathcal{A}$ by

$$\mathcal{P}_{\sigma,\mathcal{A}} := \{ \text{cycle-path } (\mathcal{C}_1, \dots, \mathcal{C}_m) | \mathcal{C}_1, \dots, \mathcal{C}_m \in \mathcal{M}(\mathcal{C}_A^+(\sigma) \backslash A), \sigma \in \mathcal{C}_1, \ \partial \mathcal{C}_m \cap \mathcal{A} \neq \emptyset \}.$$

- Given a non-empty set $\mathcal{A} \subset \mathcal{X}$ and $\sigma \in \mathcal{X}$, we constructively define a mapping $G : \Omega_{\sigma,A} \to \mathcal{P}_{\sigma,A}$. More precisely, given $\omega = (\omega_1, \ldots, \omega_n) \in \Omega_{\sigma,A}$, we set $m_0 = 1$, $\mathcal{C}_1 = \mathcal{C}_{\mathcal{A}}(\sigma)$ and define recursively

$$m_i := \min\{k > m_{i-1} | \omega_k \notin \mathcal{C}_i\} \text{ and } \mathcal{C}_{i+1} := \mathcal{C}_{\mathcal{A}}(\omega_{m_i}).$$

We note that ω is a finite sequence and $\omega_n \in \mathcal{A}$, so there exists an index $n(\omega) \in \mathbb{N}$ such that $\omega_{m_{n(\omega)}} = \omega_n \in \mathcal{A}$ and there the procedure stops. The way the sequence $(\mathcal{C}_1, \ldots, \mathcal{C}_{m_{n(\omega)}})$ is constructed shows that it is a cycle-path with $\mathcal{C}_1, \ldots, \mathcal{C}_{m_{n(\omega)}} \subset \mathcal{M}(\mathcal{X} \setminus \mathcal{A})$. Moreover, the fact that $\omega \in \Omega_{\sigma, \mathcal{A}}$ implies that $\sigma \in \mathcal{C}_1$ and that $\partial \mathcal{C}_{n(\omega)} \cap \mathcal{A} \neq \emptyset$, hence $G(\omega) \in \mathcal{P}_{\sigma, \mathcal{A}}$ and the mapping is well-defined.

- We say that a cycle-path (C_1, \ldots, C_m) is connected via typical jumps to $A \subset \mathcal{X}$ or simply vtj-connected to A if

$$\mathcal{B}(\mathcal{C}_i) \cap \mathcal{C}_{i+1} \neq \emptyset, \quad \forall i = 1, \dots, m-1, \text{ and } \mathcal{B}(\mathcal{C}_m) \cap \mathcal{A} \neq \emptyset.$$
 (4.6)

Let $J_{\mathcal{C},\mathcal{A}}$ be the collection of all cycle-path $(\mathcal{C}_1,\ldots,\mathcal{C}_m)$ vtj-connected to \mathcal{A} such that $\mathcal{C}_1=\mathcal{C}$.

- Given a non-empty set \mathcal{A} and $\sigma \in \mathcal{X}$, we define $\omega \in \Omega_{\sigma,A}$ as a typical path from σ to \mathcal{A} if its corresponding cycle-path $G(\omega)$ is vtj-connected to \mathcal{A} and we denote by $\Omega_{\sigma,A}^{\text{vtj}}$ the collection of all typical paths from σ to \mathcal{A} , i.e.,

$$\Omega_{\sigma,A}^{\text{vtj}} := \{ \omega \in \Omega_{\sigma,A} | G(\omega) \in J_{\mathcal{C}_A(\sigma),A} \}. \tag{4.7}$$

It is useful to recall the following [39, Lemma 3.12] in which the authors give the following equivalent characterization of a typical path from $\sigma \notin \mathcal{A}$ and $\mathcal{A} \subset \mathcal{X}$.

Lemma 4.1. Consider a non empty subset $A \subset \mathcal{X}$ and $\sigma \notin A$. Then

$$\omega \in \Omega_{\sigma,A}^{vtj} \iff \omega \in \Omega_{\sigma,A} \text{ and } \Phi(\omega_{i+1},A) \leq \Phi(\omega_i,A) \ \forall i=1,\ldots,|\omega|.$$
 (4.8)

In particular, this lemma shows that $\Omega_{\sigma,A}^{\text{vtj}}$ is a subset of the set of the optimal paths from σ to A.

- We define the tube of typical paths from σ to \mathcal{A} , $T_{\mathcal{A}}(\sigma)$, as the subset of states $\eta \in \mathcal{X}$ that can be reached from σ by means of a typical path which does not enter \mathcal{A} before visiting η , i.e.,

$$T_{\mathcal{A}}(\sigma) := \{ \eta \in \mathcal{X} | \exists \omega \in \Omega_{\sigma, A}^{\text{vtj}} : \eta \in \omega \}. \tag{4.9}$$

Moreover, we define $\mathfrak{T}_{\mathcal{A}}(\sigma)$ as the set of all maximal cycles and maximal extended cycles that belong to at least one vtj-connected path from $\mathcal{C}_{\mathcal{A}}(\sigma)$ to \mathcal{A} , i.e.,

$$\mathfrak{T}_{\mathcal{A}}(\sigma) := \{ \mathcal{C} \in \mathcal{M}(\mathcal{C}_{\mathcal{A}}^{+}(\sigma) \backslash \mathcal{A}) | \exists (\mathcal{C}_{1}, \dots, \mathcal{C}_{n}) \in J_{\mathcal{C}_{\mathcal{A}}(\sigma), \mathcal{A}} \text{ and } \exists j \in \{1, \dots, n\} : \mathcal{C}_{j} = \mathcal{C} \}.$$

$$(4.10)$$

Note that $\mathfrak{T}_{\mathcal{A}}(\sigma) = \mathcal{M}(T_{\mathcal{A}}(\sigma) \setminus \mathcal{A})$ and that the boundary of $T_{\mathcal{A}}(\sigma)$ consists of states either in \mathcal{A} or in the non-principal part of the boundary of some $\mathcal{C} \in \mathfrak{T}_{\mathcal{A}}(\sigma)$:

$$\partial T_{\mathcal{A}}(\sigma) \backslash \mathcal{A} \subseteq \bigcup_{\mathcal{C} \in \mathfrak{T}_{\mathcal{A}}(\sigma)} (\partial \mathcal{C} \backslash \mathcal{B}(\mathcal{C})) =: \partial^{np} \mathfrak{T}_{\mathcal{A}}(\sigma).$$
 (4.11)

For sake of semplicity, we will also refer to $\mathfrak{T}_{\mathcal{A}}(\sigma)$ as tube of typical paths from σ to \mathcal{A} .

- Given $|\mathcal{X}^s| > 2$ and $\sigma, \sigma' \in \mathcal{X}^s, \sigma \neq \sigma'$, we define the restricted-tube of typical paths between σ and σ' , $\mathcal{U}_{\sigma'}(\sigma)$, as the subset of states $\eta \in \mathcal{X}$ that can be reached from σ by means of a typical path which does not intersect $\mathcal{X}^s \setminus \{\sigma, \sigma'\}$ and does not visit σ' before visiting η , i.e,

$$\mathcal{U}_{\sigma'}(\sigma) := \{ \eta \in \mathcal{X} | \exists \omega \in \Omega_{\sigma,\sigma'}^{\text{vtj}} \text{ s.t. } \omega \cap \mathcal{X}^s \setminus \{\sigma,\sigma'\} = \emptyset \text{ and } \eta \in \omega \}.$$
 (4.12)

Moreover, we set $\mathscr{U}_{\sigma'}(\sigma)$ as the set of maximal cycles and maximal extended cycles that belong to at last one vtj-connected path from $\mathcal{C}_{\sigma'}(\sigma)$ to σ' such that does not intersect $\mathcal{X}^s \setminus \{\sigma, \sigma'\}$, i.e.,

$$\mathcal{U}_{\sigma'}(\sigma) := \{ \mathcal{C} \in \mathcal{M}(\mathcal{C}_{\{\sigma'\}}^+(\sigma) \setminus \{\sigma'\}) | \exists (\mathcal{C}_1, \dots, \mathcal{C}_m) \in J_{\mathcal{C}_{\sigma'}(\sigma), \{\sigma'\}} \text{ such that}$$

$$\bigcup_{i=1}^m \mathcal{C}_i \cap \mathcal{X}^s \setminus \{\sigma, \sigma'\} = \emptyset \text{ and } \exists j \in \{1, \dots, n\} : \ \mathcal{C}_j = \mathcal{C} \}.$$

$$(4.13)$$

Note that $\mathscr{U}_{\sigma'}(\sigma) = \mathcal{M}(\mathcal{U}_{\sigma'}(\sigma) \setminus (\mathcal{X}^s \setminus \{\sigma\}))$ and that the boundary of $\mathcal{U}_{\sigma'}(\sigma)$ consists of σ' and of states in the non-principal part of the boundary of some $\mathcal{C} \in \mathscr{U}_{\sigma'}(\sigma)$:

$$\partial \mathcal{U}_{\sigma'}(\sigma) \setminus \{ \sigma' \} \subseteq \bigcup_{\mathcal{C} \in \mathscr{U}_{\sigma'}(\sigma)} (\partial \mathcal{C} \setminus \mathcal{B}(\mathcal{C})) =: \partial^{np} \mathscr{U}_{\sigma'}(\sigma). \tag{4.14}$$

For sake of semplicity, we will also refer to $\mathscr{U}_{\sigma'}(\sigma)$ as restricted-tube of typical paths from σ to σ' .

Remark 4.1. Note that the notion of extended cycles is taken from [44]. Using also the extended cycles for defining a cycle-path vtj-connected, we get that this object is the so-called *standard cascade* in [44].

4.1.2 Model-dependent definitions and notations

In this section we add some model-dependent definitions to the list given in Section 3.1.2. For any $s, r \in \{1, \ldots, q\}$, let $\mathcal{X}(r, s)$ be the defined by

$$\mathcal{X}(r,s) := \{ \sigma \in \mathcal{X} : \sigma(v) \in \{r,s\} \ \forall v \in V \}. \tag{4.15}$$

Let $R_{\ell_1 \times \ell_2}$ be a rectangle in \mathbb{R}^2 with horizontal side of length ℓ_1 and vertical side of length ℓ_2 .

- We define

$$\overline{\mathcal{K}}(r,s) := \{ \sigma \in \mathcal{X}(r,s) : H(\sigma) = 2K + 2 + H(\mathbf{r}), \ \sigma \text{ has either a } s\text{-cluster or more}$$
s-interacting clusters and $R(C^s(\sigma)) = R_{2 \times (K-1)} \} \cup \overline{\mathcal{Q}}(\mathbf{r},\mathbf{s}) \cup \overline{\mathscr{P}}(\mathbf{r},\mathbf{s}).$ (4.16)

Note that $\overline{\mathcal{H}}(\mathbf{r}, \mathbf{s}) \subset \overline{\mathcal{K}}(r, s)$.

- We set

$$\overline{\mathcal{D}}_1(r,s) := \{ \sigma \in \mathcal{X}(r,s) : H(\sigma) = 2K + H(\mathbf{r}), \ \sigma \text{ has either a } s\text{-cluster or more}$$
s-interacting clusters such that $R(\mathbf{C}^s(\sigma)) = R_{2 \times (K-2)} \},$ (4.17)

and

$$\overline{\mathcal{E}}_1(r,s) := \{ \sigma \in \mathcal{X}(r,s) : H(\sigma) = 2K + H(\mathbf{r}), \ \sigma \text{ has either a } s\text{-cluster or more}$$

$$s\text{-interacting clusters such that } R(\mathbf{C}^s(\sigma)) = R_{1 \times (K-1)} \} \cup \overline{R}_{1,K}(r,s).$$

$$(4.18)$$

- For any $i = 2, \ldots, K - 2$, we define

$$\overline{\mathcal{D}}_i(r,s) := \{ \sigma \in \mathcal{X}(r,s) : H(\sigma) = 2K - 2i + 2 + H(\mathbf{r}), \sigma \text{ has either a } s\text{-cluster or}$$
more s -interacting clusters such that $R(\mathbf{C}^s(\sigma)) = R_{2 \times (K - (i+1))} \}, \quad (4.19)$

and

$$\overline{\mathcal{E}}_i(r,s) := \{ \sigma \in \mathcal{X}(r,s) : H(\sigma) = 2K - 2i + 2 + H(\mathbf{r}), \ \sigma \text{ has either a } s\text{-cluster or,}$$
more s-interacting clusters such that $R(C^s(\sigma)) = R_{1 \times (K-i)} \}.$ (4.20)

- Similarly, for any $i=1,\ldots,K-2$ we set $\widetilde{K}(r,s)$, $\widetilde{\mathcal{D}}_i(r,s)$, $\widetilde{\mathcal{E}}_i(r,s)$ by interchanging the role of the spins r and s, i.e., they are defined as the collection of those configurations which have either a r-cluster or more than one r-interacting clusters such that $R(C^r(\sigma))$ satisfies the same conditions given in (4.16)–(4.20) given for s.

4.2 Main results

We are now ready to state the main results on the restricted-tube of typical paths between two Potts stable configurations and on the tube of typical trajectories from a stable state to the other stable states and from a stable state to another stable configuration. In particular, we prove Theorems 4.1, 4.2 and 4.3 using [39, Lemma 3.13] and [19, Proposition 2.7].

4.2.1 Restricted-tube of typical paths between two Potts stable configurations

We briefly recall that given $\mathbf{r}, \mathbf{s} \in \mathcal{X}^s, \mathbf{r} \neq \mathbf{s}$, the restricted-tube of typical paths $\mathcal{U}_{\mathbf{s}}(\mathbf{r})$ is the set of those configurations belonging to at least a typical path $\omega \in \Omega^{\text{vtj}}_{\mathbf{r},\mathbf{s}}$ such that $\omega \cap \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\} = \emptyset$. Since in absence of external magnetic field the energy landscape between two Potts stable configurations is characterized by many extended-cycles, we describe the

restricted-tube of typical paths defined in general in (4.13). For our model, let

$$\mathcal{U}_{\mathbf{s}}(\mathbf{r}) := \bar{R}_{1,1}(r,s) \cup \bigcup_{i=1}^{K-2} (\overline{\mathcal{D}}_{i}(r,s) \cup \overline{\mathcal{E}}_{i}(r,s)) \cup \overline{\mathcal{K}}(r,s) \cup \bigcup_{h=2}^{K-2} \bar{B}_{1,K-1}^{h}(r,s) \cup \bigcup_{j=2}^{L-2} \bigcup_{h=1}^{K-1} \bar{B}_{j,K}^{h}(r,s) \cup \bigcup_{j=2}^{K-2} (\overline{\mathcal{D}}_{i}(r,s) \cup \overline{\mathcal{E}}_{i}(r,s)) \cup \tilde{R}_{1,1}(r,s).$$

$$(4.21)$$

As illustrated in the next result, $\mathscr{U}_{\mathbf{s}}(\mathbf{r})$ includes those configurations with no-vanishing probability of being visited by the Markov chain $\{X_t\}_{t\in\mathbb{N}}^{\beta}$ started in \mathbf{r} before hitting \mathbf{s} in the limit $\beta \to \infty$.

Theorem 4.1. Consider the q-state Potts model on a $K \times L$ grid Λ with $\max\{K, L\} \geq 3$ and with periodic boundary conditions. For every $\mathbf{r}, \mathbf{s} \in \mathcal{X}^s$, $\mathbf{s} \neq \mathbf{r}$, we have that $\mathcal{U}_{\mathbf{s}}(\mathbf{r})$ is the restricted-tube of typical paths for the transition $\mathbf{r} \to \mathbf{s}$. Moreover, there exists k > 0 such that for β sufficiently large

$$\mathbb{P}_{\beta}(\tau_{\partial^{n_p}\mathscr{U}_{\mathbf{c}}(\mathbf{r})}^{\mathbf{r}} \leq \tau_{\mathbf{s}}^{\mathbf{r}} | \tau_{\mathbf{s}} < \tau_{\mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}}) \leq e^{-k\beta}. \tag{4.22}$$

4.2.2 Tube of typical paths between a stable state and the other stable states

Using the results about the restricted-tube of typical paths, we prove the following results on the the tube of typical trajectories from a stable configuration to all the other stable states. We assume q > 2, since in the case q = 2 the Hamiltonian has only two global minima, $|\mathcal{X}^s| = 2$, and the result is given by Theorem 4.1.

As in Section 4.2.1, we recall the tube of typical paths defined in general in (4.10) and define $\mathfrak{T}_{\mathcal{X}^s\setminus\{\mathbf{r}\}}$ for Potts model with q>2:

$$\mathfrak{T}_{\mathcal{X}^s \setminus \{\mathbf{r}\}}(\mathbf{r}) := \bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \mathscr{U}_{\mathbf{t}}(\mathbf{r}). \tag{4.23}$$

Theorem 4.2. Consider the q-state Potts model on a $K \times L$ grid Λ with $\max\{K, L\} \geq 3$ and with periodic boundary conditions. For any $\mathbf{r} \in \mathcal{X}^s$, we have that $\mathfrak{T}_{\mathcal{X}^s \setminus \{\mathbf{r}\}}(\mathbf{r})$ is the tube of typical trajectories for the transition $\mathbf{r} \to \mathcal{X}^s \setminus \{\mathbf{r}\}$ and there exists k > 0 such that for β sufficiently large

$$\mathbb{P}_{\beta}(\tau_{\partial^{n_p}\mathfrak{T}_{\mathcal{X}^s\setminus\{\mathbf{r}\}}(\mathbf{r})}^{\mathbf{r}} \leq \tau_{\mathcal{X}^s\setminus\{\mathbf{r}\}}^{\mathbf{r}}) \leq e^{-k\beta}.$$
(4.24)

4.2.3 Tube of typical paths between a stable state and another stable state

Finally, using the results about the tube of typical paths from a stable state to the other stable configurations, we describe the set of minimal gates for the transition from a stable configuration to another stable state. Arguing like in Section 3.2.3, we describe the typical trajectories for the transition $\mathbf{r} \to \mathbf{s}$ in terms of a sequence of transitions between two stable states such that the path followed by the process does not intersect other stable configurations. We assume q > 2, otherwise when q = 2 the Hamiltonian has only two global minima and the results on the minimal gates coincide with Theorem 4.1.

As in Section 4.2.1, we recall the tube of typical paths defined in general in (4.10) and define $\mathfrak{T}_{\mathbf{s}}(\mathbf{r})$ for Potts model with q > 2:

$$\mathfrak{T}_{\mathbf{s}}(\mathbf{r}) := \bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \mathscr{U}_{\mathbf{t}}(\mathbf{r}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \mathscr{U}_{\mathbf{t}}(\mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}} \mathscr{U}_{\mathbf{t}'}(\mathbf{s}). \tag{4.25}$$

Theorem 4.3. Consider the q-state Potts model on a $K \times L$ grid Λ with $\max\{K, L\} \geq 3$ and with periodic boundary conditions. For any $\mathbf{r}, \mathbf{s} \in \mathcal{X}^s$, $\mathbf{r} \neq \mathbf{s}$ we have that $\mathfrak{T}_{\mathbf{s}}(\mathbf{r})$ is the tube of typical trajectories for the transition $\mathbf{r} \to \mathbf{s}$ and there exists k > 0 such that for β sufficiently large

$$\mathbb{P}_{\beta}(\tau_{\partial^{n_p}\mathfrak{T}_{\mathbf{s}}(\mathbf{r})}^{\mathbf{r}} \le \tau_{\mathbf{s}}^{\mathbf{r}}) \le e^{-k\beta}.$$
(4.26)

4.2.4 Tube of typical paths for the Ising model with zero magnetic field

For sake of completeness, we give the following result on the tube of typical paths for the Ising model with zero magnetic field.

As in Section 4.2.1, we recall the tube of typical paths defined in general in (4.10) and define $\mathfrak{T}_{+1}(-1)$ for Ising model:

$$\mathfrak{T}_{+1}(-1) := \bar{R}_{1,1}(-1,+1) \cup \bigcup_{i=1}^{K-2} (\overline{\mathcal{D}}_{i}(-1,+1) \cup \overline{\mathcal{E}}_{i}(-1,+1)) \cup \overline{\mathcal{K}}(-1,+1)$$

$$\cup \bigcup_{h=2}^{K-2} \bar{B}_{1,K-1}^{h}(-1,+1) \cup \bigcup_{j=2}^{L-2} \bigcup_{h=1}^{K-1} \bar{B}_{j,K}^{h}(-1,+1) \cup \bigcup_{j=2}^{L-2} \bar{R}_{j,K}(-1,+1) \cup \bigcup_{h=2}^{K-2} \tilde{B}_{1,K-1}^{h}(-1,+1)$$

$$\cup \widetilde{\mathcal{K}}(-1,+1) \cup \bigcup_{i=1}^{K-2} (\widetilde{\mathcal{D}}_{i}(-1,+1) \cup \widetilde{\mathcal{E}}_{i}(-1,+1)) \cup \widetilde{R}_{1,1}(-1,+1). \tag{4.27}$$

Corollary 4.1. Consider the Ising model on a $K \times L$ grid Λ with $\max\{K, L\} \geq 3$ and with periodic boundary conditions. Then, we have that $\mathfrak{T}_{+1}(-1)$ is the tube of typical trajectories for the transition $+1 \to -1$ and there exists k > 0 such that for β sufficiently large

$$\mathbb{P}_{\beta}(\tau_{\partial^{n_p}\mathfrak{T}_{\{+1\}}(-1)}^{\mathbf{r}} \le \tau_{+1}^{-1}) \le e^{-k\beta},\tag{4.28}$$

5 Minimal restricted-gates

In order to prove our main results on the set of minimal gates, we first describe the set of all minimal restricted-gates for the transition from $\mathbf{r} \in \mathcal{X}^s$ to $\mathbf{s} \in \mathcal{X}^s$, $\mathbf{r} \neq \mathbf{s}$. To do this, we first collect some relevant properties and results concerning the energy landscape between \mathbf{r} and \mathbf{s} by studying those optimal paths $\omega \in (\mathbf{r} \to \mathbf{s})_{opt}$ such that

$$\omega \cap \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\} = \varnothing.$$

5.1 Energy landscape between two Potts stable configurations

Let

$$\mathcal{V}_n^s := \{ \sigma \in \mathcal{X} : N_s(\sigma) = n \}, \tag{5.1}$$

be the set of configurations with n spins equal to s, with $s \in \{1, \ldots, q\}$ and $n = 0, \ldots, KL$. Note that, given two different stable configurations $\mathbf{r}, \mathbf{s} \in \mathcal{X}^s$, every optimal path from \mathbf{r} to \mathbf{s} has to intersect at least one time \mathcal{V}_n^s for any $n = 0, \ldots, KL$.

In [38, Theorem 2.1], the authors prove that the communication energy (3.2) between any $\mathbf{r}, \mathbf{s} \in \mathcal{X}^s$, with $\mathbf{r} \neq \mathbf{s}$, is given by

$$\Phi(\mathbf{r}, \mathbf{s}) = 2\min\{K, L\} + 2 + H(\mathbf{r}) = 2K + 2 + H(\mathbf{r}).$$
(5.2)

Hence, in view of (5.2) we have that any optimal path $\omega \in (\mathbf{r} \to \mathbf{s})_{opt}$ cannot pass through configurations whose energy is strictly larger than $2K + 2 + H(\mathbf{r})$.

Remark 5.1. For any $\sigma \in \mathcal{X}$

$$H(\sigma) - H(\mathbf{r}) = H(\sigma) + |E| = |E| - \sum_{(v,w)\in E} \mathbb{1}_{\{\sigma(v) = \sigma(w)\}}$$
$$= \sum_{(v,w)\in E} \mathbb{1}_{\{\sigma(v)\neq\sigma(w)\}}, \text{ for every } \mathbf{r}\in\mathcal{X}^s.$$
(5.3)

We note that the total number of disagreeing edges in a configuration $\sigma \in \mathcal{X}$, i.e., those edges which connect two vertices with different spin, represents the total perimeter of the same-spin clusters in σ . Thus, thanks to (5.2) and to (5.3), it follows that for any σ , that belongs to an optimal path $\omega \in (\mathbf{r} \to \mathbf{s})_{opt}$, the total perimeter of its clusters with the same spin value cannot be larger than 2K + 2.

The following lemma is an immediate consequence of (5.3).

Lemma 5.1. Consider the q-state Potts model on a $K \times L$ grid Λ with periodic boundary conditions. Consider $\mathbf{r}, \mathbf{s} \in \mathcal{X}^s, \mathbf{r} \neq \mathbf{s}$. Then, for every $j = 1, \ldots, L - 1$,

- (a) any $\sigma \in \bar{B}_{j,K}^h(r,s) = \tilde{B}_{L-j-1,K}^{K-h}(r,s), h = 1,...,K-1, is such that <math>H(\sigma) = H(\mathbf{s}) + 2K + 2 = \Phi(\mathbf{r},\mathbf{s});$
- (b) any $\sigma \in \bar{B}_{1,K-1}^h(r,s)$ and any $\sigma \in \tilde{B}_{1,K-1}^h(r,s)$, h = 2, ..., K-2, is such that $H(\sigma) = H(\mathbf{s}) + 2K + 2 = \Phi(\mathbf{r}, \mathbf{s})$;
- (c) any $\sigma \in \bar{R}_{i,K}(r,s) = \tilde{R}_{L-i,K}(r,s)$ is such that $H(\sigma) = H(\mathbf{s}) + 2K$;
- (d) any $\sigma \in \bar{R}_{i,K-1}(r,s) \cup \tilde{R}_{i,K-1}(r,s)$ is such that

$$\begin{cases}
H(\sigma) = H(\mathbf{s}) + 2K, & \text{if } j = 1; \\
H(\sigma) = H(\mathbf{s}) + 2K + 2 = \Phi(\mathbf{r}, \mathbf{s}), & \text{if } j = 2; \\
H(\sigma) > \Phi(\mathbf{r}, \mathbf{s}), & \text{if } j = 3, \dots, L - 1.
\end{cases}$$
(5.4)

In the next Lemma we point out which configurations communicate by one step of the dynamics along an optimal path with those states belonging to the sets defined at the beginning of Section 3.1.2.

Lemma 5.2. Consider the q-state Potts model on a $K \times L$ grid Λ with periodic boundary conditions. Consider $\mathbf{r}, \mathbf{s} \in \mathcal{X}^s$, $\mathbf{r} \neq \mathbf{s}$.

Given a configuration σ , let $\bar{\sigma}$ be a configuration which communicates with σ along an optimal path from \mathbf{r} to \mathbf{s} that does not intersect $\mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}$. For any $j = 2, \ldots, L-2$, the following properties hold:

(a) if $\sigma \in \bar{B}^h_{j,K}(r,s)$ and $N_s(\sigma) > N_s(\bar{\sigma})$, then

$$\begin{cases} \bar{\sigma} \in \bar{R}_{j,K}(r,s), & \text{if } h = 1; \\ \bar{\sigma} \in \bar{B}_{j,K}^{h-1}(r,s), & \text{if } h = 2, \dots, K-1; \end{cases}$$

(b) if $\sigma \in \bar{B}_{i,K}^h(r,s)$ and $N_s(\sigma) < N_s(\bar{\sigma})$, then

$$\begin{cases} \bar{\sigma} \in \bar{B}_{j,K}^{h+1}(r,s), & \text{if } h = 1, \dots, K-2; \\ \bar{\sigma} \in \bar{R}_{j+1,K}(r,s), & \text{if } h = K-1; \end{cases}$$

- (c) if $\sigma \in \bar{R}_{j,K}(r,s)$ and $N_s(\sigma) > N_s(\bar{\sigma})$, then $\bar{\sigma} \in \bar{B}_{j-1,K}^{K-1}(r,s)$;
- (d) if $\sigma \in \bar{R}_{j,K}(r,s)$ and $N_s(\sigma) < N_s(\bar{\sigma})$, then $\bar{\sigma} \in \bar{B}^1_{j,K}(r,s)$.

Proof. Consider $\sigma \in \bar{B}^h_{j,K}(r,s)$ for some $j=2,\ldots,L-2,\ h=1,\ldots,K-1$. Let $\bar{\sigma} \in \mathcal{X}$ and $v \in V$ be a configuration and a vertex such that flipping the spin in v we can move from σ to $\bar{\sigma}$. Thanks to (2.8) the following implications hold:

- (i) $\bar{\sigma}(v) = t \in S \setminus \{r, s\} \implies H(\bar{\sigma}) H(\sigma) \ge 2;$
- (ii) if $\sigma(v) = s$ and v has four nearest-neighbor spins s in σ , then

$$\bar{\sigma}(v) = r \implies H(\bar{\sigma}) - H(\sigma) = 4;$$

(iii) if $\sigma(v) = r$ and v has four nearest-neighbor spins r in σ , then

$$\bar{\sigma}(v) = s \implies H(\bar{\sigma}) - H(\sigma) = 4;$$

(iv) if $\sigma(v) = s$ and v has three nearest-neighbor spins s in σ , then

$$\bar{\sigma}(v) = r \implies H(\bar{\sigma}) - H(\sigma) = 2;$$

(v) if $\sigma(v) = r$ and v has three nearest-neighbor spins r in σ , then

$$\bar{\sigma}(v) = s \implies H(\bar{\sigma}) - H(\sigma) = 2.$$

Since Lemma 5.1 holds, it follows that in all the above five cases, we have $H(\bar{\sigma}) > \Phi(\mathbf{r}, \mathbf{s})$ which is not admissible. Hence, the only configurations $\bar{\sigma}$ that communicate with $\sigma \in \bar{B}^h_{j,K}(r,s)$, such that $H(\bar{\sigma}) \leq \Phi(\mathbf{r},\mathbf{s})$, are those which are obtained by flipping either a spin from s to r or a spin from r to s among the spins with two nearest-neighbor spins s and two nearest-neighbor spins r in σ . In particular, following an optimal path from $\sigma \in \bar{B}^h_{j,K}(r,s)$ to \mathbf{r} we have

$$\begin{cases} \bar{\sigma} \in \bar{R}_{j,K}(r,s), & \text{if } h = 1; \\ \bar{\sigma} \in \bar{B}_{j,K}^{h-1}(r,s), & \text{if } h = 2, \dots, K-1. \end{cases}$$

Otherwise, following an optimal path from $\sigma \in \bar{B}^h_{j,K}(r,s)$ to s, we have

$$\begin{cases} \bar{\sigma} \in \bar{B}_{j,K}^{h+1}(r,s), & \text{if } h = 1, \dots, K-2; \\ \bar{\sigma} \in \bar{R}_{j+1,K}(r,s), & \text{if } h = K-1. \end{cases}$$

When $\sigma \in \bar{R}_{j,K}(r,s)$ for some $j=2,\ldots,L-2$, the proof is similar. Indeed, in view of (2.8) we have

- (i) $\bar{\sigma}(v) = t \in S \setminus \{r, s\} \implies H(\bar{\sigma}) H(\sigma) = 4;$
- (ii) if $\sigma(v) = s$ and v has four nearest-neighbor spins s in σ , then

$$\bar{\sigma}(v) = r \implies H(\bar{\sigma}) - H(\sigma) = 4;$$

(iii) if $\sigma(v) = r$ and v has four nearest-neighbor spins r in σ , then

$$\bar{\sigma}(v) = s \implies H(\bar{\sigma}) - H(\sigma) = 4.$$

Moreover, by Lemma 5.1 we know that $H(\sigma) = 2K + H(\mathbf{r})$. Thus (i), (ii) and (iii) imply $H(\bar{\sigma}) > \Phi(\mathbf{r}, \mathbf{s})$ which is not admissible. Hence, for any $j = 2, \ldots, L-2, \ \sigma \in \bar{R}_{j,K}(r,s)$ can communicate only with configurations obtained either by flipping a spin from s to r among those spins with three nearest-neighbor spins s and one nearest-neighbor spin r in σ or by flipping a spin from r to s among those spins with three nearest-neighbor spins r and one nearest-neighbor spin s in s. Following an optimal path from s to s to s, these configurations belong to s, while along an optimal path from s to s to s.

We remark that thanks to (3.9), Lemma 5.2 may be also used for describing the transition between those configurations which belong to either some $\tilde{B}_{j,K}^h(r,s)$ or some $\tilde{R}_{j,K}(r,s)$, for $j=2,\ldots,L-2$ and $h=1,\ldots,K-1$.

5.2 Geometric properties of the Potts model with zero external magnetic field

A two dimensional polyomino on \mathbb{Z}^2 is a finite union of unit squares. The area of a polyomino is the number of its unit squares, while its perimeter is the cardinality of its boundary, namely, the number of unit edges of the dual lattice which intersect only one of the unit squares of the polyomino itself. Thus, the perimeter is the number of interfaces on \mathbb{Z}^2 between the sites inside the polyomino and those outside. We define M_n as the set of all the polyominoes with minimal perimeter among those with area n. We call minimal polyominoes the elements of M_n .

We are now able to prove some useful lemmas.

Lemma 5.3. Consider the q-state Potts model on a $K \times L$ grid Λ with periodic boundary conditions. Let $\mathbf{r}, \mathbf{s} \in \mathcal{X}^s$ be two different stable configurations and let ω be an optimal path for the transition from \mathbf{r} to \mathbf{s} such that $\omega \cap (\mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}) = \varnothing$.

Then, there exists $K^* \in [0, KL] \cap \mathbb{N}$ such that in any $\sigma \in \omega$ with $N_s(\sigma) > K^*$ at least a cluster of spins s belongs to either $\bar{R}_{j,K}(r,s)$ or $\bar{B}_{j,K}^h(r,s)$, for some $h = 1, \ldots, K-1$ and $j = 2, \ldots, L$. In other words, at least a cluster of spin s wraps around Λ .

Proof. The strategy for the proof is to construct a path $\tilde{\omega}: \mathbf{r} \to \mathbf{s}$ as a sequence of configurations in which the unique cluster of spins s is a polyomino with minimal perimeter among those with the same area. Since in [1, Theorem 2.2], the authors show that the set of minimal polyominoes of area n, M_n , includes squares or quasi-squares with possibly a bar on one of the longest sides, we define $\tilde{\omega} := (\tilde{\omega}_0, \tilde{\omega}_1, \tilde{\omega}_2, \dots)$ as the sequence of configurations in which the cluster of spins s is a polyomino with square or quasi-square shapes with possibly a bar on one of the longest sides. During this construction our aim is to understand what is the last polyomino of s with perimeter smaller or equal than 2K + 2 (see Remark 5.1).

More precisely, we set $\tilde{\omega}_0 = \mathbf{r}$ and define

$$\tilde{\omega}_1 := \tilde{\omega}_0^{(i,j),s},$$

where (i, j) denotes the vertex which belongs to the row i and to the column j of the grid Λ , for some $i = 0, \ldots, K-1$ and $j = 0, \ldots, L-1$. Then, we set

$$\tilde{\omega}_2 := \tilde{\omega}_1^{(i+1,j),s}$$

and following the clockwise direction, we consider the flipping from r to s of all the vertices that sourround (i,j) and so on with the sourrounding vertices of the next 3×3 square. In Figure 4, there is an example of this construction. The white squares have spin r, the other colors denote spin s.

We remark that at the step m, $\tilde{\omega}_m$ is a configuration with all the spins r, except those, which are s, in a cluster of area m of minimal perimeter.

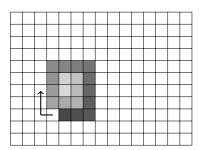


Figure 4: First steps of path $\tilde{\omega}$ on a 11×15 grid Λ . The arrow indicates the order in which the spins are flipped from r to s. The colors of the squares indicate when they have been flipped, with darker squares having been flipped later.

Since the iterative construction of $\tilde{\omega}$ implies

$$N_s(\tilde{\omega}_{j+1}) = N_s(\tilde{\omega}_j) + 1$$

for all $j=0,1,\ldots$, the perimeter of the cluster of spins s grows monotonously. Hence, necessarily at a certain point this perimeter overcomes 2K+2 and the condition of Remark 5.1 is no longer satisfied.

Define

$$K^* := \begin{cases} \frac{K^2 + 2K + 1}{4}, & \text{if } K \text{ is odd,} \\ \frac{K^2 + 2K}{4}, & \text{if } K \text{ is even,} \end{cases}$$
 (5.5)

and note that

- if K is an odd number, the configuration $\tilde{\omega}_{K^*}$ with the cluster of spins s of area $\frac{K^2+2K+1}{4}$ is the last one with energy smaller or equal to $2K+2+H(\mathbf{r})$;
- if K is an even number, then the configuration $\tilde{\omega}_{K^*}$ with the cluster of s of area $\frac{K^2+2K}{4}$ is the last one with energy smaller or equal to $2K+2+H(\mathbf{r})$.

Indeed, if K is an odd number, in $\tilde{\omega}_{K^*}$ the cluster of spins s is a square $\frac{K+1}{2} \times \frac{K+1}{2}$ and it is the last one with perimeter 2K+2; the next configuration, $\tilde{\omega}_{K^*+1}$, has energy strictly larger than $\Phi(\mathbf{r}, \mathbf{s})$ because the perimeter of the cluster of spins s grows by two edges. Similarly, if K is an even number, in $\tilde{\omega}_{K^*}$ the cluster of spins s is a rectangle $\frac{K}{2} \times (\frac{K}{2} + 1)$ and it is the last one with perimeter 2K + 2.

In view of the above discussion, it follows that when an optimal path $\omega \in (\mathbf{r} \to \mathbf{s})_{opt}$ intersects \mathcal{V}_n^s for $n > K^*$, it has to pass through a configuration in which spins s cannot form a minimal polyomino of area n. Indeed, all the minimal polyominoes which belong to M_n have the same perimeter and we have just highlighted that the perimeter of squares or quasi-squares with possibly an incomplete side is larger than 2K + 2 when their area is larger than K^* . Therefore, any other configuration in which the cluster of spin s does not wrap around Λ has energy higher that $\Phi(\mathbf{r}, \mathbf{s})$ when $n > K^*$. Indeed, since the condition of Remark 5.1 is not satisfied by those configurations in which the cluster of spins s is a minimal polyomino, it follows that there does not exist any cluster of spins s not wrapping around Λ with perimeter smaller than 2K + 2. Hence, when $n > K^*$, any $\omega \in (\mathbf{r} \to \mathbf{s})_{opt}$ can intersect \mathcal{V}_n^s only in a configuration σ which belongs to either $\bar{R}_{j,K}(r,s)$ or $\bar{B}_{j,K}^h(r,s)$, for some $t = 1, \ldots, K - 1$ and $j = 2, \ldots, L$. \square

Lemma 5.4. Consider the q-state Potts model on a $K \times L$ grid Λ with periodic boundary conditions. Consider $\mathbf{r}, \mathbf{s} \in \mathcal{X}^s, \mathbf{r} \neq \mathbf{s}$.

Then, for any $\omega \in (\mathbf{r} \to \mathbf{s})_{opt}$ such that $\omega \cap (\mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}) = \emptyset$, we have

- (a) $\omega \cap \overline{\mathscr{P}}(\mathbf{r}, \mathbf{s}) \neq \emptyset$, $\omega \cap \widetilde{\mathscr{P}}(\mathbf{r}, \mathbf{s}) \neq \emptyset$;
- (b) $\omega \cap \overline{\mathcal{Q}}(\mathbf{r}, \mathbf{s}) \neq \emptyset$, $\omega \cap \widetilde{\mathcal{Q}}(\mathbf{r}, \mathbf{s}) \neq \emptyset$;
- (c) $\omega \cap \overline{\mathscr{H}}(\mathbf{r}, \mathbf{s}) \neq \varnothing$, $\omega \cap \widetilde{\mathscr{H}}(\mathbf{r}, \mathbf{s}) \neq \varnothing$.

Proof. We begin by proving (a). We prove the statement only for $\overline{\mathscr{P}}(\mathbf{r},\mathbf{s})$ since the proof for $\widetilde{\mathscr{P}}(\mathbf{r},\mathbf{s})$ follows by switching the roles of r and s and using the symmetry of the model. Let $\omega \in (\mathbf{r} \to \mathbf{s})_{opt}$ be any optimal path between \mathbf{r} and \mathbf{s} such that $\omega \cap (\mathcal{X}^s \setminus \{\mathbf{r},\mathbf{s}\}) = \varnothing$. Thanks to Lemma 5.3, there exists $K^* \in \mathbb{N}$ such that, when $n > K^*$, every ω intersects \mathcal{V}^s_n in configurations which belong to either $\bar{B}^h_{j,K}(r,s)$ or $\bar{R}_{j,K}(r,s)$ for some $j=2,\ldots,L-2$ and $h=1,\ldots,K-1$. Moreover, in view of Lemma 5.2, it follows that ω can reach these configurations only moving among configurations belonging to either $\bar{B}^h_{j,K}(r,s)$ or $\bar{R}_{j,K}(r,s)$ with $j=2,\ldots,L-2,\ h=1,\ldots,K-1$. Note that, given an optimal path ω from either $\bar{B}^h_{j,K}(r,s)$ or $\bar{R}_{j,K}(r,s)$ to \mathbf{r} and given $\sigma \in \omega \cap \bar{R}_{2,K}(r,s)$, the only $\bar{\sigma} \in \mathcal{V}^s_{2K-1}$ which communicates with σ belongs to $\overline{\mathscr{P}}(\mathbf{r},\mathbf{s}) = \bar{B}^{K-1}_{1,K}(r,s)$, see Lemma 5.2(c). Indeed, we may move from σ to $\bar{\sigma}$ by flipping a spin from s to r and the only possibility to not overcome $\Phi(\mathbf{r},\mathbf{s})$ is to flip a spin s with three nearest-neighbor spins s.

From now on, using the reversibility of the dynamics, we prefer to study one optimal path $\omega \in (\mathbf{r} \to \mathbf{s})_{opt}$ such that $\omega \cap (\mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}) = \emptyset$ by analyzing instead its time reversal $\omega^T = (\omega_n, \dots, \omega_0)$. Indeed, a path $\omega = (\omega_0, \dots, \omega_n)$ from \mathbf{r} to \mathbf{s} is optimal if and only if the path $\omega^T = (\omega_n, \dots, \omega_0)$ is optimal.

Now we move to the proof of (b). To aid the understanding, we suggest to use Figure 5 as a reference for this part of the proof. We prove the statement only for $\overline{\mathcal{Q}}(\mathbf{r}, \mathbf{s})$ since the proof for $\widetilde{\mathcal{Q}}(\mathbf{r}, \mathbf{s})$ again follows from symmetry considerations.

Consider $\omega \in (\mathbf{r} \to \mathbf{s})_{opt}$ such that $\omega \cap (\mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}) = \varnothing$ and take $\sigma \in \overline{\mathscr{P}}(\mathbf{r}, \mathbf{s}) \cap \omega$ This exists in view of (a). Note that from Lemma 5.1 we have $H(\sigma) = \Phi(\mathbf{r}, \mathbf{s})$. Since $\sigma \in \mathcal{V}^s_{2K-1}$, we have to move from σ to $\bar{\sigma}$ by removing a spin s and the only possibility to not overcome $\Phi(\mathbf{r}, \mathbf{s})$ is to change from s to r a spin s with two nearest-neighbor spins r. Indeed, in a such a way the perimeter of the cluster with spins s does not increase and $H(\bar{\sigma})$ does not exceed $\Phi(\mathbf{r}, \mathbf{s})$, see Remark 5.1. Hence, given $\sigma \in \overline{\mathscr{P}}(\mathbf{r}, \mathbf{s})$, the only configurations $\bar{\sigma} \in \mathcal{V}^s_{2K-2}$ which communicate with σ , along an optimal path from σ to \mathbf{r} , belong to either $\bar{R}_{2,K-1}(r,s)$ or $\bar{B}^{K-2}_{1,K}(r,s)$, which are subsets of $\overline{\mathbb{Q}}(\mathbf{r}, \mathbf{s})$.

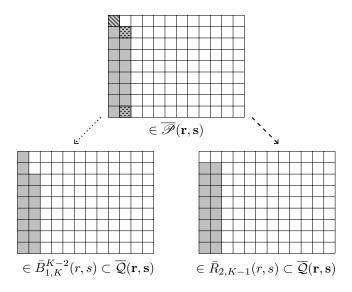


Figure 5: Example on a 9×12 grid Λ of (b). Gray vertices have spin value s, white vertices have spin value r. By flipping to r a spin s among those with the lines, the path enters into $\bar{B}_{1,K}^{K-2}(r,s) \subset \overline{\mathcal{Q}}(\mathbf{r},\mathbf{s})$; instead, by flipping to r a spin s among those with dots, the path goes to $\bar{R}_{2,K-1}(r,s) \subset \overline{\mathcal{Q}}(\mathbf{r},\mathbf{s})$.

Finally, we carry out the proof of (c). We prove the statement only for $\widetilde{\mathcal{H}}(\mathbf{r}, \mathbf{s})$ since the proof for $\widetilde{\mathcal{H}}(\mathbf{r}, \mathbf{s})$ again follows from symmetry considerations. For semplicity, we split the proof in several steps.

Step 1. We claim that, given $\bar{\sigma} \in \bar{R}_{2,K-1}(r,s) \cup \bar{B}_{1,K}^{K-2}(r,s)$, the only configurations $\hat{\sigma} \in \mathcal{V}_{2K-3}^s$ which communicate with $\bar{\sigma}$, along an optimal path from $\bar{\sigma}$ to \mathbf{r} , belong to either $\bar{B}_{1,K-1}^{K-2}(r,s)$ or $\bar{B}_{1,K}^{K-3}(r,s)$, see Figure 6.

We remark that $\bar{\sigma} \in \mathcal{V}^s_{2K-2}$ and, thanks to Lemma 5.1, that $H(\bar{\sigma}) = \Phi(\mathbf{r}, \mathbf{s})$. Hence, we have to move from $\bar{\sigma}$ to $\hat{\sigma}$ by removing a spin s without increasing the energy and the only possibility is flipping from s to r a spin s among those with two nearest-neighbor spins s. This can happen in many ways. Assume first that $\bar{\sigma} \in \bar{R}_{2,K-1}(r,s)$, then $\hat{\sigma} \in \bar{B}_{1,K-1}^{K-2}(r,s) \subset \overline{\mathscr{H}}(\mathbf{r},\mathbf{s})$ and both the proof of (c) and the proof of the claim are concluded. Otherwise, when $\bar{\sigma} \in \bar{B}_{1,K}^{K-2}(r,s)$, we can flip from s to r either

(i) a spin s with two nearest-neighbor spins s which lies on the column full of s or

(ii) a spin s among those with two nearest-neighbor spins s on the incomplete column of spins s.

In particular, in case (i), $\hat{\sigma} \in \bar{B}_{1,K-1}^{K-2}(r,s) \subset \overline{\mathscr{H}}(\mathbf{r},\mathbf{s})$ and both the proof of (c) and of the claim are completed. Otherwise, in case (ii), $\hat{\sigma} \in \bar{B}_{1,K}^{K-3}(r,s) \subset \overline{\mathcal{Q}}(\mathbf{r},\mathbf{s})$. Thus claim is verified. However it is necessary to consider another step to prove (c).

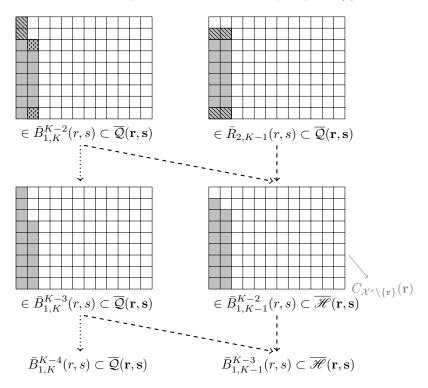


Figure 6: Example on a 9×12 grid Λ of Step 1. White vertices have spin r, gray vertices have spin s. Starting from $\bar{B}_{1,K}^{K-2}(r,s)$, the path can remain in $\overline{\mathcal{Q}}(\mathbf{r},\mathbf{s})$ by flipping a spin s to r among those with dots, otherwise it can enter into $\overline{\mathcal{H}}(\mathbf{r},\mathbf{s})$ by flipping from s to r a spin s among those with lines. Note that from $\bar{B}_{1,K-1}^{K-3}(r,s)$ the path can enter into $C_{\mathcal{X}^s\setminus\{\mathbf{r}\}}(\mathbf{r})$ in one step by flipping from s to r the spin s with three nearest-neighbor r.

Step 2. We claim that, given $\hat{\sigma} \in \bar{B}_{1,K}^{K-3}(r,s)$, the only configurations of \mathcal{V}_{2K-4}^s which communicate with $\hat{\sigma}$, along an optimal path between $\hat{\sigma}$ and \mathbf{r} , belong to either $\bar{B}_{1,K-1}^{K-3}(r,s)$ or $\bar{B}_{1,K}^{K-4}(r,s)$, see Figure (7).

Since $H(\hat{\sigma}) = \Phi(\mathbf{r}, \mathbf{s})$ (see Lemma 5.1), then in order to not increase the energy and to reduce the number of spins s, the moves (1) and (2) of Step 1 are the only possibilities. It follows that ω can pass through $\bar{B}_{1,K}^{K-3}(r,s)$ coming from a configuration that lies in $\bar{B}_{1,K-1}^{K-3}(r,s) \subset \overline{\mathscr{H}}(\mathbf{r},\mathbf{s})$ or in $\bar{B}_{1,K}^{K-4}(r,s) \subset \overline{\mathscr{Q}}(\mathbf{r},\mathbf{s})$. In any case, the claim is verified. However, we can conclude the proof of (c) only in the first case, otherwise we have to consider another step.

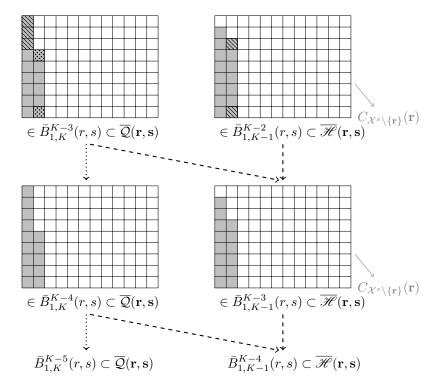


Figure 7: Example on a 9×12 grid Λ of Step 2. White vertices have spin r, gray vertices have spin s. By flipping a spin s to r among those with dots, the optimal path remains in $\overline{\mathcal{Q}}(\mathbf{r},\mathbf{s})$. Otherwise, if a spin s with lines becomes r, the path arrives for the first time in $\overline{\mathcal{H}}(\mathbf{r},\mathbf{s})$. Note that starting from $\bar{B}_{1,K-1}^{K-2}(r,s)$, the path can pass to another configuration belonging to $\overline{\mathcal{H}}(\mathbf{r},\mathbf{s})$.

Iterating the above construction, if at a certain step ω intersects \mathcal{V}_m^s , for $m=K+2,\ldots,2K-2$, in a configuration of $\bar{B}_{1,K-1}^n(r,s)\subset\overline{\mathscr{H}}(\mathbf{r},\mathbf{s})$ for some $n=3,\ldots,K-3$, then item (c) is satisfied and the proof is completed at that step. Otherwise, if ω intersects every \mathcal{V}_m^s , for $m=K+2,\ldots,2K-2$, in configurations belonging to $\overline{\mathcal{Q}}(\mathbf{r},\mathbf{s})$, then the above construction leads to a configuration that lies in $\bar{B}_{1,K}^2(r,s)\subset\overline{\mathcal{Q}}(\mathbf{r},\mathbf{s})$ and item (c) is satisfied because any $\eta\in\bar{B}_{1,K}^2(r,s)$ communicates with \mathcal{V}_{K+1}^s only through configurations belonging to either $\bar{B}_{1,K}^1(r,s)\subset\overline{\mathscr{H}}(\mathbf{r},\mathbf{s})$ or $\bar{B}_{1,K-1}^2(r,s)\subset\overline{\mathscr{H}}(\mathbf{r},\mathbf{s})$, see Figure 8. Indeed, (i) and (ii) of Step 1 are the only admissible options to move from $\bar{B}_{1,K}^2(r,s)$ to \mathcal{V}_{K+1}^s following an optimal path. \square

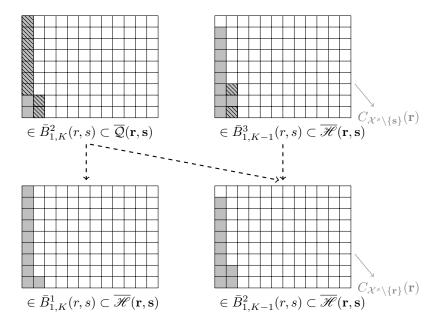


Figure 8: Example on a 9×12 grid Λ of the final step of the proof of Lemma 5.4(c). White vertices have spin r, gray vertices have spin s. If the optimal path intersects \mathcal{V}_{K+2}^s in a configuration of $\overline{B}_{1,K}^2(r,s) \subset \overline{\mathcal{Q}}(\mathbf{r},\mathbf{s})$ and it has not already passed thorugh $\overline{\mathscr{H}}(\mathbf{r},\mathbf{s})$, necessarily it arrives in this set by considering the step towards \mathcal{V}_{K+1}^s .

In the proof of [38, Proposition 2.5], the authors define a reference path ω^* between any pair of different stable configurations of a q-state Potts model on a $K \times L$ grid Λ . Before stating the last lemma of the section, we briefly introduce this path.

Definition 5.1. Given any $\mathbf{r}, \in \mathcal{X}^s$, $\mathbf{r} \neq \mathbf{s}$, the reference path ω^* is an optimal path from \mathbf{r} to \mathbf{s} that is formed by a sequence of configurations in which the cluster of spins s grows gradually column by column. During the first K steps, ω^* passes through configurations in which the spins on a particular column, say c_j for some $j=0,\ldots,L-1$, become s, then it crosses those configurations in which the spins on either c_{j+1} or c_{j-1} become s and so on. More precisely, without loss of generality we can start to flip the spins on the first column c_0 and define ω^* as the concatenation of L paths $\omega^{*(1)},\ldots,\omega^{*(L)}$ such that $\omega^{*(i)}:\eta_{i-1}\to\eta_i$, where $\eta_0:=\mathbf{r},\,\eta_L:=\mathbf{s}$ and for any $i=1,\ldots,L,\,\eta_i$ is defined as

$$\eta_i(v) := \begin{cases} s, & \text{if } v \in \bigcup_{j=0}^{i-1} c_j, \\ r, & \text{otherwise.} \end{cases}$$
 (5.6)

In particular, for any $i=1,\ldots,L,$ we define $\omega^{*(i)}=(\omega^{*(i)}_{0},\ldots,\omega^{*(i)}_{K})$ as

-
$$\omega^{*(i)}_{0} = \eta_{i-1};$$

-
$$\omega_h^{*(i)} = (\omega_{h-1}^{*(i)})^{(h-1,i),s}$$
, for $h = 1, \dots, K-1$;

-
$$\omega^*_K^{(i)} = \eta_i$$
.

Note that for any $i = 1, \ldots, L-1, h = 1, \ldots, K-1$, we have

-
$$\omega_h^{*(1)} \in \bar{R}_{1,h}(r,s);$$

-
$$\eta_i \in \bar{R}_{i,K}(r,s)$$
;

-
$$\omega_h^{*(i+1)} \in \bar{B}_{i,K}^h(r,s)$$
.

Using Lemma 5.1 and the fact that $\Phi(\mathbf{r}, \mathbf{s}) = 2K + 2 + H(\mathbf{r})$, we see, indeed, that ω^* is an optimal path.

Lemma 5.5. Consider the q-state Potts model on a $K \times L$ grid Λ with periodic boundary conditions. Let $\mathbf{r}, \mathbf{s} \in \mathcal{X}^s$, $\mathbf{r} \neq \mathbf{s}$.

For any $\sigma \in \overline{\mathcal{H}}(\mathbf{r}, \mathbf{s})$ there exists a path $\bar{\omega} = (\bar{\omega}_0, \dots, \bar{\omega}_n)$ from \mathbf{r} to σ such that

$$H(\bar{\omega}_i) < 2K + 2 + H(\mathbf{r}),\tag{5.7}$$

for any i = 0, ..., n - 1. Similarly, there exists $\tilde{\omega}$ from \mathbf{s} to any $\sigma \in \widetilde{\mathscr{H}}(\mathbf{r}, \mathbf{s})$ with the same properties of $\bar{\omega}$.

Proof. We prove that there exists $\bar{\omega}: \mathbf{r} \to \sigma$ which satisfies (5.7) for any $\sigma \in \overline{\mathscr{H}}(\mathbf{r}, \mathbf{s})$; by reversing the roles of r and s, the proof of the existence of $\tilde{\omega}$ from \mathbf{s} to any $\sigma \in \widehat{\mathscr{H}}(\mathbf{r}, \mathbf{s})$ is analogous.

The definition of $\overline{\mathcal{H}}(\mathbf{r}, \mathbf{s})$ gives rise to the two following scenarios, see (3.12). If $\sigma \in \bar{B}^1_{1,K}(r,s)$, then $\bar{\omega}$ is given by the first steps of the path ω^* depicted in Definition 5.1, i.e.,

$$\bar{\omega} = (\mathbf{r}, \omega_1^{*(1)}, \dots, \omega_K^{*(1)}, \omega_1^{*(2)} = \sigma).$$

Indeed, without loss of generality, we may consider c_0 as the column in which σ has all spins s and the construction of Definition 5.1 holds.

Otherwise, we have $\sigma \in \bar{B}_{1,K-1}^h(r,s)$ for $h=2,\ldots,K-2$. Possibly relabeling the columns, we build $\bar{\omega}$ taking into account the columns c_0,c_1 of the grid. In Figure 9 we depict an example of the path $\bar{\omega}$. For every $h=2,\ldots,K-2$ and for any odd value i from 1 to 2h-1, we set

$$\bar{\omega}_i = \bar{\omega}_{i-1}^{(\frac{i-1}{2},0),s}, \quad \bar{\omega}_{i+1} = \bar{\omega}_i^{(\frac{i-1}{2},1),s}.$$
 (5.8)

Then, we set

$$\bar{\omega}_j = \bar{\omega}_{j-1}^{(j-h,0)},\tag{5.9}$$

for any $j=2h+1,\ldots,K-1+h$. As we can see in Figure 9, after 2h steps $\bar{\omega}$ arrives in $\bar{\omega}_{2h} \in \bar{R}_{2,h}(r,s)$ and its next configurations belong to $\bar{B}_{1,j-h}^h(r,s)$ for $j=2h+1,\ldots,K-1+h$. Finally, (5.7) is satisfied in view of (5.3). \square

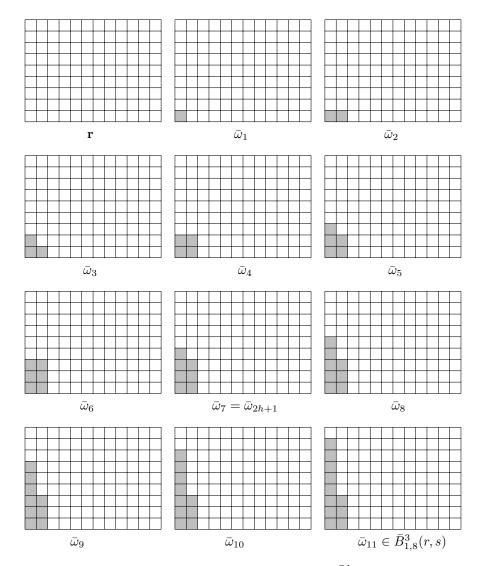


Figure 9: Example of $\bar{\omega}: \mathbf{r} \to \sigma$ of Lemma 5.5 where $\sigma \in \bar{B}_{1,K-1}^h(r,s)$ with K=9 and h=3. White vertices have spin r, gray vertices have spin s.

5.3 Study of the set of all minimal restricted-gates between two different stable states

We are now able to prove the following results concerning the set of minimal restricted-gates from $\mathbf{r} \in \mathcal{X}^s$ to $\mathbf{s} \in \mathcal{X}^s, \mathbf{s} \neq \mathbf{r}$.

Proof of Theorem 3.1. In order to prove that a set $W_{RES} \subset \mathcal{S}(\mathbf{r}, \mathbf{s})$ is a minimal restricted-gate for the transition from \mathbf{r} to \mathbf{s} we show that

- (i) W_{RES} is a restricted-gate, i.e., every $\omega \in (\mathbf{r} \to \mathbf{s})_{opt}$ such that $\omega \cap (\mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}) = \varnothing$ intersects W_{RES} ,
- (ii) for any $\eta \in \mathcal{W}_{RES}$ there exists an optimal path $\omega' \in (\mathbf{r} \to \mathbf{s})_{opt}$ such that $\omega' \cap (\mathcal{W}_{RES} \setminus \{\eta\}) = \varnothing$.

Hence, we now show that the sets defined in (a), (b), (c) and (d) of Theorem 3.1 satisfy the conditions above.

Using Lemma 5.4(a), $\overline{\mathscr{P}}(\mathbf{r}, \mathbf{s})$ and $\widetilde{\mathscr{P}}(\mathbf{r}, \mathbf{s})$ are gates for the transition from \mathbf{r} to \mathbf{s} . Next let us show that for any $\eta \in \overline{\mathscr{P}}(\mathbf{r}, \mathbf{s})$ there exists an optimal path $\omega' \in (\mathbf{r} \to \mathbf{s})_{opt}$ such that $\omega' \cap (\overline{\mathscr{P}}(\mathbf{r}, \mathbf{s}) \setminus \{\eta\}) = \varnothing$. Indeed, it is enough to consider ω' as the path ω^* of Definition 5.1

and to rewrite it in order to have $\omega' \cap \overline{\mathscr{P}}(\mathbf{r}, \mathbf{s}) = \{\eta\}$, i.e., $\omega^*_{K-1}^{(2)} = \eta$. By the symmetry of the model, we can prove similarly that there exists a such a path also for any $\eta \in \widetilde{\mathscr{P}}(\mathbf{r}, \mathbf{s})$.

Using Lemma 5.4(b), $\overline{\mathcal{Q}}(\mathbf{r}, \mathbf{s})$ and $\widetilde{\mathcal{Q}}(\mathbf{r}, \mathbf{s})$ are gates for the transition from \mathbf{r} to \mathbf{s} . Next let us show that for any $\eta \in \overline{\mathcal{Q}}(\mathbf{r}, \mathbf{s})$ there exists an optimal path $\omega' \in (\mathbf{r} \to \mathbf{s})_{opt}$ such that $\omega' \cap (\overline{\mathcal{Q}}(\mathbf{r}, \mathbf{s}) \setminus \{\eta\}) = \emptyset$. We distinguish two cases:

- (i) if $\eta \in \overline{R}_{2,K-1}(r,s)$, given $\overline{\eta} \in \overline{B}_{1,K-1}^{K-2}(r,s)$ and $\widehat{\eta} \in \overline{\mathscr{P}}(\mathbf{r},\mathbf{s})$ which communicate with η , then ω' is the optimal path given by the concatenation of
 - the path $\bar{\omega}: \mathbf{r} \to \bar{\eta}$ of Lemma 5.5;
 - the path $(\bar{\eta}, \eta, \hat{\eta})$;
 - the portion of the path ω^* in Definition 5.1 from $\omega^*_{K-1}^{(2)} = \hat{\eta}$ to s,
 - so that $\omega' \cap \overline{\mathcal{Q}}(\mathbf{r}, \mathbf{s}) = \{\eta\}.$
- (ii) if $\eta \in \overline{B}_{1,K}^h(r,s)$, for some $h=2,\ldots,K-2$, then to define ω' it is enough to consider the path ω^* of Definition 5.1 and to construct it in order to have $\omega' \cap \overline{\mathcal{Q}}(\mathbf{r},\mathbf{s}) = \{\eta\}$, i.e., $\omega^*_{b}^{(2)} = \eta$.

Thanks to the symmetry of the model, we may define ω' in an analogous way for any $\eta \in \widetilde{\mathcal{Q}}(\mathbf{r}, \mathbf{s})$.

Using Lemma 5.4(c), $\overline{\mathscr{H}}(\mathbf{r}, \mathbf{s})$ and $\widetilde{\mathscr{H}}(\mathbf{r}, \mathbf{s})$ are gates for the transition from \mathbf{r} to \mathbf{s} . Next let us show that for any $\eta \in \overline{\mathscr{H}}(\mathbf{r}, \mathbf{s})$ there exists an optimal path $\omega' \in (\mathbf{r} \to \mathbf{s})_{opt}$ such that $\omega' \cap (\overline{\mathscr{H}}(\mathbf{r}, \mathbf{s}) \setminus \{\eta\}) = \varnothing$. In particular, we have to distinguish two cases:

- (i) if $\eta \in \bar{B}^1_{1,K}(r,s)$, then ω' is given by the path ω^* of Definition 5.1 defined in order to have $\omega' \cap \overline{\mathscr{H}}(\mathbf{r},\mathbf{s}) = \{\eta\}$, i.e., $\omega^*_1^{(2)} = \eta$;
- (ii) if $\eta \in \bar{B}_{1,K-1}^h(r,s)$, for some $h=2,\ldots,K-2$, then ω' corresponds to the optimal path given by the concatenation of
 - the path $\bar{\omega}: \mathbf{r} \to \eta$ of Lemma 5.5;
 - the path $(\eta, \bar{\eta})$ with $\bar{\eta} \in \bar{B}_{1,K}^h(r,s)$, such that the bar of length h is in the same position as in η ;
 - the portion of the path ω^* in Definition 5.1 from ${\omega^*}_h^{(2)} = \bar{\eta}$ to s,

so that
$$\omega' \cap \overline{\mathscr{H}}(\mathbf{r}, \mathbf{s}) = \{\eta\}.$$

Thanks to the symmetry of the model, we may define ω' for any $\eta \in \widetilde{\mathscr{H}}(\mathbf{r}, \mathbf{s})$ following the same strategy.

From Lemma 5.3 and Lemma 5.2, we conclude that $\mathcal{W}_{j}^{(h)}(\mathbf{r},\mathbf{s})$ are gates for the transition $\mathbf{r} \to \mathbf{s}$ for any $j=2,\ldots,L-3$ and any $h=1,\ldots,K-1$. Indeed, by Lemma 5.3, there exists $K^* \in \mathbb{N}$ such that when $n>K^*$ every $\omega \in (\mathbf{r} \to \mathbf{s})_{opt}$ intersects \mathcal{V}_n^s in configurations which belong to either $\bar{R}_{j,K}(r,s)$ or $\mathcal{W}_{j}^{(h)}(\mathbf{r},\mathbf{s})=\bar{B}_{j,K}^h(r,s)$ for some $j=2,\ldots,L-3,$ $h=1,\ldots,K-1$. Moreover, by Lemma 5.2, we know that ω can reach these configurations only moving among configurations lying either in $\bar{R}_{j,K}(r,s)$ or in $\mathcal{W}_{j}^{(h)}(\mathbf{r},\mathbf{s})=\bar{B}_{j,K}^h(r,s)$. Hence, between its last visit to $\overline{\mathscr{P}}(\mathbf{r},\mathbf{s})$ and its first visit to $\widetilde{\mathscr{P}}(\mathbf{r},\mathbf{s}),$ ω passes at least once through each $\mathcal{W}_{j}^{(h)}(\mathbf{r},\mathbf{s}),$ $j=2,\ldots,L-3$. Thus, to conclude the proof we have to show that for every $\eta \in W_{j}^{(h)}(\mathbf{r},\mathbf{s}),$ there exists a path $\omega' \in (\mathbf{r} \to \mathbf{s})_{opt}$ such that $\omega' \cap (\mathcal{W}_{j}^{(h)}(\mathbf{r},\mathbf{s}) \setminus \{\eta\}) = \varnothing$. For any $j=2,\ldots,L-3$ and any $h=1,\ldots,K-1$, we can define this path ω' as the path ω^* of Definition 5.1, which we rewrite in order to have $\omega' \cap \mathcal{W}_{j}^{(h)}(\mathbf{r},\mathbf{s})$, i.e., $\omega_{h}^{*(j+1)} = \eta$. \square

Remark 5.2. A saddle $\eta \in \mathcal{S}(\sigma, \sigma')$ is unessential if for any $\omega \in (\sigma \to \sigma')_{opt}$ such that $\omega \cap \eta \neq \emptyset$ the following conditions are both satisfied:

- (a) $\{\operatorname{argmax}_{\omega} H\} \setminus \{\eta\} \neq \emptyset$,
- (b) there exists $\omega' \in (\sigma \to \sigma')_{opt}$ such that

$$\{\operatorname{argmax}_{\omega'} H\} \subseteq \{\operatorname{argmax}_{\omega} H\} \setminus \{\eta\}.$$

Proof of Theorem 3.2. In view of Theorem 3.1, we have

$$\bigcup_{j=2}^{L-3} \mathcal{W}_j(\mathbf{r},\mathbf{s}) \cup \overline{\mathscr{H}}(\mathbf{r},\mathbf{s}) \cup \widetilde{\mathscr{H}}(\mathbf{r},\mathbf{s}) \cup \overline{\mathcal{Q}}(\mathbf{r},\mathbf{s}) \cup \widetilde{\mathcal{Q}}(\mathbf{r},\mathbf{s}) \cup \overline{\mathscr{P}}(\mathbf{r},\mathbf{s}) \cup \widetilde{\mathscr{P}}(\mathbf{r},\mathbf{s}) \subseteq \mathcal{F}(\mathbf{r},\mathcal{X}^s \setminus \{\mathbf{r}\}).$$

Hence, we have only to prove the opposite inclusion. In order to do this, we use the characterization of minimal gates as essential saddles given in [35, Theorem 5.1]. Thus, if we prove that any

$$\eta \in \mathcal{S}(\mathbf{r}, \mathcal{X}^s \setminus {\mathbf{r}}) \setminus \left[\bigcup_{j=2}^{L-3} \mathcal{W}_j(\mathbf{r}, \mathbf{s}) \cup \overline{\mathcal{H}}(\mathbf{r}, \mathbf{s}) \cup \widetilde{\mathcal{H}}(\mathbf{r}, \mathbf{s}) \cup \overline{\mathcal{Q}}(\mathbf{r}, \mathbf{s}) \right] \\
\cup \widetilde{\mathcal{Q}}(\mathbf{r}, \mathbf{s}) \cup \overline{\mathcal{P}}(\mathbf{r}, \mathbf{s}) \cup \widetilde{\mathcal{P}}(\mathbf{r}, \mathbf{s}) \right]$$
(5.10)

is an unessential saddle, the proof is completed.

Consider η as in (5.10) and some $\omega \in (\mathbf{r} \to \mathbf{s})_{opt}$, $\omega = (\omega_0, \dots, \omega_n)$, such that $\eta \in \omega$. See Figure 10 for an example of ω . By Lemma 5.2 and Lemma 5.1 the condition (i) of Remark 5.2 is satisfied. Indeed, any $\omega \in (\mathbf{r} \to \mathbf{s})_{opt}$ passes through many configurations with energy value equal to $\Phi(\mathbf{r}, \mathbf{s})$. Hence, to conclude that η is an unessential saddle we have to prove that condition (b) of Remark 5.2 is verified. By Lemma 5.4(c), there exist $\bar{\eta} \in \omega \cap \overline{\mathscr{H}}(\mathbf{r}, \mathbf{s})$ and $\tilde{\eta} \in \omega \cap \overline{\mathscr{H}}(\mathbf{r}, \mathbf{s})$, where $\bar{\eta}$ is the last configuration visited by ω in $\overline{\mathscr{H}}(\mathbf{r}, \mathbf{s})$ and $\tilde{\eta}$ is the first configuration visited by ω in $\widetilde{\mathscr{H}}(\mathbf{r}, \mathbf{s})$. Moreover, Lemma 5.4(a) implies that there exist $\bar{\eta}^* \in \omega \cap \overline{\mathscr{P}}(\mathbf{r}, \mathbf{s})$ and $\tilde{\eta}^* \in \omega \cap \overline{\mathscr{P}}(\mathbf{r}, \mathbf{s})$, where $\bar{\eta}^*$ is the last configuration visited by ω in $\overline{\mathscr{P}}(\mathbf{r}, \mathbf{s})$ and $\tilde{\eta}^*$ is the first configuration visited by ω in $\widetilde{\mathscr{P}}(\mathbf{r}, \mathbf{s})$ and $\tilde{\eta}^*$ is the first configuration visited by ω in $\widetilde{\mathscr{P}}(\mathbf{r}, \mathbf{s})$.

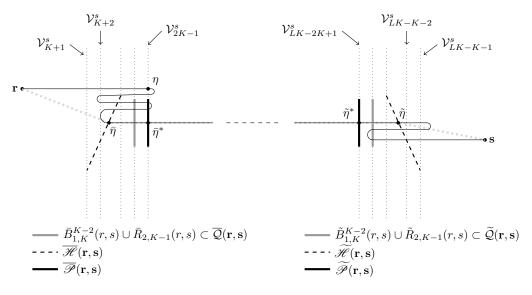


Figure 10: Example of the paths ω (solid black path) and ω' (dotted gray path) of the proof of Theorem 3.6.

In view of the proof of Lemma 5.4, after visiting $\bar{\eta}$, ω interstects $\mathcal{S}(\mathbf{r}, \mathbf{s})$ only in saddles belonging to either $\overline{\mathcal{Q}}(\mathbf{r}, \mathbf{s})$ or $\overline{\mathcal{P}}(\mathbf{r}, \mathbf{s})$ or $\mathcal{W}_j(\mathbf{r}, \mathbf{s})$, for some $j = 2, \ldots, L-3$, until it intersects

 $\mathscr{P}(\mathbf{r}, \mathbf{s})$ in $\tilde{\eta}^*$. Similarly, after the visit in $\bar{\eta}^*$ and before the arrival in $\tilde{\eta}$, ω passes only through saddles belonging to either $W_j(\mathbf{r}, \mathbf{s})$, for some $j = 2, \ldots, L-3$, or $\widetilde{\mathscr{P}}(\mathbf{r}, \mathbf{s})$ or $\widetilde{\mathscr{Q}}(\mathbf{r}, \mathbf{s})$. It follows that after $\bar{\eta}$ and before $\tilde{\eta}$, ω intersects $\mathcal{S}(\mathbf{r},\mathbf{s})$ only in those saddles which belong to $\bigcup_{j=2}^{L-3} \mathcal{W}_{j}(\mathbf{r},\mathbf{s}) \cup \overline{\mathscr{H}}(\mathbf{r},\mathbf{s}) \cup \overline{\mathscr{H}}(\mathbf{r},\mathbf{s}) \cup \overline{\mathscr{Q}}(\mathbf{r},\mathbf{s}) \cup \overline{\mathscr{Q}}(\mathbf{r},\mathbf{s}) \cup \overline{\mathscr{P}}(\mathbf{r},\mathbf{s}) \cup \overline{\mathscr{P}}(\mathbf{r},\mathbf{s}).$ Now consider the paths $\bar{\omega} : \mathbf{r} \to \bar{\eta}$ and $\tilde{\omega} : \mathbf{s} \to \tilde{\eta}$, which exist in view of Lemma 5.5, and

take the time reversal of $\tilde{\omega}$, i.e.,

$$\tilde{\omega}^T = (\omega_n = \tilde{\eta}, \tilde{\omega}_{n-1}, \dots, \omega_1, \omega_0 = \mathbf{s}).$$

Thus, if

$$\omega = (\omega_0 = \mathbf{r}, \dots, \omega_i = \bar{\eta}, \dots, \omega_i = \tilde{\eta}, \dots, \omega_n = \mathbf{s}),$$

the path $\omega' \in (\mathbf{r} \to \mathbf{s})_{opt}$, can be defined as

- $\omega' \equiv \bar{\omega}$ from \mathbf{r} to $\bar{\eta}$;
- $\omega' \equiv (\omega_i = \bar{\eta}, \dots, \omega_j = \tilde{\eta})$ from $\bar{\eta}$ to $\tilde{\eta}$;
- $\omega' \equiv \tilde{\omega}^T$ from $\tilde{\eta}$ to s.

Thus, (b) of Remark 5.2 is verified.

Proof of Corollary 3.1. Since Theorem 3.1 holds, the corollary follows by [35, Theorem [5.4].

Minimal gates 6

We are now able to carry out the proof of the main results on the minimal gates for the transitions from a stable state to the other stable configurations and from a stable state to another stable configuration.

6.1 The minimal gates from a stable state to the other stable states

Proof of Theorem 3.3. We recall that a subset $W \subset S(\mathbf{r}, \mathcal{X}^s \setminus \{\mathbf{r}\})$ is a minimal gate for the transition $\mathbf{r} \to \mathcal{X}^s \setminus \{\mathbf{r}\}$ if

- (i) \mathcal{W} is a gate, i.e., every $\omega \in (\mathbf{r} \to \mathcal{X}^s \setminus \{\mathbf{r}\})_{opt}$ intersects \mathcal{W} ,
- (ii) for any $\eta \in \mathcal{W}$ there exists an optimal path $\omega' \in (\mathbf{r} \to \mathcal{X}^s \setminus \{\mathbf{r}\})_{opt}$ such that $\omega' \cap$ $(\mathcal{W}\setminus\{\eta\})=\varnothing.$

We begin to prove that the sets depicted in (a) of Theorem 3.3 are minimal gates for the transition $\mathbf{r} \to \mathcal{X}^s \setminus \{\mathbf{r}\}\$. Consider any $\omega \in (\mathbf{r} \to \mathcal{X}^s \setminus \{\mathbf{r}\})_{opt}$ and let $\mathbf{s} \in \mathcal{X}^s \setminus \{\mathbf{r}\}$ be the first configuration visited by ω in $\mathcal{X}^s \setminus \{\mathbf{r}\}$. From Theorem 3.1(a) we have $\omega \cap \overline{\mathscr{P}}(\mathbf{r}, \mathbf{s}) \neq \emptyset$ and $\omega \cap \mathscr{P}(\mathbf{r}, \mathbf{s}) \neq \varnothing$. Thus,

$$\omega \cap \left(igcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathscr{P}}(\mathbf{r}, \mathbf{t})
ight)
eq \varnothing \quad ext{and} \quad \omega \cap \left(igcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \widetilde{\mathscr{P}}(\mathbf{r}, \mathbf{t})
ight)
eq \varnothing$$

and (i) is verified.

Now consider $\eta \in \bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathscr{P}}(\mathbf{r}, \mathbf{t})$. There exists $\mathbf{s} \in \mathcal{X}^s \setminus \{\mathbf{r}\}$ such that $\eta \in \overline{\mathscr{P}}(\mathbf{r}, \mathbf{s})$. Let $\omega' \in (\mathbf{r} \to \mathcal{X}^s \setminus \{\mathbf{r}\})_{opt}$ be the optimal path from \mathbf{r} to $\mathbf{s} \in \mathcal{X}^s \setminus \{\mathbf{r}\}$ constructed in the proof of Theorem 3.1(a), such that $\omega' \cap (\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathscr{P}}(\mathbf{r}, \mathbf{t}) \setminus \{\eta\})$

 $= \varnothing$ and $\omega' \cap \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\} = \varnothing$. Hence, (ii) is verified for $\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathscr{P}}(\mathbf{r}, \mathbf{t})$. By the symmetry of the model, we can argue similarly to prove that (ii) holds also for $\bigcup_{t \in \mathcal{X}^s \setminus \{r\}} \widehat{\mathscr{P}}(r,t)$.

Next we move to the proof that the sets depicted in (b) of Theorem 3.3 are minimal gates for the transition $\mathbf{r} \to \mathcal{X}^s \setminus \{\mathbf{r}\}$. Consider any $\omega \in (\mathbf{r} \to \mathcal{X}^s \setminus \{\mathbf{r}\})_{opt}$ and let $\mathbf{s} \in \mathcal{X}^s \setminus \{\mathbf{r}\}$ be the first configuration visited by ω in $\mathcal{X}^s \setminus \{\mathbf{r}\}$. From Theorem 3.1(b) we have $\omega \cap \overline{\mathcal{Q}}(\mathbf{r}, \mathbf{s}) \neq \emptyset$ and $\omega \cap \widetilde{\mathcal{Q}}(\mathbf{r}, \mathbf{s}) \neq \emptyset$. Thus,

$$\omega \cap \left(\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathcal{Q}}(\mathbf{r}, \mathbf{t})\right) \neq \varnothing \quad \text{and} \quad \omega \cap \left(\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \widetilde{\mathcal{Q}}(\mathbf{r}, \mathbf{t})\right) \neq \varnothing$$

and (i) is verified.

Now consider $\eta \in \bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathcal{Q}}(\mathbf{r}, \mathbf{t})$. There exists $\mathbf{s} \in \mathcal{X}^s \setminus \{\mathbf{r}\}$ such that $\eta \in \overline{\mathcal{Q}}(\mathbf{r}, \mathbf{s})$. Let $\omega' \in (\mathbf{r} \to \mathcal{X}^s \setminus \{\mathbf{r}\})_{opt}$ be the optimal path from \mathbf{r} to $\mathbf{s} \in \mathcal{X}^s \setminus \{\mathbf{r}\}$ constructed in the proof of Theorem 3.1(b), such that $\omega' \cap (\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathcal{Q}}(\mathbf{r}, \mathbf{t}) \setminus \{\eta\})$

 $= \varnothing$ and $\omega' \cap \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\} = \varnothing$. Hence, (ii) is verified for $\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathcal{Q}}(\mathbf{r}, \mathbf{t})$. By the symmetry of the model, we can argue in the same way to prove that (ii) holds also for $\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \widetilde{\mathcal{Q}}(\mathbf{r}, \mathbf{t})$.

Now we move to showing that the sets depicted in (c) of Theorem 3.3 are minimal gates for the transition $\mathbf{r} \to \mathcal{X}^s \setminus \{\mathbf{r}\}$. Consider any $\omega \in (\mathbf{r} \to \mathcal{X}^s \setminus \{\mathbf{r}\})_{opt}$ and let $\mathbf{s} \in \mathcal{X}^s \setminus \{\mathbf{r}\}$ be the first configuration visited by ω in $\mathcal{X}^s \setminus \{\mathbf{r}\}$. From Theorem 3.1(c) we have $\omega \cap \overline{\mathcal{H}}(\mathbf{r}, \mathbf{s}) \neq \emptyset$ and $\omega \cap \overline{\mathcal{H}}(\mathbf{r}, \mathbf{s}) \neq \emptyset$. Thus,

$$\omega \cap \left(\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathscr{H}}(\mathbf{r}, \mathbf{t})\right) \neq \varnothing \quad \text{and} \quad \omega \cap \left(\bigcup_{\mathbf{s} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \widetilde{\mathscr{H}}(\mathbf{r}, \mathbf{t})\right) \neq \varnothing$$

and (i) is verified.

Now consider $\eta \in \bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathcal{H}}(\mathbf{r}, \mathbf{t})$. There exists $\mathbf{s} \in \mathcal{X}^s \setminus \{\mathbf{r}\}$ such that $\eta \in \overline{\mathcal{H}}(\mathbf{r}, \mathbf{s})$. Let $\omega' \in (\mathbf{r} \to \mathcal{X}^s \setminus \{\mathbf{r}\})_{opt}$ be the optimal path from \mathbf{r} to $\mathbf{s} \in \mathcal{X}^s \setminus \{\mathbf{r}\}$ constructed in the proof of Theorem 3.1(c), such that $\omega' \cap (\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathcal{H}}(\mathbf{r}, \mathbf{t}) \setminus \{\eta\})$

 $= \varnothing$ and $\omega' \cap \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\} = \varnothing$. Hence, (ii) is verified for $\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathscr{H}}(\mathbf{r}, \mathbf{t})$. By the symmetry of the model, we can argue in the same way to prove that (ii) holds also for $\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \widetilde{\mathscr{H}}(\mathbf{r}, \mathbf{t})$.

Finally, we prove that also the sets depicted in (d) of Theorem 3.3 are minimal gates for the transition $\mathbf{r} \to \mathcal{X}^s \setminus \{\mathbf{r}\}$. Consider any $\omega \in (\mathbf{r} \to \mathcal{X}^s \setminus \{\mathbf{r}\})_{opt}$ and let $\mathbf{s} \in \mathcal{X}^s \setminus \{\mathbf{r}\}$ be the first configuration visited by ω in $\mathcal{X}^s \setminus \{\mathbf{r}\}$. From Theorem 3.1(d) for any $j = 2, \ldots, L - 3$ and any $h = 1, \ldots, K - 1$, we have

$$\omega \cap \mathcal{W}_{j}^{(h)}(\mathbf{r}, \mathbf{s}) \neq \varnothing$$

and it follows that

$$\omega \cap \left(\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \mathcal{W}_j^{(h)}(\mathbf{r}, \mathbf{t})\right) \neq \varnothing$$

and (i) is verified.

For any $j=2,\ldots,L-3$ and $h=1,\ldots,K-1$, consider $\eta\in\bigcup_{\mathbf{t}\in\mathcal{X}^s\backslash\{\mathbf{r}\}}W_j^{(h)}(\mathbf{r},\mathbf{t})$, thus there exists $\mathbf{s}\in\mathcal{X}^s\backslash\{\mathbf{r}\}$ such that $\eta\in W_j^{(h)}(\mathbf{r},\mathbf{s})$. Let $\omega'\in(\mathbf{r}\to\mathcal{X}^s\backslash\{\mathbf{r}\})_{opt}$ be the optimal path from \mathbf{r} to $\mathbf{s}\in\mathcal{X}^s\backslash\{\mathbf{r}\}$ constructed in the proof of Theorem 3.1(d) such that $\omega'\cap(\bigcup_{\mathbf{t}\in\mathcal{X}^s\backslash\{\mathbf{r}\}}W_j^{(h)}(\mathbf{r},\mathbf{t})\backslash\{\eta\})=\varnothing$ and $\omega'\cap\mathcal{X}^s\backslash\{\mathbf{r},\mathbf{s}\}=\varnothing$. Thus, (ii) is verified and $\bigcup_{\mathbf{t}\in\mathcal{X}^s\backslash\{\mathbf{r}\}}W_j^{(h)}(\mathbf{r},\mathbf{t})$ is a minimal gate for the transition from \mathbf{r} to $\mathcal{X}^s\backslash\{\mathbf{r}\}$. \square

Proof of Theorem 3.4. In view of Theorem 3.3 we have

$$\begin{split} \bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} & \left[\bigcup_{j=2}^{L-3} \mathcal{W}_j(\mathbf{r}, \mathbf{t}) \cup \overline{\mathscr{H}}(\mathbf{r}, \mathbf{t}) \cup \widetilde{\mathscr{H}}(\mathbf{r}, \mathbf{t}) \cup \overline{\mathscr{Q}}(\mathbf{r}, \mathbf{t}) \right. \\ & \left. \cup \, \widetilde{\mathcal{Q}}(\mathbf{r}, \mathbf{t}) \cup \overline{\mathscr{P}}(\mathbf{r}, \mathbf{t}) \cup \widetilde{\mathscr{P}}(\mathbf{r}, \mathbf{t}) \right] \subseteq \mathcal{G}(\mathbf{r}, \mathcal{X}^s \setminus \{\mathbf{r}\}). \end{split}$$

Hence, we only have to prove the opposite inclusion. In order to do this, we again use the characterization of minimal gates as essential saddles given in [35, Theorem 5.1]. Thus, our strategy is to prove that any

$$\eta \in \mathcal{S}(\mathbf{r}, \mathcal{X}^s \setminus {\mathbf{r}}) \setminus \bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus {\mathbf{r}}} \left[\bigcup_{j=2}^{L-3} \mathcal{W}_j(\mathbf{r}, \mathbf{t}) \cup \overline{\mathscr{H}}(\mathbf{r}, \mathbf{t}) \cup \widetilde{\mathscr{H}}(\mathbf{r}, \mathbf{t}) \cup \overline{\mathscr{Q}}(\mathbf{r}, \mathbf{t}) \right] \\
\qquad \qquad \cup \widetilde{\mathcal{Q}}(\mathbf{r}, \mathbf{t}) \cup \overline{\mathscr{P}}(\mathbf{r}, \mathbf{t}) \cup \widetilde{\mathscr{P}}(\mathbf{r}, \mathbf{t}) \right]$$
(6.1)

is an unessential saddle. In particular, for any saddle η as in (6.1) and for any $\omega \in (\mathbf{r} \to \mathcal{X}^s \setminus \{\mathbf{r}\})_{opt}$ such that $\eta \in \omega$, we have to prove that the conditions of Remark 5.2 are satisfied. Let $\mathbf{s} \in \mathcal{X}^s \setminus \{\mathbf{r}\}$ be the first stable state visited by ω . By Lemma 5.2 and Lemma 5.1 the condition (a) of Remark 5.2 is satisfied. Moreover, let $\omega' \in (\mathbf{r} \to \mathcal{X}^s \setminus \{\mathbf{r}\})_{opt}$ be the optimal path from \mathbf{r} to $\mathbf{s} \in \mathcal{X}^s \setminus \{\mathbf{r}\}$ constructed in the proof of Theorem 3.2 such that

$$\{\operatorname{argmax}_{\omega'}H\}\subseteq\{\operatorname{argmax}_{\omega}H\}\backslash\{\eta\}$$

and $\omega' \cap \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\} = \emptyset$. Thus, condition (b) of Remark 5.2 is satisfied and η is an unessential saddle. \square

Proof of Corollary 3.2. Since Theorem 3.3 holds, the corollary follows by [35, Theorem 5.4]. \Box

6.2 The minimal gates from a stable state to an other stable state

Proof of Theorem 3.5. We recall that a subset $W \subset S(\mathbf{r}, \mathbf{s})$ is a minimal gate for the transition \mathbf{r} to \mathbf{s} if

- (i) W is a gate, i.e., every $\omega \in (\mathbf{r} \to \mathbf{s})_{opt}$ intersects W,
- (ii) for any $\eta \in \mathcal{W}$ there exists an optimal path $\omega' \in (\mathbf{r} \to \mathbf{s})_{opt}$ such that $\omega' \cap (\mathcal{W} \setminus \{\eta\}) = \emptyset$.

Let us start to prove that the sets depicted in (i) are minimal gates for the transition from \mathbf{r} to \mathbf{s} . Consider any $\omega \in (\mathbf{r} \to \mathbf{s})_{opt}$ and let $\mathbf{s}' \in \mathcal{X}^s \setminus \{\mathbf{r}\}$ be the first stable configuration visited by ω in $\mathcal{X}^s \setminus \{\mathbf{r}\}$. From Theorem 3.1(a) we have $\omega \cap \overline{\mathscr{P}}(\mathbf{r}, \mathbf{s}') \neq \emptyset$ and $\omega \cap \widetilde{\mathscr{P}}(\mathbf{r}, \mathbf{s}') \neq \emptyset$. Thus,

$$\omega \cap \left(\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathscr{P}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \overline{\mathscr{P}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \overline{\mathscr{P}}(\mathbf{t}', \mathbf{s})\right) \neq \varnothing$$

and

$$\omega \cap \left(\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \widetilde{\mathscr{P}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \widetilde{\mathscr{P}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \widetilde{\mathscr{P}}(\mathbf{t}', \mathbf{s}) \right) \neq \varnothing.$$

Hence (i) is satisfied. Now consider

$$\eta \in \biggl(\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathscr{P}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \overline{\mathscr{P}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \overline{\mathscr{P}}(\mathbf{t}', \mathbf{s}) \biggr).$$

There exist $\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s, \mathbf{t} \neq \mathbf{t}'$, such that $\eta \in \overline{\mathcal{P}}(\mathbf{t}, \mathbf{t}')$. In order to define a path ω' such that

$$\omega' \cap \left[\left(\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathcal{P}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \overline{\mathcal{P}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \overline{\mathcal{P}}(\mathbf{t}', \mathbf{s}) \right) \setminus \{\eta\} \right] = \varnothing, \quad (6.2)$$

let us separate four different cases.

- If $\mathbf{t} = \mathbf{r}$ and $\mathbf{t}' = \mathbf{s}$, then let $\omega' \in (\mathbf{r} \to \mathbf{s})_{opt}$ be the optimal path from \mathbf{r} to \mathbf{s} constructed in the proof of Theorem 3.1(a) such that $\omega^{(1)} \cap \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\} = \emptyset$.
- If $\mathbf{t} = \mathbf{r}$ and $\mathbf{t}' \neq \mathbf{s}$, then let $\omega' \in (\mathbf{r} \to \mathbf{s})_{opt}$ be the optimal path defined as the concatenation of the paths $\omega^{(1)} \in (\mathbf{r} \to \mathbf{t}')_{opt}$ constructed in the proof of Theorem 3.1(a) such that $\omega^{(1)} \cap \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{t}'\} = \emptyset$ and $\omega^{(2)} \in (\mathbf{t}' \to \mathbf{s})_{opt}$ of Definition 5.1.
- If $\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}$, then let $\omega' \in (\mathbf{r} \to \mathbf{s})_{opt}$ be the optimal path defined as the concatenation of the paths $\omega^{(1)} \in (\mathbf{r} \to \mathbf{t})_{opt}$ of Definition 5.1, $\omega^{(2)} \in (\mathbf{t} \to \mathbf{t}')_{opt}$ constructed in the proof of Theorem 3.1(a) such that $\omega^{(2)} \cap \mathcal{X}^s \setminus \{\mathbf{t}, \mathbf{t}'\} = \emptyset$ and $\omega^{(3)} \in (\mathbf{t}' \to \mathbf{s})_{opt}$ of Definition 5.1.
- If $\mathbf{t} \neq \mathbf{r}$ and $\mathbf{t}' = \mathbf{s}$, then let $\omega' \in (\mathbf{r} \to \mathbf{s})_{opt}$ be the optimal path defined as the concatenation of the paths $\omega^{(1)} \in (\mathbf{r} \to \mathbf{t})_{opt}$ of Definition 5.1 and $\omega^{(2)} \in (\mathbf{t} \to \mathbf{s})_{opt}$ constructed in the proof of Theorem 3.1(a) such that $\omega^{(2)} \cap \mathcal{X}^s \setminus \{\mathbf{t}, \mathbf{s}\} = \emptyset$.

In any case (6.2) is satisfied and (ii) is verified for

$$\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathscr{P}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \overline{\mathscr{P}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \overline{\mathscr{P}}(\mathbf{t}', \mathbf{s}).$$

By the symmetry of the model, we can argue similarly to prove that (ii) holds also for

$$\bigcup_{\mathbf{t}\in\mathcal{X}^s\setminus\{\mathbf{r}\}}\widetilde{\mathscr{P}}(\mathbf{r},\mathbf{t})\cup\bigcup_{\mathbf{t},\mathbf{t}'\in\mathcal{X}^s\setminus\{\mathbf{s}\},\mathbf{t}\neq\mathbf{t}'}\widetilde{\mathscr{P}}(\mathbf{t},\mathbf{t}')\cup\bigcup_{\mathbf{t}'\in\mathcal{X}^s\setminus\{\mathbf{r},\mathbf{s}\}}\widetilde{\mathscr{P}}(\mathbf{t}',\mathbf{s}).$$

Next we move to prove that the sets depicted in (b) are minimal gates for the transition from \mathbf{r} to \mathbf{s} . Consider any $\omega \in (\mathbf{r} \to \mathbf{s})_{opt}$ and let $\mathbf{s}' \in \mathcal{X}^s \setminus \{\mathbf{r}\}$ be the first stable configuration visited by ω in $\mathcal{X}^s \setminus \{\mathbf{r}\}$. From Theorem 3.1(b) we have $\omega \cap \overline{\mathcal{Q}}(\mathbf{r}, \mathbf{s}') \neq \emptyset$ and $\omega \cap \widetilde{\mathcal{Q}}(\mathbf{r}, \mathbf{s}') \neq \emptyset$. Thus,

$$\omega \cap \left(\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathcal{Q}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \overline{\mathcal{Q}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \overline{\mathcal{Q}}(\mathbf{t}', \mathbf{s})\right) \neq \varnothing$$

and

$$\omega \cap \left(\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \widetilde{\mathcal{Q}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \widetilde{\mathcal{Q}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \widetilde{\mathcal{Q}}(\mathbf{t}', \mathbf{s})\right) \neq \varnothing.$$

Thus, (i) is verified. Now consider

$$\eta \in \biggl(\bigcup_{\mathbf{t} \in \mathcal{X}^s \backslash \{\mathbf{r}\}} \overline{\mathcal{Q}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \backslash \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \overline{\mathcal{Q}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \backslash \{\mathbf{r}, \mathbf{s}\}} \overline{\mathcal{Q}}(\mathbf{t}', \mathbf{s}) \biggr).$$

There exist $\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s, \mathbf{t} \neq \mathbf{t}'$, such that $\eta \in \overline{\mathcal{Q}}(\mathbf{t}, \mathbf{t}')$. In order to define a path ω' such that

$$\omega' \cap \left[\left(\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathcal{Q}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \overline{\mathcal{Q}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \overline{\mathcal{Q}}(\mathbf{t}', \mathbf{s}) \right) \setminus \{\eta\} \right] = \varnothing, \quad (6.3)$$

let us separate four cases.

- If $\mathbf{t} = \mathbf{r}$ and $\mathbf{t}' = \mathbf{s}$, then let $\omega' \in (\mathbf{r} \to \mathbf{s})_{opt}$ be the optimal path from \mathbf{r} to \mathbf{s} constructed in the proof of Theorem 3.1(b) such that $\omega^{(1)} \cap \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\} = \emptyset$.
- If $\mathbf{t} = \mathbf{r}$ and $\mathbf{t}' \neq \mathbf{s}$, then let $\omega' \in (\mathbf{r} \to \mathbf{s})_{opt}$ be the optimal path defined as the concatenation of the paths $\omega^{(1)} \in (\mathbf{r} \to \mathbf{t}')_{opt}$ constructed in the proof of Theorem 3.1(b) such that $\omega^{(1)} \cap \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{t}'\} = \emptyset$ and $\omega^{(2)} \in (\mathbf{t}' \to \mathbf{s})_{opt}$ of Definition 5.1.
- If $\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}$, then let $\omega' \in (\mathbf{r} \to \mathbf{s})_{opt}$ be the optimal path defined as the concatenation of the paths $\omega^{(1)} \in (\mathbf{r} \to \mathbf{t})_{opt}$ of Definition 5.1, $\omega^{(2)} \in (\mathbf{t} \to \mathbf{t}')_{opt}$ constructed in the proof of Theorem 3.1(b) such that $\omega^{(2)} \cap \mathcal{X}^s \setminus \{\mathbf{t}, \mathbf{t}'\} = \emptyset$ and $\omega^{(3)} \in (\mathbf{t}' \to \mathbf{s})_{opt}$ of Definition 5.1.

- If $\mathbf{t} \neq \mathbf{r}$ and $\mathbf{t}' = \mathbf{s}$, then let $\omega' \in (\mathbf{r} \to \mathbf{s})_{opt}$ be the optimal path defined as the concatenation of the paths $\omega^{(1)} \in (\mathbf{r} \to \mathbf{t})_{opt}$ of Definition 5.1 and $\omega^{(2)} \in (\mathbf{t} \to \mathbf{s})_{opt}$ constructed in the proof of Theorem 3.1(b) such that $\omega^{(2)} \cap \mathcal{X}^s \setminus \{\mathbf{t}, \mathbf{s}\} = \emptyset$.

In any case (6.3) is satisfied and (ii) is verified for

$$\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathcal{Q}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \overline{\mathcal{Q}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \overline{\mathcal{Q}}(\mathbf{t}', \mathbf{s}).$$

By the symmetry of the model, we can argue similarly to prove that (ii) holds also for

$$\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \widetilde{\mathcal{Q}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \widetilde{\mathcal{Q}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \widetilde{\mathcal{Q}}(\mathbf{t}', \mathbf{s}).$$

Similarly, we may prove that the sets depicted in (c) are minimal gates for the transition from \mathbf{r} to \mathbf{s} . Indeed, consider any $\omega \in (\mathbf{r} \to \mathbf{s})_{opt}$ and let $\mathbf{s}' \in \mathcal{X}^s \setminus \{\mathbf{r}\}$ be the first stable configuration visited by ω in $\mathcal{X}^s \setminus \{\mathbf{r}\}$. From Theorem 3.1(c) we have $\omega \cap \overline{\mathscr{H}}(\mathbf{r}, \mathbf{s}') \neq \emptyset$ and $\omega \cap \widetilde{\mathscr{H}}(\mathbf{r}, \mathbf{s}') \neq \emptyset$. Thus,

$$\omega \cap \left(\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathcal{H}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \overline{\mathcal{H}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \overline{\mathcal{H}}(\mathbf{t}', \mathbf{s})\right) \neq \emptyset$$

and

$$\omega \cap \left(\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \widetilde{\mathscr{H}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \widetilde{\mathscr{H}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \widetilde{\mathscr{H}}(\mathbf{t}', \mathbf{s})\right) \neq \varnothing.$$

Hence (i) is satisfied. Now consider

$$\eta \in igg(igcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathscr{H}}(\mathbf{r}, \mathbf{t}) \cup igcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t}
eq \mathbf{t}'} \overline{\mathscr{H}}(\mathbf{t}, \mathbf{t}') \cup igcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \overline{\mathscr{H}}(\mathbf{t}', \mathbf{s})igg).$$

There exist $\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s, \mathbf{t} \neq \mathbf{t}'$, such that $\eta \in \overline{\mathcal{Q}}(\mathbf{t}, \mathbf{t}')$. In order to define a path ω' such that

$$\omega' \cap \left[\left(\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathcal{H}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \overline{\mathcal{H}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \overline{\mathcal{H}}(\mathbf{t}', \mathbf{s}) \right) \setminus \{\eta\} \right] = \varnothing, \quad (6.4)$$

let us distinguish four cases.

- If $\mathbf{t} = \mathbf{r}$ and $\mathbf{t}' = \mathbf{s}$, then let $\omega' \in (\mathbf{r} \to \mathbf{s})_{opt}$ be the optimal path from \mathbf{r} to \mathbf{s} constructed in the proof of Theorem 3.1(c) such that $\omega^{(1)} \cap \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\} = \emptyset$.
- If $\mathbf{t} = \mathbf{r}$ and $\mathbf{t}' \neq \mathbf{s}$, then let $\omega' \in (\mathbf{r} \to \mathbf{s})_{opt}$ be the optimal path defined as the concatenation of the paths $\omega^{(1)} \in (\mathbf{r} \to \mathbf{t}')_{opt}$ constructed in the proof of Theorem 3.1(c) such that $\omega^{(1)} \cap \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{t}'\} = \emptyset$ and $\omega^{(2)} \in (\mathbf{t}' \to \mathbf{s})_{opt}$ of Definition 5.1.
- If $\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}$, then let $\omega' \in (\mathbf{r} \to \mathbf{s})_{opt}$ be the optimal path defined as the concatenation of the paths $\omega^{(1)} \in (\mathbf{r} \to \mathbf{t})_{opt}$ of Definition 5.1, $\omega^{(2)} \in (\mathbf{t} \to \mathbf{t}')_{opt}$ constructed in the proof of Theorem 3.1(c) such that $\omega^{(2)} \cap \mathcal{X}^s \setminus \{\mathbf{t}, \mathbf{t}'\} = \emptyset$ and $\omega^{(3)} \in (\mathbf{t}' \to \mathbf{s})_{opt}$ of Definition 5.1.
- If $\mathbf{t} \neq \mathbf{r}$ and $\mathbf{t}' = \mathbf{s}$, then let $\omega' \in (\mathbf{r} \to \mathbf{s})_{opt}$ be the optimal path defined as the concatenation of the paths $\omega^{(1)} \in (\mathbf{r} \to \mathbf{t})_{opt}$ of Definition 5.1 and $\omega^{(2)} \in (\mathbf{t} \to \mathbf{s})_{opt}$ constructed in the proof of Theorem 3.1(c) such that $\omega^{(2)} \cap \mathcal{X}^s \setminus \{\mathbf{t}, \mathbf{s}\} = \emptyset$.

In any case (6.4) is satisfied and (ii) is verified for

$$\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \overline{\mathscr{H}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \overline{\mathscr{H}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \overline{\mathscr{H}}(\mathbf{t}', \mathbf{s}).$$

By the symmetry of the model, we can argue similarly to prove that (2) holds also for

$$\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \widetilde{\mathscr{H}}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \widetilde{\mathscr{H}}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \widetilde{\mathscr{H}}(\mathbf{t}', \mathbf{s}).$$

Finally, we prove that also the sets depicted in (d) are minimal gates for the transition from \mathbf{r} to \mathbf{s} . For any $j=2,\ldots,L-3$ and h=1,K-1, consider any

$$\eta \in \left(\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \mathcal{W}_j^{(h)}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \mathcal{W}_j^{(h)}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \mathcal{W}_j^{(h)}(\mathbf{t}', \mathbf{s})\right)$$

and let $\mathbf{s}' \in \mathcal{X}^s \setminus \{\mathbf{r}\}$ be the first stable state visited by ω in $\mathcal{X}^s \setminus \{\mathbf{r}\}$. From Theorem 3.1(d) for any j = 2, ..., L - 3 and h = 1, j, K - 1, we have

$$\omega \cap \mathcal{W}_{j}^{(h)}(\mathbf{r}, \mathbf{s}') \neq \varnothing$$

and it follows that

$$\omega \cap \left(\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \mathcal{W}_j^{(h)}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \mathcal{W}_j^{(h)}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \mathcal{W}_j^{(h)}(\mathbf{t}', \mathbf{s})\right) \neq \varnothing.$$

Now for any j = 2, ..., L - 3 and h = 1, K - 1, consider

$$\eta \in \bigg(\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \mathcal{W}_j^{(h)}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \mathcal{W}_j^{(h)}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \mathcal{W}_j^{(h)}(\mathbf{t}', \mathbf{s})\bigg),$$

thus there exists $\mathbf{s}' \in \mathcal{X}^s \setminus \{\mathbf{r}\}$ such that $\eta \in \mathcal{W}_j^{(h)}(\mathbf{t}', \mathbf{s}')$. Let $\omega' \in (\mathbf{r} \to \mathbf{s})_{opt}$ be the optimal path from \mathbf{r} to \mathbf{s}' constructed in the proof of Theorem 3.1(d), such that ω' does not intersect

$$\bigg(\bigcup_{\mathbf{t}\in\mathcal{X}^s\backslash\{\mathbf{r}\}}\mathcal{W}_j^{(h)}(\mathbf{r},\mathbf{t})\cup\bigcup_{\mathbf{t},\mathbf{t}'\in\mathcal{X}^s\backslash\{\mathbf{s}\},\mathbf{t}\neq\mathbf{t}'}\mathcal{W}_j^{(h)}(\mathbf{t},\mathbf{t}')\cup\bigcup_{\mathbf{t}'\in\mathcal{X}^s\backslash\{\mathbf{r},\mathbf{s}\}}\mathcal{W}_j^{(h)}(\mathbf{t}',\mathbf{s})\bigg)\backslash\{\eta\}$$

and $\omega' \cap \mathcal{X}^s \setminus \{\mathbf{r}\} = \emptyset$. Thus (ii) is satisfied and the sets depicted in (iv) are minimal gates for the transition $\mathbf{r} \to \mathbf{s}$. \square

Proof of Theorem 3.6. Our aim is to prove that $\mathcal{G}(\mathbf{r}, \mathbf{s})$ only contains the minimal gates of Theorem 3.5. To do this, we use once again the characterization of minimal gates as essential saddles given in [35, Theorem 5.1]. Thus, our strategy is to prove that any

$$\eta \in \mathcal{S}(\mathbf{r}, \mathbf{s}) \setminus \left(\bigcup_{\mathbf{t} \in \mathcal{X}^s \setminus \{\mathbf{r}\}} \mathcal{F}(\mathbf{r}, \mathbf{t}) \cup \bigcup_{\mathbf{t}, \mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{s}\}, \mathbf{t} \neq \mathbf{t}'} \mathcal{F}(\mathbf{t}, \mathbf{t}') \cup \bigcup_{\mathbf{t}' \in \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\}} \mathcal{F}(\mathbf{t}', \mathbf{s}) \right)$$
(6.5)

is an unessential saddle. Hence, for any η as in (6.5) and for any $\omega \in (\mathbf{r} \to \mathbf{s})_{opt}$ such that $\eta \in \omega$, we have to show that both the conditions of Remark 5.2 are verified. By Lemma 5.2 and Lemma 5.1 the condition (a) of Remark 5.2 is satisfied. Next we move to prove condition (b). Let $\mathbf{t}_1, \ldots, \mathbf{t}_{m-1} \in \mathcal{X}^s$ be the stable configurations visited by ω in \mathcal{X}^s before hitting \mathbf{s} . If we set $\mathbf{t}_0 = \mathbf{r}$, $\mathbf{t}_m = \mathbf{s}$ and $\mathbf{t}_i \neq \mathbf{t}_{i+1}$ for all $i = 0, \ldots, m-1, m \in \mathbb{N}$, we may rewrite ω as the concatenation of the m paths $\omega^{(i)}: \mathbf{t}_i \to \mathbf{t}_{i+1}$. Let us assume that $\eta \in \omega^{(j)}$. Let $\omega'^{(j)} \in (\mathbf{t}_j \to \mathbf{t}_{j+1})_{opt}$ be the optimal path constructed in the proof of Theorem 3.2 such that

$$\{\operatorname{argmax}_{\omega'^{(j)}}H\}\subseteq\{\operatorname{argmax}_{\omega^{(j)}}H\}\backslash\{\eta\}$$

and $\omega'^{(j)} \cap \mathcal{X}^s \setminus \{\mathbf{t}_i, \mathbf{t}_{i+1}\} = \emptyset$. Thus we can define a path ω' such that

$$\{\operatorname{argmax}_{\omega'} H\} \subseteq \{\operatorname{argmax}_{\omega} H\} \setminus \{\eta\}$$

as the concatenation of the m paths $\omega^{(1)}, \ldots, \omega^{(j-1)}, \ldots, \omega^{(j)}, \omega^{(j+1)}, \ldots, \omega^{(m)}$. Hence, both the conditions of Remark 5.2 are satisfied and η is an unessential saddle. \square

Proof of Corollary 3.3. Since Theorem 3.5 holds, the corollary follows by [35, Theorem 5.4]. \Box

7 Restricted-tube and tube of typical paths

In this section we prove the main results on the restricted-tube of typical paths and on the tube of typical paths stated in Section 4.2.

7.1 Restricted-tube of typical paths

In order to describe the tube of typical paths for the transition from a stable state to the other stable configurations and for the transition from a stable state to an other stable configuration, we first describe a "restricted-tube" of typical paths. Indeed, we want to prove that $\mathscr{U}_{\mathbf{s}}(\mathbf{r})$ in (4.21) satisfies the following properties: it includes $\mathcal{C} \in \mathcal{M}(\mathcal{C}_{\mathbf{s}}^+(\mathbf{r}) \setminus \{\mathbf{s}\})$ that belong to at least a cycle-path $(\mathcal{C}_1, \ldots, \mathcal{C}_n) \in J_{\{\mathbf{r}\}, \{\mathbf{s}\}}, n \in \mathbb{N}$, such that $\bigcup_{i=1}^n \mathcal{C}_i \cap \mathcal{X}^s \setminus \{\mathbf{r}, \mathbf{s}\} = \varnothing$, $\mathcal{C}_1 = \mathcal{C}_{\mathbf{s}}(\mathbf{r})$ and $\mathbf{s} \in \partial \mathcal{C}_n$, see (4.1.1). More precisely, we start by studying the first descent from a trivial cycle $\{\eta\}$ for some $\xi^* \in \bar{R}_{\lfloor \frac{L}{2} \rfloor, K}(r, s)$ to \mathbf{r} , where $\lfloor n \rfloor := \max\{m \in \mathbb{Z} : m \leq n\}$. Using the symmetry of the model on Λ , we can describe similarly the first descent from the same configuration ξ^* to \mathbf{s} . Finally using reversibility, we will obtain a complete description of $\mathscr{U}_{\mathbf{s}}(\mathbf{r})$ by joining the time reversal of the first descent from $\{\xi^*\}$ to \mathbf{r} with the first discent from $\{\xi^*\}$ to \mathbf{s} .

Remark 7.1. Given a q-Potts configuration $\sigma \in \mathcal{X}$ on a grid-graph Λ , a vertex $v \in V$ and a spin value $s \in \{1, \ldots, q\}$ such that $\sigma(v) \neq s$, using (2.8) we have

$$H(\sigma) - H(\sigma^{v,s}) \in \{-4, -2, 0, 2, 4\}.$$

It follows that we can depict the principal boundary of an extended cycles \mathcal{C} in (4.16)–(4.20) is fully described by the union of those configurations $\bar{\sigma} \in \partial \mathcal{C}$ such that either

(i)
$$H(\bar{\sigma}) - H(\sigma) = -2$$
, or

(ii)
$$H(\bar{\sigma}) - H(\sigma) = -4$$
.

For sake of semplicity, we separate the description of the first descent from $\{\xi^*\}$ for some $\xi^* \in \overline{R}_{\lfloor \frac{L}{2} \rfloor, K}(r, s)$ to \mathbf{r} in more parts. We start by studying the typical trajectories followed by the process during the transition from $\{\xi^*\}$ to $\overline{R}_{2,K}(\mathbf{r}, \mathbf{s}) \subset \partial \overline{\mathcal{K}}(r, s)$, see (4.16), and then we study the typical paths followed for the first descent from $\overline{\mathcal{K}}(r, s)$ to \mathbf{r} . It is useful to remark that $\partial \mathcal{C}_{\mathbf{s}}(\mathbf{r}) \cap \overline{\mathcal{K}}(r, s) \neq \emptyset$.

Using Lemma 5.2(a) and (c), for any $i = \lfloor \frac{L}{2} \rfloor - 1, \ldots, 2$ we may define a cycle-path (C_i^0, C_i^1, C_i^2) such that

- $C_i^0 = \{ \eta_K \}$ for $\eta_K \in \bar{R}_{i+1,K}$,
- $C_i^1 = \bigcup_{j=1}^{K-1} \{\eta_j\}$ for $\eta_j \in \bar{B}_{i,K}^j$,
- $C_i^2 = {\eta_0}$ for $\eta_0 \in \bar{R}_{i,K}$,

where $\eta_{K-1}, \ldots, \eta_0$ are chosen in such a way that there exists $v \in V$ such that $\eta_i := \eta_{i+1}^{v,r}$. We note that C_i^0 and C_i^2 are non trivial cycles, while C_i^1 is a plateau. Furthermore, note that $(C_i^0, C_i^1, C_i^2) \in J_{C_i^0, C_i^2}$ since (4.6) is satisfied. Indeed, for any $i = \lfloor \frac{L}{2} \rfloor - 1, \ldots, 2$, using Lemma 5.2 we remark that for any $\sigma \in \bar{R}_{i,K}$

$$\mathscr{F}(\partial\{\sigma\}) \subset \bar{B}_{i-1,K}^{K-1} \cup \bar{B}_{i,K}^{1}.$$

Moreover, using Lemma 5.1 we also note $\{\sigma\}$ satisfies (4.2) and it follows that

$$\mathcal{B}(\{\sigma\}) = \mathcal{F}(\partial\{\sigma\}). \tag{7.1}$$

Moreover, using Lemma 5.1 and Lemma 5.2 we remark that for any $i = \lfloor \frac{L}{2} \rfloor - 1, \ldots, 2, C_i^1$ is a plateau and its principal boundary is given by

$$\mathcal{B}(\mathcal{C}_i^1) = \mathcal{C}_i^0 \cup \mathcal{C}_i^2. \tag{7.2}$$

Hence, starting from $C^0_{\lfloor \frac{L}{2} \rfloor} = \{\xi^*\}$ for some $\xi^* \in \bar{R}_{\lfloor \frac{L}{2} \rfloor,K}(r,s)$ we may depict a cycle-path vtj-connected to $C^2_2 = \{\hat{\eta}\}$ for some appropriate $\hat{\eta} \in \bar{R}_{2,K}$ as

$$(\mathcal{C}_{\lfloor \frac{L}{2} \rfloor}^{0}, \mathcal{C}_{\lfloor \frac{L}{2} \rfloor - 1}^{1}, \mathcal{C}_{\lfloor \frac{L}{2} \rfloor - 1}^{2} \equiv \mathcal{C}_{\lfloor \frac{L}{2} \rfloor - 1}^{0}, \dots, \mathcal{C}_{1}^{2} \equiv \mathcal{C}_{2}^{0}, \mathcal{C}_{2}^{1}, \mathcal{C}_{2}^{2})$$

$$(7.3)$$

Next we move to describe a cycle-path

$$(\bar{\mathcal{C}}_1, \dots, \bar{\mathcal{C}}_m) \tag{7.4}$$

vtj-connected to $\{\mathbf{r}\}$ such that $\bar{\mathcal{C}}_1 = \{\bar{\eta}^*\}$, with $\bar{\eta}^* \in \overline{\mathscr{P}}(\mathbf{r}, \mathbf{s})$ which exists in view of Lemma 5.4 and which is chosen in such a way that it is defined by a spin update in a vertex of $\hat{\eta}$. Let us begin to note that any set from (4.16) to (4.20) is an extended cycle, i.e., a maximal connected set of equielevated trivial cycles. Thus, using Remark 7.1 we prove the following lemmas on their principal boundary.

Lemma 7.1. Consider the q-state Potts model on a $K \times L$ grid Λ with periodic boundary conditions. Let $\mathbf{r}, \mathbf{s} \in \mathcal{X}^s$, $\mathbf{r} \neq \mathbf{s}$. Then,

$$\mathcal{B}(\overline{\mathcal{K}}(r,s)) = \overline{\mathcal{D}}_1(r,s) \cup \overline{\mathcal{D}}_2(r,s) \cup \overline{\mathcal{E}}_1(r,s) \cup \overline{\mathcal{E}}_2(r,s). \tag{7.5}$$

Proof. According to (4.3), we may describe the principal boundary of the extended cycle $\overline{\mathcal{K}}(r,s)$ by looking for those configurations $\bar{\sigma} \notin \overline{\mathcal{K}}(r,s)$ which communicate with some $\sigma \in \overline{\mathcal{K}}(r,s)$ by one step of the dynamics such that σ and $\bar{\sigma}$ satisfy either case (i) or case (ii) of Remark 7.1.

Let us start to consider case Remark 7.1(i). In view of (4.16), this case occurs only when σ has a spin s with three nearest-neighbor spins r and $\bar{\sigma}$ is obtained from σ by flipping from s to r this spin s. In particular, we note that $\sigma \in \overline{\mathcal{K}}(r,s)$ has such a spin s only when $\sigma \in \overline{\mathcal{K}}(r,s) \setminus [\overline{\mathcal{Q}}(\mathbf{r},\mathbf{s}) \cup \overline{\mathcal{P}}(\mathbf{r},\mathbf{s})]$, i.e., when

$$\sigma \in \overline{\mathscr{H}}(\mathbf{r}, \mathbf{s}) \cup \{ \sigma \in \mathcal{X} : \sigma(v) \in \{r, s\} \ \forall v \in V, H(\sigma) = 2K + 2 + H(\mathbf{r}), \sigma \text{ has at least two } s\text{-interacting clusters, and } R(\mathbf{C}^s(\sigma)) = R_{2 \times (K-1)} \}.$$

Hence, given $\sigma \in \overline{\mathcal{K}}(r,s)$ with a spin s, say on vertex \hat{v} , with three nearest-neighbor spins r and one nearest-neighbor spin s and defined $\bar{\sigma} := \sigma^{\hat{v},r}$, we note that

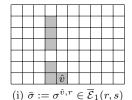
- for any $h=2,\ldots,K-2$ if $\sigma\in \bar{B}^h_{1,K-1}(r,s),$ then $\bar{\sigma}\in \bar{B}^h_{1,K-2}(r,s)\subset \overline{\mathcal{D}}_1(r,s);$
- if $\sigma \in \bar{B}_{1,K}^1(r,s)$, then $\bar{\sigma} \in \bar{R}_{1,K}(r,s) \subset \overline{\mathcal{E}}_1(r,s)$;
- if \hat{v} has its unique nearest-neighbor spin s on an adjacent column, then $\bar{\sigma} \in \overline{\mathcal{E}}_1(r, s)$, see Figure 11(i);
- if \hat{v} and its nearest-neighbor spin s lie on the same column, then $\bar{\sigma} \in \overline{\mathcal{D}}_1(r, s)$, see Figure 11(ii).

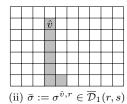
Next we move to consider case Remark 7.1(ii), that occurs only when σ has a spin s, say on vertex \hat{w} , sourrounded by four spins r and $\bar{\sigma} := \sigma^{\hat{w},r}$, i.e., when

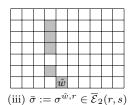
$$\sigma \in \overline{\mathcal{K}}(r,s) \setminus [\overline{\mathscr{H}}(\mathbf{r},\mathbf{s}) \cup \overline{\mathcal{Q}}(\mathbf{r},\mathbf{s}) \cup \mathscr{P}(\mathbf{r},\mathbf{s})].$$

Then, we note that

- if $R(C^s(\bar{\sigma})) = R_{1 \times (K-2)}$, i.e., if \hat{w} lies on a column where there are no other spins s, then $\bar{\sigma} \in \mathcal{E}_2(r, s)$, see Figure 11(iii);
- if $R(C^s(\bar{\sigma})) = R_{2 \times (K-3)}$, i.e., if \hat{w} lies on a column where there are other spins s, then $\bar{\sigma} \in \overline{\mathcal{D}}_2(r,s)$, see Figure 11(iv).







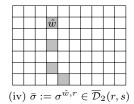


Figure 11: Examples of $\sigma \in \overline{\mathcal{K}}(r,s)$ and $\bar{\sigma} \in \mathcal{B}(\overline{\mathcal{K}}(r,s))$. We color white the vertices with spin r and gray those vertices whose spin is s.

Lemma 7.2. Consider the q-state Potts model on a $K \times L$ grid Λ with periodic boundary conditions. Let $\mathbf{r}, \mathbf{s} \in \mathcal{X}^s, \mathbf{r} \neq \mathbf{s}$. Then, for any $i = 1, \ldots, K - 4$,

$$\mathcal{B}(\overline{\mathcal{D}}_{i}(r,s)) = \overline{\mathcal{D}}_{i+1}(r,s) \cup \overline{\mathcal{D}}_{i+2}(r,s) \cup \overline{\mathcal{E}}_{i+1}(r,s) \cup \overline{\mathcal{E}}_{i+2}(r,s)$$
 (7.6)

and

$$\mathcal{B}(\overline{\mathcal{E}}_i(r,s)) = \overline{\mathcal{E}}_{i+1}(r,s) \cup \overline{\mathcal{E}}_{i+2}(r,s). \tag{7.7}$$

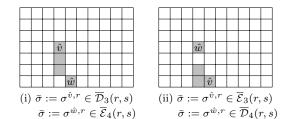
Proof. Similarly to the proof of Lemma 7.1, for any $i=1,\ldots,K-4$ we may describe the principal boundary of the extended cycles $\overline{\mathcal{D}}_i(r,s)$ and $\overline{\mathcal{E}}_i(r,s)$ by using Remark 7.1. For any $i=1,\ldots,K-4$, let us start to study the principal boundary of $\overline{\mathcal{D}}_i(r,s)$. Case Remark 7.1(i) occurs only when $\sigma\in\overline{\mathcal{D}}_i(r,s)$ has a spin s, say on vertex \hat{v} with three nearest-neighbor spins r and one nearest-neighbor spin s and $\bar{\sigma}:=\sigma^{\hat{v},r}$. Then, we note that

- if \hat{v} its unique nearest-neighbor spin s on an adjacent column, then $R(\mathbf{C}^s(\bar{\sigma})) = R_{1\times(K-(i+1))}$ and $\bar{\sigma}\in\overline{\mathcal{E}}_{i+1}(r,s)$, see Figure 12(ii);
- if \hat{v} and its nearest-neighbor spin s lie on the same column, then $R(C^s(\bar{\sigma})) = R_{2 \times (K (i+2))}$ and $\bar{\sigma} \in \overline{\mathcal{D}}_{i+1}(r,s)$, see Figure 12(i).

Regarding case Remark 7.1(ii), it occurs only when σ has a spin s, say on vertex \hat{w} , sourrounded by four spins r and $\bar{\sigma} := \sigma^{\hat{w},r}$. It follows that,

- if $R(C^s(\bar{\sigma})) = R_{1 \times (K (i+2))}$, i.e., if \hat{w} lies on a column where there are no other spins s, then $\bar{\sigma} \in \overline{\mathcal{E}}_{i+2}(r,s)$, see Figure 12(i);
- if $R(C^s(\bar{\sigma})) = R_{2 \times (K (i+3))}$, i.e., if \hat{w} lies on a column where there are other spins s, then $\bar{\sigma} \in \overline{\mathcal{D}}_{i+2}(r,s)$, see Figure 12(ii).

For any $i=1,\ldots,K-4$, next we move to describe the principal boundary of $\overline{\mathcal{E}}_i(r,s)$. Case Remark 7.1(i) occurs when $\sigma \in \overline{\mathcal{E}}_i(r,s)$ has a spin s, say on vertex \hat{v} , with three nearest-neighbor spins r and one nearest-neighbor spin s and $\bar{\sigma}:=\sigma^{\hat{v},r}$. Hence, $\bar{\sigma} \in \overline{\mathcal{E}}_{i+1}(r,s)$, see Figure 12(ii). Instead case Remark 7.1(ii) occurs only when σ has a spin s, say on vertex \hat{w} , sourrounded by four spins r and $\bar{\sigma}:=\sigma^{\hat{w},r}$. Thus $\bar{\sigma} \in \overline{\mathcal{E}}_{i+2}(r,s)$, see Figure 12(iv). \Box



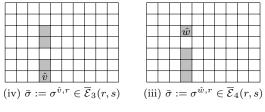


Figure 12: Examples of $\sigma \in \overline{\mathcal{D}}_2(r,s)$ and $\bar{\sigma} \in \mathcal{B}(\overline{\mathcal{D}}_2(r,s))$ in (i) and (ii); examples of $\sigma \in \overline{\mathcal{E}}_2(r,s)$ and $\bar{\sigma} \in \mathcal{B}(\overline{\mathcal{E}}_2(r,s))$ in (iii) and (iv). We color white the vertices with spin r and gray those vertices whose spin is s.

Lemma 7.3. Consider the q-state Potts model on a $K \times L$ grid Λ with periodic boundary conditions. Let $\mathbf{r}, \mathbf{s} \in \mathcal{X}^s$, $\mathbf{r} \neq \mathbf{s}$. Then,

$$\mathcal{B}(\overline{\mathcal{D}}_{K-3}(r,s)) = \overline{\mathcal{D}}_{K-2}(r,s) \cup \overline{\mathcal{E}}_{K-2}(r,s) \cup \overline{R}_{1,1}(\mathbf{r},\mathbf{s}), \tag{7.8}$$

$$\mathcal{B}(\overline{\mathcal{E}}_{K-3}(r,s)) = \overline{\mathcal{E}}_{K-2}(r,s) \cup \overline{R}_{1,1}(r,s) \tag{7.9}$$

and

$$\mathcal{B}(\overline{\mathcal{D}}_{K-2}(r,s)) = \mathcal{B}(\overline{\mathcal{E}}_{K-2}(r,s)) = \overline{R}_{1,1}(r,s). \tag{7.10}$$

Proof. First of all, we note that from (4.19) and (4.20) we have

$$\overline{\mathcal{D}}_{K-2}(r,s) = \bar{R}_{2,1}(r,s) \quad \text{and} \quad \overline{\mathcal{E}}_{K-2}(r,s) = \bar{R}_{1,2}(r,s).$$
 (7.11)

For i = K - 3, K - 2 once again we describe the principal boundary of the extended cycles $\overline{\mathcal{D}}_i(r,s)$ and $\overline{\mathcal{E}}_i(r,s)$ by using Remark 7.1.

Let us start to study the principal boundary of $\overline{\mathcal{D}}_{K-3}(r,s)$. Case Remark 7.1(i) takes place if σ has a spin s, say on vertex \hat{v} , with three nearest-neighbor spins r and one nearest-neighbor spin s and $\bar{\sigma} := \sigma^{\hat{v},r}$. Hence, it occurs only when $\sigma \in \bar{B}^1_{1,2}(r,s)$ and either $\bar{\sigma} \in \overline{\mathcal{D}}_{K-2}(r,s)$ or $\bar{\sigma} \in \overline{\mathcal{E}}_{K-2}(r,s)$, see Figure 13(i) and (ii).

Instead case Remark 7.1(ii) occurs when σ has only two spins s and they lie on the diagonal of a rectangle $R_{2\times 2}$, i.e., when $\bar{\sigma}$ is obtained by flipping from s to r one of these two spins s and $\bar{\sigma} \in \bar{R}_{1,1}(r,s)$, see Figure 13(iii).

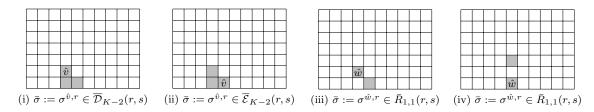


Figure 13: Examples of $\sigma \in \overline{\mathcal{D}}_{K-3}(r,s)$ and $\bar{\sigma} \in \mathcal{B}(\overline{\mathcal{D}}_{K-3}(r,s))$. We color white the vertices with spin r and gray those vertices whose spin is s.

Next we move to describe the principal boundary of $\overline{\mathcal{E}}_{K-3}(r,s)$. Case Remark 7.1(ii) occurs when $\sigma \in \overline{\mathcal{E}}_{K-3}(r,s)$ has a spin s, say on vertex \hat{v} , with three nearest-neighbor spins r and one nearest-neighbor spin s and $\bar{\sigma} := \sigma^{\hat{v},r}$. Hence, when $\sigma \in \overline{\mathcal{R}}_{1,3}(r,s)$ and $\bar{\sigma} \in \overline{\mathcal{E}}_{K-2}(r,s)$. Finally, case Remark 7.1(ii) is verified when $\sigma \in \overline{\mathcal{E}}_{K-3}(r,s)$ has two spins s with four nearest-neighbor spins r and one of them is flipped to r, i.e., when $\bar{\sigma} \in \overline{\mathcal{R}}_{1,1}(r,s)$, see Figure 13(iv).

To conclude it is enough to see that (7.10) follows by Remark 7.1 and (7.11). Indeed, both $\overline{\mathcal{D}}_{K-2}(r,s)$ and $\overline{\mathcal{E}}_{K-2}(r,s)$ are characterized by configurations in which there are two spins s with three nearest-neighbor spins r and by flipping from s to r one of these spins we obtain a configuration belonging to their principal boundary. \square

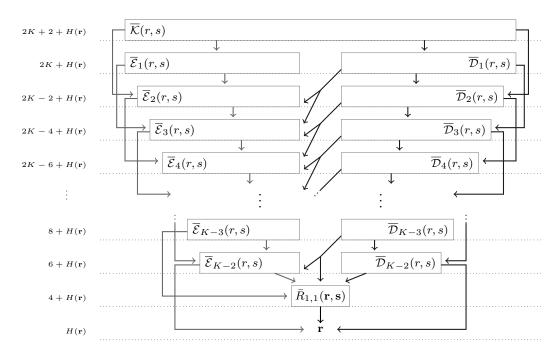


Figure 14: Illustration of the first descent from $\overline{\mathcal{K}}(r,s)$ to \mathbf{r} . The rectangles denote extended cycles, i.e., the sets of trivial equielevated cycles.

Thanks to the Lemmas 7.1, 7.2 and 7.3 we obtain that for every $i = m, \ldots, n-1$, the cycle-path (7.4) is characterized by a sequenze of cycles and extended cycles $\bar{C}_1, \ldots, \bar{C}_m$ such that

$$\bar{\mathcal{C}}_1, \dots, \bar{\mathcal{C}}_m \subset \overline{\mathcal{K}}(r,s) \cup \bigcup_{i=1}^{K-2} (\overline{\mathcal{D}}_i(r,s) \cup \overline{\mathcal{E}}_i(r,s)) \cup \bar{R}_{1,1}(r,s)$$

and $\bar{\mathcal{C}}_m = \{\mathbf{r}\}$. More precisely, using Lemmas 7.1, 7.2 and 7.3 we can say that $(\bar{\mathcal{C}}_1, \dots, \bar{\mathcal{C}}_m) \in J_{\bar{\mathcal{C}}_1,\bar{\mathcal{C}}_m}$. Indeed, it is easy to check that for any pair of consecutive cycles the condition (4.6) is satisfied. Arguing similarly, we may construct a vtj-path from $\{\xi^*\}$ to $\{\mathbf{s}\}$, i.e., we may construct the following

$$(\mathcal{C}^0_{\lfloor \frac{L}{2} \rfloor}, \mathcal{C}^1_{\lfloor \frac{L}{2} \rfloor + 1}, \mathcal{C}^2_{\lfloor \frac{L}{2} \rfloor + 1} \equiv \mathcal{C}^0_{\lfloor \frac{L}{2} \rfloor + 1}, \dots, \mathcal{C}^2_{L - 2} \equiv \mathcal{C}^0_{L - 1}, \mathcal{C}^1_{L - 1}, \mathcal{C}^2_{L - 1})$$

from $\{\xi^*\}$ to $\tilde{\eta} \in \tilde{R}_{L-2,K}(r,s)$ and $(\tilde{\mathcal{C}}_1,\ldots,\tilde{\mathcal{C}}_m)$ for the first descent from $\tilde{\eta}^* \in \widetilde{\mathcal{P}}(\mathbf{r},\mathbf{s})$ to $\{\mathbf{s}\}$.

Proof of Theorem 4.1. According to the discussion above and using reversibility, we may depict the restricted-tube of typical paths between $\bf r$ and $\bf s$ as in (4.21). Instead, (4.22) follows by [39, Lemma 3.13].

7.2 Tube of typical paths from a stable state to the other stable states

Proof of Theorem 4.2. We may generalize the discussion concerning the restricted-tube of typical paths, we may depict the tube of typical paths between \mathbf{r} and $\mathcal{X}^s \setminus \{\mathbf{r}\}$ as in (4.23). Instead, (4.24) follows by [39, Lemma 3.13]. \square

7.3 Tube of typical paths from a stable state to another stable state

Proof of Theorem 4.3. We may generalize the discussion concerning the restricted-tube of typical paths, we may depict the tube of typical paths between \mathbf{r} and \mathbf{s} as in (4.25). Instead, (4.26) follows by [39, Lemma 3.13].

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