On the essential features of metastability: tunnelling time and critical configurations

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Abstract

We consider Metropolis Markov chains with finite state space and transition probabilities of the form

$$P(\eta, \eta') = q(\eta, \eta') e^{-\beta [H(\eta') - H(\eta)]_+}$$

for given energy function H and symmetric Markov kernel q. We propose a simple approach to determine the asymptotic behavior, for large β, of the first hitting time to the ground state starting from

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a particular class of local minima for H called metastable states. We separate the asymptotic behavior of the transition time from the determination of the tube of typical paths realizing the transition. This approach turns out to be useful when the determination of the tube of typical paths is too difficult, as for instance in the case of conservative dynamics. We analyze the structure of the saddles introducing the notion of "essentiality" and describing essential saddles in terms of "gates". As an example we discuss the case of the 2D Ising Model in the degenerate case of integer $\frac{2J}{h}$.
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1 Introduction and preliminary discussion.

In recent years an increasing interest has been addressed to the rigorous study of metastability in the framework of the “pathwise approach” (see [7], [29])). After the pioneering papers [25], [26], that refer to Glauber dynamics for standard 2D Ising model, in finite volume and very low temperature, several other models have been considered, in the same asymptotic regime (see [17], [18], [11], [23], [2], [8], [9], [10], [15], [16]), aiming to describe various aspects of the transition from metastability to stability. From a physical point of view, these works refer to the study of local aspects of nucleation of the stable phase, at very low temperature. Mathematically, the metastable behavior in this regime is related to the first exit problem, from suitable domains, for a class of Freidlin-Wentzell (F-W) Markov chains (see [12], page 176). These are characterized by a finite state space and transition probabilities that are exponentially small in a large parameter β (representing, in many applications, the inverse temperature). Other, perhaps more interesting, asymptotic regimes have also been considered, like infinite volume at very low temperature (see [13], [14],[20],[21]), or fixed low temperature at very small magnetic field (see [31], [34]).

We refer to [30], [29] for a general rigorous discussion of metastability.

From the point of view of general probability theory, the first exit problem in the Freidlin Wentzell regime is nowadays well understood. A good control of the first exit time and of typical exit paths is possible in terms of the exponential rates in β of the transition probabilities via large deviation theory. While the general strategy is well known, in many applications relevant for statistical mechanics, the specific model-dependent problems are far from being solved.

In other words, the general theory is not applicable in many concrete cases, since the needed detailed control on the specific Markov chain is too difficult to obtain. This fact reopens the problem also from the point of view of the general theory, making important to understand what is the minimal information on the process that is necessary to obtain each specific result.

In this note we discuss this problem and we propose a simple approach to the study of metastability for general Metropolis Markov chains, having in mind applications to stochastic dynamics for lattice spin systems. This allows to extract from the full description of the process the most relevant information about the tunnelling time and the critical configurations by only requiring a rough analysis of the energy landscape. This approach has been recently used in some cases of conservative stochastic evolution like 3D Kawasaki dynamics (see [16]) or the anisotropic version of 2D Kawasaki dynamics (see [24]), where the conservation law makes the mechanism of decay from metastability more subtle. Here we want to systematically describe our strategy within a critical discussion of results and tools commonly used in the study of metastability. We will use the simple and well known case of Glauber-Metropolis dynamics for standard 2D Ising model, as an example to explain our approach.

Let us introduce the setup: We consider ergodic aperiodic Markov chains with finite state space $\mathcal{X}$ and transition probabilities $P(\eta,\eta')$ satisfying the detailed balance condition

$$\mu(\eta)P(\eta,\eta') = \mu(\eta')P(\eta',\eta), \tag{1.1}$$

with respect to the Gibbs measure

$$\mu(\eta) = \frac{e^{-\beta H(\eta)}}{\sum_{\eta' \in \mathcal{X}} e^{-\beta H(\eta')}}, \tag{1.2}$$

with $H : \mathcal{X} \to \mathbb{R}$ an assigned energy function.

For simplicity we consider the Metropolis choice: for $\eta' \neq \eta$ we take

$$P(\eta', \eta) = q(\eta', \eta) e^{-\beta [H(\eta) - H(\eta')]_+}, \tag{1.3}$$

where $[\cdot]_+$ denotes the positive part and $q(\eta', \eta)$ is a connectivity matrix independent of β.

We will denote by σ_t^η the Markov chain at time $t \in \mathbb{N}$ starting from η at $t = 0$.

In this context, the problem of metastability is the study of the first arrival of the process $\sigma_t^{\eta_0}$ to the stable state η^s, corresponding to the absolute minimum of H, (or to the set $\mathcal{X}^s$ of absolute minima of H) when starting from an initial local minimum η_0: we speak of *tunnelling* between η_0 and η^s.

Local minima can be ordered in terms of their increasing *stability level* i.e., the height of the barrier separating them from lower energy states. A particularly relevant case is when η_0 turns out to be in the set $\mathcal{X}^m$ of local minima of maximal stability in $\mathcal{X} \setminus \mathcal{X}^s$, also called set of "metastable states" (see (2.12) below). The study of the transition between $\mathcal{X}^m$ and $\mathcal{X}^s$ constitutes the most typical metastability problem. However, we want to stress that, establishing that a given local minimum η_0 is a metastable state (in the above sense) is one of the main points to be settled when studying the tunnelling between η_0 and $\mathcal{X}^s$.

For $\eta \in \mathcal{X}$, $\mathcal{A} \subseteq \mathcal{X}$, let

$$\tau_{\mathcal{A}}^\eta := \min\{t > 0; \, \sigma_t^\eta \in \mathcal{A}\} \tag{1.4}$$

be the first hitting time to $\mathcal{A}$ for the process σ_t^η starting from η. We call $\tau_{\mathcal{X}^s}^{\eta_0}$ *tunnelling time*.

There are, mainly, two different aspects in the problem of the decay from η_0 to $\mathcal{X}^s$:

1. The asymptotic behavior for large β of the tunnelling time, expressed as

$$\lim_{\beta\to\infty} \mathbb{P}(e^{(\Gamma-\varepsilon)\beta} \leq \tau_{\mathcal{X}^s}^{\eta_0} \leq e^{(\Gamma+\varepsilon)\beta}) = 1, \tag{1.5}$$

   for a suitable $\Gamma > 0$ and arbitrary $\varepsilon > 0$. Clearly, this corresponds to the convergence in probability (as $\beta \to \infty$) of the random variables $X_\beta := \frac{1}{\beta}\ln(\tau_{\mathcal{X}^s}^{\eta_0})$ to Γ as β tends to infinity. It is also interesting to analyze the asymptotic behavior in $\mathcal{L}^1$ and in law (with a proper normalization).

2. The tube of typical paths realizing the tunnelling.

   To describe the typical transition pattern during the first excursion between η_0 and $\mathcal{X}^s$, we are interested in determining the minimal tube of paths going for the first time from η_0 to $\mathcal{X}^s$, still having a probability exponentially close to one.

The general approach to the first exit problem for F-W Markov chains ([12], [6], [27] [28], [32]) is based on the notion of *cycle*, i.e., a maximal connected component of the set of states lying below a given energy (see 2.7 for a formal definition). A cycle $\mathcal{C}$ is characterized by the property that, with a probability exponentially close to one, starting from any state $\eta \in \mathcal{C}$, our process visits every state in $\mathcal{C}$ before exiting from $\mathcal{C}$. It is possible to control the asymptotic behavior, for large β, of the first exit time from a cycle, in probability, in $\mathcal{L}^1$ and in law, in terms of the *depth* of the cycle, i.e., the difference between the minimal energy in the external boundary $\partial\mathcal{C}$ (i.e. the set in $\mathcal{C}^c$ connected to $\mathcal{C}$ in one step of the dynamics) and the energy of the ground state of the cycle. Moreover, it is also possible to give significant estimates on the probability distribution of the first exit state (see Theorem 2.17 below).

By regarding single states as trivial cycles, given a set $\mathcal{A} \subset \mathcal{X}$, we can consider the decomposition of the set $\mathcal{X}\backslash\mathcal{A}$ into maximal cycles. A sequence of cycles of this decomposition, in which each cycle is connected with the following one in the sequence, is called a *cycle-path*. It is natural to associate to a given cycle-path a tube of trajectories (of single states) defined as the set of trajectories visiting the ordered sequence of cycles given by the cycle-path. Cycle-paths describe tubes of trajectories in which only the sequence of visited cycles is fixed while the time spent in each cycle, and the corresponding piece of trajectory in the cycle, is somehow free.

In [6], the notion of cycle-path has been introduced and developed in the general non reversible case, and large deviation principles have been proved for cycle-paths.

A cycle-path is called *downhill* if the *height* of the cycles (i.e. the minimal energy on their boundary) is non-increasing. In [27] particular sets of downhill cycle-paths, called "standard cascades" are introduced and it is shown that they define, via time-reversal, the tube of typical trajectories exiting from a given cycle.

An alternative construction of typical first-exit cycle-paths is obtained in [28] for the general non reversible case, starting from the renormalization procedure in [32]. This procedure was introduced in order to describe phenomena taking place in suitable, exponentially increasing, time scales. For this purpose a complete classification of the states in $\mathcal{X}$ was introduced, in terms of increasing stabilities, related to the increasing time-scales. Starting from this classification, a sequence of renormalized Markov chains, corresponding to the sequence of time scales, was introduced and, in [28], paths of the renormalized chain were associated to cycle-paths.

By using cycles and cycle-paths one can study the tunnelling time and the tube of typical tunnelling paths. Indeed, let $\mathcal{C}(\eta_0)$ be the maximal cycle containing η_0 such that $\mathcal{C}(\eta_0) \cap \mathcal{X}^s = \emptyset$. We will call *escape time* the first exit time $\tau^{\eta_0}_{(\mathcal{C}(\eta_0))^c}$ from the cycle $\mathcal{C}(\eta_0)$.

Obviously, the escape time is smaller than the tunnelling time. In order to study the escape time we can use well developed results about the first exit from cycles (see Theorem 2.17 below), giving, in this way, a lower estimate of the tunnelling time. On the other hand, an upper estimate easily follows once we know that, after the escape time, with high probability for large β, the process hits $\mathcal{X}^s$ in a relatively short time. So, we get that escape and tunnelling times are of the same order, once we are able to prove that, with high probability for large β, the cycles visited by the process σ_t for $t \in (\tau^{\eta_0}_{(\mathcal{C}(\eta_0))^c}, \tau^{\eta_0}_{\mathcal{X}^s})$ have a depth smaller than or equal to the one of $\mathcal{C}(\eta_0)$. This is not true in general: in the case of the dynamical Blume-Capel model, for suitable values of the parameters (see [11]), it happens that the process, after escaping from $\mathcal{C}(\eta_0)$, typically visits very deep wells (deeper than $\mathcal{C}(\eta_0)$) so that the asymptotics of the tunnelling time is exponentially larger (in β), than the one of the escape time.

This suggests two possible ways of proving that escape and tunnelling times are of the same order: the first one requires the total absence of deep wells in the whole space $\mathcal{X}$; the second one needs a good control on the tube $\mathcal{T}$ of typical paths[1] exiting from $\mathcal{C}(\eta_0)$ where the process typically stays confined and requires that $\mathcal{T}$ does not contain deep wells. The first way involves a global control on the energy landscape, everywhere in $\mathcal{X}$, while the second one involves a detailed knowledge of the typical trajectories realizing the transition.

The second way was adopted in many previous works on metastability and, indeed, the lack of a global control of deep wells was the main reason why in the previous approaches to metastability the two issues of the asymptotics and the tube of typical paths were strictly connected. As we will discuss later on, the presence of deep wells can induce different asymptotics in probability and in $\mathcal{L}^1$.

We are now at the main point of the problem: How to construct, for a concrete model, the cycle $\mathcal{C}(\eta_0)$? how to find the tube of typical paths reaching $\mathcal{X}^s$? In other words, even if general tools to study metastability are well developed, there is a highly non trivial model-dependent problem to solve, in order to apply the general results on cycles and cycle-paths, when discussing a concrete example.

Let us describe the basic features of the approach commonly used in previous works on metastability. In [17], [18], [11], [23], [9], [10], $\mathcal{X}^s$ consists of a unique state, η_s and an important step is to find a special set of states $\mathcal{D}$, representing in practice the *subcritical* states, i.e. initial states starting from which the process visits η_0 before η^s, with high probability. The process, while performing the tunnelling, has to cross, with high probability, the boundary of $\mathcal{D}$ in a particular set of states, say $\mathcal{P}$, where the energy equals the communication height (see (2.5)) between η_0 and η^s.

[1] i.e. the set of cycle–paths typically followed during the tunnelling.

Successively, it goes towards η^s, following a well defined family of trajectories, never being trapped inside deep cycles, so that the descent to η^s is relatively fast.

The set of trajectories realizing this descent can be described in terms of a downhill cycle-path $\mathcal{C}_1, \ldots, \mathcal{C}_n$ starting from $\mathcal{C}_1 \equiv \mathcal{C}(\eta_0)$ and ending in a cycle $\mathcal{C}_n$ connected to $\mathcal{X}_s$. A complete control of typical paths from $\mathcal{P}$ to $\mathcal{X}_s$ amounts to know all downhill cycle-paths emerging from $\mathcal{C}(\eta_0)$.

We can say that the approach above heavily relies on a precise knowledge of the set $\mathcal{P}$ (that represents a narrow gate for the transition from η_0 to η^s) and of all typical future evolutions starting from *any* state in $\mathcal{P}$. In other words we need to know in detail the tube of typical trajectories going from $\mathcal{P}$ to η^s .

A different strategy was used in [2], to find the asymptotics in probability of the tunnelling time and the tube of typical paths. This strategy is based on the analysis of the state space by means of its foliation into manifolds at fixed number of plus spins. By looking at the minimal energy barrier between contiguous manifolds, one obtains a control of the energy landscape sufficient to find $\mathcal{C}(\eta_0)$ and the tube of typical paths. This kind of model-dependent discussion is sufficiently simple in cases, as the isotropic Glauber dynamics, where there are strong symmetries in the problem, but becomes much more complicated in more general cases (we will discuss this point in more detail in the final section).

Both these strategies require a very detailed knowledge of the energy landscape; however, only a local analysis is needed around the typical tube and no global control.

It is clear that without controlling the deep wells outside the tube, it is impossible to conclude about the asymptotic behavior of the tunnelling time in $\mathcal{L}^1$. Indeed, it is possible that with a small probability the process visits a very deep well outside the tube, in such a way that, the asymptotics in $\mathcal{L}^1$ becomes strictly larger than the one in probability. This is possible when the probability to visit a deep well times the excess waiting time is sufficiently large.

In the final section of this paper we will discuss in more detail these approaches in connection with the ideas developed in the present paper.

In this note we discuss the different model-dependent inputs necessary to obtain the different results and propose a simpler approach to solve the problem of the asymptotics of the exit time and find partial results about the tube. This approach is related to some of the ideas developed in [32]. An important ingredient there, was a recurrence property of the process on the set of states of a given stability in the corresponding exponentially long time scale. In the present paper we do not need the whole detailed analysis developed in [32] but we still exploit the idea of proving a global recurrence to a suitable set of states. Indeed we show that absence of deep wells has the effect of partially separating the problem of the asymptotics from the problem of the typical tube. The absence of deep wells here is obtained by proving a global recurrence. Indeed the total absence of deep wells is equivalent to saying that η_0 is a metastable state since the depth of $\mathcal{C}(\eta_0)$ is the maximal depth of the cycles not intersecting $\mathcal{X}^s$.

We will show that to study the tunnelling time, starting from a state η_0, it is sufficient (i) to solve the global min-max problem, i.e. to find the height of the energy barrier between η_0 and $\mathcal{X}^s$ and (ii) to prove that for any state $\eta \notin \{\eta_0\} \cup \mathcal{X}^s$ the energy barrier towards lower energy states is lower than the energy barrier between η_0 and $\mathcal{X}^s$, which is equivalent to saying that $\eta_0 \in \mathcal{X}^m$. This means that we are able to separate the control of the tunnelling time (i.e. point 1) from the much more difficult control of the tube of typical paths (i.e. point 2).

Recurrence property actually gives a control on the distribution tail of the tunnelling time which implies the property of uniform integrability, necessary to give also a control of the asymptotic behavior in $\mathcal{L}^1$. In this sense, we can say that with our approach the model-dependent input is minimized.

We observe that inputs (i) and (ii) (together with some additional non-degeneracy assumptions) correspond to the hypotheses required in [5], to apply the general method introduced in [3] to Glauber dynamics. This method is based on a very sharp control of the Laplace transforms of the tunnelling times and does not even take into account the description of typical trajectories. As we will see in section 6.3, the results obtained in [3], [5] are restricted to the tunnelling times and are for some respects stronger than those obtained with our method. The relationship between the two strategies is interesting by itself and we will come back to the topic in the final section.

In the framework of our pathwise approach it is natural to study the typical trajectories realizing the tunnelling between η_0 and $\mathcal{X}^s$. These can be described at different levels of detail, corresponding to different levels of detail in the analysis of the energy landscape.

A central role in this description is played by the *optimal paths*, i.e. the set of paths realizing the minimal value of the maximal energy in the paths going from η_0 to $\mathcal{X}^s$.

A first basic notion is the set of *saddles* $\mathcal{S}$ defined as the set of all maxima in the optimal paths between η_0 and $\mathcal{X}^s$. In this note, we focus on the subsets of saddles that are typically visited during the last excursion from η_0 to $\mathcal{X}^s$. To this end, we introduce the *gates* from metastability to stability, defined as the subsets of $\mathcal{S}$ that are visited by all the optimal paths.

We will see that the process, while performing the tunnelling, is likely to follow one of the optimal paths. Therefore, gates are subsets of $\mathcal{S}$ that are typically visited during the tunnelling.

The configurations in the *minimal gates* (minimal by inclusion) have the physical meaning of "critical configurations" and are central objects both from a probabilistic and from a physical point of view.

The structure of the minimal gates and their geometrical characterization is therefore a crucial point in the description of the typical trajectories. On the other hand, the hypotheses needed to discuss the gates are weaker than the ones necessary to completely characterize the tube of typical paths.

We remark that in several models analyzed in the literature in the context of F-W Markov chains, the minimal gate was unique but, in general, there may exist many minimal sets with the gate property, either distinct or overlapping. In the present paper we shall analyze in detail the set of minimal gates in some examples, without assuming, like in [5], additional non–degeneracy hypothesis, that simplify the structure of the gates.

It is clear that a crucial point in this analysis is to find out the minimality of a given gate. To this end, we will provide a sufficient criterion in section 5.

We provide also a characterization of the set $\mathcal{G} \subset \mathcal{S}$, defined as the union of minimal gates, in terms of *essential saddles*. These are defined as the states in $\mathcal{S}$ that cannot be avoided with a short-cut of an optimal path (where a short-cut of a path ω is a path ω' whose set of maxima is a subset of the set of maxima in ω).

As an example to illustrate the treatment of gates, we will discuss in detail the 2D Ising model in the high degenerate case corresponding to $2J/h$ integer. In this case we will find the set of all essential saddles and its decomposition into minimal gates, revealing a quite complicated structure (see fig. 4, page 53).

The analysis of the properties of the minimal gates becomes particularly interesting when related to the results about the pre-factors of the mean tunnelling time given in [5]. This is an open problem posed by our analysis and, though not completely solved in the present paper, it is widely discussed in the final section. From this discussion, we can conclude, quite surprisingly, that unessential saddles, not characterizing the typical behavior of the process, may contribute to the pre-factors and that a weaker notion of essentiality is needed to control the $\mathcal{L}_1$ estimates.

The rest of the paper is organized as follows:

- In Section 2 we give definitions and preliminary results.
- In section 3 we study "recurrence property":
  - In Theorem 3.1 we show that for any $V > 0, \varepsilon > 0$, uniformly in the starting state, the process typically visits within time $e^{\beta(V+\varepsilon)}$ the set of local minima with "stability level" larger than or equal to V (see (2.9));
  - In Corollary 3.5 we discuss the implications of Theorem 3.1 on uniform integrability.

- We use these results to control the tunnelling time, between a metastable state and the set of stable states, in terms of the stability level of the metastable states:
  - In Theorem 4.1 we control the tunnelling time in probability;
  - In Theorem 4.9 we give the corresponding result in $\mathcal{L}_1$;
  - In Theorem 4.15, under the additional hypothesis of uniqueness of the metastable state, we show that the (suitably normalized) tunnelling time converges in law to a mean one exponential random variable.
- In order to implement these model–independent results in a specific case, we give in Section 4.2 a general method to compute the communication height and to verify that a specific state is metastable.
- As an example, we apply this method to the case of 2-d Ising model with Metropolis dynamics in Section 4.3.
- In order to give a partial characterization of the tube of typical paths realizing the tunnelling, we discuss in Section 5 the notions of minimal gate and essential saddle:
  - In Theorem 5.1 we relate these two concepts;
  - In Theorem 5.4 we show that the process typically visits the gates during the tunnelling.
- Our strategy to give a decomposition into minimal gates of the set of essential saddles is based on:
  - a necessary and sufficient condition for a gate to be minimal, given in Section 5.3;

    - a necessary condition for a saddle to be essential, given in Proposition 5.8.

- In Section 5.4 we apply this strategy to study the 2-d Ising model with Metropolis dynamics; in the degenerate case ($2J/h$ integer) we find a surprisingly rich structure of the minimal gates.

- In Section 6 we relate our results with other approaches:

    - In Section 6.1 we compare our new approach with previous ones, discussing in detail why the problems of the tunnelling time and of the tube of typical paths were interconnected;

    - In Section 6.2 we remark the differences between Glauber and Metropolis dynamics;

    - In Section 6.3 we relate our results about gates with the results in [5]about pre-factors of the mean tunnelling time; we propose a conjecture that should be useful to give a weaker notion of essentiality that characterizes the pre-factors.

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2 Definitions and preliminary results.

We need some definitions.

- A **path** is a sequence $\omega = (\omega_1, \dots, \omega_k)$, $k \in \mathbb{N}$, $\omega_i \in \mathcal{X}$ for $i = 1, \dots, k$, such that $q(\omega_i, \omega_{i+1}) > 0$ for $i = 1, \dots, k-1$.

  We write $\omega\colon\ \eta \to \eta'$ to denote a path from η to η'.

  Given $\zeta \in \mathcal{X}$, we write $\zeta \in \omega$ when ω visits ζ.

- A set $\mathcal{A} \subseteq \mathcal{X}$ with $|\mathcal{A}| > 1$ is **connected** if and only if for all $\eta, \eta' \in \mathcal{A}$ there exists a path $\omega\colon\ \eta \to \eta'$ such that $\omega_i \in \mathcal{A}$ for all i. Every singleton is connected.

  We use $A \subset B$ to mean A strictly contained in B.

- Given a non-empty set $\mathcal{A} \subset \mathcal{X}$, define its (external) **boundary** as

$$\partial\mathcal{A} := \{\zeta \notin \mathcal{A}\colon\ q(\zeta, \eta) > 0 \text{ for some } \eta \in \mathcal{A}\} \tag{2.1}$$

  and its internal boundary as

$$\partial^{-}\mathcal{A} := \partial(\mathcal{A}^c), \tag{2.2}$$

  where $\mathcal{A}^c := \mathcal{X} \setminus \mathcal{A}$.

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

$$\mathcal{F}(\mathcal{A}) = \Big\{\eta \in \mathcal{A}\colon\ H(\eta) = \min_{\zeta \in \mathcal{A}} H(\zeta)\Big\}. \tag{2.3}$$

- For a set $\mathcal{A}$ whose points have the same energy, we denote (by an abuse of notation) this energy by $H(\mathcal{A})$.

- Given a function $f : \mathcal{X} \to \mathbb{R}$ and a subset $\mathcal{A} \subseteq \mathcal{X}$, we denote by

$$\arg\max\nolimits_{\mathcal{A}} f := \Big\{\eta \in \mathcal{A} :\ f(\eta) = \max_{\xi \in \mathcal{A}} f(\xi)\Big\} \tag{2.4}$$

  the set of points where the maximum of f in $\mathcal{A}$ is reached.

- The **communication height** between a pair $\eta, \eta' \in \mathcal{X}$ is

$$\Phi(\eta, \eta') = \min_{\omega:\ \eta \to \eta'} \max_{\zeta \in \omega} H(\zeta). \tag{2.5}$$

  Given two non-empty sets $\mathcal{A}, \mathcal{B} \subseteq \mathcal{X}$, put

$$\Phi(\mathcal{A}, \mathcal{B}) = \min_{\eta \in \mathcal{A},\, \eta' \in \mathcal{B}} \Phi(\eta, \eta') \tag{2.6}$$

- A **non-trivial cycle** is a connected set $\mathcal{C}$ such that

$$\max_{\sigma \in \mathcal{C}} H(\sigma) < H(\mathcal{F}(\partial \mathcal{C})). \tag{2.7}$$

  Any singleton that is not a non-trivial cycle is called **trivial cycle**.

- The following structure Lemma is a well-known fact (see e.g. [27] Prop. 3.2):

  Lemma 2.8 For any pair of cycles $\mathcal{C}$, $\mathcal{C}'$ such that $\mathcal{C} \cap \mathcal{C}' \neq \emptyset$, either $\mathcal{C} \subseteq \mathcal{C}'$ or $\mathcal{C} \supset \mathcal{C}'$.

- We call **stability level** of a state $\zeta \in \mathcal{X}$ the energy barrier

$$V_\zeta := \Phi(\zeta, \mathcal{I}_\zeta) - H(\zeta) \tag{2.9}$$

  where $\mathcal{I}_\zeta$ is the set of states with energy below $H(\zeta)$:

$$\mathcal{I}_\zeta := \Big\{ \eta \in \mathcal{X} :\ H(\eta) < H(\zeta) \Big\} \tag{2.10}$$

  We set $V_\zeta := \infty$ if $\mathcal{I}_\zeta$ is empty.

- We call **stability level of a state** $\zeta \in \mathcal{X}$ **in a set** $\mathcal{A}$ the energy barrier

$$V_\zeta^{\mathcal{A}} := \Phi(\zeta, \mathcal{I}_\zeta \cap \mathcal{A}) - H(\zeta), \tag{2.11}$$

  setting $V_\zeta^{\mathcal{A}} := \infty$ if $\mathcal{I}_\zeta \cap \mathcal{A}$ is empty.

- The set $\mathcal{X}^s := \mathcal{F}(\mathcal{X})$ of the global minima of the hamiltonian is called set of **stable states**.

- The set of **metastable states** is given by

$$\mathcal{X}^m := \{\eta \in \mathcal{X} : \quad V_\eta = \max_{\zeta \in \mathcal{X} \setminus \mathcal{X}^s} V_\zeta\} \tag{2.12}$$

- We call **metastable set at level** V the set of all states with stability level larger than V:

$$\mathcal{X}_V := \{\eta \in \mathcal{X} : \quad V_\eta > V\}. \tag{2.13}$$

  We denote by Γ the stability level of the states in $\mathcal{X}^m$.

- The **depth** of a cycle $\mathcal{C}$ is given by

$$D(\mathcal{C}) := [H(\mathcal{F}(\partial\mathcal{C})) - H(\mathcal{F}(\mathcal{C}))]_+. \tag{2.14}$$

- For a non-trivial cycle $\mathcal{C}$, we set $U(\mathcal{C}) := \mathcal{F}(\partial\mathcal{C})$; for a trivial cycle $\mathcal{C}$, we set $U(\mathcal{C}) := \mathcal{C}$. We call $H(U(\mathcal{C}))$ **height** of the cycle $\mathcal{C}$.

- We call **maximal internal resistance** $\Theta(\mathcal{C})$ the maximal depth of the sub-cycles of $\mathcal{C}$ that do not contain the whole $\mathcal{F}(\mathcal{C})$:

$$\Theta(\mathcal{C}) := \max_{\substack{\text{cycles } \mathcal{C}' \subset \mathcal{C}; \\ \mathcal{C}' \not\supset \mathcal{F}(\mathcal{C})}} D(\mathcal{C}') \tag{2.15}$$

An immediate consequence of the definition of cycles is that for any η, η' in a given cycle $\mathcal{C}$

$$\Phi(\eta, \eta') < \Phi(\mathcal{C}, \mathcal{C}^c) \tag{2.16}$$

It is possible to show that this implies that, with probability exponentially close to one, every state in the cycle is visited before the exit from the cycle, and that the exit time is of order $e^{\beta D(\mathcal{C})}$. More precisely, the main result of [27] Prop. 3.7 is contained in the following

Theorem 2.17 Let us consider a non–trivial cycle $\mathcal{C}$ and let $D := D(\mathcal{C})$ be its depth. For any $\eta \in \mathcal{C}$, $\xi \in \partial\mathcal{C}$ $\varepsilon, \varepsilon' > 0$, $\delta \in (0, \varepsilon)$, for $\tau^{\eta}_{\partial\mathcal{C}}$ as in (1.4), and all sufficiently large β

$$\mathbb{P}\left(\tau^{\eta}_{\partial\mathcal{C}} < e^{\beta(D+\varepsilon)}\ ;\ \tau^{\eta}_{\partial\mathcal{C}} = \tau^{\eta}_{\xi}\right) \geq e^{-\beta(H(\xi)-H(U(\mathcal{C}))+\varepsilon')} \tag{2.18}$$

$$\mathbb{P}\left(\tau^{\eta}_{\partial\mathcal{C}} > e^{\beta(D-\varepsilon)}\right) \geq 1 - e^{-\beta\delta} \tag{2.19}$$

Moreover there exists $\kappa > 0$ such that for all $\eta, \eta' \in \mathcal{C}$ and all sufficiently large β:

$$\mathbb{P}\left(\tau^{\eta}_{\eta'} < \tau^{\eta}_{\partial\mathcal{C}}\right) \geq 1 - e^{-\beta\kappa}. \tag{2.20}$$

See [27] for the proof; see also [12], [28], [6] for similar results.

We need here some other definitions.

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

$$\mathcal{S}(\eta,\eta') = \Big\{\zeta \in \mathcal{X} :\ \ \exists\omega : \eta \to \eta',\ \omega \ni \zeta :\ \ \max_{\xi\in\omega} H(\xi) = H(\zeta) = \Phi(\eta,\eta')\Big\}. \tag{2.21}$$

$$\mathcal{S}(\mathcal{A},\mathcal{B}) = \bigcup_{\substack{\eta\in\mathcal{A},\ \eta'\in\mathcal{B}:\\ \Phi(\eta,\eta')=\Phi(\mathcal{A},\mathcal{B})}} \mathcal{S}(\eta,\eta'). \tag{2.22}$$

- We write

$$(\mathcal{A} \to \mathcal{B})_{opt} \tag{2.23}$$

  to denote the **set of optimal paths** i.e. the set of all paths from $\mathcal{A}$ to $\mathcal{B}$ realizing the min-max in $\mathcal{X}$ between $\mathcal{A}$ and $\mathcal{B}$.

- Given a pair $\eta, \eta' \in \mathcal{X}$, we say that $\mathcal{W} \equiv \mathcal{W}(\eta,\eta')$ is a **gate** for the transition $\eta \to \eta'$ if $\mathcal{W}(\eta,\eta') \subseteq \mathcal{S}(\eta,\eta')$ and $\omega \cap \mathcal{W} \neq \emptyset$ for all $\omega \in (\eta \to \eta')_{opt}$.

- We say that $\mathcal{W}$ is a **minimal gate** for the transition $\eta \to \eta'$ if it is a gate and for any $\mathcal{W}' \subset \mathcal{W}$ there exists $\omega' \in (\eta \to \eta')_{opt}$ such that $\omega' \cap \mathcal{W}' = \emptyset$. In words, a minimal gate is a minimal (by inclusion) subset of $\mathcal{S}(\eta, \eta')$ that is visited by all optimal paths.

  For a given pair η, η', there may be several disjoint minimal gates. We denote by $\mathcal{G}(\eta, \eta')$ the union of all the minimal gates:

$$\mathcal{G}(\eta, \eta') = \bigcup_{\mathcal{W}:\ \mathcal{W} \text{ minimal gate for } (\eta,\eta')} \mathcal{W}. \tag{2.24}$$

  Obviously, $\mathcal{G}(\sigma, \sigma') \subseteq \mathcal{S}(\sigma, \sigma')$ and $\mathcal{S}(\sigma, \sigma')$ is a gate (but in general it is not minimal). The configurations $\zeta \in \mathcal{S}(\eta, \eta') \setminus \mathcal{G}(\eta, \eta')$ (if any) are called **dead-ends**.

- A saddle $\zeta \in \mathcal{S}(\eta, \eta')$ is called **unessential** if for any $\omega \in (\eta \to \eta')_{opt}$ such that $\omega \cap \zeta \neq \emptyset$ we have $\{\arg\max_\omega H\} \setminus \{\zeta\} \neq \emptyset$ and there exists $\omega' \in (\eta \to \eta')_{opt}$ such that $\{\arg\max_{\omega'} H\} \subseteq \{\arg\max_\omega H\} \setminus \{\zeta\}$ (see (2.4) for the definition of $\arg\max$).

- A saddle $\zeta \in \mathcal{S}(\eta, \eta')$ is called **essential** if it is not unessential, i.e. if either

  (i) there exists $\omega \in (\eta \to \eta')_{opt}$ such that $\{\arg\max_\omega H\} = \{\zeta\}$ or

  (ii) there exists $\omega \in (\eta \to \eta')_{opt}$ such that $\{\arg\max_\omega H\} \supset \{\zeta\}$ and $\{\arg\max_{\omega'} H\} \not\subseteq \{\arg\max_\omega H\} \setminus \{\zeta\}$ for all $\omega' \in (\eta \to \eta')_{opt}$.

- Given $\mathcal{A} \subset \mathcal{X}$ and $\eta \in \mathcal{X} \setminus \mathcal{A}$, we consider the sets

$$\mathcal{C}_{\mathcal{A}}(\eta) := \eta \cup \Big\{\zeta :\ \Phi(\eta, \zeta) < \Phi(\eta, \mathcal{A})\Big\}. \tag{2.25}$$

  These sets are either trivial cycles coinciding with η (in case $\Phi(\eta, \mathcal{A}) = H(\eta)$) or non-trivial cycles containing η (in case $\Phi(\eta, \mathcal{A}) > H(\eta)$).

Notice that $H(U(\mathcal{C}_{\mathcal{A}}(\eta))) \equiv \Phi(\eta, \mathcal{A})$ and that $\mathcal{C}_{\mathcal{A}}(\eta) \subseteq \mathcal{X} \setminus \mathcal{A}$. We immediately see that if $\eta' \in \mathcal{C}_{\mathcal{A}}(\eta)$ then $\mathcal{C}_{\mathcal{A}}(\eta') = \mathcal{C}_{\mathcal{A}}(\eta)$.

Lemma 2.26 Given $\mathcal{A} \subset \mathcal{X}$, the sets $\left\{\mathcal{C}_{\mathcal{A}}(\eta)\right\}_{\eta \in \mathcal{X} \setminus \mathcal{A}}$ in (2.25) form the partition into maximal cycles of $\mathcal{X} \setminus \mathcal{A}$:

$$\bigcup_i \mathcal{C}_i = \mathcal{X} \setminus \mathcal{A}, \;\; \mathcal{C}_i \cap \mathcal{C}_j = \emptyset \; \forall i \neq j \text{ and } \; \forall i \; \exists \eta \text{ s.t. } \mathcal{C}_i = \mathcal{C}_{\mathcal{A}}(\eta). \tag{2.27}$$

Proof. It is immediate to see that for any $\zeta \in \mathcal{X} \setminus \mathcal{A}$, $\zeta \in \mathcal{C}_{\mathcal{A}}(\zeta)$. We know by Lemma 2.8, that two overlapping cycles either coincide or are included into each other. Thus, to conclude the proof it is sufficient to show that $\mathcal{C}_{\mathcal{A}}(\eta)$ are maximal cycles in $\mathcal{X} \setminus \mathcal{A}$. For, suppose $\mathcal{C}'$ be a cycle strictly containing $\mathcal{C}_{\mathcal{A}}(\eta)$, we necessarily have $\mathcal{C}' \cap \mathcal{A} \neq \emptyset$, contradicting the fact that $\mathcal{C}' \subset \mathcal{X} \setminus \mathcal{A}$. Indeed, $\mathcal{C}'$ contains a point ζ in $\partial \mathcal{C}_{\mathcal{A}}(\eta)$ with $H(\zeta) \geq \Phi(\eta, \mathcal{A})$ and every optimal path $\omega \in (\eta \to \mathcal{A})_{opt}$ is contained in $\mathcal{C}'$, since $H(U(\mathcal{C}')) > \Phi(\eta, \mathcal{A})$ and $\mathcal{C}' \ni \eta$.

□

We refer to [6] for a definition of decomposition into maximal cycles in a more general setting.

- A sequence of cycles $\mathcal{C}_0, \ldots, \mathcal{C}_n$ is called **downhill cycle-path** if the cycles are pairwise connected with decreasing height; namely, such that $H(U(\mathcal{C}_i)) \geq H(U(\mathcal{C}_{i+1}))$ for each $i \in \{0, \ldots, n-1\}$. Notice that the predecessor and the successor of a non-trivial cycle in a cycle path must be trivial cycles.

  Notice that the probability that the process exiting from $\mathcal{C}_i$ goes to $\mathcal{C}_{i+1}$ is not exponentially small: when $\mathcal{C}_i$ is a non–trivial cycle this fact can be seen by using Theorem 2.17, if $\mathcal{C}_i$ is a trivial cycle, it is a direct consequence of the definition of the dynamics.

The key property of the partition in (2.27) is that, any $\mathcal{C}_0$ in the partition can be joined with $\mathcal{A}$ by a downhill cycle-path made of cycles in the partition.

Lemma 2.28 For any $\eta \in \mathcal{X}$ and $\mathcal{A} \subset \mathcal{X}$, there exists a finite downhill cycle-path $\mathcal{C}_0, \ldots, \mathcal{C}_n$ such that $\eta \in \mathcal{C}_0$ and $\mathcal{C}_n$ is a singleton in $\mathcal{A}$.

Proof. We consider the case where $\eta \notin \mathcal{A}$, otherwise there is nothing to prove. We give an algorithm to construct the aforementioned downhill cycle-path by using the partition in (2.27). More precisely, we construct a path $\omega : \eta \to \mathcal{A}$ by joining pieces of optimal paths $\omega^{(i)} \in (\eta_i \to \eta_{i+1})_{opt}$ for suitably defined $\{\eta_i\}_{i\in\mathbb{N}}$. The sets $\mathcal{C}_\mathcal{A}(\eta_i)$ will form our downhill cycle-path:

1. SET $\eta_0 := \eta$
2. pick a self-avoiding[2] optimal path $\omega^{(1)} \in (\eta_0 \to \mathcal{A})_{opt}$
3. FOR $i \geq 1$
4. SET $\eta_i := \omega_k^{(i)}$, where $k := \min\{n : \omega_n^{(i)} \notin \mathcal{C}_\mathcal{A}(\eta_{i-1})\}$
5. IF $\eta_i \in \mathcal{A}$, STOP
6. IF $\Phi(\eta_i, \mathcal{A}) = \Phi(\eta_{i-1}, \mathcal{A})$, THEN
   $\omega_n^{(i+1)} := \omega_{k+n}^{(i)}$;
   ELSE
   pick a self-avoiding optimal path $\omega^{(i+1)} \in (\eta_i \to \mathcal{A})_{opt}$

[2] Self-avoiding paths can be obtained from general paths by removing the loops in the order they appear.

7. NEXT i

The key point in this construction is that we keep using the same path until the communication height $\Phi(\eta_{i+1}, \mathcal{A})$ changes; since self-avoiding paths are finite, condition 6. can hold for a finite number of indices i for each of these paths. When changing the path, $\Phi(\eta_{i+1}, \mathcal{A})$ must decrease since η_i and η_{i+1} belong to the same optimal path $\omega^{(i)} \in (\eta_i \to \mathcal{A})_{opt}$, implying

$$\Phi(\eta_i, \mathcal{A}) = \max\left\{\Phi(\eta_i, \eta_{i+1}), \Phi(\eta_{i+1}, \mathcal{A})\right\} \geq \Phi(\eta_{i+1}, \mathcal{A}). \qquad (2.29)$$

By the finiteness of $\mathcal{X}$ and the monotonicity of $\Phi(\eta_i, \mathcal{A})$, we see that the whole sequence of cycles $\{\mathcal{C}_{\mathcal{A}}(\eta_i)\}_i$ is finite.

□

- A function $\beta \to f(\beta)$ is called **super-exponentially small** (SES) if

$$\lim_{\beta\to\infty} \frac{1}{\beta} \log f(\beta) = -\infty \qquad (2.30)$$

2.1 The Ising model.

We will use the standard 2D Ising model with Metropolis dynamics as an example to clarify our approach. Let us give some definitions:

- For $x = (x_1, x_2) \in \mathbb{Z}^2$, we will use the norms $||x||_n := (|x_1|^n + |x_2|^n)^{\frac{1}{n}}$ and $||x||_\infty := \max_{i=1,2} |x_i|$.

- Let Λ be a two dimensional torus with a sufficiently large side-length L. A configuration is a function $\sigma : \Lambda \to \{-1, +1\}$. With each configuration $\sigma \in \mathcal{X}_I := \{-1, +1\}^\Lambda$ we associate an energy given by the Hamiltonian

$$E(\sigma) := -\frac{J}{2} \sum_{\substack{\{x,y\}\subset\Lambda: \\ ||x-y||_1=1}} \sigma(x)\sigma(y) - \frac{h}{2}\sum_{x\in\Lambda}\sigma(x), \tag{2.31}$$

We take the external magnetic field $\frac{h}{2} > 0$ and $J > 0$.

We set

$$H(\sigma) := E(\sigma) - E(-\mathbf{1}) \tag{2.32}$$

- The dynamics is defined via the Metropolis algorithm given in (1.3), where $q(\sigma, \eta)$, for all $\sigma \neq \eta$, is

$$q(\sigma,\eta) := \begin{cases} \frac{1}{|\Lambda|} & \text{if } \exists x \in \Lambda : \sigma^x = \eta, \\ 0 & \text{otherwise} \end{cases} \tag{2.33}$$

where

$$\sigma^x(z) = \begin{cases} \sigma(z) & \text{if } z \neq x, \\ -\sigma(x) & \text{if } z = x. \end{cases} \tag{2.34}$$

- Let

$$N^+(\sigma) = \sum_{x\in\Lambda} \frac{\sigma(x)+1}{2} \tag{2.35}$$

be the number of plus spins in the configuration σ.

- Given a configuration $\sigma \in \mathcal{X}_I$, consider the set $C(\sigma) \subseteq \mathbb{R}^2$ defined as the union of the closed unit cubes centered at sites x such that $\sigma(x) = 1$. The maximal connected components $C_1, \dots, C_m$, $m \in \mathbb{N}$, of $C(\sigma)$ are called **clusters** of σ. We often identify σ with $C(\sigma)$.

- We denote by ∂C the boundary of C as a subset of the two dimensional torus of side length L in $\mathbb{R}^2$. For $\sigma \in \mathcal{X}_I$, let $\gamma(\sigma) = \bigcup_{i=1}^m \partial C_i$ be the **boundary** of σ and $|\gamma(\sigma)| := \sum_{i=1}^m |\partial C_i|$ the **perimeter** of σ. $|\gamma(\sigma)|$ equals the number of pairs of n.n. sites with opposite spin in σ. It is immediate to see that the energy of a configuration in the Ising model is

$$H(\sigma) = J|\gamma(\sigma)| - hN^+(\sigma). \tag{2.36}$$

- $-\mathbf{1}, \mathbf{1}$ are respectively the configurations in which all the spins have value -1, $+1$.

3 Recurrence to $\mathcal{X}_V$.

A crucial property of our Markov chains is that with probability super-exponentially close to one, starting from any point in $\mathcal{X}$ the process visits $\mathcal{X}_V$ (the metastable set at level V defined in (2.13)) within a time of order $e^{\beta V}$. We will prove this result in Theorem 3.1, by using Theorem 2.17.

This recurrence property can be considered the key ingredient of our results on metastability.

Theorem 3.1 For any $\varepsilon > 0$ and sufficiently large β

$$\sup_{\eta \in \mathcal{X}} \mathbb{P}\left(\tau^{\eta}_{\mathcal{X}_V} > e^{\beta(V+\varepsilon)}\right) = \text{SES} \tag{3.2}$$

Proof.

We use the partition in (2.27) with $\mathcal{A} = \mathcal{X}_V$ and Lemma 2.28 to show that there exists a finite downhill cycle-path from $\mathcal{C}_{\mathcal{X}_V}(\eta)$ to $\mathcal{X}_V$. Since none of the cycles in the downhill cycle-path can contain states in $\mathcal{X}_V$, all these cycles have depth not larger than V.

By using Theorem 2.17 we get that the probability to reach $\mathcal{X}_V$ within $e^{\beta(V+\varepsilon/2)}$ is uniformly larger than $e^{-\beta\varepsilon'}$ for any $\varepsilon' > 0$ and sufficiently large β. Indeed, the cycles in the downhill cycle-path are pairwise connected in such a way that the probability to pass from an element of the cycle-path to the following one, within a time $e^{\beta(V+\varepsilon/4)}$, is larger than $e^{-\beta\varepsilon''}$ for any $\varepsilon'' > 0$ and sufficiently large β; moreover, their number is bounded independently of β by $|\mathcal{X}|$. So that by Theorem 2.17 we get

$$\mathbb{P}\left(\tau^{\eta}_{\mathcal{X}_V} < e^{\beta(V+\frac{\varepsilon}{2})}\right) \geq e^{-\beta\varepsilon'} \tag{3.3}$$

A standard iteration of this estimate (based on Markov property) proves (3.2):

$$\mathbb{P}\left(\tau^{\eta}_{\mathcal{X}_V} > e^{\beta(V+\varepsilon)}\right) \leq \left(\sup_{\eta'\notin\mathcal{X}_V} \mathbb{P}\left(\tau^{\eta'}_{\mathcal{X}_V} > e^{\beta(V+\frac{\varepsilon}{2})}\right)\right)^{e^{\beta\frac{\varepsilon}{2}}} = \text{SES}. \tag{3.4}$$

□

An immediate consequence of the previous theorem, applied to $V = \Gamma := V_{\mathcal{X}^m}$, is the following:

Corollary 3.5 For any $\delta > 0$, the variables $Y^{\eta}_{\beta} := \tau^{\eta}_{\mathcal{X}^s} e^{-(\Gamma+\delta)\beta}$ are uniformly integrable that is, there exists β_0 sufficiently large such that for any $\varepsilon > 0$ there exists $K \in [0, \infty)$ such that for any $\beta > \beta_0$

$$\sup_{\eta\in\mathcal{X}} \mathbb{E}\left(Y^{\eta}_{\beta}\mathbf{1}_{\{Y^{\eta}_{\beta}>K\}}\right) < \varepsilon \tag{3.6}$$

Proof. It is sufficient to have an exponential control on the tail of the distribution:

$$\sup_{\eta\in\mathcal{X}} \mathbb{P}(\tau^{\eta}_{\mathcal{X}^s} e^{-(\Gamma+\delta)\beta} > n) < 2^{-n} \tag{3.7}$$

for any sufficiently large β. This estimate can be obtained as in (3.4), since $\mathcal{X}_{\Gamma} = \mathcal{X}^s$ and $\forall\delta > 0$

$$\sup_{\eta\in\mathcal{X}} \mathbb{P}(\tau^{\eta}_{\mathcal{X}^s} e^{-(\Gamma+\delta)\beta} > n) \leq \left(\sup_{\eta'\notin\mathcal{X}^s} \mathbb{P}\left(\tau^{\eta'}_{\mathcal{X}^s} > e^{(\Gamma+\delta)\beta}\right)\right)^{n} < 2^{-n}, \tag{3.8}$$

where we used Theorem 3.1 to get the last inequality. □

Remark 3.9 We note that it is possible to prove a recurrence result similar to theorem 3.1 also if we consider the recurrence to a given state in $\mathcal{X}^s$. This is important when studying the tunnelling problem between stable states. More precisely, let $\eta_1 \in \mathcal{X}^s$ and let $\Theta = \Theta(\mathcal{X})$ the maximal internal resistance defined in 2.15. By using Lemma 2.28 and the arguments of proof of Theorem 3.1, we can prove that

$$\sup_{\eta \in \mathcal{X}} \mathbb{P}\left(\tau_{\eta_1}^{\eta} > e^{\beta(\Theta+\varepsilon)}\right) = \mathrm{SES} \tag{3.10}$$

for any $\varepsilon > 0$ and β sufficiently large.

4 Asymptotics of tunnelling time.

In this section we give results on the asymptotics of the tunnelling time. We first obtain general results and then we discuss how to apply them to concrete models. We conclude this section by discussing the example of the Ising model.

4.1 General results.

We study the tunnelling time $\tau_{\mathcal{X}^s}^{\eta_0}$ by giving results in probability (in Theorem 4.1 and Theorem 4.5), on the asymptotics of the expectation (in Theorem 4.9) and on the convergence in law (in Theorem 4.15).

Notice that in some cases where a global description of the energy landscape is not given it is still possible to give results in probability, but neither in law nor in $\mathcal{L}_1$.

Let us first consider the case $\eta_0 \in \mathcal{X}^m$.

Theorem 4.1 Let $\eta_0 \in \mathcal{X}^m$ and $\Gamma := V_{\eta_0}$ Then, for any $\delta > 0$, there exist β_0 and $K > 0$ such that for any $\beta > \beta_0$

$$\mathbb{P}\left(\tau^{\eta_0}_{\mathcal{X}^s} < e^{\beta(\Gamma-\delta)}\right) < e^{-K\beta} \tag{4.2}$$

$$\mathbb{P}\left(\tau^{\eta_0}_{\mathcal{X}^s} > e^{\beta(\Gamma+\delta)}\right) = \mathrm{SES} \tag{4.3}$$

Proof. (4.2) is a consequence of (2.19) when $\mathcal{C} = \{\xi : \Phi(\xi, \eta_0) < \Phi(\eta_0, \mathcal{X}^s)\}$, since $\tau^{\eta_0}_{\mathcal{X}^s} > \tau^{\eta_0}_{\partial\mathcal{C}}$.

(4.3) is just a particular case of Theorem 3.1 when $V = \Gamma$. In this case $\mathcal{X}_V$ coincides with $\mathcal{X}^s$. $\square$

Remark 4.4 As noted at the end of the previous section, in the case of several stable states, we can obtain a similar result for the tunnelling time $\tau^{\eta_0}_{\eta_1}$ between stable states η_0, η_1, by substituting Γ with the maximal internal resistance $\Theta(\mathcal{X})$.

In some cases, where a global characterization of the metastable sets is missing, we can use a slightly weaker version of Theorem 4.1. The idea is to control stable and metastable states only locally. More precisely, suppose to be able to find a *habitat*, defined as a set $\mathcal{A}$ such that there exist $K_{\mathcal{A}} > 0$, $\beta_0 > 0$ such that for any $\eta \in \mathcal{A} \setminus \mathcal{F}(\mathcal{A})$ and $\mathbb{P}\left(\tau^{\eta}_{\mathcal{F}(\mathcal{A})} < \tau^{\eta}_{\partial\mathcal{A}}\right) \geq 1 - e^{-K_{\mathcal{A}}\beta}$ for all $\beta > \beta_0$. Notice that, by definitions (2.9) and (2.11), for any η in a habitat $\mathcal{A}$ either $V^{\mathcal{A}}_{\eta} = \infty$ or $V^{\mathcal{A}}_{\eta} = V_{\eta}$. Indeed, if $V^{\mathcal{A}}_{\eta} > V_{\eta}$, we immediately see that the cycle $\mathcal{C}_{\mathcal{I}_\eta \cap \mathcal{A}}(\eta)$ has non–empty intersection with $\mathcal{I}_\eta \cap \mathcal{A}^c$. By Theorem 2.17 $\mathbb{P}(\tau^{\eta}_{\mathcal{F}(\mathcal{C}_{\mathcal{I}_\eta\cap\mathcal{A}}(\eta))} < \tau^{\eta}_{\mathcal{I}_h \cap \mathcal{A}}) \to 1$, contradicting the definition of habitat. Examples of habitats are given by basins of attraction, cycles and suitable sets of downhill cycle paths.

Theorem 4.5 Let $\mathcal{A}$ be a habitat and let $V(\mathcal{A}) := \max_{\eta \in \mathcal{A}\setminus F(\mathcal{A})} V^{\mathcal{A}}_{\eta}$ be the maximal stability level in $\mathcal{A}$. Let $\eta \in \mathcal{A}$ with $V^{\mathcal{A}}_{\eta} = V(\mathcal{A})$.

Then, for some $\kappa > 0$ and β sufficiently large

$$\mathbb{P}\left(e^{\beta(V(\mathcal{A})-\varepsilon)} < \tau^{\eta}_{\mathcal{F}(\mathcal{A})} < e^{\beta(V(\mathcal{A})+\varepsilon)}\right) \geq 1 - e^{-\beta\kappa} \tag{4.6}$$

that is, η "plays the role of a metastable state relatively to $\mathcal{A}$".

Proof. Let us start to prove that $\mathbb{P}\left(\tau^{\eta}_{\mathcal{F}(\mathcal{A})} \geq e^{\beta(V+\varepsilon)}\right)$ is exponentially small. The proof is very similar to that of Theorem 3.1.

$$\begin{aligned} \mathbb{P}\left(\tau^{\eta}_{\mathcal{F}(\mathcal{A})} > e^{\beta(V+\varepsilon)}\right) \quad \leq \quad & \mathbb{P}\left(\tau^{\eta}_{\mathcal{F}(\mathcal{A})} = \tau^{\eta}_{\mathcal{F}(\mathcal{A})\cup\partial\mathcal{A}} > e^{\beta(V+\varepsilon)}\right) + \\ & \mathbb{P}\left(\tau^{\eta}_{\partial\mathcal{A}} < \tau^{\eta}_{\mathcal{F}(\mathcal{A})}\right). \end{aligned} \tag{4.7}$$

By Lemma 2.28, there exists $\delta > 0$ such that

$$\mathbb{P}\left(\tau^{\zeta}_{\mathcal{F}(\mathcal{A})} < \tau^{\zeta}_{\partial\mathcal{A}}\ ;\ \tau^{\zeta}_{\mathcal{F}(\mathcal{A})} < e^{\beta(V+\frac{\varepsilon}{2})}\right) \geq e^{-\beta\delta}. \tag{4.8}$$

Hence, a standard iteration argument like in (3.4) shows that the first term in (4.7) is super-exponentially small; the second one is the leading term and it is exponentially small by definition of habitat.

On the other hand, since for any ξ in $\mathcal{F}(\mathcal{A})$ the depth of $\mathcal{C}_\xi(\eta)$ is V, by (2.19) we see that $\mathbb{P}(\tau^{\eta}_{\mathcal{F}(\mathcal{A})} < e^{\beta(V-\varepsilon)}) \leq \mathbb{P}(\tau^{\eta}_{\partial\mathcal{C}_\xi(\eta)} < e^{\beta(V-\varepsilon)}) \leq e^{-\beta\delta}$ for any $\delta \in (0,\varepsilon)$ and sufficiently large β. $\square$

A different characterization of the tunnelling time is given by the following Theorem:

Theorem 4.9 For any $\eta_0 \in \mathcal{X}^m$,

$$\lim_{\beta\to\infty} \frac{1}{\beta} \log \mathbb{E}\tau^{\eta_0}_{\mathcal{X}^s} = \Gamma \tag{4.10}$$

Proof. By theorem 4.1 we know that, for each $\delta > 0$, the variables $Y_\beta := \tau^{\eta}_{\mathcal{X}^s} e^{-(\Gamma+\delta)\beta}$ tend to zero in probability, moreover by Corollary 3.5

they are uniformly integrable. This implies that they tend to zero also in $\mathcal{L}^1$, that is

$$\mathbb{E}(|Y_\beta^{\eta_0}|) \to 0. \tag{4.11}$$

Hence, there exists β_0 such that for any $\beta > \beta_0$

$$\mathbb{E}\tau_{\mathcal{X}^s}^{\eta_0} < e^{(\Gamma+\delta)\beta}. \tag{4.12}$$

The estimate

$$\mathbb{E}\tau_{\mathcal{X}^s}^{\eta_0} > e^{(\Gamma-\delta)\beta}, \tag{4.13}$$

valid for any $\delta > 0$ and sufficiently large β, immediately follows by theorem 4.1 since

$$\mathbb{E}\tau_{\mathcal{X}^s}^{\eta_0} > e^{(\Gamma-\delta)\beta}\mathbb{P}(\tau_{\mathcal{X}^s}^{\eta_0} > e^{(\Gamma-\delta)\beta}) \geq e^{(\Gamma-\delta)\beta}(1-e^{-K\beta}). \tag{4.14}$$

By using that δ is arbitrary, by (4.12) and (4.13) we obtain (4.10).

$\square$

We remark that in the previous Theorem the hypothesis $\eta_0 \in \mathcal{X}^m$ (often called "absence of deep wells") is not necessary and can be easily substituted by η_0 is such that $\forall \eta \notin \mathcal{X}^s$ with $V_\eta > V_{\eta_0},\ H(\eta) > H(\eta_0)$ that can be called "absence of dangerous wells". This property is also "global" since it requires the analysis of the whole energy landscape.

Theorem 4.15 Suppose there exists a state η_0, such that $T_\beta := \inf\{n \geq 1 :\ \mathbb{P}\left(\tau_{\mathcal{X}^s}^{\eta_0} \leq n\right) \geq 1-e^{-1}\}$ tends to infinity with β. Moreover suppose that there exist T'_β and δ_β such that for all $\eta \in \mathcal{X}$

$$\mathbb{P}(\tau_{\{\eta_0,\mathcal{X}^s\}}^{\eta} > T'_\beta) \leq \delta_\beta \quad \text{with} \quad \lim_{\beta\to\infty}\frac{T'_\beta}{T_\beta} = 0 \quad \text{and} \quad \lim_{\beta\to\infty}\delta_\beta = 0, \tag{4.16}$$

then, for any $\delta > 0$,

$$\lim_{\beta\to\infty} \mathbb{P}(\tau^{\eta_0}_{\mathcal{X}^s} > tT_\beta) = e^{-t} \tag{4.17}$$

and

$$\lim_{\beta\to\infty} \frac{\mathbb{E}(\tau^{\eta_0}_{\mathcal{X}^s})}{T_\beta} = 1 \tag{4.18}$$

Proof.

Let $\tau^*(t) := \inf\{s \geq tT_\beta : \ \sigma_s \in \{\eta_0, \mathcal{X}^s\}\}$ be the first hitting time to $\{\eta_0, \mathcal{X}^s\}$ after tT_β.

$$\begin{aligned}
&\mathbb{P}\left(\tau^{\eta_0}_{\mathcal{X}^s} > (t+s)T_\beta\right) = \\
&\mathbb{P}\left(\tau^{\eta_0}_{\mathcal{X}^s} > (t+s)T_\beta \ ; \ \tau^*(t) \leq tT_\beta + T'_\beta\right) + \mathbb{P}\left(\tau^{\eta_0}_{\mathcal{X}^s} > (t+s)T_\beta \ ; \ \tau^*(t) > tT_\beta + T'_\beta\right) \\
&\ \text{r.h.s of (4.19)} = \\
&\sum_{u=0}^{T'_\beta} \mathbb{P}\left(\tau^*(t) = tT_\beta + u \ ; \ \tau^{\eta_0}_{\mathcal{X}^s} > tT_\beta + u\right) \mathbb{P}\left(\tau^{\eta_0}_{\mathcal{X}^s} > sT_\beta - u\right) + \\
&\sum_{\eta \in \{\eta_0, \mathcal{X}^s\}^c} \mathbb{P}\left(\tau^{\eta_0}_{\mathcal{X}^s} > tT_\beta \ ; \ \sigma_{tT_\beta} = \eta\right) \mathbb{P}\left(\tau^{\eta}_{\mathcal{X}^s} > sT_\beta \ ; \ \tau^{\eta}_{\{\eta_0, \mathcal{X}^s\}} > T'_\beta\right),
\end{aligned} \tag{4.19}$$

where we used Markov property at time $tT_\beta + u$, and the fact that $\tau^{\eta_0}_{\mathcal{X}^s} > \tau^*(t)$ implies $\sigma_{\tau^*(t)} = \eta_0$.

Clearly, by (4.16),

$$\begin{aligned}
&\text{l.h.s. of (4.19)} \geq \\
&\left[\mathbb{P}\left(\tau^{\eta_0}_{\mathcal{X}^s} > tT_\beta + T'_\beta\right) - \mathbb{P}\left(\tau^{\eta_0}_{\mathcal{X}^s} > tT_\beta + T'_\beta \ ; \ \tau^*(t) > tT_\beta + T'_\beta\right)\right] \mathbb{P}\left(\tau^{\eta_0}_{\mathcal{X}^s} > sT_\beta\right) \geq \\
&\left[\mathbb{P}\left(\tau^{\eta_0}_{\mathcal{X}^s} > tT_\beta + T'_\beta\right) - \delta_\beta\right] \mathbb{P}\left(\tau^{\eta_0}_{\mathcal{X}^s} > sT_\beta\right)
\end{aligned} \tag{4.20}$$

and

$$\text{l.h.s. of (4.19)} \leq \mathbb{P}\left(\tau^{\eta_0}_{\mathcal{X}^s} > tT_\beta\right) \left[\mathbb{P}\left(\tau^{\eta_0}_{\mathcal{X}^s} > sT_\beta - T'_\beta\right) + \delta_\beta\right]. \tag{4.21}$$

Let β_0 be such that $T'_\beta \leq T_\beta$ for all $\beta \geq \beta_0$. Thus for any integer $k \geq 2$ we write

$$\mathbb{P}(\tau^{\eta_0}_{\mathcal{X}^s} > (k+2)T_\beta) \leq \mathbb{P}(\tau^{\eta_0}_{\mathcal{X}^s} > kT_\beta)(\delta_\beta + \mathbb{P}(\tau^{\eta_0}_{\mathcal{X}^s} > T_\beta)) \tag{4.22}$$

and taking $r := 2e^{-1}$ we may assume that $\delta_\beta + \mathbb{P}(\tau^{\eta_0}_{\mathcal{X}^s} > T_\beta) \leq \delta_\beta + e^{-1} \leq r < 1$, for each $\beta \geq \beta_0$. Thus, for each $\beta \geq \beta_0$ and each $k \geq 3$ we get

$$\mathbb{P}\big(\tau^{\eta_0}_{\mathcal{X}^s} > kT_\beta\big) \leq r^{[k/2]} \tag{4.23}$$

which immediately implies the tightness of the family $\{\tau^{\eta_0}_{\mathcal{X}^s}/T_\beta\}$, on $[0,+\infty)$. Let us call ϑ_β the family of random variables $\frac{\tau^{\eta}_{\mathcal{X}^s}}{T_\beta}$.

From (4.21) it follows that if the random variable $\hat{\vartheta}$ is the limit in distribution of a subsequence ϑ_{β_k} then

$$\mathbb{P}(\hat{\vartheta} > t+s) = \mathbb{P}(\hat{\vartheta} > t)\mathbb{P}(\hat{\vartheta} > s) \tag{4.24}$$

for any $s, t > 0$ which are continuity

points

for the distribution of $\tau^{\eta_0}_{\mathcal{X}^s}$. From the density of such points, and the right-continuity of the distribution function, we conclude the validity of (4.24) for all $s, t \geq 0$, and consequently that $\mathbb{P}(\hat{\vartheta} > t) = e^{-at}$, for all $t > 0$, where $a = -\log \mathbb{P}(\hat{\vartheta} > 1) \in (0, +\infty]$. The case $a = +\infty$ corresponds to $\hat{\vartheta}$ identically null; in our case this is excluded from the definition of T_β, which implies at once:

$$\mathbb{P}(\hat{\vartheta} < 1) = \lim_{k \to +\infty} \mathbb{P}(\vartheta_{\beta_k} < 1) \leq 1 - e^{-1} \leq \lim_{k \to +\infty} \mathbb{P}(\vartheta_{\beta_k} \leq 1) = \mathbb{P}(\hat{\vartheta} \leq 1), \tag{4.25}$$

and since $\mathbb{P}(\hat{\vartheta} \leq 1) = \mathbb{P}(\hat{\vartheta} < 1)$, we conclude that $a = 1$.

To conclude the proof of the theorem we write

$$\frac{\mathbb{E}\tau^{\eta_0}_{\mathcal{X}^s}}{T_\beta} = \frac{1}{T_\beta}\int_0^{+\infty} \mathbb{P}(\tau^{\eta_0}_{\mathcal{X}^s} > s)ds = \int_0^{+\infty} \mathbb{P}(\tau^{\eta_0}_{\mathcal{X}^s} > T_\beta s)\, ds. \tag{4.26}$$

Due to (4.23) we may apply the dominated convergence theorem, and so

$$\lim_{\beta\to+\infty}\frac{\mathbb{E}\tau_{\mathcal{X}^s}^{\eta_0}}{T_\beta}=\int_0^{+\infty}\lim_{\beta\to+\infty}\mathbb{P}(\tau_{\mathcal{X}^s}^{\eta_0}>T_\beta s)ds=\int_0^{+\infty}e^{-s}ds=1. \quad (4.27)$$

□

We remark that if $\mathcal{X}^m=\{\eta_0\}$, hypothesis (4.16) is immediately verified. Moreover if $\mathcal{C}_{\mathcal{X}^s}(\eta_0)$ i.e., the maximal cycle containing η_0 and not intersecting $\mathcal{X}^s$ (see (2.25)), is the unique cycle of maximal depth in the decomposition of $\mathcal{X}\setminus\mathcal{X}^s$ (see lemma 2.26), hypothesis (4.16) holds for any η in this cycle. In general, when there are many metastable states hypothesis (4.16) is not satisfied. More than that, it is possible to find examples where even the statement of the theorem does not hold, namely, the asymptotic law of the renormalized tunnelling time is not exponential. An example where we expect an asymptotic gamma distribution can be found in the framework of the probabilistic cellular automaton studied in [10]. However, in the general case of many metastable states
1) there are examples of η_0 that does not satisfy the hypothesis of the theorem, but nevertheless, we have asymptotic exponentiality of the tunnelling time.
2) we always have an exponential tail of the distribution and the convergence in $\mathcal{L}^1$.

4.2 The model-dependent input.

We note that in order to apply the previous results to some concrete model we need essentially two model-dependent inputs:

I) to determine the communication height $\Phi(\eta_0,\mathcal{X}^s)$.

II) to verify the hypothesis $\eta_0 \in \mathcal{X}^m$;

As far as point I) is concerned, a general criterion is to find a set of states $\mathcal{B}$ satisfying the following:

(a) $\mathcal{B}$ is a connected set containing η_0 with $\mathcal{B} \cap \mathcal{X}^s = \emptyset$

(b) there is a *reference path* $\omega^* : \eta_0 \to \mathcal{X}^s$; namely, a path such that

$$\{\arg\max_{\omega^*} H\} \cap \mathcal{F}(\partial\mathcal{B}) \neq \emptyset \tag{4.28}$$

i.e. such that the maximum of the energy in ω^* is reached in $\mathcal{F}(\partial\mathcal{B})$.

Indeed, point (a) gives the lower bound $\Phi(\eta_0, \mathcal{X}^s) \geq H(\mathcal{F}(\partial\mathcal{B}))$, while the path ω^*, joining η_0 with $\mathcal{X}^s$, gives the upper bound $\Phi(\eta_0, \mathcal{X}^s) \leq \max_i H(\omega_i^*)$; by eq. (4.28) the two bounds coincide.

As we will show in the next section, this criterion can also be used to determine the gates.

Notice that there is no need to determine the domain of attraction of $\mathcal{X}^m$ or $\mathcal{X}^s$ (i.e. the set of initial configurations s.t. the process typically hits $\mathcal{X}^m$ before, resp. after, $\mathcal{X}^s$). This is a crucial point since such a detailed description of the energy landscape is often not possible. Instead, a rather simple analysis can be used to find a suitable set $\mathcal{B}$ satisfying the above mentioned criterion.

One of the ideas that were used to carry out this preliminary analysis in some cases consists in a suitable *foliation* of the state space $\mathcal{X}$ into manifolds according to a given parameter (for instance the number of pluses of the configuration, for the Ising model) so that the solution of point I) can be reduced to solve the min-max problems between contiguous manifolds of the foliation. This method (used in [22], [2], [5], [15], [16]) suggests the choice of the set $\mathcal{B}$ that we will make in the next subsection to treat the Ising model.

As observed above, point II) can be verified even locally in a habitat; actually this is the way followed in many cases in the literature. Our proposal in this paper is to find a global solution to this problem. We note that the statement $\eta_0 \in \mathcal{X}^m$ is equivalent to the absence of too deep energy wells in the sense that saying $V_\eta \leq V_{\eta_0}$ for each $\eta \notin \mathcal{X}^s$, is equivalent to saying that the maximal depth of the cycles of the decomposition of $\mathcal{X}\backslash\mathcal{X}^s$, is V_{η_0}. In many physically interesting cases (as shown for the Ising model) if one guesses correctly the metastable state, it is easy to solve this point with a very rough argument by constructing for each configuration $\eta \notin \mathcal{X}^s$ a "reducing path" $\omega : \eta \to \eta'$ with $H(\eta) > H(\eta')$ for which $\max_i H(\omega_i) - H(\eta) \leq V_{\eta_0}$. Moreover, if the last inequality is strict for each $\eta \notin \eta_0 \cup \mathcal{X}^s$, then we have that η_0 is the unique metastable state, and we can also apply Theorem 4.15.

4.3 The Ising model.

As an example, we apply the above procedure to the well known case of 2D Ising model (see §2.1 for definitions). Without loss of generality, we set, here and in subsection 5.4, $J = 1$.

The first step is the determination of the communication height. We use the criterion proposed in the previous section.

Theorem 4.29 $\Phi(-\mathbf{1}, \mathbf{1}) = -h(\ell^*(\ell^* - 1) + 1) + 4\ell^*$.

Proof. We start by defining our reference path. Equation (2.36) suggests that the best paths from $-\mathbf{1}$ to $\mathbf{1}$ are sequences of configurations that are increasing clusters "as close as possible to squares".

We define the reference path $\omega^* : \mathbf{-1} \to \mathbf{1}$ by flipping the spin at the origin and then filling (flipping the spins from minus to plus) consecutively the shells

$$S_i := \Big\{ x \in \Lambda : \ ||x||_\infty = i \Big\}, \tag{4.30}$$

starting from the point $(i, i-1)$ and continuing clockwise so that $N^+(\omega^*_k) = k$.

All configurations in this path consist of a rectangle (either a square $l \times l$ or a "quasi-square" $l \times (l-1)$) possibly with one of the longest sides not completely filled.

The maximum of the energy in ω^* between consecutive rectangles is achieved in the configuration where the incomplete side contains exactly one plus. For these configurations, the number of pluses is either $k = l^2 + 1$ and $H(\omega^*_k) = -hl^2 + 4l + 2 - h$ or $k = l(l-1) + 1$ and $H(\omega^*_k) = -hl^2 + hl + 4l + 2 - h$.

It is immediate to see that the maximum energy among these configurations is achieved in $k^* := \ell^*(\ell^* - 1) + 1$, where $\ell^* := \lceil 2/h \rceil$. If $2/h$ is non–integer , this is the only maximum, otherwise $k = \ell^{*2} + 1$ corresponds to the same energy.

We take the side-length L of the torus larger than $k^* + 1$.

We define[3]

$$\mathcal{B} := \{ \xi : \ N_+(\xi) < k^* \}, \tag{4.31}$$

The Theorem is proven once we show that $H(\mathcal{F}(\partial \mathcal{B})) = H(\omega_{k^*})$.

[3]This set is suggested by the fact that our reference path ω^* crosses all manifolds $\{\xi : \ N_+(\xi) = k\}$ (for $k = 0, \dots, L$) in a state with minimal energy in that manifold. However, we stress once again that we do not need to analyze the whole foliation but we can focus only on the critical manifold.

It is easy to show that the minimum of the energy on the manifolds with fixed number of pluses is achieved only in configurations consisting of a single cluster.[4]

Moreover, it is immediate to see that the perimeter of a cluster is larger than or equal to the perimeter of the rectangle circumscribed to the cluster (this property can even be extended to configurations that wrap around the torus, but we do not need to consider such configurations since $L > k^* + 1$).

The perimeter of the cluster of pluses in $\omega^*_{k^*}$ is $4\ell^*$. In order to prove $\omega^*_{k^*} \in \mathcal{F}(\partial\mathcal{B})$, we only have to show that there is no configuration with k^* pluses that is contained in a rectangle with perimeter $4\ell^* - 2$ or smaller, but this is immediate since $4\ell^* - 2 < 4\sqrt{k^*}$, being $\sqrt{k^*}$ the side-length of the square with area k^* (that is, the rectangle in $\mathbb{R}^2$ of minimal perimeter among that of area k^*).

$\square$

Our next step is to show that $-\mathbf{1} \in \mathcal{X}^m$, namely the absence of deep wells:

Theorem 4.32 $V_\eta < V_{-\mathbf{1}}$ for any $\eta \notin \{-\mathbf{1}, \mathbf{1}\}$ i.e., $\mathcal{X}^m = \{-\mathbf{1}\}$.

Proof. It is sufficient to focus on the local minima of the energy, namely configurations where the pluses form rectangles (possibly encircling the torus) such that the minimal distance $||x - y||_1$ between sites in different rectangles (if they exist) is at least 2.

We distinguish two cases:

[4]This fact can be proved by using a suitable map that associates to a configuration with a set of clusters a new configuration where the same clusters are attached to each other.

1. If there exists a rectangle of pluses with a side-length l strictly smaller than ℓ^*, we consider the path that flips the spins in that side consecutively starting from one corner and ending with the other corner. The energy gap between the final and the initial configuration is $lh-2<0$. Each step increases the energy by h, except the last one that lowers the energy by $2-h$. Since the energy gap between the highest point in the path and the starting configuration is $h(l-1)<2-h$, for all these configurations $V_\eta \le h(\ell^*-2)<2-h$.

2. If there exists a rectangle of pluses with all sides larger than or equal to ℓ^*, consider the path that flips consecutively the minus spins near this side. The first step increases the energy by $2-h$, while each consecutive step lowers the energy by h. If the maximal side-length l is strictly larger than ℓ^*, this path reduces the energy since $2-lh<0$. Otherwise, for a square $\ell^* \times \ell^*$, the final configuration of the above-defined path has the same energy as η and contains a rectangle $\ell^* \times (\ell^*+1)$ full of pluses. Now, either this rectangle does not interact with any other rectangle and we are in the case already considered (so that we can decrease the energy by iterating the construction), or it does interact and the energy can be decreased by flipping one further minus to plus. The maximum energy of the path is reached at the first step showing that $V_\eta \le 2-h$ for all these configurations.

Since every local minimum different from $-\mathbf{1}$ and from $\mathbf{1}$ falls in at least one of the two cases above, we see that $\max_{\eta\in\mathcal{X}\setminus\{-\mathbf{1},\mathbf{1}\}} V_\eta \le 2-h$. This implies that $-\mathbf{1}=\mathcal{X}^m$.

□

5 Gate.

In this section we first discuss the relation between gates and essential configurations. Then, we show that the process passes through a gate with high probability and we discuss the minimality of the gates. We conclude again with the example of the Ising model.

5.1 Essential saddles and gates.

The following Theorem shows that unessential configurations are dead-ends:

Theorem 5.1 $\zeta \in \mathcal{S}(\eta, \eta')$ is essential if and only if $\zeta \in \mathcal{G}(\eta, \eta')$.

Proof. Abbreviate $\mathcal{S} = \mathcal{S}(\eta, \eta')$, $\mathcal{G} = \mathcal{G}(\eta, \eta')$, $\Omega = (\eta \to \eta')_{opt}$.

We first prove that $\zeta \in \mathcal{G}$ implies ζ essential.

For, let $\mathcal{W}$ be a minimal gate containing ζ. It is immediate to see that there exists a path $\omega \in (\eta \to \eta')_{opt}$ such that $\omega \cap \mathcal{W} = \zeta$; indeed, otherwise ζ would not be pivotal for the minimal gate $\mathcal{W}$.

We have either $\{\arg\max_\omega H\} = \{\zeta\}$ and then ζ is essential, or $\{\arg\max_\omega H\} \supset \{\zeta\}$, with $\{\arg\max_\omega H\} \cap \mathcal{W} \setminus \{\zeta\} = \emptyset$. In this last case no $\omega' \in (\eta \to \eta')_{opt}$ can exist with $\{\arg\max_{\omega'} H\} \subset \{\arg\max_\omega H\} \setminus \{\zeta\}$ since all optimal paths going from η to η' must cross the gate $\mathcal{W}$; thus, again, ζ is essential.

Next, we prove that $\zeta \in \mathcal{S}$ essential implies $\zeta \in \mathcal{G}$, i.e. there exists a minimal gate $\mathcal{W}$ containing ζ.

If there exists $\omega \in \Omega$ such that $\{\arg\max_\omega H\} = \zeta$, then ζ must belong to all minimal gates and hence to $\mathcal{G}$. Thus, we may assume that, for all $\omega \in \Omega$ with $\omega \ni \zeta$, we have $\{\arg\max_\omega H\} \setminus \{\zeta\} \neq \emptyset$. Since ζ is essential, we know that there exists $\bar{\omega} \ni \xi$ such that $\{\arg\max_{\bar{\omega}} H\} \setminus \{\zeta\} \not\supseteq \{\arg\max_{\omega'} H\}$ for any $\omega' \in \Omega$.

Partition

$$\Omega = \Omega_\zeta \cup \Omega_\zeta^c \tag{5.2}$$

with $\Omega_\zeta = \{\omega \in \Omega \colon \omega \ni \zeta\}$, $\Omega_\zeta^c = \Omega \setminus \Omega_\zeta$.

We may assume that $\Omega_\zeta^c \neq \emptyset$, otherwise ζ is obviously a minimal gate and we are done. We know that $\omega' \cap \mathcal{S}' \neq \emptyset$ for all $\omega' \in \Omega_\zeta^c$, where $\mathcal{S}' := \mathcal{S} \setminus \{\arg\max_{\bar{\omega}} H\} \neq \emptyset$. Let $\mathcal{W}'$ be a *minimal gate for* Ω_ζ^c *in* $\mathcal{S}'$, i.e.

$$\begin{aligned} &\mathcal{W}' \subseteq \mathcal{S}', \\ &\omega' \cap \mathcal{W}' \neq \emptyset \ \forall \omega' \in (\Omega_\zeta)^c, \\ &\forall\, \mathcal{W}'' \subset \mathcal{W}' \ \exists\, \omega'' \in (\Omega_\zeta)^c \colon \ \omega'' \cap \mathcal{W}'' = \emptyset. \end{aligned} \tag{5.3}$$

Such a $\mathcal{W}'$ certainly exists, since trivially $\mathcal{S}'$ is a gate for Ω_ζ^c in $\mathcal{S}'$ and we can always extract from it a minimal gate in $\mathcal{S}'$. We claim that $\mathcal{W} = \zeta \cup \mathcal{W}'$ is a minimal gate. Indeed, $\omega \cap \mathcal{W} \neq \emptyset$ for all $\omega \in \Omega$, since any $\omega \in \Omega$ not passing through $\mathcal{W}'$ must pass through ζ. Moreover, $\mathcal{W}'$ is minimal because we cannot exclude any configuration from $\mathcal{W}'$ without destroying the minimal gate property, nor can we exclude ζ, since $\bar{\omega} \cap \mathcal{W}' = \emptyset$ because $\mathcal{W}' \subseteq \mathcal{S}'$ and $\{\arg\max_{\bar{\omega}} H\} \cap \{\ S'\} = \emptyset$. $\square$

5.2 Crossing the gates.

Theorem 5.4 For any pair of states η, ξ, for any gate $\mathcal{W} \equiv \mathcal{W}(\eta, \xi) \subseteq \mathcal{S}(\eta, \xi)$ there exists $c > 0$ such that

$$\mathbb{P}\left(\tau_{\mathcal{W}}^\eta > \tau_\xi^\eta\right) \leq e^{-\beta c} \tag{5.5}$$

for sufficiently large β.

Proof. We can suppose the set of non–optimal paths $\omega : \eta \to \xi$ non–empty, otherwise $\mathbb{P}\left(\tau^{\eta}_{\mathcal{W}} > \tau^{\eta}_{\xi}\right) = 0$; then,

$$\delta_o := \min_{\substack{\omega:\eta\to\xi \\ \omega\notin(\eta\to\xi)_{opt}}} \max_{\zeta\in\omega} H(\zeta) - \min_{\omega\in(\eta\to\xi)_{opt}} \max_{\zeta\in\omega} H(\zeta) \tag{5.6}$$

is strictly larger than zero.

We consider the cycle $\mathcal{C} := \left\{\zeta : \ \Phi(\zeta,\eta) \le H(\mathcal{W}) + \frac{\delta_o}{2})\right\}$. By definition this cycle contains both η and ξ. Moreover, it is impossible to go from η to ξ without crossing $\mathcal{W}$ or exiting the cycle. Indeed, if $\omega \in (\eta \to \xi)_{opt}$ then ω crosses $\mathcal{W}$, and if $\omega \notin (\eta \to \xi)_{opt}$ then by definition of δ_0, ω leaves the cycle $\mathcal{C}$.

We have:

$$\mathbb{P}\left(\tau^{\eta}_{\mathcal{W}} > \tau^{\eta}_{\xi}\right) \le \mathbb{P}\left(\tau^{\eta}_{\xi} > \tau^{\eta}_{\partial\mathcal{C}}\right) \le e^{-\beta c}, \tag{5.7}$$

where in the last inequality we used the cycle property in Theorem 2.17, and c is a suitable constant. $\square$

5.3 Reducing the gates.

A crucial information on the tube of critical paths is given by the set $\mathcal{G}$ defined in (2.24).

The method proposed in Section 4.2 to implement the model-dependent input, i.e. to find a set $\mathcal{B}$ satisfying (4.28), provides a gate given by $\mathcal{W} = \mathcal{F}(\partial\mathcal{B}) \cap \mathcal{S}$. In general $\mathcal{W}$ is neither minimal nor unique; however, we can try to extract from it a minimal gate by eliminating dead–ends.

The criterion used in this analysis is based on the observation that a gate $\mathcal{W}$ is minimal if and only if $\forall\eta \in \mathcal{W}\ \exists\ \omega \in (\mathcal{X}^m \to \mathcal{X}^s)_{opt}$ with $\omega \cap \mathcal{W} = \eta$.

In more complex situations, we can make use of Theorem 5.1 and identify the unessential saddles.

For $\zeta \in \mathcal{S}(\eta, \eta')$, we call *bypassing set* of ζ with respect to the transition $\eta \to \eta'$ a set $\mathcal{A} \equiv \mathcal{A}_{\eta,\eta'}(\zeta) \in \mathcal{X}$ with the following properties:

1. $\mathcal{A} \ni \zeta$
2. $\mathcal{A} \not\supset \{\eta, \eta'\}$
3. $H(\mathcal{F}(\partial\mathcal{A})) = \Phi(\eta, \eta')$
4. $\forall \zeta', \zeta'' \in \mathcal{F}(\partial\mathcal{A}) \cup (\mathcal{A} \cap \{\eta, \eta'\})\ \exists \hat{\omega} \in (\zeta' \to \zeta'')_{opt}$ with $\arg\max_{\hat{\omega}} H = \{\zeta', \zeta''\} \setminus (\mathcal{A} \cap \{\eta, \eta'\})$.

Proposition 5.8 A saddle $\zeta \in \mathcal{S}(\eta, \eta')$ is unessential if there exists a bypassing set $\mathcal{A}_{\eta,\eta'}(\zeta)$

Proof. It is sufficient to show that for any path $\omega \in (\eta \to \eta')_{opt}$ with $\zeta \in \omega$ there exists $\omega' \in (\eta \to \eta')_{opt}$ with $\arg\max_{\omega'} H \subseteq \{\arg\max_{\omega} H\} \setminus \{\zeta\}$.

Let ζ' and ζ'' be the first and the last states in $\partial\mathcal{A} \cup (\mathcal{A} \cap \{\eta, \eta'\})$ hit by ω, respectively.

Since ω is optimal, ζ' and ζ'' are in $\mathcal{F}(\partial\mathcal{A}) \cup (\mathcal{A} \cap \{\eta, \eta'\})$. We define ω' by substituting the sub-path of ω that connects ζ' and ζ'' with $\hat{\omega}$.

$\square$

We stress that this condition is not necessary (see fig 1).

5.4 Gates for the Ising model.

The Ising model provides an excellent example of the procedures that can be used to reduce the gate (see Theorem 5.10 below). Besides the well

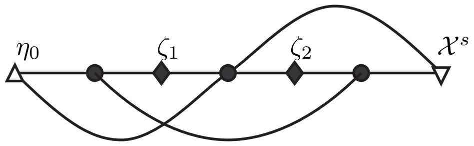


Figure 1: A counterexample where a bypassing set containing the unessential saddles ζ_1 or ζ_2 does not exist. $H(\bullet) = H(\blacklozenge) > H(\triangle) > H(\triangledown)$.

known case $2/h$ non–integer (where the Ising model has a unique minimal gate), we analyze here the case $2/h$ integer, where the structure of the gates is rather complex (see fig. 4).

We consider the Ising model in a torus with side-length $L > k^*$.

Let $\mathcal{P}_m$ (resp. $\mathcal{P}'_m$) be the set of configurations where the pluses form a rectangle $\ell^* \times m$ with a unitary protuberance attached to one of the longest (resp. shortest) sides (for $m = \ell^*$, when the rectangle is a square, we set $\mathcal{P}_{\ell^*} = \mathcal{P}'_{\ell^*}$).

Let

$$\mathcal{W}_{\ell^*-1} := \mathcal{P}_{\ell^*-1}. \tag{5.9}$$

Theorem 5.10 For $2/h$ non–integer , $\mathcal{W}_{\ell^*-1}$ is the unique minimal gate, so that $\mathcal{G} \equiv \mathcal{W}_{\ell^*-1}$.

Proof. We consider the set $\mathcal{B}$ defined in 4.31 and prove that $\mathcal{P}_{\ell^*-1}$ is a gate in two steps:

i) every optimal path in $(-\mathbf{1} \to \mathbf{1})_{opt}$ hits $\partial\mathcal{B}$ in $\mathcal{P}_{\ell^*-1} \cup \mathcal{P}'_{\ell^*-1}$.

ii) for any ζ in $\mathcal{P}'_{\ell^*-1}$ there is no optimal path in $\omega \in (\zeta \to \mathbf{1})_{opt}$ such that $\omega \cap \mathcal{B} = \emptyset$.

From i), ii) we conclude that $\mathcal{P}_{\ell^*-1}$ is a gate. Indeed, from i) we have that every optimal path exiting from $\mathcal{B}$ visits the set $\mathcal{P}_{\ell^*-1} \cup \mathcal{P}'_{\ell^*-1}$, on the other hand, from ii) we can conclude that in its last exit from $\mathcal{B}$ before the first arrival to $\mathbf{1}$, every optimal path has to hit $\mathcal{P}_{\ell^*-1}$. Thus, $\mathcal{P}_{\ell^*-1}$ is a gate.

i) We use the fact that the minimum of the energy in the manifold $\{\eta : N_+(\eta) = k^*-1\} \equiv \partial^- \mathcal{B}$ is unique (up to rotations and translations).[5]

   Indeed, we know that the minimum of the energy must be a single cluster. The perimeter of the cluster of the pluses is larger than or equal to the perimeter of the circumscribed rectangle. Let l_1 and l_2 be the side-lengths of this rectangle. The minima of the energy are the configurations that minimize $l_1 + l_2$ with $l_1 l_2 \geq k^* - 1$.

   It is easy to see that these configurations are rectangles $\ell^* \times (\ell^* - 1)$.

   The gap with every other configuration in $\partial^- \mathcal{B}$ is at least 2 because the perimeter is an even number.

   But the energy gap between the rectangle $\ell^* \times (\ell^* - 1)$ and the saddle is $2 - h$; thus, all configurations in $\partial^- \mathcal{B}$ except the quasi-square $\ell^* \times (\ell^* - 1)$ have energy higher than $\Phi(-\mathbf{1}, \mathbf{1})$.

   Hence, only the configurations in $\partial \mathcal{B}$ that are neighbors of this quasi-square can be essential saddles.

   Among these, the only configurations with energy equal to $\Phi(-\mathbf{1}, \mathbf{1})$ are in $\mathcal{P}_{\ell^*-1} \cup \mathcal{P}'_{\ell^*-1}$.

ii) By contradiction, let $\zeta \in \mathcal{P}'_{\ell^*-1}$ and let $\omega : \zeta \to \mathbf{1}$ be the optimal path lying outside $\mathcal{B}$.

[5]We will refer at this technique as "focusing".

Let n be the first time when ω_n has a plus spin outside the rectangle R circumscribed to the pluses in ζ.

We see that $H(\omega_n) - H(\omega_{n-1}) \geq 2 - h$ because a minus with at most one plus neighbor is flipped in the transition.

On the other hand, $k^* \leq N_+(\omega_{n-1}) \leq (\ell^* - 1)(\ell^* + 1)$ and the perimeter of ω_{n-1} is at least equal to the perimeter $2((\ell^*-1)+(\ell^*+1))$ of the rectangle R because the minuses in the rectangle are strictly less than $\ell^* - 1$ since $\omega_k \notin \mathcal{B}$ for any k.

Thus, $H(\omega_{n-1}) \geq -h(\ell^{*2} - 1) + 4\ell^*$ and $H(\omega_n) \geq -h\ell^{*2} + 4\ell^* + 2 > \Phi(-\mathbf{1}, \mathbf{1})$.

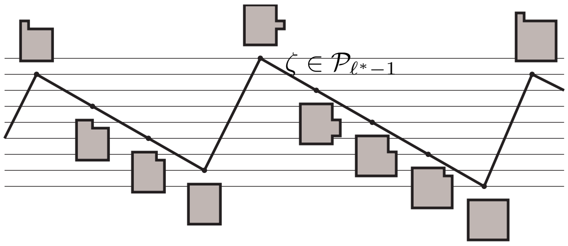


Figure 2: Energy vs. volume for the (modified) reference path for $h = 4/9$. The maximal energy is reached only in ζ.

To show that $\mathcal{P}_{\ell^*-1}$ is a minimal gate it is sufficient to exhibit for each $\zeta \in \mathcal{P}_{\ell^*-1}$ an optimal path that touches $\partial\mathcal{B}$ only in ζ. Clearly, such a family of paths can be obtained by modifying the updating order of the reference path ω^* between the quasi-square $\ell^* \times (\ell^* - 1)$ and the square $\ell^* \times \ell^*$ (see fig. 2).

Since $2/h$ is non–integer, $\mathcal{P}_{\ell^*-1}$ is the only minimal gate because the above defined reference paths reach the energy $\Phi(-\mathbf{1}, \mathbf{1})$ only in $\mathcal{P}_{\ell^*-1}$.

$\square$

Let us now consider the case where $2/h$ is integer, all rectangles with a side of length $2/h$ have the same energy $4/h = 2(2/h + l) - h(2l/h)$. This will give rise to a rich gate structure we are going to analyze.

Let

$$\begin{aligned} \mathcal{W}_{\ell^*} &:= \mathcal{P}_{\ell^*} \\ \mathcal{W}_m &:= \bigcup_{n=\ell^*+1}^{m} \mathcal{P}_n \cup \mathcal{P}'_m \quad \text{for } m \in \{\ell^*+1, \dots, L-1\} \end{aligned} \tag{5.11}$$

We set

$$\mathcal{H} := \bigcup_{m \in \{\ell^*-1, \dots, L-2\}} \mathcal{W}_m. \tag{5.12}$$

We will prove in Theorems 5.27, 5.28 that the $\mathcal{W}_m$'s are minimal gates and $\mathcal{G} = \mathcal{H}$.

A simple argument could have been used in order to prove just the identification $\mathcal{G} = \mathcal{H}$. Indeed it is possible to show that the configurations in $\bigcup_{m \in \{\ell^*-1, \dots, L-2\}} \mathcal{W}_m$ are essential saddles by using suitable modifications of the reference path that cannot be short-cut. These paths can be obtained modifying the reference path after reaching the square $\ell^* \times \ell^*$ by adding the protuberances on the shortest sides instead of on the longest sides, when needed (see fig.3). However, this description is not sufficient to investigate the structure of the set $\mathcal{G}$ and to show that the $\mathcal{W}_m$'s are minimal gates.

The more detailed analysis that we perform in order to get the minimality of the $\mathcal{W}_m$ allows a satisfactory characterization of the set of critical droplets and more generally of the tube of typical paths followed by the system during the transition. Indeed the critical droplets can be identified with the sets $\mathcal{W}_m$. It turns out that the supercritical growth of the stable **1** phase can begin starting from any rectangle $l^* \times m$ with arbitrary

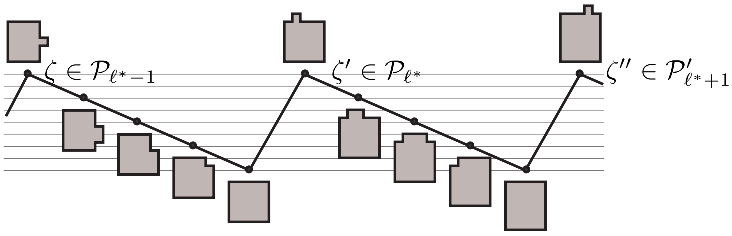


Figure 3: Energy vs. volume for the (modified) reference path for $h = 2/5$. The maximal energy is reached in ζ, ζ', ζ''.

$m \in (l^*, \dots, L-2)$. It is remarkable that the degeneracy generated by the choice $2/h \in \mathbb{N}$ gives rise to this arbitrariness in the shape of the critical rectangles. Before touching $\mathcal{W}_{l^*-1}$ and after leaving $\mathcal{H}$ the system behaves similarly to the case $2/h \notin \mathbb{N}$.

As we will argue in section 6.4, the structure of $\mathcal{G}$ is crucial for the computation of the pre-factor of the expectation of the tunnelling time as outlined in [5].

Unfortunately, the simple method used in Theorem 5.10 only allows to show that $\mathcal{W}_{\ell^*-1}$, $\mathcal{W}_{\ell^*}$ and $\mathcal{W}_{\ell^*+1}$ are minimal gates; for larger m's the manifolds at fixed magnetization cease to be a good approximation of the boundary of the "domain of attraction" of $-\mathbf{1}$.

We introduce the *bootstrap percolation* map in order to define suitable sets $\mathcal{B}_m$ such that the gates $\mathcal{W}_m$ coincide with $\mathcal{F}(\partial \mathcal{B}_m)$.
Given a configuration $\eta \in \mathcal{X}_I$, we consider the configuration obtained by flipping all the minus spins that have at least two plus nearest neighbors; we iterate this procedure and, since the map is monotonic and the volume is finite, we reach the final configuration (denoted by $\bar{\eta}$) in a finite number of iterations. The map $\eta \to \bar{\eta}$ is called *bootstrap*.

It is clear that there exists a downhill path $\omega : \eta \to \bar{\eta}$.

It is immediate to see that

$$H(\bar{\eta}) \leq H(\eta) - h\, d(\eta, \bar{\eta}), \tag{5.13}$$

where $d(\eta, \eta')$ is the number of sites x where $\eta(x) \neq \eta'(x)$. Indeed, $\eta(x) \leq \bar{\eta}(x)$ for every x while in each step of the updating procedure the perimeter does not increase. Another direct consequence of the definition of bootstrap is that the pluses in $\bar{\eta}$ (if any) form *non–interacting rectangles* namely, rectangles such that no site x in Λ exists with two n.n. contained in these two rectangles. Moreover, all the configurations η' where the set of occupied sites is intermediate between the sets of occupied sites in η and in $\bar{\eta}$, give the same $\bar{\eta'} \equiv \bar{\eta}$; thus, we are allowed to change the order in the updating procedure without affecting the final configuration.

For $l \leq m < L$, we consider the sets

$$\begin{aligned} \mathcal{B}_{l,m} := \Big\{ \eta :\ & \bar{\eta} \text{ contains only rectangles of pluses with} \\ & \text{smallest side-length} \leq l \text{ and largest side-length } \leq m \Big\} \end{aligned} \tag{5.14}$$

The bootstrap percolation map, used in [17] for the "anisotropic Ising model" gives a very deep insight into the structure of the gates and no reduction is needed. On the other hand, the analysis of the minima on the sets $\partial\mathcal{B}_{l,m}$ defined with the help of this map is rather difficult.

In order to show that for $\ell^* - 1 \leq m \leq L - 2$, $\mathcal{F}(\partial\mathcal{B}_{\ell^*,m}) \equiv \mathcal{W}_m$, we start proving the following

Lemma 5.15 Let $\mathcal{R}_{l,m}$ be the set of configurations in $\mathcal{B}_{l,m}$ that consist of a set of non-interacting rectangles $\{a_1^i \times a_2^i\}_{i \leq n}$ with the following properties:

$$\max_{e=1,2} \sum_{i \leq n} a_e^i > m - n \tag{5.16}$$

or

$$\sum_{i\le n} a_1^i + a_2^i > 2l \tag{5.17}$$

or both.

Then, for $l \le \ell^* \le m \le L-2$, we have $H(\mathcal{F}(\mathcal{R}_{l,m})) = -hl(l+1)+4l+2$ and the configurations in $\mathcal{F}(\mathcal{R}_{l,m})$ consist of a single rectangle $l \times \hat{m}$, where

$$\begin{aligned} \hat{m} &= l+1 && \text{if } \ l < \ell^* \le m \\ \ell^*+1 \le \hat{m} &\le m && \text{if } \ l = \ell^* < m \end{aligned} \tag{5.18}$$

Proof.

Let us denote by $H(a,b) := -hab + 2(a+b)$ the energy associated to a rectangle $a \times b$. Notice that

$$\frac{\partial}{\partial a} H(a,b) = -hb + 2 \ge 0 \ \Leftrightarrow b \le \ell^* \ (= 0 \Leftrightarrow b = \ell^*) \tag{5.19}$$

We will compare the energy of a generic $\eta \in \mathcal{R}_{l,m}$ with the energy associated to a particular rectangle in $\mathcal{R}_{l,m}$ of the form $(l-\delta) \times m$ or $l \times (l+1+\delta)$, where $\delta \in \mathbb{N}$.

- For η verifying (5.16), we compare it with a rectangle $(l-\delta)\times m$: Let $l^i := \min\{a_1^i, a_2^i\}$ and $m^i := \max\{a_1^i, a_2^i\}$. We set $l_{max} := \max_{i\le n} l^i$.

$$\begin{aligned} H(\eta) &= -h\sum_{i\le n} l^i m^i + 2\sum_{i\le n}(l^i + m^i) \\ &\ge -hl_{max}\sum_{i\le n} m^i + 2\Big(l_{max} + (n-1) + \sum_{i\le n} m^i\Big) \end{aligned} \tag{5.20}$$

By adding and subtracting $2m + hl_{max}m$, we have

$$\text{r.h.s. of eq. (5.20)} =$$
$$-hl_{max}m + 2(l_{max}+m) - (2 - hl_{max})\Big(m - \sum_{i\le n} m^i\Big) + 2(n-1) \tag{5.21}$$

By (5.16), $\sum_{i\leq n} m^i > m-n$ and thus, using that $l_{max}\leq l^*$,

$$\text{r.h.s. of (5.21)} \geq H(l_{max},m)+(n-1)hl_{max}. \tag{5.22}$$

Hence, the set of configurations of minimal energy in $\mathcal{R}_{l,m}$ verifying (5.16) must contain a single rectangle of pluses, with maximum side-length m. By (5.19), we get that the minimum of the energy associated to rectangles $(l-\delta)\times m$ is $-hlm+2l+2m$ and is associated to rectangles $l\times m$. If $m>\ell^*$, these are the only minima, otherwise if $m=l^*$ all rectangles $(l-\delta)\times m$ are associated to the same energy.

- For η verifying (5.17), we compare it with a rectangle $l\times(l+1+\delta)$:

  Let us assume (without loss of generality) that $\sum_{i\leq n} a_1^i \leq \sum_{i\leq n} a_2^i$, so that $\sum_{i\leq n} a_2^i \geq l+1$. Let $b^i := \min\{a_1^i, l\}$. Since, by definition of $\mathcal{R}_{l,m}$, $a_1^i > l$ implies $a_2^i \leq l \leq \ell^*$, by (5.19) we have

$$H(\eta)=\sum_{i\leq n} H(a_1^i,a_2^i) \geq \sum_{i\leq n} H(b^i,a_2^i) = -h\sum_{i\leq n} b^i a_2^i + 2\sum_{i\leq n}(b^i+a_2^i) \tag{5.23}$$

  Notice that $\sum_{i\leq n} b^i + a_2^i > 2l$ since either $a_1^i \equiv b^i$ or $\sum_{i\leq n} a_2^i > \sum_{i\leq n} b^i \geq l$.

  We set $r := l - \sum_{i\leq n} b^i$ and distinguish two cases:

  - if $r<0$, by using $b_i \leq l$ we have

$$\begin{aligned} \text{r.h.s of (5.23)} &\geq -hl\sum_{i\leq n} a_2^i + 2\Big(l - r + \sum_{i\leq n} a_2^i\Big) \\ &= H\Big(l, \sum_{i\leq n} a_2^i\Big) + 2|r| > H\Big(l, \sum_{i\leq n} a_2^i\Big) \end{aligned} \tag{5.24}$$

– if $r \geq 0$, we use that

$$
\begin{aligned}
l\Big(\sum_{j\leq n} a_2^j - r\Big) &= \sum_{i,j\leq n} b^i a_2^j + r\Big(\sum_{i\leq n}(a_2^i - b^i) - r\Big) \\
= \sum_{i\leq n} b^i a_2^i + \sum_{i\neq j\leq n} b^i a_2^j &+ r\Big(\sum_{i\leq n}(a_2^i + b^i) - 2l + r\Big) \\
&\geq \sum_{i\leq n} a_2^i b^i + n(n-1) + r^2, \qquad (5.25)
\end{aligned}
$$

where we used (5.17) and we estimated the sum of the off-diagonal terms by $n(n-1)$. By 5.25, we can estimate $-h\sum_{i\leq n} a_2^i b^i$ so we have

$$
\begin{aligned}
\text{r.h.s of (5.23)} \quad &\geq \quad -hl\Big(\sum_{i\leq n} a_2^i - r\Big) + hn(n-1) + hr^2 + 2\Big(l - r + \sum_{i\leq n} a_2^i\Big) \\
&= \quad H\Big(l, \sum_{i\leq n} a_2^i - r\Big) + hn(n-1) + hr^2. \qquad (5.26)
\end{aligned}
$$

Since $\sum_{i\leq n} a_2^i - r \geq l+1$, we see that the minimum of the energy among configurations verifying (5.17) can only be achieved in a configuration consisting of a single rectangle $l \times (l+1+\delta)$.

By (5.19), we get that the minimum of the energy associated to rectangles $l \times (l+1+\delta)$ is $-hl(l+1) + 4l + 2$ and is reached for $\delta = 0$. If $l < \ell^*$, these are the only minima and the energy of these configurations is lower than the one of the rectangles $l \times m$ if $m > l+1$. Otherwise, if $l = \ell^*$, all rectangles $l \times (l+1+\delta)$ are associated to the same energy.

$\square$

Theorem 5.27 If $2/h$ is integer, for any $m \in \{\ell^* - 1, \dots, L-2\}$ the set $\mathcal{W}_m$ (see (5.9), (5.11)) is a minimal gate for the transition $-\mathbf{1} \to \mathbf{1}$.

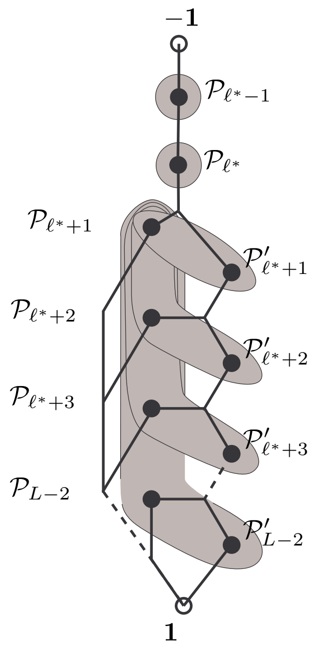


Figure 4: Structure of the minimal gates when $2/h$ is integer. The grey areas denote minimal gates.

Proof. Our strategy is to prove that $\mathcal{F}(\partial\mathcal{B}_{\ell^*-1,L-2}) = \mathcal{W}_{\ell^*-1}$ and $\mathcal{F}(\partial\mathcal{B}_{\ell^*,m}) = \mathcal{W}_m$ for any $m \in \{\ell^*, \ldots, L-2\}$.

Let ξ^x denote the configuration obtained from ξ by flipping the spin at site x.

Let us consider $\eta \in \mathcal{B}_{l,m}$ with $\eta^x \in \mathcal{F}(\partial\mathcal{B}_{l,m})$.

Obviously, $\bar{\eta}(x) = -1$.

We observe that $\eta = \bar{\eta}$. Otherwise, $H(\eta^x) > H(\eta^x) - H(\eta) + H(\bar{\eta}) > H(\bar{\eta}^x)$ while $\bar{\eta} \in \mathcal{B}_{l,m}$ and $\bar{\eta}^x \in \partial\mathcal{B}_{l,m}$ contradicting that $H(\eta^x) \in \mathcal{F}(\partial\mathcal{B}_{l,m})$.

Now, let R be a rectangle of pluses in η interacting with x. We see that x must be a protuberance attached to R. Otherwise, there would exist a protuberance y adjacent to x attached to R and either $\eta^y \in \partial\mathcal{B}_{l,m}$ with $H(\eta^y) < H(\eta^x)$ or $\eta^y \in \mathcal{B}_{l,m}$, $\overline{\eta^y}^x \in \partial\mathcal{B}_{l,m}$ with $H(\overline{\eta^y}^x) < H(\eta^x)$. Hence, $H(\eta^x) = H(\eta) + 2 - h$.

Recall that $\mathcal{R}_{l,m}$ has been defined in lemma 5.15, we see that $\eta \in \mathcal{R}_{l,m}$: indeed, $\overline{\eta^x}$ contains either a rectangle $(l+a)\times(l+b)$ with $a, b \geq 1$ or a rectangle $a \times (m+b)$ with $a, b \geq 1$.

In the first case,

$$|\gamma(\eta^x)| = |\gamma(\eta)| + 2 = 2\sum_{i\leq n}(a_1^i + a_2^i) + 2 \geq 4l + 4;$$

in the second case, we assume (without loss of generality) that the length of the north side of the rectangle is $m+b$. Then, there exists an interval larger than or equal to $m+b$ where each pair of adjacent columns contains at least one plus in η^x. Hence,

$$\sum_{i\leq n} a_1^i + n > m + b \geq m + 1.$$

We can use Lemma 5.15 to conclude the proof:

- For $l = \ell^* - 1$, $m = L - 2$, η is a rectangle $(\ell^* - 1)\times\ell^*$ and $\eta^x \in \mathcal{P}_{\ell^*-1}$, since $\mathcal{P}'_{\ell^*-1} \subset \mathcal{B}_{\ell^*-1,L-2}$.

- For $m = l = \ell^*$, η is a square $\ell^* \times \ell^*$ and $\mathcal{F}(\partial\mathcal{B}_{\ell^*,\ell^*}) = \mathcal{P}^*_{\ell}$.

- For $m > l = \ell^*$, η is a rectangle $\ell^* \times \hat{m}$ where $\hat{m} \in \{\ell^* + 1, m\}$. If $\hat{m} < m$, $\mathcal{P}'_{\hat{m}} \subset \mathcal{B}_{\ell^*,m}$, if $\hat{m} = m$ we get $\mathcal{F}(\partial\mathcal{B}_{\ell^*,m}) = \mathcal{W}_m$.

This concludes the proof that $\mathcal{F}(\partial\mathcal{B}_{\ell^*-1,L-2}) = \mathcal{W}_{L-2}$ and $\mathcal{F}(\partial\mathcal{B}_{\ell^*,m}) = \mathcal{W}_m$. To prove that the $\mathcal{W}_m$'s are minimal gates, we exhibit, for any $\zeta \in \mathcal{W}_m$, an optimal path that crosses $\mathcal{W}_m$ only in ζ. These paths can be obtained by the following rule:

$\omega' \in (\zeta \to -\mathbf{1})_{opt}$ is defined by flipping the plus protuberance and then sequentially eroding the pluses on the shortest sides of the rectangles $\bar{\omega}'_k$. $\omega'' \in (\zeta \to \mathbf{1})_{opt}$ is defined by completing the side where the protuberance is and then sequentially flipping the minuses in the layer near one of the longest sides of the rectangles of pluses.

□

Theorem 5.28

$$\mathcal{G} = \mathcal{H} \tag{5.29}$$

Proof. We have shown in Theorem 5.27 that $\mathcal{H} \subseteq \mathcal{G}$, to conclude the proof we show that $\mathcal{H} \supseteq \mathcal{G}$. By Theorem 5.1, this is equivalent to show that every $\eta \in \mathcal{S}(-\mathbf{1}, \mathbf{1}) \setminus \mathcal{H}$ is unessential.

To this end, we use the sufficient condition given in Proposition 5.8 and exhibit a bypassing set $\mathcal{A}_{-\mathbf{1},\mathbf{1}}(\eta)$ for any saddle η in $\mathcal{S}(-\mathbf{1}, \mathbf{1}) \setminus \mathcal{H}$.

The configuration $\bar{\eta}$ consists of a set of rectangles of pluses (possibly degenerate) $l^i \times m^i$ where $l^i \leq m^i$. Let $l(\bar{\eta}) := \max_i l^i$ and $m(\bar{\eta}) := \max_i m^i$.

We distinguish three cases:

a) If $l(\bar{\eta}) < \ell^*$ and $m(\bar{\eta}) < L - 1$, we set $\mathcal{A} := \mathcal{B}_{\ell^*-1, L-2}$.

b) If $l(\bar{\eta}) = \ell^*$ and $m(\bar{\eta}) < L-1$, we set $\mathcal{A}$ as the set of all configurations ξ with $\bar{\xi} = \bar{\eta}$ and such that every row and column of the rectangles of pluses in $\bar{\eta}$ has at least two plus sites in η.

c) If $l(\bar{\eta}) > \ell^*$ or $m(\bar{\eta}) \geq L - 1$, we set $\mathcal{A}$ as $(\mathcal{B}_{\ell^*, L-2} \cup \partial\mathcal{B}_{\ell^*, L-2})^c$.

We now show that $\mathcal{A}$ is a bypassing set $\mathcal{A}_{-\mathbf{1},\mathbf{1}}(\eta)$.

In cases a), properties 1) and 2) in the definition of bypassing set can be readily checked. In case c) to prove property 1) we notice that $\eta \notin \partial\mathcal{B}_{l^*, L-2}$, otherwise by theorem 5.27 and by $\eta \notin \mathcal{H}$ we have $H(\eta) > \Phi(-\mathbf{1}, \mathbf{1})$, against the hypothesis $\eta \in \mathcal{S}(-\mathbf{1}, \mathbf{1})$. Properties 3) and 4) have already been proved in the proof of Theorem 5.27: we have that $\mathcal{F}(\partial\mathcal{A}) = \mathcal{W}_{\ell^*-1}$ in case a) and $\mathcal{F}(\partial\mathcal{A}) = \mathcal{W}_{L-2}$ in case c). Moreover, we showed that for any $\zeta \in \mathcal{F}(\partial\mathcal{A})$ there exists a suitable modification of the reference paths $\omega'(\zeta) \in (\zeta \to -\mathbf{1})_{opt}$ such that $\{\arg\max_{\omega'} H\} = \{\zeta\}$ (resp. $\omega''(\zeta) \in (\zeta \to \mathbf{1})_{opt}$ such that $\{\arg\max_{\omega''} H\} = \{\zeta\}$); by joining these paths we obtain the paths $\hat{\omega}(\zeta', \zeta'')$ for any pair $\{\zeta', \zeta''\} \subseteq \mathcal{F}(\partial\mathcal{A}) \cup (\mathcal{A} \cap \{-\mathbf{1}, \mathbf{1}\})$..

Let us focus on case b). The point here is to show that $\eta \in \mathcal{A}$. We start showing that $\bar{\eta}$ contains a single cluster of pluses. Since η is a saddle, it is not a local minimum and its energy is $\Phi(-\mathbf{1}, \mathbf{1})$.

$$H(\eta) = 2\ell^* + 2 - h > \sum_n H(l^n, m^n) = \sum_{i:\ l^i = \ell^*} H_i + H', \tag{5.30}$$

where H' is the energy associated with the rectangles with $l^j < \ell^*$ and $H_i \equiv 2\ell^*$ is the energy associated with the ith rectangle when $l^i = \ell^*$. We immediately get $|\{i:\ l^i = \ell^*\}| = 1$ and, since the energy associated to the rectangles with $l^j < \ell^*$ is larger than $4 - h$ no such rectangle can exist.

Now we observe that every row and column of the rectangle $\ell^* \times m(\bar{\eta})$, that is full of pluses in $\bar{\eta}$, has at least two pluses in η. By (5.13),

$$H(\eta) = 2\ell^* + h(\ell^* - 1) \geq H(\bar{\eta}) + hd(\eta, \bar{\eta}) \tag{5.31}$$

By using $H(\bar{\eta}) = 2\ell^*$, from the previous inequality, we get

$$d(\eta, \bar{\eta}) \leq \ell^* - 1. \tag{5.32}$$

By direct inspection we see that the configurations with energy $\Phi(-\mathbf{1}, \mathbf{1})$ with only one plus in a row or column of the rectangle $\ell^* \times m(\bar{\eta})$ are in $\mathcal{H}$.

Property 2) of the bypassing set $\mathcal{A}$ can be immediately checked. To prove properties 3) and 4) we show that $\mathcal{F}(\partial\mathcal{A}) \subset \mathcal{H}$ and that from each

$\zeta' \in \mathcal{F}(\partial\mathcal{A})$ there exists a downhill path going to the configuration $\hat{\eta} := \mathcal{F}(\mathcal{A})$ consisting of a rectangle $\ell(\bar{\eta})\times m(\bar{\eta})$) by joining these paths we obtain the paths $\hat{\omega}(\zeta', \zeta'')$.

Let $\zeta \in \mathcal{F}(\partial\mathcal{A}(\eta))$ we distinguish two cases:

1. if ζ is a neighbor of a configuration $\zeta^x \in \mathcal{A}$ with $\zeta^x(x) = -1$, we immediately see that $H(\zeta) \geq H(\ell^*, m(\bar{\eta})) + 2 - h$ and the minima are only for $\zeta \in \mathcal{P}_{m(\eta)} \cup \mathcal{P}'_{m(\eta)}$; the path $\tilde{\omega} : \zeta \to \hat{\eta}$ consists in only one step.

2. if ζ is a neighbor of a configuration $\zeta^x \in \mathcal{A}$ with $\zeta^x(x) = +1$, there exists in ζ a row or column with only one plus. Clearly, $H(\zeta) \geq 2 - h + H(l, m)$, where $l = \ell^* - 1$ or $m = m(\bar{\eta}) - 1$. The minima are only for $\zeta \in \mathcal{P}'_{m(\bar{\eta})-1}$; namely, the pluses in η form a rectangle $\ell^* \times (m(\bar{\eta}) - 1)$ with a protuberance on one of the shortest sides. The path $\tilde{\omega} : \zeta \to \hat{\eta}$ consists in filling the incomplete side of the rectangle $\ell^* \times m(\bar{\eta})$.

$\square$

6 Final discussion.

As already discussed in the introduction, this paper is mainly motivated by the need to give partial results about the metastable behavior of some models where we could not get a sufficiently good control of the energy landscape. The effort of determining the weaker hypothesis at the basis of these partial results allowed to clarify many aspects of the problem.

Indeed, we separated the hypotheses needed to control the tunnelling time from the ones needed to control the tube of typical paths.

As far as tunnelling time is concerned, we separated the hypotheses to get convergence in probability, in $\mathcal{L}_1$ and in law of the variables $X_\beta := \frac{1}{\beta}\ln \tau^{\eta_0}_{\mathcal{X}^s}$.

Concerning the tube of typical paths, we propose to give a partial characterization (the most important one from a physical point of view) by identifying the minimal gates.

This better understanding of the problem allows to clarify the relationship among the different approaches to metastability in the Freidlin-Wentzell regime. This section is devoted to discuss in more details the differences between the approach proposed in this paper and previous results.

6.1 Why in some previous approaches tunnelling time and exit tube came jointly.

We want now to discuss the approach followed in several previous papers (see [17], [18], [11], [23], [9], [10]), treating metastability for different lattice models and to make a comparison with the method in the present note. In those papers a common strategy was used. A key ingredient was the possibility to find a connected set $\mathcal{D}$ containing η_0 and not intersecting $\mathcal{X}^s$ satisfying the following conditions:

(a) There exists a path $\omega^* : \eta_0 \to \mathcal{X}^s$ such that $\{\arg\max_{\omega^*} H\} \subseteq \mathcal{F}(\partial\mathcal{D})$

(b) Let $\mathcal{P} = \mathcal{F}(\partial D)$ and let $\Gamma = H(\mathcal{P}) - H(\eta_0)$. For any $\eta \in \mathcal{D}$ we have

$$\lim_{\beta\to\infty} \mathbb{P}\left(\tau^{\eta}_{\eta_0} < \tau^{\eta}_{\partial\mathcal{D}} \text{ and } \tau^{\eta}_{\eta_0} < e^{\beta\Gamma_0}\right) = 1 \tag{6.1}$$

where $\Gamma_0 < \Gamma$.

(c) Let

$$\bar{\mathcal{P}} = \{\eta \notin (\mathcal{D} \cup \partial\mathcal{D}) : \exists \sigma \in \mathcal{P} \text{ downhill communicating with } \eta\} \quad (6.2)$$

For any $\eta \in \bar{\mathcal{P}}$ we have

$$\lim_{\beta\to\infty} \mathbb{P}\left(\tau^{\eta}_{\mathcal{X}^s} < e^{\beta\Gamma_0}\right) = 1 \quad (6.3)$$

where $\Gamma_0 < \Gamma$.

The above conditions characterizing the set $\mathcal{D}$ are a strengthening of the previous hypotheses characterizing the set $\mathcal{B}$ introduced at the beginning of Section 4.2 (see 4.28)

$\mathcal{D}$ represents, in practice, the subcritical states, namely the ones typically evolving towards η_0 before hitting $\mathcal{X}^s$. Condition (b) says that from any configuration in $\mathcal{D}$ the system recurs in η_0 before exiting $\mathcal{D}$, in a time exponentially smaller than $e^{\beta\Gamma}$. From (a) it is easy to deduce that the communication height between η_0 and $\mathcal{X}^s$ is $H(\mathcal{P})$. It is easily seen that $\mathcal{C}_{\mathcal{X}^s}(\eta_0)$ is contained in $\mathcal{D}$ so we can use the exit time from $\mathcal{C}_{\mathcal{X}^s}(\eta_0)$ to get a lower estimate of the tunnelling time.

With high probability when our process crosses the boundary $\partial\mathcal{D}$, during the first excursion from η_0 to $\mathcal{X}^s$, it passes through $\mathcal{F}(\partial\mathcal{D}) = \mathcal{P}$. This follows from condition (b) and eq. (2.18), using that, by reversibility we have

$$\lim_{\beta\to\infty} \mathbb{P}\left(\tau^{\eta}_{\zeta} < e^{\beta(H(\zeta)-H(\eta)-\delta)}\right) = 0 \quad (6.4)$$

for any $\eta, \zeta \in \mathcal{X}$ and $\delta > 0$.

Then, possibly after many attempts, the process will eventually exit downhill from $\mathcal{D} \cup \partial\mathcal{D}$ passing through $\bar{\mathcal{P}}$. Condition (c) ensures that from $\bar{\mathcal{P}}$ the first hitting time in $\mathcal{X}^s$ is exponentially shorter than $e^{\beta\Gamma}$, so the $\tau_{\mathcal{X}^s}$ and $\tau_{\partial\mathcal{D}}$ are of the same order. In this way it is possible to get an upper estimate of the tunnelling time without supposing total absence of deep wells.

In order to use this method, in many of the previous works, the authors needed a precise knowledge of the set $\mathcal{P}$. Then, to verify condition (c), they used other very detailed model-dependent information, namely they determined the set $\bar{\mathcal{P}}$ and were able to control the tube of typical path to $\mathcal{X}^s$ emerging from states in $\bar{\mathcal{P}}$.

We clearly see that in this approach the problem of tunnelling time is solved jointly with the one of the tube of typical paths.

In the language developed in section 4 we can say that the tube of typical paths from $\bar{\mathcal{P}}$ to $\mathcal{X}^s$ is a habitat without deep cycles. This requires a local detailed analysis of the energy landscape instead of a rough but global analysis as the one used to prove recurrence to $\{\eta_0 \cup \mathcal{X}^s\}$ in a sufficiently short time. On the other hand, this local information is enough to get the result in probability, but not in $\mathcal{L}_1$ since, for this purpose, it is necessary to have a global control of deep wells in the whole energy landscape.

As we discussed before, in [17], [18], [11], [23], [8], [9], [10], due to the strong conditions required in the definition of the set $\mathcal{D}$, it was easy to get that $\mathcal{P} := \mathcal{F}(\mathcal{D})$ is a minimal gate.

This approach could be probably extended to cases with many minimal gates by relaxing hypothesis (c). Anyway, we remark that the structure of the gates and the behavior of the process, when crossing them, is a key point in the description of the tube of typical paths.

In this note, we call the attention on these sets and give general results on their structure. The strategy we use consists in observing the process when it crosses suitable target manifolds (the sets $\partial\mathcal{B}$ with $\mathcal{B}$ as in (4.28)).

In order to complete the picture and give the full information on the tube of typical paths, we should follow all the optimal paths emerging from any essential saddle until they reach a new essential saddle or $\mathcal{X}^s \cup \mathcal{X}^m$. This involves a model-dependent analysis that is often quite delicate. However the approach proposed in this paper could have some advantages:

1) the analysis needed to find a set $\mathcal{B}$ with the properties in (4.28) requires just a description of the energy landscape whereas (6.1), which is formulated in terms of probabilities of hitting times is, at least in principle, a stronger condition;

2) the general notions and structure properties concerning the gates that we develop, turn out to be useful in the perspective of determining the typical tube. Indeed, for example, the preliminary knowledge of the minimal gates allows to restrict the search of optimal paths to the subpaths emerging from essential saddles.

6.2 An example: 3DK versus 3DG.

In order to give an example and a concrete comparison between the approach proposed in this paper and more powerful but more difficult theories, we discuss here the differences between the analysis of metastability in non-conservative and conservative dynamics, having in mind the results on the 3D Glauber and Kawasaki dynamics in finite volume, [2] and [16] respectively.

Let us first briefly recall the main ideas used in [2] for the case of Glauber dynamics. We introduce the Glauber dynamics for the 3D Ising model in complete analogy to what we did in section 2.1 for the 2D case. We still assume $h > 0$. It is easy to see that, as in dimension 2, the configuration

$+\mathbf{1}$, with all spin plus, is the stable state, i.e. the unique absolute minimum of the energy $H(\sigma)$, while the configuration with all spins minus, $-\mathbf{1}$, for $h < 2$ is a local minimum. To study the asymptotics of the tunnelling time, it is important to determine the communication height $\Phi(-\mathbf{1}, +\mathbf{1})$. To this purpose one can use the strategy already explained in the previous section in the example of the 2D Ising model, see Theorem 5.10. Indeed, as before, to every configuration σ it is possible to associate the union of unitary cubes corresponding to plus spins of σ, this region is called a *polyomino* in [2]. The energy of the configuration σ can be easily written in terms of the area, $a(\sigma)$, and the volume, $v(\sigma)$, of the corresponding polyomino: $H(\sigma) = Ja(\sigma) - hv(\sigma)$. This remark suggests that, in order to determine the communication height between states or set of states, it is useful to consider the foliation of the state space in terms of volumes of the corresponding polyominoes. Indeed, every path going from $-\mathbf{1}$ to $+\mathbf{1}$ has to cross every manifold corresponding to fixed volume. In this way the solution of the min-max problem is reduced to minimize the area at fixed volume. Following [1], we call quasi-cube a parallelepiped with sides m, $(m+\delta)$, $(m+\theta)$, with $\delta, \theta \in \{0, 1\}$, a quasi-square a parallelepiped with sides l, $(l+\alpha), 1$, with $\alpha \in \{0, 1\}$ and a bar a parallelepiped with sides $k, 1, 1$. We define *minimal polyomino* a configuration with minimal surface among all those with the same volume, and *principal polyomino* a configuration whose single cluster is a quasi-cube with a quasi-square attached to one face of the quasi-cube and with a bar attached to one side of the quasi-square (see [1] for more details).

Since for each $n \in \mathbb{N}$ there exists a unique 6-tuple $(m, l, k, \delta, \vartheta, \alpha)$ such that:

$$n = m(m+\delta)(m+\vartheta) + l(l+\alpha) + k. \tag{6.5}$$

where $m, l, k \in \mathbb{N}_0$, $\delta, \vartheta, \alpha \in \{0, 1\}$, and $\delta \leq \vartheta$, $k < l + \alpha$, $l(l + \alpha) + k < (m + \delta)(m + \vartheta)$, then it is natural to associate with each $n \in \mathbb{N}$ a principal polyomino.

The following discrete isoperimetric inequality is a key ingredient in the analysis.

Theorem 6.6 Alonso and Cerf [1], Theorems 3.1.and 3.6)
(a) All principal polyominoes are minimal polyominoes.
(b) The set of minimal polyominoes of volume n coincides with the set of principal polyminoes of volume n if and only if n is of the form "quasi-cube + quasi-square" or "quasi-cube -1".

Item (a) of Proposition 6.6 was in fact already proved by Neves [22]. This first result is sufficient to find the communication height $\Phi(-\mathbf{1}, +\mathbf{1})$. Indeed, it turns out that the maximal energy of principal polyominoes, as a function of the volume, is obtained for a critical value of the volume, $v(\sigma) = n_c$, where n_c is a suitable function of h. Call Γ this energy. Since it is possible to exhibit a reference path $\omega : -\mathbf{1} \to +\mathbf{1}$ with $\max_i H(\omega_i) = \Gamma$, we can conclude that Γ is the communication energy.

Item (b) is the crucial ingredient to complete the analysis of the asymptotics and of the tube of typical paths. For the *magic numbers* corresponding to volumes of "quasi-cube + quasi-square" the minimal polyominoes are just given by the principal polyominoes. Note that this is no longer true for "general" volumes. However, the information at magic numbers is sufficient to completely solve the problem. This is the 3D analog of what we called "focusing" in the discussion of the 2D Ising model (in theorem 5.10). In fact if we consider the maximal cycle $\mathcal{C}_{+\mathbf{1}}(-\mathbf{1})$ containing $-\mathbf{1}$ but not containing $+\mathbf{1}$, it is possible to show that the configuration of minimal energy on its boundary are principal polyominoes of volume n_c. In other words, since n_c is of the form magic number $+1$, the complete information on configurations minimizing the energy on the manifold corresponding to the volume given by the magic number $n_c - 1$, is sufficient to obtain a geometrical characterization of the configuration of minimal energy on the boundary of $\mathcal{C}_{+\mathbf{1}}(-\mathbf{1})$.

By means of the above model-dependent analysis ben Arous and Cerf are able to apply the theory developed in [6], to determine the tube of typical path after exiting $\mathcal{C}_{+\mathbf{1}}(-\mathbf{1})$ from which the the asymptotics of tunnelling time, can be derived in probability.

Notice that this proof does not need a control of stability of configurations far away from the tube, and thus the evaluation of the mean value of the tunnelling time is not done.

Let us now consider a "local version" of 3D Kawasaki dynamics introduced in [16]. Consider a lattice gas in a finite box $\Lambda \subset \mathbb{Z}^3$ with each configuration $\eta \in \{0,1\}^\Lambda$ we associate a grand-canonical hamiltonian

$$H(\eta) = -U \sum_{(x,y)} \eta(x)\eta(y) + \Delta \sum_{x\in\Lambda} \eta(x) \tag{6.7}$$

where $-U < 0$ is a binding energy, the first sum is on pairs (x,y) of n.n. sites inside Λ_-, the interior of Λ, obtained by removing the internal boundary $(\partial^-\Lambda)$ from Λ, i.e. $\Lambda_- := \Lambda \backslash \partial^-\Lambda$ and $\Delta > 0$ is an activity parameter. The standard Kawasaki dynamics is usually defined in an infinite volume given by a Metropolis Markov chain where the occupation variables of each pair of n.n. sites, (x,y), are exchanged with a rate

$$e^{-\beta[H(\eta^{(x,y)})-H(\eta)]_+} \tag{6.8}$$

with $\eta^{(x,y)}$ the configuration obtained from η by interchanging the occupation number at x, y. The local version introduced in [16] is the following: inside the box moves are Kawasaki exchange and on the boundary a process of creation and annihilation of particles takes place at rates $e^{-\Delta\beta}$ and 1, respectively. Here $e^{-\Delta\beta}$ represent the gas density in the limit of large β.

By using the transformation $\eta = \frac{1+\sigma}{2}$, it is immediate to verify that this lattice gas hamiltonian corresponds to the Ising hamiltonian with $J = \frac{U}{2}$ and $h = 2U - \Delta$. As in the case of the spin variables, we can write the energy in terms of the area and the volume of the associated polyomino of occupied sites in Λ_- and the number of particles in $\partial^-\Lambda$: $H(\eta) = \frac{U}{2}a(\eta) - (3U - \Delta)v(\eta) + \Delta\sum_{x\in\partial^-\Lambda}\eta(x)$. The unique ground state is then $\mathbf{1}$, the configuration with ones precise in Λ_- and empty in $\partial^-\Lambda$, and $\mathbf{0}$, the empty configuration, is a local minimum for $\Delta < 3U$.

Arguments similar to those used in 3DG, can be used in 3DK to evaluate the communication height $\Phi(\mathbf{0}, \mathbf{1})$. Actually the same idea of foliation of the state space in terms of the volume of the cluster, with the associated results by [1], can be used in the conservative case to find the solution of the min-max problem. Let $\Gamma := \Phi(\mathbf{0}, \mathbf{1})$. Again the result on magic numbers produces an effect of focusing. However the min-max problem between contiguous manifolds happens to be much more complicated as a consequence of conservativity of the dynamics so the gate of the transition is much larger. Indeed, as explained in details in [16], Kawasaki moves produce a motion of matter along the boundary of the cluster that takes place with high probability before the growth or the shrinking of the cluster. This motion, at fixed number of particles, is a conservative effect producing a sensitive enlargement of the gate in the transition from the $\mathbf{0}$ to $\mathbf{1}$. In other words, due to this conservation there is a large degeneracy of states at the same minimal energy on the boundary of $\mathcal{C}_{\mathbf{1}}(\mathbf{0})$. For this reason it becomes really very hard to determine the typical evolution after leaving $\mathcal{C}_{\mathbf{1}}(\mathbf{0})$, as done in the non–conservative case.

However, with a very simple argument, we can prove that in 3DK there are no deep wells. More precisely in [16] it is proven that there exists $\Gamma_0 < \Gamma$ such that $\mathcal{X}_{\Gamma_0} = \{\mathbf{0}, \mathbf{1}\}$. This is proved by finding, for each configuration η different from $\mathbf{0}$, a suitable path starting at η and reaching $\mathbf{1}$ within an energy Γ_0.

Using this result we can apply the approach proposed in this paper to obtain asymptotic estimates on the tunnelling time $\tau_{\mathbf{1}}^{\mathbf{0}}$ in probability and in $\mathcal{L}^1$ and we can prove its asymptotic exponential distribution. Actually in [16] the results in $\mathcal{L}^1$ and in law are not derived. An example of a gate configuration is given in the picture.

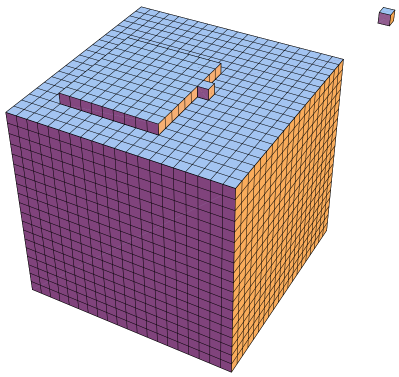


Figure 5: A critical configuration with $m_c = 20$, $l_c = 10$ and $\delta_c = 0$.

6.3 Gates and pre-factors.

One of the main aspects in this paper is to focus the attention on the notion of minimal gate, a partial but central description of the tube of typical paths.

Unlike the preceding works, we analyze here the general situation where we can have many minimal gates. This fact poses many new and interesting questions.

We discuss here the relationship between the gates and the results in [5]: [5] is the application of the powerful method developed in [3] to study metastability in a quite general setting where the state-space $\mathcal{X}_\beta$ may depend on a parameter β of the system. Contrary to our approach, where $\mathcal{L}_1$ estimates are deduced by probability estimates on cycle-paths, in the approach in [3] the results in probability are obtained via a very sharp control of the Laplace transforms of the tunnelling time. The tunnelling time is described at the level of its mean value and distribution in terms of the quantities

$$\mathbb{P}\left(\tau_\xi^\eta \leq \tau_\eta^\eta\right) \tag{6.9}$$

to be computed directly from the stochastic matrix P that defines the dynamics.

In the context of [3], metastability is characterized by the existence of a sequence of sets $\{\mathcal{M}_\beta\}_\beta$ with the property

$$\sup_{\substack{\eta,\eta'\in\mathcal{M}_\beta \\ \zeta\in\mathcal{X}_\beta}} \frac{\mathbb{P}\left(\tau_{\eta'}^\eta < \tau_\eta^\eta\right)}{\mathbb{P}\left(\tau_{\mathcal{M}_\beta}^\zeta < \tau_\zeta^\zeta\right)} \underset{\beta\to\infty}{\longrightarrow} 0. \tag{6.10}$$

Under the non-degeneracy hypothesis that for any pair $\eta, \eta' \in \mathcal{M}_\beta$ and any set $\mathcal{I} \subset \mathcal{M}_\beta \setminus \{\eta, \eta'\}$ the ratio

$$\frac{\mathbb{P}\left(\tau_{\mathcal{I}}^{\eta} < \tau_{\eta}^{\eta}\right)}{\mathbb{P}\left(\tau_{\mathcal{I}}^{\eta'} < \tau_{\eta'}^{\eta'}\right)} \tag{6.11}$$

either tends to zero or to infinity as β goes to infinity, the following Theorem is proven (among other results characterizing the low lying spectrum of the Markov generator):

Theorem 6.12 [from Theorem 1.3 in [3]]

Let $\mathcal{M}_\beta$ be a set with properties (6.10), (6.11).

For any $\eta \in \mathcal{M}_\beta$, let $\mathcal{M}_\beta(\eta) := \mathcal{M}_\beta \cap \mathcal{I}_\eta$ (see (2.10) for the definition of $\mathcal{I}_\eta$),)

$$\mathbb{E}(\tau_{\mathcal{M}_\beta(\eta)}^{\eta}) = k\left(\mathbb{P}\left(\tau_{\mathcal{M}_\beta(\eta)}^{\eta} < \tau_{\eta}^{\eta}\right)\right)^{-1}(1+o(1)) \tag{6.13}$$

and, for any $t > 0$,

$$\mathbb{P}\left(\tau_{\mathcal{M}_\beta(\eta)}^{\eta} > t\mathbb{E}(\tau_{\mathcal{M}_\beta(\eta)}^{\eta})\right) = e^{-t(1+o(1))}(1+o(1)) \tag{6.14}$$

The constant k is explicitly given and can be read as the degeneracy of the bottom of the cycle $\mathcal{C}_{\mathcal{I}_\eta}(\eta)$.

Results about the typical paths are not taken into account in this approach.

All model-dependent aspects of the problem are somehow hidden in the probability $\mathbb{P}(\tau_{\mathcal{M}_\beta(\eta)}^{\eta} < \tau_{\eta}^{\eta})$ and the strength of this method relies on the precision in the computation of this quantity. In the case of Metropolis dynamics in the Friedlin-Wentzell regime, quantities like this can be directly computed by using the well known Dirichlet representation (see e.g. [19] Theorem 6.1)

$$\mathbb{P}\left(\tau_{\xi}^{\eta} < \tau_{\eta}^{\eta}\right) = \frac{1}{2}e^{\beta H(\eta)} \inf_{h \in \mathcal{H}_{\xi}^{\eta}} \sum_{\zeta,\zeta' \in \mathcal{X}} q(\zeta,\zeta')e^{-\beta \max\{H(\zeta),H(\zeta')\}}\left(h(\zeta)-h(\zeta')\right)^2, \tag{6.15}$$

where $\mathcal{H}_\xi^\eta := \{h : \mathcal{X} \to [0,1];\ h(\eta) = 0,\ h(\xi) = 1\}$.

By taking $h(\zeta)$ as the characteristic function of $\mathcal{C}_\xi(\eta)$, we immediately get

$$\mathbb{P}\left(\tau_\xi^\eta < \tau_\eta^\eta\right) \le C_1 e^{-\beta(\Phi(\eta,\xi)-H(\eta))}, \tag{6.16}$$

where $C_1 \le |\partial\mathcal{C}_\xi(\zeta)| \max_{\zeta,\zeta'\in\mathcal{X}} q(\zeta,\zeta')$. On the other hand, the simple one-dimensional argument used in [5] eq. (4.5) gives

$$\mathbb{P}\left(\tau_\xi^\eta < \tau_\eta^\eta\right) \ge C_2 e^{-\beta(\Phi(\eta,\xi)-H(\eta))}, \tag{6.17}$$

with $C_2 \ge |\mathcal{X}|^{-1} \min_{\zeta,\zeta'\in\mathcal{X}}\{q(\zeta,\zeta') :\ q(\zeta,\zeta') > 0\}$.

We remark that by (6.16), (6.17) it is not difficult to show that (6.10) is the dynamical counterpart of $\eta_0 \in \mathcal{X}^m$ and corresponds to

$$\sup_{\substack{\eta,\eta'\in\mathcal{M}_\beta \\ \zeta\in\mathcal{X}_\beta}} [(\Phi(\eta,\eta') - H(\eta)) - (\Phi(\zeta,\mathcal{M}_\beta) - H(\zeta))] > 0 \tag{6.18}$$

The non–degeneracy hypothesis (6.11) of Theorem 6.12 implies that $\eta_0 = \mathcal{X}^m$ and is needed to ensure the exponentiality of the law of $\tau_{\mathcal{X}^s}^{\eta_0}/\mathbb{E}(\tau_{\mathcal{X}^s}^{\eta_0})$ (see Theorem 4.15).

The estimate on the mean tunnelling time given by (6.16), (6.17) via Theorem 6.12 are considerably stronger than the corresponding (4.10) given by our method and can be pushed to $C_1 = C_2 + o(\beta)$ with a finer analysis.

As noticed in [5], this computation can be done under general hypotheses and was carried out in the case of a unique minimal gate with the further simplifying hypothesis that the states in the gate are not connected to any other in one step.

We want now to give a result that reformulates and slightly generalizes Lemma 3.2 in [5]:

Theorem 6.19 If $\eta_0 = \mathcal{X}^m$ and the minimal gate $\mathcal{W}$ between η_0 and $\mathcal{X}^s$ is unique and made of isolated points (i.e. $q(\zeta,\zeta') \equiv 0$ for all $\{\zeta,\zeta'\} \subset \mathcal{W}$).

Let $\mathcal{Q} := \Big\{\eta \in \mathcal{X} : \ \Phi(\eta,\eta_0) \leq \Gamma = \Phi(\eta,\mathcal{X}^s)\Big\} \setminus \mathcal{S}(\eta_0,\mathcal{X}^s)$ and $\check{p}_\zeta := \sum_{\xi\in\mathcal{C}_{\mathcal{X}^s}(\eta_0)} P(\zeta,\xi)$, $\hat{p}_\zeta := \sum_{\xi\notin\mathcal{C}_{\mathcal{X}^s}(\eta_0)} P(\zeta,\xi)$

Then,

$$\mathbb{P}\left(\tau^{\eta_0}_{\mathcal{X}^s} < \tau^{\eta_0}_{\eta_0}\right) = K_{\eta_0} e^{\beta(\Phi(\eta_0,\mathcal{X}^s)-H(\eta_0))}(1+o(1)) \tag{6.20}$$

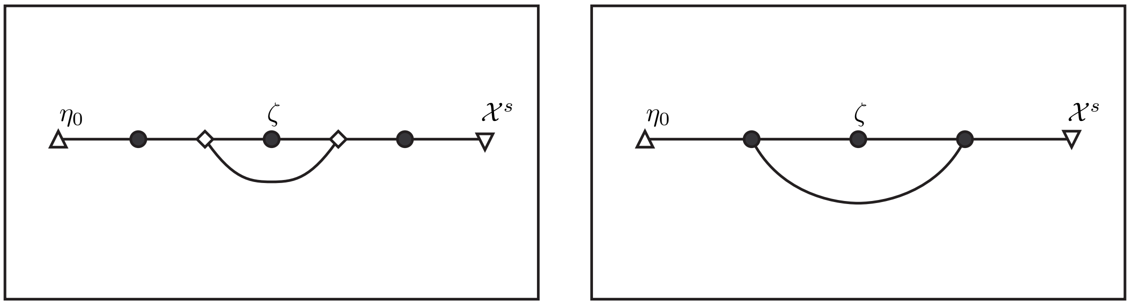
With

$$K_{\eta_0}^{-1} = \sum_{\zeta\in\mathcal{S}(\eta_0,\mathcal{X}^s)} \frac{\hat{p}_\zeta\check{p}_\zeta}{\hat{p}_\zeta+\check{p}_\zeta}(1+o(1)) = \sum_{\zeta\in\mathcal{W}(\eta_0,\mathcal{X}^s)} \frac{\hat{p}_\zeta\check{p}_\zeta}{\hat{p}_\zeta+\check{p}_\zeta}. \tag{6.21}$$

Proof. The proof is based on the notion of minimal gate that turns out to be crucial for the analysis of the structure of the set of saddles. It can be obtained along the same lines as the ones of Lemma 3.2 in [5] to which we refer: here we only outline some specific points. it is easy to see that the hypothesis of uniqueness of the minimal gate implies that $\mathcal{W} \subseteq \partial\mathcal{C}_{\mathcal{X}^s}(\eta_0)$. Suppose first all the saddles are essential; in this case we can directly apply Lemma 3.2 in [5] to get the result. On the other hand, if there are unessential saddles, it becomes crucial to use in our construction the set $\mathcal{Q}$. that contains $\mathcal{C}_{\mathcal{X}^s}(\eta_0)$ together with all cycles that can be connected to $\mathcal{C}_{\mathcal{X}^s}(\eta_0)$ through unessential saddles. Using this set $\mathcal{Q}$ it is possible to reduce the study of the pre-factor to the analysis of single steps of the dynamics as it is needed in the definitions of $\check{p}_\zeta$ and $\hat{p}_\zeta$ that involve only the one-step transition probabilities. □

It is immediate to see that $\hat{p}_\zeta$ is exponentially small if ζ is unessential, showing that only the states in the minimal gate $\mathcal{W}$ (supposed unique) contribute to the pre-factor in (6.21).

It is a very remarkable fact that the set $\mathcal{W}$ emerges in this context as the crucial set to be investigated. A natural conjecture arises: is it the case that unessential saddles do not contribute to the pre-factor K_{η_0} in (6.21) also in the case we drop the hypothesis of uniqueness of the minimal gate? As we already said, the answer is negative:



a) b)

Figure 6: Two examples where $H(\bullet) > H(\diamond) > H(\triangle) > H(\triangledown)$. Only in case a) the unessential saddle ζ does not influence the pre-factor $C_{-\mathbf{1}}$.

In figure 6, we give two examples, apparently very similar. Only in the first case though, the unessential saddle ζ does not influence the pre-factor.

We conjecture that ζ does not influence the pre-factor whenever there exists a cycle $\mathcal{C} \not\supset \mathcal{X}^s \cup \eta_0$ that is crossed by every optimal path $\omega \in (\zeta \to \{\mathcal{X}^s \cup \eta_0\})$. Heuristically, this property entails that the process when reentering $\mathcal{C}$ looses memory of its visit to ζ. More precisely, there exists $\delta > 0$ such that for any $\xi \in \mathcal{C}$,

$$\mathbb{P}\left(\tau^{\xi}_{\mathcal{X}^s} < \tau^{\xi}_{\eta_0}\right) = \mathbb{P}\left(\tau^{\xi}_{\mathcal{X}^s} < \tau^{\xi}_{\eta_0} \mid \tau^{\xi}_{\mathcal{X}^s \cup \eta_0} < \tau^{\xi}_{\zeta}\right)(1 + O(e^{-\beta\delta})) \qquad (6.22)$$

Indeed,

$$\mathbb{P}\left(\tau^{\xi}_{\mathcal{X}^s} < \tau^{\xi}_{\eta_0}\right) = \mathbb{P}\left(\tau^{\xi}_{\mathcal{X}^s} < \tau^{\xi}_{\eta_0\cup\zeta}\right) + \mathbb{P}\left(\tau^{\xi}_{\zeta} < \tau^{\xi}_{\mathcal{X}^s\cup\eta_0}\right)\mathbb{P}\left(\tau^{\zeta}_{\mathcal{X}^s} < \tau^{\zeta}_{\eta_0}\right) =$$
$$\mathbb{P}\left(\tau^{\xi}_{\mathcal{X}^s} < \tau^{\xi}_{\eta_0\cup\zeta}\right) + \mathbb{P}\left(\tau^{\xi}_{\zeta} < \tau^{\xi}_{\mathcal{X}^s\cup\eta_0}\right)\Big[\mathbb{P}\left(\tau^{\zeta}_{\xi} < \tau^{\zeta}_{\mathcal{X}^s\cup\eta_0}\right)\mathbb{P}\left(\tau^{\xi}_{\mathcal{X}^s} < \tau^{\xi}_{\eta_0}\right) +$$
$$\mathbb{P}\left(\tau^{\zeta}_{\mathcal{X}^s} < \tau^{\zeta}_{\eta_0\cup\xi}\right)\Big] \tag{6.23}$$

Since all optimal paths $\omega \in (\zeta \to \mathcal{X}^s \cup \eta_0)_{opt}$ must enter $\mathcal{C}$, by the same argument used in the proof of theorem 5.4 and by Theorem 2.17 we get $\mathbb{P}\left(\tau^{\zeta}_{\xi} < \tau^{\zeta}_{\mathcal{X}^s\cup\eta_0}\right) = 1 - O(e^{-2\beta\delta})$ for suitable δ.

Hence,

$$\text{l.h.s. of (6.23)} \;=\; \mathbb{P}\left(\tau^{\xi}_{\mathcal{X}^s} < \tau^{\xi}_{\eta_0\cup\zeta}\right) + \mathbb{P}\left(\tau^{\xi}_{\zeta} < \tau^{\xi}_{\mathcal{X}^s\cup\eta_0}\right)\Big[(1 - O(e^{-2\beta\delta}))\mathbb{P}\left(\tau^{\xi}_{\mathcal{X}^s} < \tau^{\xi}_{\eta_0}\right) + O(e^{-2\beta\delta})\Big] \tag{6.24}$$

and

$$\mathbb{P}\left(\tau^{\xi}_{\mathcal{X}^s} < \tau^{\xi}_{\eta_0}\right) = \frac{\mathbb{P}\left(\tau^{\xi}_{\mathcal{X}^s} < \tau^{\xi}_{\eta_0\cup\zeta}\right)\left(1 + O(e^{-2\beta\delta})\frac{\mathbb{P}\left(\tau^{\xi}_{\zeta} < \tau^{\xi}_{\eta_0\cup\mathcal{X}^s}\right)}{\mathbb{P}\left(\tau^{\xi}_{\mathcal{X}^s} < \tau^{\xi}_{\eta_0\cup\zeta}\right)}\right)}{\mathbb{P}\left(\tau^{\xi}_{\mathcal{X}^s\cup\eta_0} < \tau^{\xi}_{\zeta}\right)\left(1 + O(e^{-2\beta\delta})\frac{1-\mathbb{P}\left(\tau^{\xi}_{\mathcal{X}^s\cup\eta_0} < \tau^{\xi}_{\zeta}\right)}{\mathbb{P}\left(\tau^{\xi}_{\mathcal{X}^s\cup\eta_0} < \tau^{\xi}_{\zeta}\right)}\right)} \tag{6.25}$$

Now, since $\Phi(\zeta, \mathcal{X}^s \cup \eta_0) \leq H(\zeta)$, by Theorem 2.17 $\mathbb{P}\left(\tau^{\xi}_{\mathcal{X}^s\cup\eta_0} < \tau^{\xi}_{\zeta}\right) \geq e^{-\beta\delta}$ and $\mathbb{P}\left(\tau^{\xi}_{\mathcal{X}^s} < \tau^{\xi}_{\eta_0\cup\zeta}\right) \geq e^{-\beta\varepsilon}$ for any ε. (6.22) follows.

In the example of figure 6, we see that while in case a) the trajectories leaving ζ must enter the cycle given by the two states denoted with the symbol $\diamond$, in case b) the visit to the state ζ must be taken into account in the computation of the transition probability.

We will further explore the connection between gates ad pre-factors in a forthcoming paper.

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