



UNIVERSITÀ
DEGLI STUDI
FIRENZE



UNIVERSITÀ
DEGLI STUDI
DI PERUGIA

[INdAM]
Istituto Nazionale
di Alta Matematica

Università di Firenze, Università di Perugia, INdAM consorziate nel CIAFM

**DOTTORATO DI RICERCA
IN MATEMATICA, INFORMATICA, STATISTICA
CURRICULUM IN MATEMATICA
CICLO XXIX**

Sede amministrativa Università degli Studi di Firenze
Coordinatore Prof. Graziano Gentili

**Metastability for Lattice Gas
Model under
Kawasaki Dynamics**

Settore Scientifico Disciplinare MAT/06

Dottorando:
Majid Alamdari

Majid Alamdari

Tutor
Prof. Francesca Romana Nardi

Francesca Romana Nardi

Coordinatore
Prof. Graziano Gentili

Contents

1		7
1.1	Metastability	7
1.2	Anisotropic Kawasaki dynamics	8
1.3	Different approaches to metastability	12
1.4	Application overview	13
1.5	Outline	14
2		15
2.1	Path-wise approach: model independent results	15
2.1.1	Initial discussion	17
2.2	Definitions and notations	18
2.3	Main results	24
2.4	Escape from the boundary of a transient cycle	25
2.5	Asymptotic exponentiality of the exit time	26
2.6	The exit tube	27
2.7	Asymptotic in probability of tunneling times	31
2.8		31
2.9	Recurrence to $\mathcal{X}_V$	35
2.10	Asymptotic of tunneling time	36
2.10.1	General results	36
2.11	The Model-Dependent Input	39
2.12	Gate	40
2.12.1	Essential Saddles and Gates	40
2.12.2	Crossing the Gates	41
3		43
3.1	The standard stochastic Ising model in two dimensions	45
3.2	The local minimum	49
3.3	Sub-critical and super-critical rectangles	52
3.4	Subcritical configurations and global saddles	53
3.5	Alternative method to determine $\Phi(-\underline{1}, +\underline{1})$	65
4		69
4.1	The Van Der Waals-Maxwell theory	69
4.2	Isotropic dynamics	72
4.2.1	Dynamics in two dimensions	76
4.3	Local Kawasaki Dynamics	77
4.3.1	Definition of the Model	77

4.3.2	Kawasaki dynamics	78
4.3.3	Rough description of nucleation in two dimensions	79
4.4	Results for Ising-Kawasaki Model	80
4.4.1	Critical droplets	80
4.4.2	Sharp description of nucleation in two dimensions	82
4.5	Geometry in two dimensions	84
4.5.1	Some geometric definitions	84
4.5.2	Protocritical droplets: Proof of Theorem 4.6	85
4.6	Structure of the communication level set	88
4.6.1	Optimal paths	88
4.6.2	Motion on C^*	92
4.6.3	Graph structure of the energy landscape	95
4.6.4	Two global geometric facts	95
5		97
5.1	Definition of the Model and Main Result	97
5.1.1	Clusters, projections, and vacancies	98
5.1.2	Standard and Domino Rectangles	100
5.1.3	Main Results for transition time	101
5.1.4	Main Results for the Gate	102
5.2	Heuristics	103
5.2.1	Metastability: Static Heuristics	103
5.2.2	Dynamic Heuristics	105
5.3	Proof of the Theorems for the Transition time	111
5.3.1	Configurations of Minimal Energy at s Fixed	113
5.3.2	Reference Path	116
5.3.3	The Exit from the Set	123
5.3.4	Communication Height and Gate	130
5.4	Theorems for the Gate	131
5.4.1	Reduction	131
5.4.2	Proof of Theorem 5.3	134
6		137
6.1	Definition of the Model and Main Results	137
6.1.1	Horizontal and Vertical Rectangles	138
6.1.2	Main Results for transition time	138
6.1.3	Main Results of the Gate	140
6.2	Heuristics	141
6.2.1	Dynamic Heuristics	141
6.3	Proofs of the theorems for the Transition time	147
6.3.1	Construction of the reference path	147
6.3.2	The Exit from the Set $\mathcal{B}_{sa}$	154
6.3.3	Communication Height and Gate	163
6.4	Theorems for the Gate	163
6.4.1	Reduction	163
6.4.2	Stable and Metastable States	165
6.4.3	Proof of Theorem 6.5	165

ACKNOWLEDGMENTS

I would like to express my warm thanks to my thesis supervisor, Prof. Francesca Romana Nardi, for her helps and supports. She helped me choose a very interesting and important topic for investigation and making progress. With her encouragement, I was able to overpass all the difficulties in my career and complete this project.

I would like to thank Prof. Carlo Casolo for his advises and helps in finding the right direction and his kinds regards during my career.

I also would like to thank Prof. Graziano Gentili for his patience. All the students of Department of Mathematics for their guidance. I also want to thank my family for moral, financial support and for their patience during my PhD's study.

I am very thankful to Professor Nardi for her knowledge and critical guidance, for the endless hours she spent reviewing and editing my thesis, and for her kindness in accommodating my schedule.

Chapter 1

Introduction

1.1 Metastability

The phenomenon of metastability is defined by the following scenario: (i) a system is "trapped" for an abnormally long time in a state: the metastable state different from the eventual equilibrium state that is consistent with the thermodynamical parameters. (ii) In the metastable state the system behaves as if it were in regular equilibrium. (iii) Subsequently, the system undergoes a sudden transition at a random time from the metastable to the stable state. The mathematical study of this phenomenon has been a standing issue since the foundation of Statistical Mechanics, but only in the 80's rigorous mathematical approaches started to be developed and, due to the great interest of the subject, they then proliferated to a multitude of different approaches. These mathematical approaches; however, are not completely equivalent as they rely on different definitions of metastable states and thus involve different properties of hitting and escape times. The situation is particularly delicate for evolution of infinite volume systems and for irreversible systems. The proliferation of definitions and hypotheses on metastable behavior arises from the diversity of the physical situations in which the phenomenon appears. This diversity results in contrasting demands on the appropriate mathematical theory. The main issues confronted by the mathematical treatment of metastability can be grouped into three categories.

Conservative vs non conservative dynamics. This dichotomy applies to dynamics for statistical mechanical models of fluids or magnets. Non conservative dynamics are those that do not conserve the total number of particles or the total magnetization. They include Glauber (that is, single spin flip) dynamics (used to model metastable ferromagnets) and many probabilistic cellular automate (that is, parallel dynamics). In contrast, conservative dynamics are suitable to the study of supersaturated gases. Its study poses enormous challenges because particle or magnetization conservation introduces non local effects.

Finite vs infinite configuration space. Two extreme types of metastability studies can be distinguished. In the finite space case, the configuration space remains fixed (or bounded) while the drift towards (metastable) configurations

is increased (e.g., temperature goes to zero). In the infinite space setup, the size of the configuration space grows in an unbounded fashion, while drifts are kept approximately constant. In many instances both parameters (drift and size of the space) change simultaneously, but usually these changes are coupled so one of the effects is dominant. Mathematically, the distinction stems from the possibility of entropic effects in the infinite volume case that changes the scale at which distribution laws must be controlled. The iconic case is the thermodynamic limit of spin or gas models, see for instance [61, 37, 31, 32, 58]. In these models, exit from metastability requires nucleation, that is the formation of a critical droplet. The probability of such an event in a large volume must include the entropic contribution” due to the fact that the nucleation can take place anywhere in the volume.

Parallel dynamics and cost functions. Following the matrix imposed by Metropolis and Glauber dynamics, stochastic transition rates are written as exponential of cost functions. For reversible single spin flip dynamics these costs are determined by the difference of energy between the two states involved in the move. This is not true for parallel dynamics (for instance for Probabilistic Cellular Automata [7, 20, 22]) in which, at each step, all spins are independently tested. In such evolution, costs are a possibly complicated function of the different patterns of spin flips connecting the relevant states. In these cases it is therefore necessary to dissociate energy profiles from energy barriers. The former are associated to invariant measures and determine the set of stable and metastable configurations. The latter are associated to transition rates and determine drifts and exit times.

Three main questions that are analyzed in Metastability studies,

- (1) . The first hitting time on the stable set for a chain that starts at a metastable state, namely,

$$\tau_{\mathcal{X}_s}^x = \inf\{t \in \mathcal{N} : \mathbf{X}_0 = x, \mathbf{X}_t \in \mathcal{X}_s\}$$

where x is a metastable states and $\mathcal{X}_s$ is the set of energy global minima. Results can be given in probability, $\mathcal{L}^1$ or exponential and distribution.

- (2) . The droplets of nucleation namely the critical configuration that the process must visit with high probability before reaching the set of stable states.
- (3) . The typical trajectories of the process, namely the tube trajectories that the process must follow with high probability during the transition time, from metastable state to the set of stable states.

1.2 Anisotropic Kawasaki dynamics

In this thesis we study the metastable behavior of the two-dimensional anisotropic Ising lattice gas subject to Kawasaki dynamics. We consider the local version of the model, where particles live and evolve in a conservative way on a finite box Λ and are created respectively annihilated at the boundary of this box in a way that reflects an infinite gas reservoir. In this way the number of particles

is not globally conserved and the equilibrium will be described by means of a grand-canonical Gibbs measure with a chemical potential which is related to the rate of creation of particles at the boundary. In [32, 38] the local isotropic version of the model with the same interaction with vertical and horizontal model was studied and results about the transition time and critical configurations were derived. Moreover, the authors show how to obtain results for the model with periodic boundary conditions from the ones of the local version. Using the latter and the results for the local weakly anisotropic model in ref. [48], one could obtain results for weak anisotropic model with boundary conditions. The innovative results of this thesis concern the model with strong anisotropy.

We introduce a stochastic dynamics given by a discrete time Markov chain Metropolis algorithm (we refer to (4.43), see also [56]). In particular the detailed balance condition is satisfied with respect to the Gibbs grand-canonical measure corresponding to the Ising Hamiltonian (see equation (5.1)). We call U_1, U_2 the binding energy between two nearest neighbor particles in the horizontal and vertical direction, respectively. Without loss of generality we always suppose $U_1 \geq U_2$. We consider the asymptotic regime corresponding to fixed volume and chemical potential in the limit of large inverse temperature β . The above setup gives rise to a reversible Freidlin Wentzell Markov chain (see [56, 43]).

In [36] there is the study of typical trajectories for the local model with isotropic interaction $U_1 = U_2$. In [36], the three-dimensional isotropic case was considered and the results for about transition time and gate are proven. In [40, 36, 8, 48] the parameters were chosen so that the empty and full configurations are naturally associated to the metastable and stable states. The authors identify the size and shape of the critical droplet and the time of its creation in the limit of low temperature. These results are comparable with but less complete than those obtained in [40] for the anisotropic Ising model subject to Glauber dynamics where there are results about all the three questions of metastability. Note that, for the treatment of anisotropic Ising model with Glauber dynamics, there is no need to distinguish between weak and strong anisotropy, results and proofs are both valid. In this thesis we consider the same model but impose strong anisotropy. Consequently, we find different results about the size and the shape of the critical droplet and the time of its creation with respects to corresponding ones in [48]. Kawasaki dynamics has its own characteristics, which need to be handled in the description of the nucleation. Particles conservation in the interior of the box represent a serious obstacle in controlling the growing and the shrinking of droplets.

It will turn out that a complete description of the metastable behavior, as given in [40] for Glauber dynamics, is much more complicated for Kawasaki dynamics. The isotropic case is simpler but still quite complicated. In this context in [36], a description of the tube of typical trajectories is given. In the present paper we do not obtain such a complete description. We remark that in many previous papers [4, 39, 40, 20, 47, 41, 26] the asymptotic of the tunneling time and the tube of typical trajectories realizing the transition were treated simultaneously by exploiting a detailed control of the landscape of energy in connection with the paths allowed by the dynamics.

In this thesis, as in [48], we follow the strategy proposed in [43] and to determine the asymptotic behavior in probability, for large β , of the transition time between the empty and full configuration. Indeed using ref. [43] the control of the transition time can be obtained on the basis of relatively weak hypotheses: the knowledge of the energy of the global saddles between the metastable and the stable state together with the absence of too deep wells.

We also have for strong anisotropy some partial information on the typical trajectories realizing the transition between metastability and stability. Indeed we discuss the critical droplet representing the gate to the stable state. This results are the analogue for strong anisotropy of those in [48]. Let us now discuss the motivations and the specific features of our model by outlining the main results. In the Freidlin Wentzell regime it is natural to call Wulff shape the one minimizing the energy of a droplet at fixed volume. Indeed at low temperature only the energy is relevant not entropy. In model the Wulff shape is a rectangle with horizontal and vertical sides proportional, respectively, to the corresponding coupling constants U_1 and U_2 (see [56]).

The main question that is natural to address concerns the relevance of Wulff shape in the nucleation pattern. It turns out that particles can move along the border of a droplet more rapidly than they can arrive from the boundary of the container by inducing the growth of the droplet.

One could be tempted to conjecture that this displacement along the border of the growing droplet should be able to establish the equilibrium shape at fixed volume namely, the Wulff shape. However, a careful comparison between time scales subsection 6.2.1 of contraction, growth and of different types of movements on the border, shows that the above conjecture is false as one can see in chapter 5 and 6. The critical configurations are different and more complicated than the ones for Ising spins under Glauber dynamics (even in the anisotropic case).

We observe very different behavior of our model for weak or strong anisotropy, corresponding, roughly speaking, to U_1 smaller or larger than $2U_2$ (weak anisotropy and strong anisotropy. In [48] for weak anisotropy, a rigorous result that is proven is that the critical droplet is close to the Wulff shape (with a highly degenerate and complicated microscopic structure), whereas there are strong indications that during the other stages of nucleation, namely both in the sub-critical and super-critical part, the shape of the growing droplet is not Wulff. Actually large super-critical droplets tend to have a squared shape contrary to what happens for the non-conservative Glauber dynamics.

In this thesis we show that for strong anisotropy the critical droplet is not Wulff and the Wulff shape is accidentally crossed during the supercritical growth. In both cases the Wulff shape is not relevant in the nucleation pattern, similarly to what came out in the Glauber case (see [41, 40]). In subsection 6.2.1 in order to predict, at least at the heuristic level the nucleation pattern, we have to analyze the various mechanisms of modification of a rectangular droplet. We restrict ourselves to rectangles since, as is easy to verify, every cluster is transformed with high probability into a rectangle in a relatively short time. Suppose we

are given a rectangle with horizontal side l_1 and vertical side l_2 . Suppose that the occupied sites are precisely the ones contained inside the rectangle. The typical mechanisms to add or remove a row, or a column from a rectangle are similar to the corresponding mechanisms occurring in non-conservative Glauber dynamics; but now, in our locally conservative dynamics, an important role is played by an additional mechanism involving the displacement of particles along the border of the rectangle. It consists either

(I) of the loss of a row with the simultaneous gain of a column: $(l_1, l_2) \longrightarrow (l_1 + 1, l_2 - 1)$; or

(II) of the loss of a column with the simultaneous gain of a row: $(l_1, l_2) \longrightarrow (l_1 - 1, l_2 + 1)$

(I) and (II) can also involve, beyond locally conservative moves, creation or annihilation of particles at the boundary of the container to get the final rectangle. It is reasonable to expect that the mechanism (I) is preferred when l_2 is sufficiently large in terms of l_1 whereas (II) is preferred in the opposite case. The characteristic shape corresponding to a balance between the two mechanisms gives rise to a sort of equilibrium that corresponds to a minimum of the energy at fixed perimeter and that is not Wulff. For sufficiently large rectangles, this balance takes place when $l_1 - l_2 \approx \bar{l}$ with $\bar{l}$ a suitable constant depending on the coupling constants of the model (see (5.13)). A rectangle with such a shape is called standard (see subsection 5.1.2) for a precise definition).

As discussed heuristically in subsection 5.1.2, *for weak anisotropy*, we expect that, after an initial stage which we are going to describe in a while, the nucleation pattern consists of a growing sequence of standard rectangles. The critical droplet belongs to this sequence, and it happens that it is, at the same time, standard and Wulff but this has to be considered as an accident. Clearly, large super critical standard rectangles are almost squared. This behavior is very different with respect to the one of non conservative dynamics where, for any degree of anisotropy, the super critical growth is highly anisotropic (see [40]). Quite surprisingly, in the early stage of nucleation we have a growth along domino shape with $l_1 \approx l_2$ independently on the parameters of the interaction (see subsection 5.1.2).

In the case of *strong anisotropy* $U_1 > 2U_2$ in subsection 6.1.2, we develop the above heuristic discussion coming to the conclusion that the growth follows the domino shape up to the critical droplet which is not Wulff. Indeed in this case the ratio between the side lengths of a Wulff rectangle is larger than 2, the value corresponding to domino shape. Let $\hat{l}_1, \hat{l}_2$ be the horizontal and vertical sides, respectively, of the critical droplet. In this strongly anisotropic case the super-critical growth follows a sequence of rectangles with $l_2 = \hat{l}_2$ and $l_1 = \hat{l}_2 + m$, with $m = 1, 2, \dots$ up to $l_1 = L$ the side of the container (that we called l_2^* -horizontal in definition). During this epoch, the nucleation pattern crosses the Wulff shape. Finally, after the formation of a strip $\hat{l}_2 \times L$ (called $-$ horizontal in definition (6.2)) the system starts growing in the vertical direction up to the full configuration.

This behavior in the strongly anisotropic case is more similar to what happens in the corresponding Glauber case for any degree of anisotropy. See [40].

1.3 Different approaches to metastability

Early approaches to metastability were based on the computation of expected values with respect to restricted equilibrium states [57]. This paradigm is still influential in physics, see e.g. [42]. The influence of Probability on Statistical Mechanics led to an alternative pattern of thoughts based on stochastic dynamics and focused on their spectral properties and on the behavior of their typical trajectories. This point of view has given rise to different theoretical constructions that can be classified, roughly, in three major groups.

(I) *Classical approach*: Hitting times of Markov chains. The escape time from metastability is determined, by the visiting or hitting time to a set of states of very small (invariant) measure, when most of the measure is carried by a different, somehow reduced, set of states (see, e.g. [29]). Similar problems were confronted in reliability theory where typical states were called good and those concerned by the hitting times were called bad. The exponential character of good-to-bad transitions is due to the existence of two different time scales: long times are needed to go from good to bad states, while the return to good states from anywhere (except, perhaps, the bad states) is much shorter. As a result, a system in a good state can reach the bad ones only through a large fluctuation bringing it all the way to the bad state. Indeed, any "intermediate" fluctuation would be followed by an unavoidable return to the good states, where, by Markovianity, the process would start afresh independently of previous attempts. Hence, the escape time is made of a large number of independent returns to the good states followed by a final successful excursion to badness that must happen without hesitation, in a much shorter time. The exit time is, therefore, a geometric random variable with extremely small success probability. In the limit exponentiality is found.

(II) *Large deviations of trajectory distributions*. Freidlin and Wentzel [33] were the first to use the large deviation machinery to study the problem of exit times from an attractive domain. Their theory applies to stochastic differential equations with a deterministic driving gradient force and a small Brownian stochastic term. The deterministic part of the dynamics is responsible for the fast return to good states" while the stochastic contribution provides the escape mechanism. The smallness of this last contribution leads to very long time scales for the visit to "bad" states. Typical trajectories are described using a graphical method built out of two basic ingredients: cycles (associated to metastable pieces of trajectories) and exit tubes (describing typical escape trajectories).

The Freidlin and Wentzel theory evolved into two related schools that we shall call the graphical [15] and the path-wise [14] approach. The former relies on a refinement of Freidlin and Wentzel's graphical methods allowing for a detailed study of exit paths via a decomposition into cycles and saddle points traversed from cycle to cycle. The exit time also decomposes into the time spent at each point of the exit path. This graphical approach has been applied to re-

versible Metropolis dynamics and to simulated annealing in [15, 19, 62, 61]. The path-wise approach, on the other hand, proposed in [14], was introduced as an adaptation of the ideas of Freidlin and Wentzel to Metropolislike dynamics, with all notions and properties expressed in terms of an energy profile associated to the invariant measure. This provides a clearer and physically appealing picture. In particular, absolute energy minima identify stable states and "deep" local energy minima lead to metastability. The two time scales within each energy well correspond, respectively, to fast "downhill" and infrequent uphill trajectories. In the limit of very steep wells (temperature tending to zero), the theory yields rather precise information on: (i) the transition time, i.e., the time needed to arrive to the stable equilibrium, which is determined by the height of the largest energy barrier separating metastable from stable states. (ii) The typical exit tube, i.e., the sequences of configurations along which the formation of the stable phase takes place. This is the physically relevant mechanism that, in gas or spin systems, is mediated by the appearance of a critical droplet after which the system quickly relaxes to equilibrium.

The full power of this method was first exploited in [53] and comprehensively reviewed in [62]. It has been extended to nonreversible Markov processes in [53] (though irreversibility brings back to the graphical approach). The approach was further simplified in [47] where transition times are determined on the basis of a ranking of stability levels, without requiring detailed knowledge of typical trajectories.

(III) *Potential theoretical approach*: spectral properties of Markov transition matrices. In the early eighties Aldous and Brown [1] proposed a new approach to the hittingtime theory based on spectral properties of the transition matrix and the use of the Dirichlet form. This approach has the advantage of leading to quite precise error bounds for the exponential approximation. The current version of this strategy is the potentialtheoretic approach developed in [12] (see [13] for reviews). Besides exponential laws, this method gives more precise estimates of the expected value of the transition time, including a pre factor that cannot be found with alternative approaches. The determination of this pre factor, however, requires the knowledge of the critical droplet and neighboring configurations; information that has to be imported from more detailed path-wise studies. In ref. [12] another use of spectral and potential theoretical techniques is proposed in which only visits to well bottoms are registered. Upon time re scaling, a continuous-time Markov process is obtained whose transition rates encode the information on transition times. (See also [5, 6] for recent development).

1.4 Application overview

We outline briefly some applications of the theories described above. The aim is not to be exhaustive, but rather to list references useful in relation to the definitions and comparisons to follow.

The general theory [15, 16, 60, 43, 56, 53, 62] and metastability studies in the nineties (see [14, 19, 21, 53, 4, 26, 39, 47, 53] for the path-wise approach

and [19, 62, 61] for the graphical approach) refer to single spin flip dynamics (Metropolis, Glauber) of Ising-like models (including meanfield versions) in finite volume and at low temperature. Studies within the general potential theoretical approach refer both to a general Markov process point of view [10, 11] and applications to meanfield and Ising model [12, 13].

The study of metastability for conservative dynamics started a decade after and initially involved nearest neighbor lattice gases at low temperature and density inside finite boxes with open boundary conditions mimicking infinite reservoirs fixing particle density. Relevant references are [28, 32, 36, 49] for the path-wise approach and [8, 31, 29] for the potential theoretic approach.

Models with parallel dynamics were studied first from a numerical point of view in [7] and then rigorously in [20, 25, 24] (path-wise approach) and [53] (potential theoretic approach).

The more involved infinite volume limit, at low temperature or vanishing magnetic field, was first studied via large deviations techniques in [18, 44, 45, 59, 27, 58] and potential theoretically in ref. [9]. These references dealt with Ising and Blume-Capel models under Glauber dynamics. The Ising lattice gas model subjected to Kawasaki dynamics was studied in [37, 32, 38] and [9] (potential theoretic approach) in the limit of temperature and volume growing exponentially fast to infinity.

1.5 Outline

In chapter 2 we give the general model independently results that can be obtained using path wise approach. In chapter 3 we define the Ising model evolving under Glauber dynamics. In chapter 4 we discuss Kawasaki Isotropic Ising model its critical droplet its asymptotic results and exit tubes. In chapter 5 we discuss Kawasaki anisotropic model under weak anisotropic conditions. In chapter 6 we discuss Kawasaki anisotropic model under strong anisotropic conditions.

Chapter 2

Metastability for spin models under Glauber dynamics

2.1 Path-wise approach: model independent results

We start by defining the Markov chains that we want to study in the present chapter. After general *FreidlinWentzell* Markov chains, we move on to the simple and interesting particular case of reversible FreidlinWentzell Markov chains; finally we introduce the more particular case of Metropolis Markov chains which constitute the main object of our study in this chapter. We also introduce particular Markov chains satisfying a non-degeneracy condition which further simplifies the theory.

Condition FW (FreidlinWentzell) We say that an ergodic aperiodic Markov chain on a finite state space $\mathcal{X}$ satisfies condition FW if its transition probabilities $P(x, y)$ decay exponentially fast in a large parameter β , satisfying the following estimates:

$$\exp[\beta(\Delta(x, y) + \gamma(\beta))] \leq P(x, y) \leq \exp[\beta(\Delta(x, y) - \gamma(\beta))]$$

where Δ is a non-negative matrix

$$\Delta : \mathcal{X} \times \mathcal{X} \longrightarrow R^+ \cup \{+\infty\}$$

and $\gamma(\beta) \rightarrow 0$ as $\beta \rightarrow \infty$.

The elements of $\mathcal{X}$ will be called indifferently points or states. FW Markov chains can be regarded as small random perturbations of $\beta = \infty$ dynamics, where only transitions with $\Delta(x, y) = 0$ are allowed.

Condition R (reversibility) We say that a Markov chain on a finite state

space $\mathcal{X}$ satisfies condition R if, considering the set $\mathcal{V}_0 := \{(x, y) : x \in \mathcal{X}, y \in \mathcal{X}, x \neq y\}$ of pairs of distinct states,

- (i) there exists a connectivity function $q : \mathcal{V}_0 \rightarrow [0, 1]$ satisfying
 - for any $x, y \in \mathcal{X}$, $\sum_{x \neq y} q(x, y) \leq 1$ (normalizability)
 - for any $x, y \in \mathcal{X}$, $q(x, y) = q(y, x)$ (symmetry)
 - for any $x, y \in \mathcal{X}$ there exists $n \in \mathbb{N}$ and $x_0, \dots, x_n \in \mathcal{X}$ with $x_0 = x$, $x_n = y$ and $q(x_i, x_{i+1}) > 0$, $i = 0, \dots, n-1$ (irreducibility),
- (ii) there exists an energy function $H : \mathcal{X} \rightarrow \mathbf{R}$,
- (iii) let $\mathcal{V}$ be the set of pairs of communicating states $\mathcal{V} = \{(x, y) \in \mathcal{V}_0 : q(x, y) > 0\}$, then there exists a function $\tilde{H} : \mathcal{V} \rightarrow \mathbf{R}$ such that $\tilde{H}(x, y) = \tilde{H}(y, x)$ and $\tilde{H}(x, y) \geq H(x) \vee H(y)$, so that the transition probabilities $P(x, y)$ of the Markov chain are given by

$$P(x, y) = \begin{cases} q(x, y) \exp(-\beta[\tilde{H}(y, x) - H(x)]) & \text{if } x \neq y \\ 1 - \sum_{z \neq x} P(x, z) & \text{if } x = y \end{cases} \quad (2.1)$$

Condition R is a particular case of FW with

$$\Delta(x, y) = \tilde{H}(x, y) - H(x) \quad (2.2)$$

The above choice corresponds to a reversible Markov chain:

$$\forall x, x' \in \mathcal{X} \quad \mu(x)P(x, x') = \mu(x')P(x', x) \quad (2.3)$$

with

$$\mu(x) = \frac{\exp(-\beta H(x))}{\sum_{z \in \mathcal{X}} \exp(-\beta H(z))}$$

It is natural to interpret β as the inverse temperature and μ as the Gibbs measure. From (2.3) one immediately deduces that μ is the unique invariant probability measure of the chain.

Condition M (Metropolis) We say that a Markov chain on a finite state space $\mathcal{X}$ with transition probabilities $P(x, y)$ satisfies condition M if there exists a connectivity function q satisfying (i) in condition R and an energy function $H : \mathcal{X} \rightarrow \mathbf{R}$, so that:

$$P(x, y) = \begin{cases} q(x, y) \exp(-\beta[H(y) - H(x)]^+) & \text{if } x \neq y \\ 1 - \sum_{z \neq x} P(x, z) & \text{if } x = y \end{cases} \quad (2.4)$$

The above defined Metropolis Markov chains are a particular case of reversible Markov chains: they correspond to the choice $\tilde{H}(x, y) = H(x) \vee H(y)$. In this case the $\beta = \infty$ dynamics only allows transitions that lower the energy.

2.1.1 Initial discussion

We now discuss the first exit problem from a general set G for a general Metropolis Markov chain with finite state space, in the limit of large β . It turns out that the most relevant case corresponds to G given by a cycle (see definition 2.5 below), namely a set whose internal points, for large β , are typically visited many times by our process before exiting. As we shall see, some specific difficulties arise when G contains many stable equilibrium, namely many local minima for the energy, which can be considered as attractors with respect to the $\beta = \infty$ dynamics (where only moves decreasing the energy are allowed).

In the case of a set G completely attracted by a unique stable point, it turns out that the exit from G , when it occurs, follows a quite fast path, taking place in an interval of time T independent of β , without hesitation. The exponentially long (in β) time needed by the process to exit from G is a consequence of the exponentially small probability that an excursion outside G takes place in a finite time independent of β . So the typical time needed to see the first excursion outside G is very long as a consequence of a very long series of unlikely attempts before the successful one, but the time spent during this first excursion is relatively short.

On the contrary, in the case of a set G containing many minima for the energy, the time needed to see the first excursion is still exponentially large in β but, in general, also the time spent during the first excursion from G will typically be exponentially large in β , even though with a smaller rate. Indeed the first excursion will involve random fluctuations inside suitable permanence sets during exponentially long random intervals of time (resistance times). As will appear clear, a mechanism of exit in a finite interval of time and without hesitation is, in general, very low in probability.

We shall see that when G contains many minima for H , even the formulation of the problem of determination of typical paths of exit from G changes drastically with respect to the case of completely attracted domains. Whereas in the completely attracted case we have to determine single optimal paths of exit, in the general case we have to introduce generalized paths given by sequences of permanence sets with relative permanence times. The single trajectory inside a permanence set cannot be specified. The specification of a typical tube of exit from a general domain G is intrinsically stochastic: the exit from a permanence set is exponentially long in β and tends to be unpredictable for large β ; moreover the behavior inside a permanence set is well described by a restricted equilibrium (conditional Gibbs) measure.

Let us start with a list of basic definitions. As we said before, for the sake of simplicity of the exposition, we shall consider Metropolis Markov chains. Our definitions and results can be easily extended to the case of general reversible Markov chains; here we only give explicitly, in this case, the crucial definition of cycle (see definition 2.5) and an estimate of the first exit time (see lemma 2.21). The case of general non-reversible Markov chains is much more difficult

2.2 Definitions and notations

Consider a Markov chain $\mathcal{X}_t$ satisfying condition M. As usual we denote by P_x the law of the process starting at $x \in \mathcal{X}$.

A *path* is a sequence $\omega = (\omega_0, \dots, \omega_N)$, with $N \in \mathcal{N}$ with $\omega_i, \omega_j, j = 1, \dots, N-1$, communicating states (i.e. $P(\omega_i, \omega_j) > 0$). We often write $\omega : x \rightarrow y$ to denote a path joining x to y to denote a path joining x to y . Given $G_1 \subseteq \mathcal{X}, G_2 \subseteq \mathcal{X}$, we write $\omega : G_1 \rightarrow G_2$ to denote a path joining x to y for some $x \in G_1, y \in G_2$. If ω is a path and $\omega_i = x$ for some i , then we say $x \in \omega$.

We denote by $\Omega \subseteq \mathcal{X}^{\mathcal{N}}$ the set of all possible paths.

A path $\omega = (\omega_0, \dots, \omega_k)$ is called downhill (strictly downhill) if $H(\omega_{i+1}) \leq H(\omega_i)$, ($H(\omega_{i+1}) < H(\omega_i)$) for $i = 0, \dots, k-1$.

We say that a state x is downhill connected (strictly downhill connected) to a state y if there exists a downhill (strictly downhill) path $\omega : x \rightarrow y$.

A set $G \subseteq \mathcal{X}$ is connected if for any $x, x' \in G$ there exists a path $\omega : x \rightarrow x'$ totally contained in G .

Definition 2.1. Given $G \subseteq \mathcal{X}$, we define

(i) *its exterior boundary*

$$\partial^+ G := \{y \notin G, P(x, y) > 0 \text{ for some } x \in G\}$$

(ii) *its interior boundary*

$$\partial^- G := \{y \in G, P(x, y) > 0 \text{ for some } x \notin G\} \quad (2.5)$$

Definition 2.2. Given $G \subseteq \mathcal{X}$ we denote by $F = F(G)$ the set of all absolute minima of the energy on G :

$$F(G) = \{y \in G; \min_{x \in G} H(x) = H(y)\} \quad (2.6)$$

The set $F(G)$ is called the ground of G .

Definition 2.3. A maximal connected set of equal energy states is called a plateau.

Given $z \in \mathcal{X}$ we denote by $D(z)$ the plateau containing z .

Definition 2.4. We say that the real positive function $\beta \rightarrow f(\beta)$ is super exponentially small and we use the notation $f(\beta) = SES$, if $\lim_{\beta \rightarrow \infty} \beta^{-1} \log f(\beta) = -\infty$.

Notation Given a set G on which H is constant, $H(x) = H_0$, for any $x \in G$, we write by abuse of notation $H(G)$ for the common value.

A plateau D such that $H(F(\partial^+ D)) > H(D)$ is said to be stable; otherwise it is called transient. In particular the set of local minima for the energy

$$M = \{x : H(F(\partial^+ \{x\})) > H(x)\} \quad (2.7)$$

is made of stable points.

We denote by $\bar{M}$ the collection of all stable plateaux in $\mathcal{X}$.

Definition 2.5. A connected set $C \subseteq S$ which satisfies $C \subseteq \mathcal{X}$ which satisfies

$$\max_{x \in C} H(x) < \min_{z \in \partial C} H(z) = H(F(\partial C)) \quad (2.8)$$

is called a non-trivial cycle.

Notice that in our definition a singleton $\{x\}$ is a non-trivial cycle if and only if it is a local minimum $x \in M$.

Remark 2.6. (i) Given a non-trivial cycle C we write

$$U(C) = F(\partial^+ C) \quad (2.9)$$

For a trivial cycle $\{x\}$, we set $U(\{x\}) \equiv x$.

(ii) The height of a non-trivial cycle A is given by

$$\Phi(C) = H(U(C)) \quad (2.10)$$

(iii) The depth of a non-trivial cycle C is given by

$$\Gamma(C) = \Phi(C) - H(F(C)) = H(U(C)) - H(F(C)) \quad (2.11)$$

(iv) For a trivial cycle $\{x\}$ we set $\Phi(x) = H(\{x\})$ and $\Gamma(\{x\}) = 0$.

We now give some propositions (in addition to other definitions). Most of the propositions refer to simple properties of the cycles. They are relevant in view of the basic results given in theorem 2.22. For some of them the proof is immediate and we omit it.

Proposition 2.7. Given a state $\bar{x} \in \mathcal{X}$ and a real number c , the set of all points x connected to $\bar{x} \in \mathcal{X}$ by paths whose points have an energy strictly less than c , if non-empty, either coincides with $\mathcal{X}$ or is a non-trivial cycle C containing $\bar{x} \in \mathcal{X}$ with $\Phi(C) \geq c$.

Proof. Immediate. $\square$

Lemma 2.8. Consider two cycles C_1, C_2 with $C_1 \cap C_2 \neq \emptyset$. Then either $C_1 \subset C_2$ or $C_2 \subset C_1$.

Proof. It suffices to check that $\partial^+ A_1 \cap A_2 \neq \emptyset$ simultaneously with $\partial^+ A_2 \cap A_1 \neq \emptyset$ is impossible. For this, just notice that if $x_1 \in \partial^+ A_1 \cap A_2$ and $x_2 \in \partial^+ A_2 \cap A_1$ we should have, at the same time, $H(x_1) < H(x_2)$ as well as $H(x_2) < H(x_1)$. $\square$

The above proposition 2.8 establishes a partial ordering among cycles. Notice that the cycles containing a given point x are totally ordered by inclusion.

Definition 2.9. For each pair of states $x, y \in \mathcal{X}$ we define their communication height $\Phi(x, y)$ as follows:

$$\Phi(x, y) = \min_{\omega: x \rightarrow y} \max_{z \in \omega} H(z).$$

Given a subset Q of S containing both x and y , we write

$$\Phi(x, y)_Q = \min_{\omega: x \rightarrow y, \omega \subseteq Q} \max_{z \in \omega} H(z) \quad (2.12)$$

to denote the communication height between x and y in Q .

Definition 2.10. (i) The set of minimal saddles $S(x, y)$ from x to y in $\mathcal{X}$ is given by:

$$S(x, y) = \{z; \exists \omega; x \rightarrow y, \text{ such that } z \in \omega \text{ and } H(z) = \max_{u \in \omega} H(u) = \Phi(x, y)\} \quad (2.13)$$

(ii) The set of optimal paths between x and y , that we denote by $(x \rightarrow y)_{\text{opt}}$, is given by

$$(x \rightarrow y)_{\text{opt}} := \{\omega : x \rightarrow y, \text{ such that } \max_{z \in \omega} H(z) = \Phi(x, y)\} \quad (2.14)$$

(iii) A set $W \subseteq S$ is called a gate for the transition $x \rightarrow y$ if for any $\omega \in (x \rightarrow y)_{\text{opt}}$, one has $\omega \cap W \neq \emptyset$. A gate W is called a minimal gate if for any $W' \subseteq W$ there exists $\omega^* \in (x \rightarrow y)_{\text{opt}}$ such that $\omega^* \cap W' = \emptyset$.

In other words, a minimal gate is a minimal (by inclusion) subset of $S(x, y)$ that is crossed by all optimal paths.

(iv) For a given transition $x \rightarrow y$, there can be many different minimal gates. Let $\mathcal{W}$ be the set of minimal gates. We denote by $\mathcal{G}(x, y)$ the union of minimal gates:

$$\cup_{W \in \mathcal{W}} W := \mathcal{G}(x, y) \subseteq S(x, y) \quad (2.15)$$

(v) The configurations in $S(x, y) \setminus \mathcal{G}(x, y)$ (if any) are called dead-ends.

(vi) Given $z \in S(x, y)$, we say that it is unessential if for any $\omega \in (x \rightarrow y)_{\text{opt}}$ such that $\omega \cap z \neq \emptyset$, defining $B(\omega) = [\omega \cap S(x, y)] \setminus z$, we have:

(i) $B(\omega) \neq \emptyset$ and

(ii) there exists a path $\omega' \in (x \rightarrow y)_{\text{opt}}$ with $\omega' \cap S(x, y) \subseteq B(\omega)$.

(vii) We say that $z \in S(x, y)$ is essential if it is not unessential, namely if either

(i) there exists a path $\omega' \in (x \rightarrow y)_{\text{opt}}$ such that $\omega' \cap S(x, y) \equiv \{z\}$, i.e. $B(\omega') = [\omega' \cap S(x, y)] \setminus \{z\} = \emptyset$, or

(ii) there exists a path $\omega \in (x \rightarrow y)_{\text{opt}}$ such that $B(\omega) \neq \emptyset$ and $\omega' \cap S(x, y) \subseteq B(\omega)$ for all $\omega' \in (x \rightarrow y)_{\text{opt}}$.

*Unessential configurations are indeed **dead-ends** for the transition $x \rightarrow y$ and, in a certain sense, can be skipped. This is the result of the following.*

It will be made clear by proposition 2.11, given any path $\omega \in (x \rightarrow y)_{opt}$ passing through a dead-end $z \in S(x, y)$, there exists another path ω' playing the role of a short-cut for going to y by skipping z .

The set $S(x, y)$ is a trivial gate for the transition $x \rightarrow y$, but in general it is not a minimal gate. Actually, it can contain configurations that are *unessential* in the following sense.

Proposition 2.11. *$z \in S(x, y)$ is essential if and only if $z \in G(x, y)$.*

Proof. Done in [56]. □

We can have the absence of any energy barrier between a pair x and y . In this case the minima problem has a trivial solution and $x \in S(x, y)$ or $y \in S(x, y)$. This cannot happen if x and y belong to different stable plateaux.

Proposition 2.12. *If A is a non-trivial cycle then:*

(i) *for any $x, y, z \in A$ and $W \in A^c$,*

$$\Phi(x, y) \leq \Phi(z, \omega)$$

(ii) *for any $x \in A$ the set $S(x, A^c)$ does not depend on x and contains $U(A)$.*

Proof. By definition of a non-trivial cycle, for any $x, y \in A$ there exists a path $\omega : x \rightarrow y$ contained in A such that for any $\omega_i \in Wy$ one has $H(\omega_i) < \Phi(A)$; this proves (i). On the other hand any path joining $z \in A$ to $\omega \in \partial^+ A$ maximizes H in $\partial^+ A$.

Thus we have, for any $x \in A$

$$\min_{\omega \in \partial^+ A} \Phi(\omega, x) = \Phi(A)$$

which implies (ii). □

Definition 2.13. *A cycle A such that for each $z \in U(A)$ the states x to which the plateau $D(z)$ is strictly downhill connected belong to A , is called a stable or attractive cycle. A cycle A which is not stable is called transient.*

Suppose that the cycle A is transient, then there exists $y^* \in U(A)$ with $D(y^*)$ strictly downhill connected to some point x in A^c ; given a transient cycle A the points y^* downhill connected to A^c are called minimal saddles of A . The set of all minimal saddles of a transient cycle A is denoted by $S(A)$.

Notice that besides $S(A) \subseteq U(A)$, we also have $S(A) \subseteq S(A, A^c)$; for a trivial transient cycle $\{x\}$, we set $S(\{x\}) = U(\{x\}) = \{x\}$.

Definition 2.14. *A transient cycle A such that there exist $\bar{x} \in A^c$ with $H(\bar{x}) \leq H(F(A))$ ($H(\bar{x}) \leq H(F(A))$), $y^* \in S(A)$ and a declining path $\omega : y^* \rightarrow \bar{x}$, is called metastable (strictly metastable).*

Definition 2.15. Given a stable plateau D (see definition 2.3 and before (2.7)), we define the following basins for D :

(i) the wide basin of attraction of D

$$\hat{B}(D) = \{z ; \exists \text{ downhill path } \omega : z \rightarrow D\} \quad (2.16)$$

(ii) the basin of attraction of D given by

$$\bar{B}(D) = \{z : \text{every downhill path starting from } z \text{ and ending in } \bar{M}, \text{ ends in } D\}, \quad (2.17)$$

(iii) the strict basin of attraction of D , $B(D)$, given by the whole set of states S if $\bar{B}(D)$ coincides with S , otherwise

$$B(D) = \{z \in \bar{B}(D) : H(z) < H(F(\partial^+ \bar{B}(D)))\} \quad (2.18)$$

Definition 2.16. Given a non-trivial cycle C , we call a non-trivial saddle internal to A any saddle between a pair of stable plateaux contained in C .

Proposition 2.17. suppose that there exist a subset G of $\mathcal{X}$ and two points x, x' with $x \in G$, $x' \notin G$, with the following properties:

- (i) G is connected,
- (ii) for some $y^* \in F(\partial^+ G)$ with $H(x') < H(y^*)$ there exists a declining path $y^* \rightarrow x$, $\omega \setminus y^* \subseteq G$,
- (iii) there exists a declining path $\omega' : y^* \rightarrow x'$, $\omega' \cap G = \emptyset$. Then, if $A = \{z : \exists \tilde{\omega} : z \rightarrow x : \forall y \in \tilde{\omega}, H(y) < H(y^*)\}$, $A' = \{z' : \exists \tilde{\omega} : z' \rightarrow x' : \forall y' \in \tilde{\omega}, H(y') < H(y^*)\}$ so that $C(C') \equiv$ maximal connected set containing $x(x')$ with energy less than $H(y^*)$.

Then:

- (1) C, C' are non-trivial cycles and $C \subseteq G$, $C' \subseteq S \setminus G$,
- (2) $\Phi(x, x') = \Phi(G, S \setminus G) = H(y^*)$, moreover $y^* \in S(x, x')$,
- (3) every path in $(x \rightarrow x')_{\text{opt}}$ has to cross $\partial^+ G$ in $F(\partial^+ G)$ so that $F(\partial^+ G)$ contains a minimal gate for the transition $x \rightarrow x'$.
If, moreover, we have the following strict inequality, $H(z) < H(y^*)$ for any $z \in (\omega \cup \omega') \setminus y^*$,
then
- (4) $y^* \in U(C) \cap U(C')$.

Proof. Immediate. □

Given a cycle C containing several stable plateaux, we consider some smaller cycles C_i contained in C , by looking at the internal non-trivial saddles between these plateaux in C . Let us start with an immediate corollary of proposition 2.12.

Proposition 2.18. *If a cycle C contains an internal non-trivial saddle y , then it contains all the cycles C_j such that $y \in \cup_{z \in (C_j)} D(z)$.*

Proof. Immediate. $\square$

Proposition 2.19. *Let A be a non-trivial cycle and suppose that it is not contained in the strict basin of attraction of any stable plateau (i.e. $C(A)$ is non-empty). Then the following are true.*

- (i) *The cycle A can be decomposed as the union of the highest internal transient cycles and the highest internal saddles $\bar{C}(A)$ plus, possibly, a part attracted by this union, namely*

$$A = \tilde{A} \cup \bar{C}(A) \cup V, \quad (2.19)$$

$$\tilde{A} = A_1 \cup \dots \cup A_k, \quad (2.20)$$

where $A_1, \dots, A_k$ are transient cycles with $\Phi(A_i) = H_0 := H(\bar{C}(A))$, $i = 1, \dots, k$ and for any $x_i \in A_i, x_j \in A_j$, $S(x_i, x_j) \subseteq \bar{C}(A)$.

- (ii) $F(A) \subseteq \{\cup_j A_j\}$ so that at least one of the A_j s must contain points in $F(A)$.

- (iii) *The set V , if it is non-empty, is made of points with energy greater than H_0 , does not contain non-trivial saddles and is completely attracted by the set $A \cup \bar{C}(A)$, namely*

$$V \cap \bar{M} = \emptyset, \quad V \subseteq \bar{B}(\tilde{A} \cup \bar{C}(A)).$$

- (iv) *For all $y \in \bar{C}(A)$ there exists a declining path $\omega : y \rightarrow F(A)$, $\omega \subseteq \tilde{A} \cup \bar{C}(A)$.*

Proof. Since A is a cycle then $\Phi(A) > H_0$. By proposition 2.7 and proposition 2.18 the maximal connected components $A_1, \dots, A_k \subseteq A$ of states in A with energy strictly less than H_0 are cycles contained in A with $\Phi(A_i) = H_0$.

Given A_i, A_j , for any $x_i \in A_i, x_j \in A_j$, by proposition 2.12 $S(x_i, x_j)$ takes the same value for every $x_i \in A_i$ and $x_j \in A_j$; moreover, for any $x_i \in A_i, x_j \in A_j$, $S(x_i, x_j) = S(F(A_i), F(A_j)) \subseteq \bar{C}(A)$.

From this, points (i), (ii), (iii) immediately follow.

Point (iv) easily follows from the fact that for any $x \in A \cap \bar{M}$, we have $\Phi(x, F(A)) \leq H_0$ since $\bar{C}(A)$ contains the internal non-trivial saddles with maximal energy. $\square$

Definition 2.20. *Given a non-trivial cycle C we speak of its maximal internal barrier $\Theta(C)$ given by the maximal depth of the cycles C' contained in C which do not contain entirely the ground $F(C)$.*

2.3 Main results

Recall now a simple but useful result based on the stationarity of μ providing a lower bound in probability to the first hitting time to a particular state.

Lemma 2.21. *For any pair of states y, x such that $H(y) > H(x)$ and any positive $\epsilon < H(y) - H(x)$, we have:*

$$P_x(\tau_y \leq \exp[\beta(H(y) - H(x) - \epsilon)]) \leq \exp(-\beta\epsilon)\{1 + \exp(-\beta[H(y) - H(x) - \epsilon])\}.$$

Proof. See the proof of proposition 4.7 in [56]. $\square$

We now give a simple lower bound in probability to the first exit time from a cycle, for a reversible, not necessarily Metropolis, Markov chain. It is useful to extend to general reversible Markov chains the results we are giving on the first exit problem for Metropolis Markov chains.

Let us go back to Markov chains satisfying condition M . The following theorem contains the basic results on the first exit from a cycle. These results are less immediate than the previous ones. We provide here, in the reversible case, a proof based on the analysis of typical paths. We use a simple intuitive argument involving the construction of appropriate events taking place on suitable, generally exponentially large in β , intervals of time. We see here the appearance of what can be called the resistance times and why they play an important role in providing an efficient mechanism of escape.

Theorem 2.22. *Consider a Markov chain satisfying condition M . Given a nontrivial cycle C :*

- (i) *for all $\epsilon > 0$, there exist $\beta_0 > 0$ and $k > 0$ such that for any $\beta > \beta_0$, $x \in C$*

$$P_x(\tau_{\partial^+ C} > \exp(\beta[\Gamma(C) - \epsilon])) \geq 1 - e^{-k\beta};$$

- (ii) *for all $\epsilon > 0$ there exist $\beta_0 > 0$ and $k' > 0$ such that for any $\beta > \beta_0$ and for any $x \in C$*

$$P_x(\tau_{\partial^+ C} < \exp(\beta[\Gamma(C) + \epsilon])) \geq 1 - e^{-k'\beta};$$

- (iii) *there exist $\kappa = \kappa(C) > 0$, $\beta_0 > 0$ and $k'' > 0$ such that for all $\beta > \beta_0$ and for any $x, x' \in C$*

$$P_x(\tau_{x'} < \tau_{\partial^+ C}; \tau_{x'} < \exp(\beta[\Gamma(C) - \kappa])) \geq 1 - e^{-k''\beta};$$

- (iv) *there exists $c > 0$ such that for any $x \in C$, $\hat{y} \in \partial^+ C$ and β sufficiently large*

$$P_x(X_{\tau_{\partial^+ C}} = \hat{y}) \geq c \exp(\beta[H(\hat{y}) - \Phi(C)]).$$

Proof. Done in [56]. $\square$

Corollary 2.23. *Given a non-trivial cycle C , let $\Theta(C)$ be its maximal internal barrier (see definition 2.20). Then for all $\epsilon > 0$, there exists $\hat{k} > 0$ such that for any $x \in C$, $z \in F(C)$ and β sufficiently large,*

$$P_x(\tau_z > e^{\beta(\Theta(C) + \epsilon)}) < e^{-\beta\hat{k}}. \quad (2.21)$$

Proof. The proof can be obtained easily by re adapting the proof of point (iii) in theorem 2.22. $\square$

Corollary 2.24. *Given a non-trivial cycle C there exists $\bar{\kappa} > 0$ such that*

$$\sup_{x \in A} P_x(X_{\partial^+ C} \notin U(C)) < e^{-\bar{\kappa}\beta} \quad (2.22)$$

Proof. The proof is the use theorem 2.22 instead of the iterative hypothesis. $\square$

We want now to give a result concerning a lower bound on the probability of the rare event consisting in exiting from a non-trivial cycle C too early, passing through a given point $y \in \partial^+ C$.

This is contained in the following proposition which provides a counterpart to theorem 2.22 (i) and extends theorem 2.22 (iv).

Proposition 2.25. *Given a non-trivial cycle C and a positive number k ,*

$$\Theta(C) < k \leq \Gamma(C)$$

we have for any $x \in C$, $y \in \partial^+ C$, $\varepsilon > 0$ and β sufficiently large:

$$P_x(\tau_{\partial^+ C} < e^{\beta k}, X_{\tau_{\partial^+ C}} = y) \geq e^{-\beta(H(y)H(F(C)) - k + \varepsilon)}. \quad (2.23)$$

Proof. Done in [56]. $\square$

2.4 Escape from the boundary of a transient cycle

The author of [56] wants now to state and prove a proposition referring to the first escape from a transient cycle C and saying, roughly, that, under general hypotheses, with high probability, after many attempts, sooner or later our process will really escape from C entering into another different cycle by passing through one of the minimal saddles of the boundary of C .

The time for this transition has the same asymptotic, in the sense of logarithmic equivalence, as the first hitting time to the boundary of C .

The proposition is, in fact, a simple consequence of the Markov property but we think that it is useful to provide an explicit proof.

Given a transient cycle C , consider the set $U(C) = F(\partial^+ C)$ and the set $S(A) \subseteq U(C)$ of the minimal saddles of C .

Let

$$\bar{\partial}^+ C := \cup_{z \in \partial^+ C} D(z) \quad (2.24)$$

Let $U^- = U^-(C)$ be the subset of A to which some point in $U(C)$ is downhill connected:

$$U^-(C) := \{x \in C \text{ such that } \exists z \in U(C) \text{ with } P(z, x) > 0\}. \quad (2.25)$$

Let $S^+ = S^+(C)$ be the analogue of U^- outside C :

$$S^+(C) := \{x \notin C : \exists z \in S(C), y \in D(z) \text{ such that } H(x) < H(y), P(x, y) > 0\}. \quad (2.26)$$

In words, $S^+(C)$ is the set of points x outside $C \cup \partial^- C$ such that there exists a downhill path starting from some point $z \in S(C)$ and staying inside the plateau $D(z)$ up to the exit from $\partial^- C$ through x . We set:

$$S^- = S^-(C) := U^-(C) \cup S^+(C). \quad (2.27)$$

Proposition 2.26. *Consider a transient cycle C . Given $\varepsilon > 0$ let*

$$T(\varepsilon) := \exp \beta(S(C)) - H(F(C)) + \varepsilon]. \quad (2.28)$$

Then, for every $\varepsilon > 0$, $x \in C$,

$$\lim_{\beta \rightarrow \infty} P_x(\tau_{(C \cup \partial^- C)^c} > T(\varepsilon)) = 0, \quad (2.29)$$

and

$$\lim_{\beta \rightarrow \infty} P_x(\tau_{(C \cup \partial^- C)^c} \in S^+(C)) = 1. \quad (2.30)$$

Proof. Done in [56]. □

2.5 Asymptotic exponentiality of the exit time

The author now analyze, in more detail, the first exit from a non-trivial cycle C . In particular, following the ideas developed in the framework of the path-wise approach to metastability, we prove the asymptotic exponentiality of the properly re normalized first exit time from any non-trivial cycle, in the limit $\beta \rightarrow \infty$. Then we deduce the asymptotic behavior of the expectation of this exit time; notice that the methods developed in the previous part of this chapter led naturally only to estimates in probability of the exit times but, as we shall see, we can even get good control on the tails of the distribution of these random variables and this will allow us to get the asymptotic of the averages.

Let C be a given non-trivial cycle. Given a point $x \in C$, let the time $T_\beta = T_\beta(x)$ be defined by

$$T_\beta(x) := \min\{T \in \mathbf{N}; P(\tau_{\partial^+ C}^x \leq T) \geq 1 - e^{-1}\} \quad (2.31)$$

where, given $G \subseteq S$, τ_G^x represents the first hitting time to G under P_x ; so that

$$P_x(\tau_{\partial^+ C} < T_\beta(x)) < 1 - e^{-1} \leq P_x(\tau_{\partial^+ C} \leq T_\beta(x)) \quad (2.32)$$

The above definition is interesting since T_β does not depend on $x \in C$, in the sense of logarithmic equivalence; namely, as a consequence of theorem 2.22 (i), (ii), we have for any $x, y \in C$:

$$\lim_{\beta \rightarrow \infty} \log[T_\beta(x)] = \Phi(C) - H(F(C)); \quad \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \frac{T_\beta(x)}{T_\beta(y)} = 0 \quad (2.33)$$

Moreover, for any $x, y \in C$, $\varepsilon > 0$,

$$\lim_{\beta \rightarrow \infty} (P_x(T_P \beta(y) e^{-\varepsilon \beta} < \tau_{\partial^+ C} < P_x(T_P \beta(y) e^{\varepsilon \beta}) = 1. \quad (2.34)$$

The following theorem states the asymptotic exponentiality of the properly re-normalized exit time from a non-trivial cycle C .

Theorem 2.27. *Let $T_\beta^* = T_\beta(x^*)$ where x^* is a particular point in C chosen once for all. Then for any $x \in C$, $\tau_{\partial^+ C}^x \setminus T_\beta^*$ converges in law to a unit mean exponential random time; in particular, for any $s \in \mathcal{R}^+$*

$$\lim_{\beta \rightarrow \infty} P_x\left(\frac{\tau_{\partial^+ C}}{T_\beta^*} > s\right) = e^{-s}. \quad (2.35)$$

Moreover, for any $x \in C$,

$$\lim_{\beta \rightarrow \infty} \frac{\tau_{\partial^+ C}}{T_\beta^*} = 1. \quad (2.36)$$

Proof. Done in [56]. □

Remark 2.28. *In particular, it follows from the above theorem that for every $x \in C$ and $\varepsilon > 0$, we have for β large enough:*

$$\exp(\beta[\Gamma(C) - \varepsilon]) < E_x(\tau_{\partial^+ C}) < \exp(\beta[\Gamma(C) + \varepsilon]). \quad (2.37)$$

To get the above estimate on the expectation of the exit time it was necessary to have the control (2.37) on the tail of the distribution.

2.6 The exit tube

This section is devoted to the study of the typical trajectories of the first excursion outside a non-trivial cycle C .

The author start by considering the first descent from any point y_0 in C to $F(C)$. Then we analyze the problem of the typical tube of first exit trajectories. It will turn out, using reversibility, that this tube is simply related, via a time reversal transformation, to the typical tube followed by the process during the first descent to the bottom $F(C)$ of C starting from suitable points in $\partial^- C$.

In order to define the tube of typical trajectories of this first descent, the basic objects will be what we call standard cascades emerging from y_0 . They specify the geometric characteristics of the tube; roughly speaking these cascades consist in sequences of minimaxes $y_1, \dots, y_n$ towards $F(C)$, decreasing in energy, intercommunicated by sequences of downhill paths $\omega^{(1)}, \dots, \omega^{(n)}$ and permanence sets $Q_1, \dots, Q_n$ which are a sort of generalized cycle.

More generally $\omega_{(i)}$ has to be seen as a downhill sequence of transient plateaux. We call p-path a sequence $\omega = D_1, \dots, D_k$ with D_i communicating with D_{i+1} ; it can also be identified with the set of usual paths following the sequence of plateaux $D_1, \dots, D_k$. A p-path is said to be downhill if $H(D_{i+1}) \leq H(D_i)$, $i = 1, \dots, k$. Indeed a downhill p-path, due to the maximality in the definition

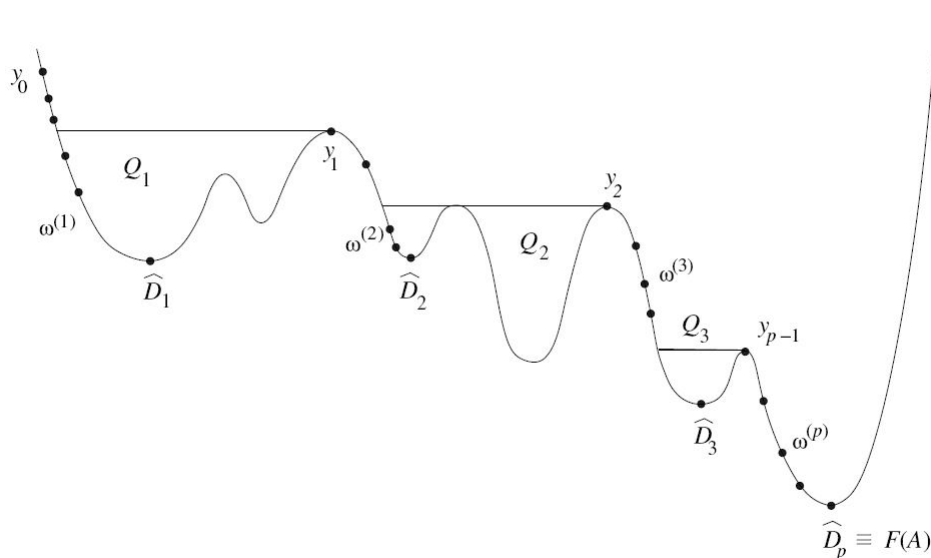


Figure 2.1:

of plateau, is strictly downhill and the corresponding paths are declining.

We prove that during its first descent to $F(C)$, with high probability, our system will follow one of the possible standard cascades; moreover we also give information about the temporal law of the descent by specifying the typical values of the random times spent inside each one of the sets Q_i .

Given any point y_0 in C and a downhill p-path $\omega^{(1)}$ starting from y_0 , we define a set $Q_1 = Q_1(y_0, \omega^{(1)})$. This set Q_1 is a union of cycles with pairwise common minimal saddles of the same height or, more generally, with minimal saddles sharing, pairwise, the same plateau. Q_1 represents the first set where our process, during its first excursion to $F(C)$, is captured if it follows the path $\omega^{(1)}$; after entering into Q_1 it will spend some time inside it before leaving through a minimal saddle, to enter, after another downhill p-path $\omega^{(1)}$, into another similar set of lower height Q_2 and so on, until it enters a cycle containing part of $F(C)$.

Let $y_0 \in C$; suppose first that y_0 does not belong to the union $\bar{M}$ of stable plateaux. Consider a downhill p-path $\omega^{(1)}$ starting from y_0 (such a path certainly exists since $y_0 \notin \bar{M}$). We stress that this path is not, in general, unique. This means that the whole construction we are making must be repeated for each path.

Let $\hat{D}_1$ be the first plateau in $\omega^{(1)}$ with $H(\hat{D}_1) < H(y_0)$ and belonging to $\bar{M}$ (see Fig 2.1 as an example). If, instead, $y_0 \in \bar{M}$, we take $\hat{D}_1 = D(y_0)$. If $\hat{D}_1$ is contained in $F(C)$, then y_0 belongs to the wide basin of attraction $\hat{B}(\hat{D}_1)$. We set $\hat{D}_1 = D^*$; this connected component of $F(C)$ depends on $C, y_0, \omega^{(1)}$. In

this degenerate case we set $Q_1 := D^*$ and the cascade of saddles $y_0, y_1, \dots, y_n$ reduces to y_0 .

Let us now suppose that $\hat{D}_1 \not\subseteq F(C)$. Let H_1 be the communication height between $\hat{D}_1$ and $F(C)$:

$$\Phi(\hat{D}_1, F(C)) = H_1. \quad (2.38)$$

We call Q_1 the maximal connected set, containing $\hat{D}_1$, such that $\Phi(\hat{D}_1, F(C)) = H_1$. We have:

$$Q_1 = \{y \text{ such that } \exists \omega : y \rightarrow \hat{D}_1 \text{ with } \max_{z \in \omega} H(z) \leq H_1 \text{ and } \Phi(\hat{D}_1, F(C)) = H_1\}. \quad (2.39)$$

It is seen immediately that Q_1 is of the form

$$Q_1 = (\cup_j C_j^{(1)}) \cup (\cup_i D_i) \quad (2.40)$$

where

- $C_j^{(1)}$ are disjoint cycles with $\Phi(C_j^{(1)}) = H_1$,
- D_i are plateaux such that $H(D_i) = H_1$, $D_i \cap (\cup_j U(C_j^{(1)})) \neq \phi$,
- one of the $C_j^{(1)}$, say $C_1^{(1)}$, contains $\hat{D}_1$,
- $C_j^{(1)} \cap F(C) = \phi$.

We can also write:

$$Q_1 = \cup_j [(C_j^{(1)}) \cup (\cup_{z \in U(C_j^{(1)})} D(z))]. \quad (2.41)$$

In other words Q_1 is the maximal connected union, containing $\hat{D}_1$, of cycles (trivial and non-trivial) with height H_1 (see (2.10)) and not intersecting $F(C)$. We decompose $\partial^+ Q_1$ as

$$\partial^{+d} Q_1 = \partial^{+u} Q_1 \cup \partial^{+d} Q_1, \text{ with } \partial^{+u} Q_1 \cap \partial^{+d} Q_1 = \phi \quad (2.42)$$

where $H(x) > H_1$ for $x \in \partial^{+u} Q_1$; $H(x) < H_1$ and $\Phi(x, F(C)) < H_1$, for $x \in \partial^{+d} Q_1$; each point $y \in \partial^{+d} Q_1$, belongs to some cycle C' containing points in $F(C)$ and such that $\Phi(C') = H_1$.

Let S_1 be the subset of Q_1 downhill connected to $\partial^{+d} Q_1$. Choose a point $y_1 \in S_1$ and consider a downhill p-path $\omega^{(2)}$ emerging from y_1 with $(\omega^{(2)} \setminus y_1) \cap Q_1 = \phi$ (such a path certainly exists by construction); let $\hat{D}_2$ be the first plateau in $\omega^{(2)}$ belonging to $\bar{M}$ and let

$$H_2 := \Phi(\hat{D}_2, F(C)). \quad (2.43)$$

We can now repeat exactly the previous construction and get the sets Q_2, S_2 , depending on the choice of $\omega^{(2)}$; we decompose Q_2 as $Q_2 = \cup_j [(C_j^{(2)}) \cup (\cup_{z \in U(C_j^{(2)})} D(z))]$ where the disjoint cycles $C_j^{(2)}$ have properties analogous to those of the $C_j^{(1)}$. We continue in this way and recursively construct a sequence of the form $\omega^{(3)}, Q_3, \omega^{(4)}, \dots$, where $\omega^{(i)} : y_{i-1} \rightarrow \hat{D}_i$ with $y_i \in S_i$, $\hat{D}_i \in \bar{M}$,

$H_i := \Phi(\hat{D}_i, F(C)) = H(y_i) > \Phi(\hat{D}_{i+1}, F(C)) = H(y_{i+1})$. Certainly this procedure ends up with some $y_{p1}, \omega^{(p)}$, for some finite p , with $\hat{D}_p$ being a connected component D^* of $F(C)$ (see Figure 2.1).

Suppose that a particular choice is made of $y_0, \omega^{(1)}, \omega^{(2)}, \dots, \omega^{(p)}$, compatible with the above construction.

Then, automatically, $\hat{D}_2, \dots, \hat{D}_{p-1}, \hat{D}_p, Q_1, \dots, Q_{p-1}, Q_p$ are given. Let

$$\mathcal{T}(y_0, \omega^{(1)}, \omega^{(2)}, \dots, \omega^{(p)}) = y_0 \cup \omega^{(1)} \cup Q_1 \cup \omega^{(2)} \cup Q_{p-1} \cup \omega^{(p)} \cup Q_p. \quad (2.44)$$

Any sequence like $\Gamma(y_0, \omega^{(1)}, \omega^{(2)}, \dots, \omega^{(p)})$, obtained via the above construction, will be called a *standard cascade*; it can be visualized as a sequence of falls and communicating lakes.

Notice that, by construction, $F(Q_1), \dots, F(Q_{p-1})$ are strictly higher, in energy, than $F(C)$.

A particularly simple case is when each Q_j is just given by a single cycle C_j . Notice that when C is completely attracted (in the $\beta = \infty$ dynamics) by a unique plateau $D^*F(C)$, every standard cascade is just given by a downhill p-path and we always have $p = 1, Q_1 = D^*$.

Now the author can state the main result.

Theorem 2.29. *Given a non-trivial cycle C , for every $y_0 \in C, y_0 \notin F(C)$.*

- (i) *With a probability tending to one as β goes to infinity, the following happens: there exists a sequence $y_0, \omega^{(1)}, \omega^{(2)}, \dots, \omega^{(p)}$ such that our process, starting at $t = 0$ from y_0 , between $t = 0$ and $t = \tau_{F(A)}$, belongs to $\Gamma(y_0, \omega^{(1)}, \omega^{(2)}, \dots, \omega^{(p)})$; moreover after having followed the initial downhill p-path $\omega^{(1)}$, it visits sequentially the sets $Q_1, Q_2, \dots, Q_{p-1}$ exiting from Q_j through $y_j \in S_j$ and then following the p-path $\omega^{(j+1)}$ before entering Q_{j+1} .*
- (ii) *For every $\epsilon > 0$ with a probability tending to one as $\beta \rightarrow \infty$, the process spends inside each plateau of the p-paths $\omega^{(1)}, \dots, \omega^{(p)}$ a time shorter than $e^{\epsilon\beta}$ and inside each Q_j a time lying in the interval*

$$[\min_k \exp(\beta\{H(y_j) - H(F(C_k^{(j)})) - \epsilon\}), \\ \max_k \exp(\beta(y_j) - H(F(C_k^{(j)})) + \epsilon)];$$

before exiting from Q_j it can perform an arbitrary sequence of passages through the cycles $C_k^{(j)}$ belonging to Q_j . Each transition between different cycles $C_k^{(j)}$ is made through a minimal saddle z_j in the boundary of $C_k^{(j)}$ ($H(z_j) = H_j$); once the process enters into a particular $C_k^{(j)}$, it spends there a time T such that

$$\exp([\beta H_j - H(F(F(C_k^{(j)})) - \epsilon]) < T < \exp(\beta[H_j - H(F(F(C_k^{(j)})) + \epsilon]),$$

whereas it spends at most a time $e^{\beta\epsilon}$ inside the plateaux of Q_j , at height H_j .

Proof. The proof follows immediately by theorem 2.22, corollary 2.24 and proposition 2.26. $\square$

2.7 Asymptotic in probability of tunneling times

We want now to give an application to the evaluation of the tunneling time between an element x_m of a stable plateau and the set $F(\mathcal{X})$ of the absolute minima (in the full state space $\mathcal{X}$) of H . The following theorem states that the typical value of the first hitting time to $F(\mathcal{X})$ starting from x_m will be $\sim e^\beta$ provided $\{x_m\} \cup F(\mathcal{X}) \equiv S_{\Gamma_0}$ for some $\Gamma \leq \Gamma_0$ and that $\Phi(x_m, F(\mathcal{X})) = \Gamma$.

Theorem 2.30. *Suppose that (i) the communication height between x_m and $F(S)$ is $\Phi(x_m, F(S)) = H(x_m) + \Gamma$ and (ii) there exists $\Gamma \leq \Gamma_0$ such that every state $x \in S \setminus (\{x_m\} \cup F(S))$ is Γ_0 -reducible in the sense that there exists $x' \in S$ such that $H(x') < H(x)$, $\Phi(x, x') \leq H(x) + \Gamma_0$. Then, for any $\delta > 0$:*

$$\lim_{\beta \rightarrow \infty} P_{x_m}(e^{\beta(\Gamma-\delta)} \leq \tau_{F(S)} \leq e^{\beta(\Gamma+\delta)}) \quad (2.45)$$

Proof. Let C_{x_m} be the cycle given as the maximal connected set containing x_m with energy smaller than $H(x_m) + \Gamma$. We have

$$\tau_{\partial^+ C_{x_m}} < \tau_{F(S)}. \quad (2.46)$$

The lower bound on $\tau_{F(S)}$ in (2.45) follows immediately from (2.46) and from theorem 2.22 (i). The upper bound on $\tau_{F(S)}$ follows immediately by taking $\nu = \Gamma$ and noticing that in this case $S_\nu \equiv F(S)$. Indeed in this way we prove that for any $x \in S, \delta > 0$:

$$P_x(\tau_{F(S)} \leq e^{\beta(\Gamma+\delta)}) = 1 - SES. \quad (2.47)$$

$\square$

2.8 Simplified path-wise approach: model independent results

The authors of [43] propose a simple approach to determine the asymptotic behavior, for large β , of the first hitting time to the ground state starting from a particular class of local minima for H called metastable states. They 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 $2\frac{J}{h}$.

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 tunneling 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 (3.30) later). 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 tunneling between η_0 and $\mathcal{X}^s$.

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

$$\tau_A = \min \{t \geq 0; \sigma_t^\eta \in A\} \quad (2.48)$$

be the first hitting time to A for the process σ_t^η starting from η . We call $\sigma_{\mathcal{X}^s}^{\eta_0}$ *tunneling 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 tunneling time, expressed as

$$\lim_{\beta \rightarrow \infty} P(e^{(\tau-\varepsilon)\beta} \leq \sigma_{\mathcal{X}^s}^{\eta_0} \leq e^{(\tau+\varepsilon)\beta}) = 1 \quad (2.49)$$

for a suitable $\tau \geq 0$ and arbitrary $\varepsilon \geq 0$. Clearly, this corresponds to the convergence in probability (as $\beta \rightarrow \infty$) of the random variables $X_\beta := \frac{1}{\beta} \ln(a_{\mathcal{X}^s}^{\eta_0})$ to τ 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 tunneling. 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 [15, 33, 55, 54, 59] is based on the notion of cycle, i.e., a maximal connected component of the set of states lying below a given energy (for a formal definition). A cycle C is characterized by the property that, with a probability exponentially close to one, starting from any state $\eta \in C$, our process visits every state in C before exiting from 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 $\partial^+ C$ (i.e., the set in C^c connected to 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.

By regarding single states as trivial cycles, given a set $A \subset \mathcal{X}$, we can consider the decomposition of the set $\mathcal{X} \setminus A$ 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.

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

Obviously, the escape time is smaller than the tunneling time. In order to study the escape time we can use well developed results about the first exit from cycles (see theorem 2.36 later), giving, in this way, a lower estimate of the tunneling 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 tunneling 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 $t \in (\tau_{(C(\eta_0))^c}^{\eta_0}, \tau_{\mathcal{X}^s}^{\eta_0})$ have a depth smaller than or equal to the one of $C(\eta_0)$.

This is not true in general: in the case of the dynamical BlumeCapel model, for suitable values of the parameters (see [26]), it happens that the process, after escaping from $C(\eta_0)$, typically visits very deep wells (deeper than $C(\eta_0)$) so that the asymptotic of the tunneling time is exponentially larger (in β), than the one of the escape time.

This suggests two possible ways of proving that escape and tunneling 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 exiting from $C(\eta_0)$ where the process typically stays confined and requires that Γ 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.

Definition 2.31. *We call stability level of a state $\zeta \in \mathcal{X}$ the energy barrier*

$$V_\zeta := \Phi(\zeta, \psi_\zeta) - H(\zeta) \quad (2.50)$$

where ψ_ζ is the set of states with energy below $H(\zeta)$:

$$\psi_\zeta := \{\eta \in \mathcal{X} : H(\zeta) \leq H(\eta)\} \quad (2.51)$$

We set $V_\zeta = \infty$ if ψ_ζ is empty.

Definition 2.32. *We call stability level of a state $\zeta \in \mathcal{X}$ in a set A the energy barrier.*

$$V_\zeta^A := \Phi(\zeta, \psi_\zeta \cap \zeta) - H(\zeta) \quad (2.52)$$

setting $V_\zeta^A = \infty$ if $\psi_\zeta \cap \zeta$ is empty.

Definition 2.33. The set $\mathcal{X}^s = F(\mathcal{X})$ of the global minima of the Hamiltonian is called set of **stable states**.

Definition 2.34. The set of metastable states is given by

$$\mathcal{X}^m := \{\eta \in \mathcal{X}; V_\eta = \max_{\zeta \in \mathcal{X} \setminus \mathcal{X}^s} V_\zeta\} \quad (2.53)$$

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

$$\mathcal{X}_V := \{\eta \in \mathcal{X}; V_\eta \geq V\} \quad (2.54)$$

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

Definition 2.35. We call **maximal internal resistance** $\Theta(C)$ the maximal depth of the sub-cycles of C that do not contain the whole $F(C)$:

$$\Theta(C) = \max_{C' \subset C; F(C') \subset C} D(C') \quad (2.55)$$

An immediate consequence of the definition of cycles is that for any η, η' in a given cycle C

$$(\eta, \eta') \leq \Theta(C, C') \quad (2.56)$$

It is possible to show that this implies that, with a probability one, every state in the cycle is visited before the exit from the cycle, and that the exit time is of order $e^{\beta D(C)}$.

More precisely, the main result is contained in the following:

Theorem 2.36. Let us consider a non-trivial cycle C and let $D := D(C)$ be its depth. For any $\eta \in C$, $\varepsilon \in \partial^+ C$, $\epsilon, \epsilon' > 0$, $\delta \in (0, \epsilon)$, for $\tau_{\partial^+ C}^\eta$ as in (2.48), and all sufficiently large β

$$P(\tau_{\partial^+ C}^\eta \leq e^{\beta(D+\epsilon)}; \tau_{\partial^+ C}^\eta = \tau_\zeta^\eta) \geq e^{-\beta(H(\zeta) - H(U(c) + \epsilon'))} \quad (2.57)$$

$$P(\tau_{\partial^+ C}^\eta \geq e^{\beta(D+\epsilon)}) \geq 1 - e^{-\beta\delta} \quad (2.58)$$

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

$$P(\tau_{\eta'}^\eta \leq \tau_{\partial^+ C}^\eta) \geq 1 - e^{-\beta\kappa} \quad (2.59)$$

Proof. Done in [56]. □

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

$$\mathcal{G}_A : (\eta) = \eta \cup \{\zeta : \Phi(\eta, \zeta) < \Phi(\eta, A)\}. \quad (2.60)$$

These sets are either trivial cycles coinciding with η (in case $\Phi(\eta, A) = H(\eta)$) or non-trivial cycles containing η (in case $\Phi(\eta, A) > H(\eta)$). Notice that $H(U(\mathcal{G}_A(\eta))) \equiv \Phi(\eta, A)$ and that $\mathcal{G}_A(\eta) \subseteq \mathcal{X} \setminus A$. We immediately see that if $\eta' \in \mathcal{G}_A(\eta)$ then $\mathcal{G}_A(\eta') = \mathcal{G}_A(\eta)$.

Lemma 2.37. Given $A \subset \mathcal{X}$, the sets $\{\mathcal{G}_A(\eta)\}_{\eta \in \mathcal{X} \setminus A}$ in (2.61) form the partition into maximal cycles of $\mathcal{X} \setminus A$:

$$\cup_i \mathcal{G}_i = \mathcal{X} \setminus A, \quad \mathcal{G}_i \cap \mathcal{G}_j = \emptyset, \quad \text{and } \forall i \exists \eta \text{ such that } \mathcal{G}_i \equiv \mathcal{G}_A(\eta) \quad (2.61)$$

Proof. It is immediate to see that for any $\zeta \in \mathcal{X} \setminus A$, $\zeta \in \mathcal{G}_A(\eta)$.

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 $\mathcal{G}_A(\eta)$ are maximal cycles in $\mathcal{X} \setminus A$. For, suppose $\mathcal{G}'$ be a cycle strictly containing $\mathcal{G}_A(\eta)$, we necessarily have $\mathcal{G}' \cap A \neq \emptyset$, contradicting the fact that $\mathcal{G}' \subset \mathcal{X} \setminus A$. Indeed, $\mathcal{G}'$ contains a point ζ in $\partial^+ \mathcal{G}_A(\eta)$ with $H(\zeta) \geq \Phi(\eta, A)$ and every optimal path $\omega \in (\eta \rightarrow A)_{opt}$ is contained in $\mathcal{G}'$, since $H(U(\mathcal{G}')) > \Phi(\eta, A)$ and $\eta \in \mathcal{G}'$. $\square$

Lemma 2.38. *For any $\eta \in \mathcal{X}$ and $A \subset \mathcal{X}$, there exists a finite downhill cycle-path $C_0, \dots, C_n$ such that $\eta \in C_0$ and C_n is a singleton in A .*

Proof. Done in [48]. $\square$

Remark 2.39. *A function $\beta \rightarrow f(\beta)$ is called **super-exponentially small** (SES) if*

$$\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \log(\beta) = -\infty \quad (2.62)$$

2.9 Recurrence to $\mathcal{X}_V$

A crucial property of our Markov chains is that with probability superexponentially close to one, starting from any point in $\mathcal{X}$ the process visits $\mathcal{X}_V$ (the metastable set at level V defined in (2.54)) within a time of order $e^{\beta V}$. We will prove this result in theorem 2.40, by using theorem 2.36.

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

Theorem 2.40. *For any $\epsilon > 0$ and sufficiently large β*

$$\sup_{\eta \in \mathcal{X}} P(\tau_{\mathcal{X}_V}^\eta \geq e^{\beta(V+\epsilon)}) = SES \quad (2.63)$$

Proof. We use the partition in (2.61) with $A = \mathcal{X}_V$ and lemma 2.38 to show that there exists a finite downhill cycle-path from $C_{\mathcal{X}_V}(\eta)$ 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 2.36 we get that the probability to reach $\mathcal{X}_V$ within $e^{\beta(V+\epsilon/2)}$ is uniformly larger than $e^{-\beta\epsilon'}$ for any $\epsilon' > 0$ 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 $e^{\beta(V+\epsilon/4)}$, is larger than $e^{-\beta\epsilon''}$ for any $\epsilon'' > 0$ and sufficiently large β ; moreover, their number is bounded independently of β by $|\mathcal{X}|$. So that by theorem 2.36 we get

$$P(\tau_{\mathcal{X}_V}^\eta \leq e^{\beta(V+\epsilon/2)}) \geq e^{-\beta\epsilon'} \quad (2.64)$$

A standard iteration of this estimate (based on Markov property) proves (2.63).

$$P(\tau_{\mathcal{X}_V}^\eta \geq e^{\beta(V+\epsilon)}) \leq (\sup_{\eta' \in \mathcal{X}_V^c} P(\tau_{\mathcal{X}_V}^{\eta'} \geq e^{\beta(V+\frac{\epsilon}{2})}))^{e^{\beta\frac{\epsilon}{2}}} = SES \quad (2.65)$$

We refer to [15] for a definition of decomposition into maximal cycles in a more general setting. $\square$

Corollary 2.41. *For any $\delta > 0$, the variables $Y_\beta^\eta := \tau_{\mathcal{X}^s}^\eta e^{-(\gamma+\delta)\beta}$ 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 $\beta > \beta_0$*

$$\sup_{\eta \in \mathcal{X}} \mathbf{E}(Y_\beta^\eta \mathbf{1}_{\{Y_\beta^\eta > K\}}) < \varepsilon \quad (2.66)$$

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

$$\sup_{\eta \in \mathcal{X}} P(\tau_{\mathcal{X}^s}^\eta e^{-(\gamma+\delta)\beta} > n) < 2^{-n} \quad (2.67)$$

for any sufficiently large β . This estimate can be obtained as in (2.65), since $\mathcal{X}\gamma = \mathcal{X}_s$ and $\forall \delta > 0$

$$\sup_{\eta \in \mathcal{X}} P(\tau_{\mathcal{X}^s}^\eta e^{-(\gamma+\delta)\beta} > n) \leq \left(\sup_{\eta' \notin \mathcal{X}^s} P(\tau_{\mathcal{X}^s}^{\eta'} e^{-(\gamma+\delta)\beta} > n) \right)^n < 2^{-n} \quad (2.68)$$

where we used theorem 2.40 to get the last inequality. $\square$

Remark 2.42. *We note that it is possible to prove a recurrence result similar to theorem 2.40 also if we consider the recurrence to a given state in $\mathcal{X}^s$. This is important when studying the tunneling problem between stable states. More precisely, let $\eta_1 \in \mathcal{X}^s$ and let $\Theta = \Theta(\mathcal{X}^s)$ the maximal internal resistance defined in (2.55). By using lemma 2.38 and the arguments of proof of theorem 2.40, we can prove that*

$$\sup_{\eta \in \mathcal{X}} P(\tau_{\eta_1}^\eta > e^{(\Theta+\varepsilon)\beta}) = SES \quad (2.69)$$

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

2.10 Asymptotic of tunneling time

In this section we give results on the asymptotic of the tunneling 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.

2.10.1 General results

We study the tunneling time $\tau_{\mathcal{X}^s}^{\eta_0}$ s by giving results in probability (in theorems 2.43 and 2.45), on the asymptotic of the expectation (in theorem 2.46 and on the convergence in law in theorem 2.47.

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 2.43. *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 $\beta > \beta_0$*

$$P(\tau_{\mathcal{X}^s}^{\eta_0} < e^{\beta(\Gamma-\delta)}) < e^{-K\beta} \quad (2.70)$$

$$P(\tau_{\mathcal{X}^s}^{\eta_0} < e^{\beta(\Gamma+\delta)}) = SES \quad (2.71)$$

Proof. (2.70) is a consequence of (2.58) when $C = \{\zeta : \Phi(\zeta, \eta_0) < \Phi(\eta_0, \mathcal{X}^s)\}$, since $\tau_{\mathcal{X}^s}^{\eta_0} > \tau_{\mathcal{X}^s}^{\partial^+ C}$.

(2.71) is just a particular case of theorem 2.40 when $V = \Gamma$. In this case $\mathcal{X}_V$ coincides with $\mathcal{X}^s$. $\square$

Remark 2.44. *As noted at the end of the previous section, in the case of several stable states, we can obtain a similar result for the tunneling time $\tau_{\eta_1}^{\eta_0}$ 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 2.43. 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 A such that there exist $K_A > 0$, $\beta_0 > 0$ such that for any $\eta \in A \setminus F(A)$ we have $P(\tau_{F(A)}^\eta < \tau_{\partial^+ A}^\eta) \geq 1 - e^{-K_A \beta}$ for all $\beta > \beta_0$. Notice that, by definitions 2.50 and (2.52), for any η in a habitat A either $V_\eta^A = \infty$ or $V_\eta^A = V_\eta$. Indeed, if $V_\eta^A > V_\eta$, we immediately see that the cycle $\mathcal{G}_{\phi_\eta \cap A}(\eta)$ has non-empty intersection with $\phi_\eta \cap A^c$. By theorem 2.36, $P(\tau_{F(\mathcal{G}_{\phi_\eta \cap A}(\eta))} < \tau_{\phi_h \cap A}) \rightarrow 1$, contradicting the definition of habitat. Examples of habitats are given by basins of attraction, cycles and suitable sets of downhill cycle paths.

Theorem 2.45. *Let A be a habitat and let $V(A) := \max_{\eta \in A \setminus F(A)} V_\eta^A$ be the maximal stability level in A . Let $\eta \in A$ with $V_\eta^A = V(A)$.*

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

$$P(e^{\beta(V(A)-\varepsilon)} < \tau_{F(A)}^\eta < e^{\beta(V(A)+\varepsilon)}) \geq 1 - e^{-(\beta\kappa)} \quad (2.72)$$

that is, η plays the role of a metastable state relatively to A .

Proof. Let us start to prove that $P(\tau_{F(A)}^\eta \geq e^{\beta(V+\varepsilon)})$ is exponentially small. The proof is very similar to that of theorem 2.40.

$$P(\tau_{F(A)}^\eta > e^{\beta(V+\varepsilon)}) \leq P(\tau_{F(A)}^\eta = \tau_{F(A)}^\eta \geq e^{\beta(V+\varepsilon)} + P(\tau_{\partial^+ A}^\eta < \tau_{F(A)}^\eta) \quad (2.73)$$

By lemma 2.38, there exists $\delta > 0$ such that

$$P(\tau_{F(A)}^\zeta < \tau_{\partial^+ A}^\zeta; \tau_{F(A)}^\zeta < e^{\beta(v+\frac{\varepsilon}{2})}) \geq e^{-\beta\delta} \quad (2.74)$$

Hence, a standard iteration argument like in (2.66) shows that the first term in (2.73) 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 $F(A)$ the depth of $\mathcal{G}_\xi(\eta)$ is V , by (2.59)

we see that $P(\tau_{F(A)}^\eta < e^{\beta(V-\varepsilon)}) \leq P(\tau_{\partial+\mathcal{G}_\varepsilon(\eta)}^\eta < e^{\beta(V-\varepsilon)})$ for any $d \in (0, \varepsilon)$ and sufficiently large β .

Different characterization of the tunneling time is given by the following theorem: $\square$

Theorem 2.46. *For any $\eta_0 \in \mathcal{X}^m$,*

$$\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \log E \tau_{\mathcal{X}^s}^{\eta_0} = \Gamma \quad (2.75)$$

Proof. By theorem 2.43 we know that, for each $\delta > 0$, the variables $Y_\beta := \tau_{\mathcal{X}^s}^\eta e^{-(\Gamma+\delta)\beta}$ tend to zero in probability, moreover by corollary 2.41 they are uniformly integrable. This implies that they tend to zero also in L^1 , that is

$$E(|Y_\beta^{\eta_0}|) \rightarrow 0 \quad (2.76)$$

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

$$E \tau_{\mathcal{X}^s}^{\eta_0} < e^{(\Gamma+\varepsilon)\beta} \quad (2.77)$$

The estimate

$$E \tau_{\mathcal{X}^s}^{\eta_0} > e^{(\Gamma-\varepsilon)\beta} \quad (2.78)$$

valid for any $\delta > 0$ and sufficiently large β , immediately follows by theorem 2.43 since

$$E \tau_{\mathcal{X}^s}^{\eta_0} > e^{(\Gamma-\delta)\beta} P(\tau_{\mathcal{X}^s}^{\eta_0} > e^{(\Gamma-\delta)\beta}) \geq (1 - e^{-K\beta}) \quad (2.79)$$

By using that d is arbitrary, by (2.77) and (2.78) we obtain (2.75). $\square$

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 $\forall \eta \in \mathcal{X}^s$ 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 2.47. *Suppose there exists a state η_0 such that $T_\beta := \inf\{n \geq 1 : P(\tau_{\mathcal{X}^s}^{\eta_0} \leq n) \geq 1 - e^{-1}\}$ tends to infinity with β . Moreover suppose that there exists T'_β and δ_β such that for all $\eta \in \mathcal{X}$.*

$$P(\tau_{\{\eta_0, \mathcal{X}^s\}}^\eta \geq T'_\beta) \leq \delta_\beta \text{ with } \lim_{\beta \rightarrow \infty} \frac{T'_\beta}{T_\beta} = 0 \text{ and } \lim_{\beta \rightarrow \infty} \delta_\beta = 0, \quad (2.80)$$

then, for any $\delta > 0$,

$$\lim_{\beta \rightarrow \infty} P(\tau_{\mathcal{X}^s}^\eta > t T_\beta) = e^{-t}, \quad (2.81)$$

and

$$\lim_{\beta \rightarrow \infty} \frac{E(\tau_{\mathcal{X}^s}^{\eta_0})}{T_\beta} = 1. \quad (2.82)$$

Proof. Done in [43]. $\square$

2.11 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 $\omega^* : \eta_0 \rightarrow \mathcal{X}^s$; namely, a path such that

$$\{\arg \max_{\omega^*} H\} \cap F(\partial^+ \mathcal{B}) \neq \emptyset \quad (2.83)$$

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

Indeed, point (a) gives the lower bound $\Phi(\eta_0, \mathcal{X}^s) \geq H(F(\partial^+ \mathcal{B}))$, 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 (2.83) 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 [4, 13, 28, 32]) 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 $\eta \in \mathcal{X}^s$, is equivalent to saying that the maximal depth of the cycles of the decomposition of $\mathcal{X} \setminus \mathcal{X}^s$, 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 $\eta_0 \in \mathcal{X}^s$ a reducing path $\omega : \eta \rightarrow \eta_0$ with $H(\eta) > H(\eta_0)$ for which $\max_i H(\omega_i) - H(\eta) \leq V_{\eta_0}$. Moreover, if the last

inequality is strict for each $\eta \in \eta_0 \cup \mathcal{X}^s$, then we have that η_0 is the unique metastable state, and we can also apply theorem 2.47.

2.12 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.

2.12.1 Essential Saddles and Gates

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

Theorem 2.48. $\zeta \in \mathcal{S}(\eta, \eta')$ is essential if and only if $\zeta \in \mathcal{G}(\eta, \eta')$.

Proof. Abbreviate $\mathcal{S} = \mathcal{S}(\eta, \eta')$, $\mathcal{G} = \mathcal{G}(\eta, \eta')$, $\Omega = (\eta \rightarrow \eta')_{opt}$. 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 $\omega \in (\eta \rightarrow \eta')_{opt}$ such that $\omega \cap \mathcal{W} = \zeta$; indeed, otherwise ζ would not be pivotal for the minimal gate $\mathcal{W}$.

We have either $\{argmax_{\omega} H\} = \{\zeta\}$ and then ζ is essential, or $\{\zeta\} \subset \{argmax_{\omega} H\}$, with $\{argmax_{\omega} H\} \cap \mathcal{W} \setminus \{\zeta\} = \phi$. In this last case no $\omega' \in (\eta \rightarrow \eta')_{opt}$ can exist with $\{argmax_{\omega'} H\} \subset \{argmax_{\omega} H\} \setminus \{\zeta\}$ 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 $\{argmax_{\omega} H\} = \zeta$, then ζ must belong to all minimal gates and hence to $\mathcal{G}$. Thus, we may assume that, for all $\omega \in \Omega$ with $\zeta \in \omega$, we have $\{argmax_{\omega} H\} \setminus \{\zeta\} \neq \phi$.

Since ζ is essential, we know that there exists $\zeta \in \bar{\omega}$ such that $\{argmax_{\omega'} H\} \subset \{argmax_{\omega} H\} \setminus \{\zeta\}$ for any $\omega' \in \Omega$.

Partition

$$\Omega = \Omega_{\zeta} \cup \Omega_{\zeta}^c \quad (2.84)$$

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

We may assume that $\Omega_{\zeta}^c \neq \phi$, otherwise ζ is obviously a minimal gate and we are done. We know that $\Omega' \cap \mathcal{S}' \neq \phi$ for all $\omega' \in \Omega_{\zeta}^c$, where $\mathcal{S}' := \mathcal{S} \setminus \{argmax_{\bar{\omega}} H\}$.

Let $\mathcal{W}'$ be a minimal gate for Ω_{ζ}^c in $\mathcal{S}'$, i.e.,

$$\mathcal{W}' \subseteq \mathcal{S}'$$

$$\begin{aligned} \omega' \cap \mathcal{W}' &\neq \phi, \forall \omega' \in \Omega_\zeta^c \\ \mathcal{W}'' \subset \mathcal{W}', \exists \omega'' \in \Omega_\zeta^c; \omega'' \cap \mathcal{W}'' &\neq \phi. \end{aligned} \quad (2.85)$$

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, $\omega \cap \mathcal{W} \neq \phi$ 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 $\bar{\omega} \cap \mathcal{W}' \neq \phi$ because $\mathcal{W}' \subseteq \mathcal{S}'$ and $\{\operatorname{argmax}_{\bar{\omega}} H\} \cap \{\mathcal{S}'\} = \phi$. $\square$

2.12.2 Crossing the Gates

Theorem 2.49. *For any pair of states ζ, η , for any gate $\mathcal{W} \equiv \mathcal{W}(\eta, \xi) \subseteq \mathcal{S}(\xi, \eta)$ there exists $c > 0$ such that*

$$P(\tau_{\mathcal{W}}^\eta > \tau_\xi^\eta) \leq e^{-\beta c} \quad (2.86)$$

for sufficiently large β .

Proof. We can suppose the set of non-optimal paths $\omega : \eta \rightarrow \xi$ nonempty, otherwise $P(\tau_{\mathcal{W}}^\eta > \tau_\xi^\eta) = 0$; then,

$$\delta_0 = \min_{\omega: \eta \rightarrow \xi} \max_{\xi \in \omega} H(\xi) - \min_{\omega: \eta \rightarrow \xi} \max_{\xi \in \omega} H(\xi) \quad (2.87)$$

is strictly larger than zero. We consider the cycle $\mathcal{G} := \{\zeta : \Phi(\zeta, \eta) \leq H(\mathcal{W}) + \frac{\delta_0}{2}\}$. 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 $\omega \in (\eta \rightarrow \xi)_{\text{opt}}$ then ω crosses $\mathcal{W}$, and if $\omega \notin (\eta \rightarrow \xi)_{\text{opt}}$ then by definition of δ_0 , ω leaves the cycle $\mathcal{G}$.

We have

$$P(\tau_{\mathcal{W}}^\eta > \tau_\xi^\eta) \leq P(\tau_\xi^\eta > \tau_{\partial^+ \mathcal{G}}^\eta) \leq e^{-\beta c} \quad (2.88)$$

where in the last inequality we used the cycle property in theorem 2.36, and c is a suitable constant. $\square$

Chapter 3

Metastable behaviour for lattice spin models at low temperature

In this chapter Olivieri and Vares discuss metastability and nucleation for several short range lattice spin systems at low temperature. The case of the Curie Weiss model is already analysed in [56]. Due to the fact that the intermolecular interaction does not decay at infinity, the Curie Weiss model exhibits a mean field behavior without any spatial structure; the configurations are well described, especially for large volumes, by the values of a unique macroscopic order parameter, i.e. the magnetization, so that the configuration space becomes one-dimensional. In contrast, for short range stochastic Ising models the geometrical aspects are particularly relevant. In this last case the configuration space can be viewed as a space of families of contours and it tends to be infinite dimensional in the thermodynamic limit. Indeed it is well known that the description of pure coexisting equilibrium phases at low temperature is naturally given in terms of a gas of contours (see proposition 3.30 of [56]). It is clear that in the analysis of dynamical phenomena taking place in large finite systems, the geometrical description in terms of contours will also play a relevant role.

The central question in the description of the decay from a metastable to a stable phase for short range stochastic Ising models is, in addition to determination of the typical escape time, the characterization of the typical nucleation pattern namely the typical sequences, in shape and size, of droplets along which nucleation of the stable phase takes place.

The Curie Weiss model and short range stochastic Ising models share many characteristic features of metastable behavior but, at the same time, they show some very relevant differences.

To be concrete let us consider the prototype of the class of short range models analyzed in this chapter: the two-dimensional Metropolis standard stochastic Ising model with small but fixed, say positive, magnetic field h in a large but fixed squared domain Λ with periodic boundary conditions, in the limit of large

inverse temperature β . A continuous time version was already introduced in [56]. A precise definition of the discrete time version will be given later on.

Let us denote by $-\underline{1}$, $+\underline{1}$ the configurations with all spins $-\underline{1}$, $+\underline{1}$ in Λ , respectively. By choosing a positive and sufficiently small h we see immediately that $-\underline{1}$ is a local minimum whereas $+\underline{1}$ is the absolute minimum for the energy, so they are naturally associated with the metastable and stable equilibrium, respectively.

As will emerge from our analysis, in the case of low temperature short range stochastic Ising models, it is natural to introduce a sort of basin of metastability, namely a set of configurations where our system will be confined before transition to the stable situation. The configurations in the basin of metastability will be close to $-\underline{1}$. The meaning of closeness in this case is not, a priori, clear at all; intuitively we expect that close to $-\underline{1}$ means without too large droplets of pluses.

The equivalent notion of metastable basin for the Curie Weiss model simply refers to configurations whose global magnetization is close, in the usual metric on $\mathcal{R}$, to the local minimum $m(\beta, h)$ of the canonical free energy $f_{\beta, h}(m)$. In both Curie Weiss and short range Ising models the system spends a very long time performing random fluctuations in the metastable basin before an almost unpredictable jump leads eventually to the stable situation. In both Curie Weiss and short range Ising models there is a notion of coercive field $\hat{h} = \hat{\beta}$ representing the threshold to instability. For $h > \hat{h}$ no metastability is possible: the state that was metastable for $h < \hat{h}$ now becomes unstable. In the Curie Weiss model $\hat{h}$ is the maximal value of h for which the canonical free energy $f_{\beta, h}(m)$ has double well behavior; for $h > \hat{h}$, $f_{\beta, h}(m)$ has only one well and for $h = \hat{h}$ it has a horizontal inflection point. For the short range Ising model the coercive field can be identified as the minimal value of h for which even the smallest possible droplets have a tendency to grow. It will turn out that for both models the lifetime increases as h decreases.

Let us discuss the differences. Whereas for the Curie Weiss model the free energy barrier to be overcome is already implicit in the dynamics as it is given by the (unphysical) double well structure of the canonical free energy, in the short range Ising model this barrier is not directly related to the microscopic single spin-flip elementary process of the dynamics but, rather, comes from the collective behaviour of the system. The height and location in the configuration space of this barrier are not given at all a priori, and they have to be determined by looking at the whole, geometrically complicated, configuration space. This is somehow reminiscent of the equilibrium description of phase transitions for short range systems where, in general, the equilibrium coexistence line is unknown as its location is a result of the collective behavior of the system. The description of how a short range Ising model spends its time in the metastable basin before the jump to stable equilibrium is much more complicated than the corresponding description for the Curie Weiss model. In both cases the fraction of time spent in the different subsets of the metastable basin before the jump tends to be proportional to an almost stationary measure: the restricted Gibbs ensemble (see [56] chapter 4 and chapter 6). In the case of the short range Ising

model this is a measure on a complicated configuration space whereas in the case of the Curie Weiss model we have a simple measure on the line. Moreover the exit path from the metastable basin in the Curie Weiss model is determined almost immediately, using reversibility, whereas in the short range Ising model it involves complicated geometrical considerations.

The crucial point is that the basin of metastability for short range Ising systems will contain many stable equilibrium configurations, namely many local minima of the energy H . These minima will correspond to particular sets of stable isolated droplets; for the standard Ising model they will be rectangles of pluses in a sea of minuses.

Before the decay to the stable situation, characterized by a sea of pluses with small islands of minuses, the system will visit many times configurations with a sea of minuses with small droplets of pluses.

Since β is very large, only moves that decrease the energy will typically take place; our system will spend the largest part of its time in the local minima for the energy. Sometimes, moves against the drift, with an increase of energy, will take place and, when entering into the basin of attraction of some local minimum, the system will typically take a suitable exponentially long (in β) time to get out of it. On a smaller time scale, a situation similar to the global escape from metastability will occur, at a local level, in the escape from the basin of attraction of a local minimum. It will also occur that, during the first excursion from -1 to $+1$, namely during the decay from the metastable to stable situation, the system will typically visit many basins of local minima, remaining exponentially long intervals of time there. This is the main new difficulty with respect to the description of the first escape from a completely attracted domain. To treat this phenomenon we make use of conceptual categories and results developed in Chapter 2 for Freidlin Wentzell reversible Markov chains.

3.1 The standard stochastic Ising model in two dimensions

Let us now define the standard stochastic Ising model. It is a discrete time stochastic dynamics given by a Metropolis Markov chain, reversible with respect to the Gibbs measure for a standard Ising model, when the elementary process is a single spin-flip.

We shall take our Ising spin system enclosed in a two-dimensional torus Λ of edge L namely, an $L \times L$ square with periodic boundary conditions. Other boundary conditions can be considered as well: this point will be discussed later on.

With any lattice site $x \in \Lambda$ we associate a spin variable $\sigma(x)$ taking values $+1, -1$: the configuration space is $\mathcal{X} := \{-1, +1\}^\Lambda$. The energy $H(\sigma)$, associated with the configuration $\sigma \in \mathcal{X}$, is given by:

$$H(\sigma) = -\frac{J}{2} \sum_{(x,y) \in \Lambda, |x-y|=1} \sigma(x)\sigma(y) - \frac{h}{2} \sum_{x \in \Lambda} \sigma(x) \quad (3.1)$$

Notice that in this chapter we use the notation $J/2$ for the coupling constant and $h/2$ for the external magnetic field. We take $J > 0$ (ferromagnetic case). The external magnetic field $h/2$ is taken positive. Notice that at $h = 0$, with our parametrization, the energy necessary to break a bond, namely to pass from a parallel pair of nearest neighbor spins to an opposite pair, is J .

The transition probabilities of our IsingMetropolis Markov chain are given, for $\sigma \neq \sigma'$, by:

$$P(\sigma, \sigma') = \begin{cases} \frac{1}{|\Lambda|} \exp(-\beta[H(\sigma) - H(\sigma^{(x)})]_+) & \text{if } \sigma' = \sigma^{(x)} \text{ for some } x \in \Lambda \\ 0 & \text{if } \sigma' \neq \sigma^{(x)} \text{ for all } x \in \Lambda \end{cases} \quad (3.2)$$

where

$$\sigma^x(y) = \begin{cases} \sigma(y) & \text{if } y \neq x \\ -\sigma(x) & \text{if } y = x \end{cases} \quad (3.3)$$

For $\sigma' = \sigma$ we set:

$$P(\sigma, \sigma) = 1 - \sum_{\sigma' \in \mathcal{X}, \sigma' \neq \sigma} P(\sigma, \sigma') \quad (3.4)$$

This is a particular case of Markov chains in the Freidlin Wentzell regime which are characterized by finite state space and transition probabilities exponentially decreasing in a large parameter β . More specifically it is a particular case of a dynamics satisfying condition M of Chapter 6; indeed it is commonly called the Metropolis algorithm. It corresponds to the following updating rule: given a configuration σ at time t we choose at random a site $x \in \Lambda$ and compute the increment of energy, $[H(\sigma) - H(\sigma^{(x)})]_+$; if this quantity is non-positive we flip the spin at x ; otherwise, if it is strictly positive, we flip it with a probability $\exp(-\beta[H(\sigma) - H(\sigma^{(x)})]_+)$. We denote by σ_t our stochastic trajectory.

We consider a situation in which h, J, L , are fixed in such a way that $0 < h < 2J < h(L-3)$ and we take the limit of large β . The condition $h < 2J$ means critical length larger than two (twice the spacing of the lattice) whereas $2J < h(L-3)$ means that the side of the box Λ exceeds the critical length by at least three units. Notice that with our choice of parameters J, h we always have, $[H(\sigma) - H(\sigma^{(x)})]_+ \neq 0$. From a physical point of view the above described asymptotic regime corresponds to analyzing local aspects of nucleation at very low temperature.

Other asymptotic regimes will be quoted at the end of this chapter. We want to note that in our finite volume system, at equilibrium, for large β the energy dominates with respect to the entropy so that the Gibbs measure is a small perturbation of a δ -mass concentrated on the unique ground state.

As we have already said in the introduction, it is easily seen that this unique ground state is given by the configuration $+\underline{1}$ where all spins are plus, whereas the natural candidate to describe the metastable situation is the configuration $-\underline{1}$ where all spins are minus.

Definition 3.1. Given a set of configurations $G \subseteq \mathcal{X}$ we denote, as usual, by τ_G the first hitting time to G :

$$\tau_G := \min\{t > 0; \sigma_t \in G\} \quad (3.5)$$

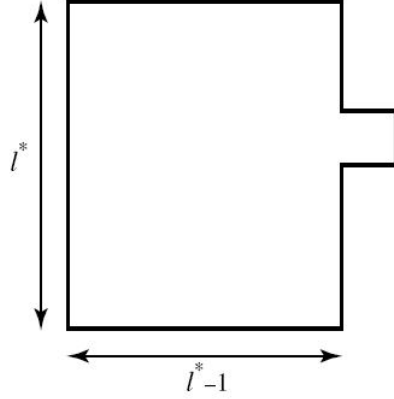


Figure 3.1:

We are interested in the asymptotic behavior, for large β , of the first hitting time $\tau_{+\underline{1}}$ to the configuration $+\underline{1}$, starting from $-\underline{1}$. A particularly interesting set of configurations that we call critical configurations and denote by $\mathcal{P}$, is the set of configurations in which the plus spins are precisely the spins contained in a polygon given by a rectangle with sides l^* , $l^* - 1$ plus a unit square protuberance attached to one of the longest sides (see Figure 3.1). Here

$$l^* = \left\lceil \frac{2J}{h} \right\rceil + 1 \quad (3.6)$$

where $\lceil \cdot \rceil$ denotes the integer part. We always suppose that $2J/h$ is not an integer.

Definition 3.2. We denote by Γ the formation energy of a critical droplet:

$$\Gamma := H(\mathcal{P}) - H(-\underline{1}) = 4Jl^* - h(l^*)^2 + h(l^* - 1) \quad (3.7)$$

Definition 3.3. $\theta_{-\underline{1}, +\underline{1}}$ is the last instant in which $\sigma_t = -\underline{1}$ before $\tau_{+\underline{1}}$:

$$\theta_{-\underline{1}, +\underline{1}} := \max\{t < \tau_{+\underline{1}}; \sigma_t = -\underline{1}\} \quad (3.8)$$

Definition 3.4. $\theta_{-\underline{1}, \mathcal{P}, +\underline{1}}$ is the first instant after $\theta_{-\underline{1}, +\underline{1}}$ in which the process visits $\mathcal{P}$:

$$\theta_{-\underline{1}, \mathcal{P}, +\underline{1}} := \min\{t > \theta_{-\underline{1}, +\underline{1}}; \sigma_t \in \mathcal{P}\}. \quad (3.9)$$

The main result is contained in the following theorem.

Theorem 3.5. Let $h < 2J$, $\frac{2J}{h} \notin \mathcal{N}$. $L \geq l^* + 3$; then for every $\delta > 0$

$$(i) \lim_{\beta \rightarrow \infty} P_{-\underline{1}}(\exp[\beta(\Gamma - \delta)] < \tau_{+\underline{1}} < \exp[\beta(\Gamma + \delta)]) = 1;$$

$$(ii) \lim_{\beta \rightarrow \infty} P_{-\underline{1}}(\theta_{-\underline{1}, \mathcal{P}, +\underline{1}} < \tau_{+\underline{1}}) = 1.$$

Proof. We present a proof based on proposition 2.17 and theorem 2.22. The main point is the determination of the communication height between $-\underline{1}$ and $+\underline{1}$. See definition 2.9 in chapter 2. $\square$

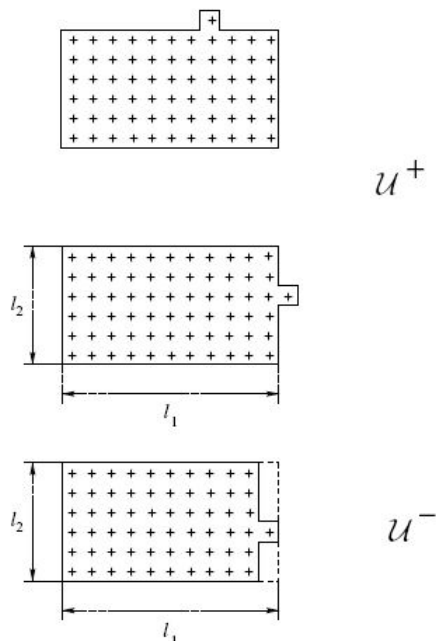


Figure 3.2:

We make a geometrical construction from which we deduce that $S(-\underline{1}, +\underline{1})$ contains $\mathcal{P}$, which indeed is a gate for the transition $-\underline{1} \rightarrow +\underline{1}$. See definition 2.10 in chapter 2.

For didactical purposes we present here a quite general approach that can be extended to various stochastic Ising models with different Hamiltonians. In the specific case of the standard Ising model there are simpler methods exploiting the peculiarities of the model. We quote the essential aspects of this simple approach later on.

Our strategy is based on three steps: we first determine the set of local minima for the energy; they will be characterized geometrically as sets of isolated, sufficiently large rectangles. When we say that a configuration is given by a set of rectangles, more generally by a set of closed polygons, we mean that in that configuration the set of plus spins is given precisely by the set of sites lying in the interior of these polygons. In the following we give more detailed definitions.

Second, we study the basins of attraction (with respect to the $\beta = \infty$ dynamics) of these minima, in particular we determine the saddles between them. This will allow us to characterize the rectangles that have a tendency to shrink and those that have a tendency to grow; the value l will emerge from this analysis as the critical length that discriminates between growing, i.e. supercritical, and shrinking, i.e. subcritical, rectangles. The heuristics behind this is related to a comparison between the speed of growth and the speed of contraction of a given rectangle R . The mechanism of growth implies the formation of a unit square

protuberance from the exterior, adjacent to one of the edges of R (see Figure 3.2). Let us call $U^+ = U^+(R)$ the class of configurations obtained in this way. The corresponding positive increment in energy is $2J - h$ so that the typical time needed to reach U^+ is of the order $\exp[\beta(2J - h)]$. U^+ is a saddle configuration. Indeed, starting from $\sigma \in U^+$, two transitions with negative $\Delta_x(H)$ can take place: a spinflip of a minus adjacent both to the unit square protuberance and to R , leading to the formation of a stable 1×2 protuberance attached to R , which would lead into the basin of attraction of a larger rectangle; or the flip of the plus spin inside the unit square protuberance, leading back to R . On the other hand, it is not difficult to convince oneself that the best mechanism of contraction is the corner erosion corresponding to $\Delta_x H = h$, all other mechanisms implying at least $\Delta_x H = 2J + h$. The minimal saddle configurations in the direction of contraction correspond to erosion of all but one unit squares adjacent to the interior to one of the edges of R of minimal length l . Let us call $U^- = U^-(R)$ the class of configurations obtained in this way (see Figure 3.2). The best way of going from R to U^- appears to be a sequence, ascending in energy, of corner erosions. This implies a cost in energy of $h(l - 1)$ and then a typical time of order $\exp[\beta(h(l - 1))]$. This typical time becomes longer than the time needed for the growth, $\exp[\beta(2J - h)]$, when $l \geq l^*$ (see (3.6)); this explains the tendency to grow of rectangles with minimal side length $l \geq l^*$.

The third and final step consists in the introduction of a sort of generalized basin of attraction of $-\underline{1}$ playing the role of the set G of proposition 2.17. It will be given by the set of all sub-critical configurations which, roughly speaking, are those that, taken as initial configurations, give rise with high probability to a hitting time $\tau_{-\underline{1}}$ strictly shorter than $\tau_{+\underline{1}}$. The set of minima of the energy on the boundary of this generalized basin will be given precisely by the set $\mathcal{P}$; this fact will easily imply that $\mathcal{P}$ is a gate between $-\underline{1}$ and $+\underline{1}$.

3.2 The local minimum

We start by introducing a geometrical description of spin configurations. Given $\sigma \in \mathcal{X}$ let $C(\sigma)$ be the subset of $\mathcal{R}^2$ given as the union of the closed unit cubes centered at the sites x of $\mathcal{Z}^2$ where the spin is plus one. The boundary of $C(\sigma)$ can be seen as a (generally not connected) polygon (Peierls contour) lying on the dual lattice $\mathcal{Z}^2 + (1/2, 1/2)$. Given $C(\sigma)$, let us decompose it into maximal connected components $C(\sigma) = C_1 \cup \dots \cup C_k$. The C_i are called clusters of σ . The sites of the original lattice $\mathcal{Z}^2$ lying inside a C_i form a $*$ -cluster in the sense of site percolation; namely they are connected via nearest and next to nearest neighbors. Of course there is a one-to-one correspondence between the spin configurations and the set of collections of non-overlapping clusters.

We often identify a configuration σ with the set of unit cubes centered at the sites containing plus spins. Actually, with an abuse of notation, we denote by the same symbol $C_1, C_2, \dots, C_k$ a set of non-overlapping clusters and the configuration where the plus spins are precisely those sitting on the sites internal to $C_1 \cup \dots \cup C_k$.

The total boundary $\partial C(\sigma)$ of a configuration σ is given as the union of the

boundaries of the clusters of σ ; it consists of a collection of unit segments with extrema in the dual lattice $\mathbb{Z}^2 + (1/2, 1/2)$ with the property that at each site of $\mathbb{Z}^2 + (1/2, 1/2)$ an even number of segments (0, 2 or 4) converge. We write

$$p(\sigma) := |\partial C(\sigma)| = \sum_{i=1}^k |\partial C(i)| \quad (3.10)$$

we call $p(\sigma)$ the perimeter of σ ; it equals the total number of pairs of n.n. sites with opposite spins in σ . The energy $H(\sigma)$.

$$H(\sigma) = H(-\underline{1}) + Jp(\sigma) - h \sum_{i=1}^k |C_i| \quad (3.11)$$

We also consider the partition of the boundary $\partial C(\sigma)$ into connected components:

$$\partial C(\sigma) = \cup_{i=1}^m \gamma_i \quad (3.12)$$

where the γ_i are called contours of σ . Of course we have

$$\cup_{i=1}^m \gamma_i = \cup_{i=1}^k \partial C_i = \partial C, \text{ and } p(\sigma) = \sum_{i=1}^m |\gamma_i|. \quad (3.13)$$

Definition 3.6. A configuration $\sigma \in \mathcal{X}$ is called *non-winding* if all its clusters are not encircling the torus i.e. connecting two opposite sides of Λ . We denote by X_{nw} the set of all non-winding configurations.

For any non-winding configuration we have a well defined sea of minuses given by the unique component of minus sites encircling the torus; inside this sea the C_i can be seen as islands possibly having in their interior lakes with possibly other islands in their interiors and so on.

Given a non-winding configuration $\sigma \in X_{nw}$, the maximal connected components of its boundary $\partial C(\sigma)$ that are all made by unit segments touching the sea of minuses are called *outer contours*.

Definition 3.7. We denote by $\hat{R}(l_1, l_2)$ the set of configurations whose plus spins are precisely those sitting on the sites internal to some rectangle $R(l_1, l_2)$ with edges parallel to the lattice axes (and vertices on the dual lattice $\mathbb{Z}_2 + (1/2, 1/2)$) of horizontal and vertical side lengths l_1, l_2 , respectively.

We want to stress that by $R(l_1, l_2)$ we mean a particular rectangle with side lengths l_1, l_2 and a particular location, for example centered at the origin, but we do not make the location explicit in the notation. Using the identification of $\sigma \in \mathcal{X}$ with $C(\sigma)$, $\hat{R}(l_1, l_2)$ can be viewed as an equivalence class of a given rectangle $R(l_1, l_2)$, modulo translations.

Let

$$l := l_1 \wedge l_2, \quad m := l_1 \vee l_2 \quad (3.14)$$

be, respectively, the minimal and maximal sides of a rectangle $R(l_1, l_2)$.

Definition 3.8. A rectangle $R(l_1, l_2)$ with $|l_1 - l_2| \leq 1$ is called a *quasi-square*.

Notation We write

$$R(l_1, l_2) = \hat{R}(l_1, l_2) \cup \hat{R}(l_2, l_1) \quad (3.15)$$

to denote the set of configurations whose plus spins are precisely those lying inside some rectangle with side lengths l_1 and l_2 (independently of the orientation).

We now give some definitions concerning rectangles seen as geometrical objects; from now on we only consider rectangles (seen as closed subsets of $\mathcal{R}^2$) with sides parallel to the lattice axes and vertices in the dual lattice.

Definition 3.9. *Two disjoint rectangles R, R' are mutually isolated if there does not exist any site $x \in \mathcal{Z}^2 \setminus (R \cup R')$ having two distinct nearest neighbor sites y, y' lying inside R, R' respectively.*

In other words R, R' are mutually isolated if, given $x \in \mathcal{Z}^2 \cup R, x' \in \mathcal{Z}^2 \cup R'$, the Euclidean distance $|x - x'|$ is $|x - x'| \geq \sqrt{5}$; thus, given two isolated rectangles R, R' either they lie at a distance greater than one or the minimal distance is one but it is realized only on two of their vertices. $R_1, \dots, R_n$ form a set of isolated rectangles if they are pairwise mutually isolated.

Definition 3.10. *We call stable the rectangles with $m \leq L-2$ and $2 \leq l \leq L-2$ or with $m = L$ (encircling the torus) and any l such that $1 \leq l \leq L-2$. A rectangle with $l = 1$ and $m \leq L-1$ (segment) is said to be ephemere.*

Notice that a configuration $\bar{\sigma}$ containing a unique segment with $l = 1$ and $m = L-1$ can be connected by a downhill path to two distinct local minima: the circle with $l = 1$ and $m = L$ or the configuration $-\underline{1}$. Thus $\bar{\sigma}$ is a saddle configuration.

Definition 3.11. *We say that a single cluster is monotonous if it is simply connected (does not have holes) and it has a perimeter equal to that of the circumscribed rectangle (see Figure 3.3).*

Definition 3.12. *Two rectangles R and R' are said to be interacting if one of the following two circumstances occurs:*

- (i) *the rectangles R and R' intersect, or*
- (ii) *R and R' are disjoint but not mutually isolated so that there exists a site $x \in \Lambda \setminus (R \cup R')$ having two distinct nearest neighbor sites y, y' lying inside R, R' respectively.*

Lemma 3.13. *The set of local minima for the energy is given precisely by the set of collections of isolated stable rectangles including the degenerate cases of $\underline{1}$ (absence of rectangles) and $+\underline{1}$ (unique rectangle $\equiv \Lambda$).*

Proof. σ is stable if for all $x \in \Lambda$, $\Delta_x H(\sigma)$ is positive (recall that, with our choice of parameters, the quantity $\Delta_x H(\sigma)$ is never zero). Let us look at the catalog of all possible positive increments

$$\Delta_x H(\sigma) = 2\sigma(x) \left[\frac{J}{2} \sum_{y \in \Lambda: |x-y|=1} \sigma(y) + \frac{h}{2} \right]$$

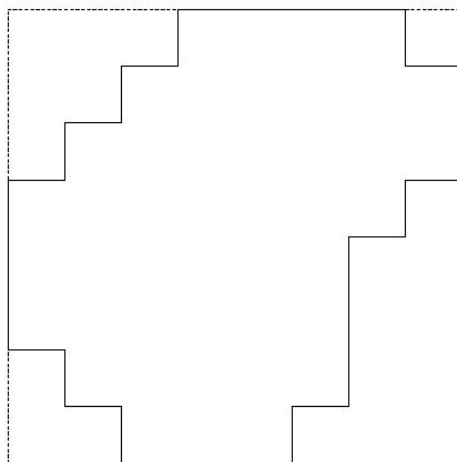


Figure 3.3:

in increasing value; we get $h, 2J - h, 2J + h, 4J - h, 4J + h$. We see that the only possibility for σ to be stable is that all minus spins have at least three positive nearest neighbors, whereas all plus spins have at least two positive nearest neighbors. From this we have the following:

- (1) Every single cluster C of a local minimum configuration σ must be a stable rectangle (possibly encircling the torus). Indeed, if C does not coincide with its circumscribed rectangle, certainly there is a minus spin in σ with less than three negative neighboring spins, that can flip into plus by strictly decreasing the energy. C cannot be ephemere, otherwise the two extreme plus spins can flip into minus by decreasing the energy. Finally C cannot be a rectangle with $m = L - 1$, namely almost encircling (and then self-interacting, otherwise there would be sites containing 1 spins and adjacent to the exterior to two opposite sides of C , that could flip by decreasing the energy (self-coalescence of C).
- (2) Every rectangular cluster of σ must be isolated from the others, otherwise there would exist, between two rectangles, a minus spin with less than three negative neighboring spins that could flip by strictly decreasing the energy; in other words an energetically favorable coalescence between two rectangles could take place.

This proves the assertion of the lemma.

□

3.3 Sub-critical and super-critical rectangles

In order to discriminate between rectangles having a tendency to shrink (sub-critical) and those having a tendency to grow (super-critical) we make use of

methods and results developed in Chapter 2. The main model dependent problem that we have to solve concerns the determination of the set of minimal saddles between a given rectangle and the others. The result is contained in the following.

Lemma 3.14. *Let $\bar{B} = \bar{B}(R(l_1, l_2))$ be the basin of attraction (see definition 2.15 in Chapter 2) of a non-winding configuration whose unique cluster is the stable rectangle $R = R(l_1, l_2)$ (with a specific location, say centered at the origin). Then, recalling $l = l_1 \wedge l_2$, the set $U = U(l_1, l_2)$ of minima of the energy in the boundary of $\bar{B}(R(l_1, l_2))$ is given*

- (a) *for $l < l^*$ by the set $\mathcal{U}^- = \mathcal{U}^-(R(l_1, l_2))$ of clusters obtained from $R(l_1, l_2)$ by eroding $l - 1$ unit squares adjacent to the interior to one of the edges of R of minimal length l ,*
- (b) *for $l \geq l^*$ by the set $\mathcal{U}^+ = \mathcal{U}^+(R(l_1, l_2))$ of clusters obtained from $R(l_1, l_2)$ by attaching a unit square protuberance to one of its edges (see Figure 3.2).*

Proof. Done in [43]. □

The above lemma justifies the following

Definition 3.15. *We call a rectangle $R(l_1, l_2)$ super-critical if either $l = l_1 \wedge l_2 \geq l^*$ or $m = l_1 \vee l_2 \geq L - 1$, ($R(l_1, l_2)$ is encircling or almost encircling the torus). A rectangle that is not super critical is called sub-critical.*

Notice that the case of an ephemere almost encircling rectangle is considered here to be super-critical even though, as we have already said, it is easily seen to be a saddle configuration between $-\underline{1}$ and $+\underline{1}$.

Remark We notice that given any rectangle encircling the torus (winding configuration) $R(l_1, l_2)$, with $m = L$ and $1 \leq l \leq L - 2$, we have that $U(l_1, l_2)$ is given by the set $\mathcal{U}^+$ obtained from $R(l_1, l_2)$ by attaching a unit square protuberance to one of its edges of length L .

3.4 Subcritical configurations and global saddles

We call global saddles the elements of $S(-1, +1)$.

Claim 3.16. *A set G exists satisfying the stronger version of the properties introduced in proposition 2.17 i.e., recalling $\mathcal{P}$ has been defined before (3.6),*

- (a) $-\underline{1} \in G$, $+\underline{1} \notin G$
- (b) G is connected,
- (c) $\mathcal{P} \subseteq \partial G$, $\forall \eta \in \mathcal{P}$ there exists a path $\omega : -\underline{1} \longrightarrow \eta$, $\omega \setminus \eta \subseteq G$, with

$$H(\zeta) < H(\eta) \quad \forall \zeta \in \omega, \zeta \neq \eta$$

moreover there exists a path $\omega' : \eta \longrightarrow +\underline{1}$, $\omega' \cap G = \emptyset$ with

$$H(\zeta) < H(\eta) \quad \forall \zeta \in \omega, \zeta \neq \eta$$

$$(d) \mathcal{P} \equiv F(\partial G).$$

Then, taking this claim for granted, it easily follows by proposition 2.23 that if $A_{-\underline{1}} = \{\zeta : \exists \omega : \zeta \longrightarrow -\underline{1}; \forall \eta \in \omega, H(\eta) < H(\mathcal{P})\} \equiv$ maximal connected set containing $-\underline{1}$ with energy less than $H(\mathcal{P})$, $A_{+\underline{1}} = \{\zeta : \exists \omega : \zeta \longrightarrow +\underline{1}; \forall \eta \in \omega, H(\eta) < H(\mathcal{P})\} \equiv$ maximal connected set containing $+\underline{1}$ with energy less than $H(\mathcal{P})$, then

- (1) $A_{-\underline{1}} \subseteq G, A_{+\underline{1}} \subseteq \mathcal{X} \setminus G,$
- (2) $A_{-\underline{1}}, A_{+\underline{1}}$ are cycles with $P \subseteq U(A_{-\underline{1}}), U(A_{+\underline{1}}),$
- (3) $H(\mathcal{P}) = \Phi(-\underline{1}, +\underline{1}). P \subseteq S(-\underline{1}, +\underline{1}).$

Moreover, from the strong property $F(\partial G) \equiv \mathcal{P}$, we deduce that P is a gate for the transition $-\underline{1} \rightarrow +\underline{1}$.

The idea in constructing such a G is to find a criterion to decide whether or not a given configuration η is subcritical, namely whether $\Phi(\eta, -\underline{1}) < \Phi(\eta, +\underline{1})$. It is clear that a natural candidate for G is the set of all configurations that are subcritical according to that criterion. Using lemma 3.14 and the remark following definition 3.15, we are already able to decide whether or not a configuration with a single rectangle is subcritical or supercritical, similarly for a set of noninteracting rectangles. It is clear that the set $\mathcal{X}$ of all configurations is just a finite set that, however, tends to be geometrically very complicated for large volumes Λ : indeed for large Λ it tends to be an infinite dimensional space whose elements are sets of polygons (the boundaries of the clusters). Thus it is convenient to introduce a rough description of a generic configuration in terms of isolated rectangles. We stress that the set G will be just an *estimate* of the true set of subcritical configurations.

We introduce a map F on the set $\mathcal{X}_{nw}$ of non-winding configurations (see definition 3.6) with values in the set of configurations whose set of clusters are collections of isolated rectangles and for $\sigma \in \mathcal{X}_{nw}$ we write

$$\hat{\sigma} = F_{\sigma}. \quad (3.16)$$

F will satisfy the properties:

- (i) F decreases the energy

$$H(\hat{\sigma}) \leq H(\sigma), \quad (3.17)$$

- (ii) F increases the set of pluses

$$\sigma \prec \hat{\sigma} \quad (3.18)$$

where $\sigma \prec \eta$ means $\sigma(x) \leq \eta(x), \forall x \in \Lambda,$

- (iii) F is a monotonous increasing map

$$\hat{\sigma} \prec \hat{\eta} \text{ for } \sigma \prec \eta. \quad (3.19)$$

For a set Q given as the union of disjoint clusters $Q = C_1 \cup \dots \cup C_k$, we denote by $R(Q)$ its rectangular envelope given by the smallest rectangle containing Q . Notice that every edge of $R(Q)$ contains at least one unit segment belonging to the boundary of Q .

Now, for any non-winding σ , we construct the new (not necessarily nonwinding) configuration

$$\hat{\sigma} = F_\sigma$$

by filling up and gluing together some of its rectangular envelopes. To this end we first introduce the notion of chains of rectangles.

A set of rectangles $R_1, \dots, R_m$ is said to form a *chain* $\mathbf{E}$ if every pair (R_i, R_j) of them can be linked by a sequence $\{R_{i_1}, \dots, R_{i_n}\}$ of pairwise interacting rectangles from $\mathbf{E}$; $R_{i_1} = R_i$, $R_{i_n} = R_j$, and $R_{i_s}, R_{i_{s+1}}$ are interacting pairs for all $s = 1, \dots, n-1$.

Given a collection of chains $\mathbf{E}_1, \dots, \mathbf{E}_n$ we start the following iterative procedure:

- (1) the chains $\mathbf{E}_j^{(1)}$ of the first generation are identical to $\mathbf{E}_j$; $j = 1, \dots, n$;
- (2) having defined $\mathbf{E}_j^{(j)} \mathbf{E}_j^{(1)}$, $j = 1, \dots, n_r$, we construct rectangular envelopes $R_j^{(1)}$ of the sets

$$\bigcup_{R \in \mathbf{E}_j^{(1)}} R$$

and the maximal chains $\mathbf{E}_j^{(1)}$ of them ($j = 1, \dots, n_{r+1}$).

The procedure ends once we reach a set of chains, each consisting of a single rectangle. Notice that every pair from the resulting set is non-interacting.

Starting now from any non-winding configuration σ , we apply the above construction on chains of rectangular envelopes of its outer contours and define $\hat{\sigma}$ as the configuration obtained by placing the spin $+1$ at all sites inside the resulting rectangles $\bar{R}_1, \dots, \bar{R}_s$ (filling up the rectangles).

Notice that it may happen that a configuration σ is non-winding but, by the above construction, we get some rectangles $R(l_1, l_2)$ encircling or almost encircling the torus; we recall that by almost encircling the torus we mean that the maximal side length $m := l_1 \vee l_2$ equals $L-1$ and thus, so to speak, $R(l_1, l_2)$ interacts with itself. If we do not have any such rectangles we define $\hat{\sigma} = \tilde{\sigma}$, otherwise we complete our construction in the following way. First change into pluses the residual minuses sitting on sites x having two of its neighbors in one of the above rectangles. If the new configuration obtained in this way contains only non-interacting rectangles we stop our construction and set $\hat{\sigma} = \tilde{\sigma}'$. However it may happen that $\tilde{\sigma}'$ contains pairs of interacting rectangles made of an ephemere and a winding rectangle. In this case we continue our construction in terms of chains like before and in this way we finally obtain the configuration $\hat{\sigma}$ containing neither interacting nor self-interacting rectangles. Notice that $\hat{\sigma}$

does not necessarily correspond to a minimum for H ; indeed it may contain ephemere rectangles. Moreover, we repeat, in $\hat{\sigma}$ we may have rectangles encircling the torus but we cannot have rectangles almost encircling the torus.

The above construction can be easily described in terms of bootstrap percolation. Consider the following updating rule that can be seen as a deterministic cellular automaton. Given a configuration $\sigma \in \mathcal{X}$ at time t , the configuration σ' at time $t + 1$ is obtained as follows:

- (i) occupied sites (i.e. sites $x \in \Lambda$ such that $\sigma(x) = +1$) remain occupied,
- (ii) if an empty site has two or more occupied nearest neighbors it becomes occupied. Otherwise it stays empty.

It is easy to see that for every $x \in \Lambda$ there exists $T = T(\sigma)$ such that if we repeat T times the above updating we end up with exactly the same invariant configuration $\hat{\sigma}$ that we have defined before, containing a finite set of non-interacting and non-self-interacting rectangles, some of which can encircle the torus. Notice that $+1$ is a particular case of $\hat{\sigma}$. We have given the definition of $\hat{\sigma}$ also in terms of a hierarchy of chains because this approach can be extended to different models whereas bootstrap is a notion specifically relevant only for the standard Ising model. The property $H(\sigma) \geq H(\hat{\sigma})$ is verified immediately.

Indeed, given any configuration giving rise to a single cluster C not coinciding with its rectangular envelope, certainly there exists a sequence of spin-flips decreasing the energy and increasing the plus spins, that leads to $\hat{\sigma}$. Moreover whenever a configuration σ has clusters C' , C'' with interacting rectangular envelopes $R' = R(C')$, $R'' = R(C'')$, we decrease the energy by filling the rectangular envelope of the union of R' and R'' . This is evident in both cases (i) and (ii) of the definition of interacting rectangles (see definition 3.12), since the number of broken bonds (i.e. pairs of nearest neighbour opposite spins) is non-increasing, whereas the volume occupied by plus spins is increasing. Using this observation in an iterative manner, we can construct a sequence of configurations of decreasing energy starting with σ and ending with $\hat{\sigma}$. The monotonicity of the map F is also evident.

Now we are ready to define the set G , namely, we introduce G as the set of all non-winding configurations σ such that every resulting rectangle $\bar{R}(l_1, l_2)$ from the configuration $\hat{\sigma}$ is subcritical ($l = l_1 \wedge l_2 < l^*$ and $m = l_1 \vee l_2 < L - 1$) and not interacting with any other rectangle. Notice that whenever $\hat{\sigma} = \tilde{\sigma}$, i.e. $\tilde{\sigma}$ contains almost winding rectangles, then certainly σ is out of G . Thus we could have avoided introduction of the completion $\hat{\sigma}$ of $\tilde{\sigma}$; we did it just to be completely coherent with the bootstrap transformation of Aizenman and Lebowitz. The required property (a) of claim 3.16 G is obvious; property (b) saying that G is connected is easily verified since, given $\sigma, \eta \in G$ it is easy to construct a path $\hat{\omega} : \sigma \rightarrow \eta$, $\hat{\omega} \subseteq G$; indeed it suffices to note that there exist two paths $\bar{\omega} : \sigma \rightarrow -1$, $\tilde{\omega} : \eta \rightarrow -1$, $\bar{\omega}, \tilde{\omega} \in G$; such paths $\bar{\omega}, \tilde{\omega}$ are obtained by successively flipping all plus spins of ω, η , respectively, following a sequence of corner erosions.

It is also immediate to verify that $\mathcal{P} \subseteq \partial G$; moreover the path ω whose ex-

istence is required in property (c) is, for example, a step by step contraction of $\mathcal{P}$ obtained by successively eliminating, using only the corner erosion mechanism, all its plus spins whereas ω' is a growth obtained by successively creating plus spins, around a unique cluster, up to total invasion of the whole Λ . More explicitly, given a configuration in $\mathcal{P}$, the first step in ω consists in removing the unit square protuberance, by gaining an amount $2J - h$ of energy. Subsequently, we erode, by corners, all but one of the plus spins adjacent to the interior to a side of the rectangle of length $l = l^* - 1$ (notice that the length of the side to which the unit square protuberance was adjacent is l^*). In this way, we increase the energy an amount $h(l^* - 2) < 2J - h$ so we stay strictly below $\mathcal{P}$ in energy. Continuing in this way we reach -1 always remaining below $H(\mathcal{P})$.

Given $\sigma \in \mathcal{P}$, the first step in ω' consists in flipping into plus one of the minus spins adjacent to the rectangle with $l = l^* - 1, m = l^*$ and to the unit square protuberance, by getting, in this way, a stable 2×1 rectangular protuberance, attached to the rectangle with $l = l^* - 1, m = l^*$. Then we continue by successively flipping the minus spins adjacent to the growing protuberance and to the rectangle, until we get to a configuration consisting of the square $l^* \times l^*$. In this way we decrease the energy an amount $h(l^* - 1)$. Then we create a unit square protuberance adjacent to the exterior of one of the four sides, by paying an amount $2J - h < h(l^* - 1)$ of energy; thus we stay below $\mathcal{P}$. Then we continue in the same way up to $+1$. Note that joining the time reversal of ω with ω' we get a *reference path* according to the definition in equation (3.42) below.

Our next task is to analyse the boundary ∂G and to prove property (d). Recall that L is only supposed to be strictly larger than $l^* + 2$; it will appear clear from what follows that choosing L much larger than l^* would simplify the treatment of those configurations in ∂G that correspond to supercriticality given by the case $m = l_1 \vee l_2 \in \{L - 1, L\}$.

Let $\eta \in \partial G$; then there exists $\sigma \in G$ and $x \in \Lambda$ such that $\eta = \sigma^{(x)} \notin G$. As a consequence of the monotonicity of the map F , $\sigma(x)$ is necessarily 1; otherwise $\sigma \in G$ would imply also $\eta \in G$. Moreover, for the same reason, the site x lies outside of all rectangles $\bar{R}_1, \dots, \bar{R}_s$ corresponding to $\hat{\sigma}$. Among the rectangles corresponding to $\hat{\eta}$ there exists a rectangle $\bar{R}(l_1, l_2)$ with the following properties:

- (i) $\bar{R}$ is supercritical,
- (ii) it contains the site x and several rectangles $\bar{R}_i$, say, $\bar{R}_1, \dots, \bar{R}_k$, corresponding to $\hat{\sigma}$; the remaining rectangles $\bar{R}_{k+1}, \dots, \bar{R}_s$ are also rectangles of $\hat{\sigma}$.

Our aim now is to prove that

$$H(\eta) - H(-1) \geq \Gamma = 4Jl^* - h[(l^*)^2 - l^* + 1] \quad (3.20)$$

Consider first the configuration $\tilde{\eta}$, $H(\eta) \geq H(\tilde{\eta})$, whose set of plus spins consists of the site x and the rectangles $\bar{R}_1, \dots, \bar{R}_k$ (the energy decreases when skipping the subcritical rectangles $\bar{R}_{k+1}, \dots, \bar{R}_s$). Further, consider the set $C^{(0)}$ consisting of the union of the unit square $q(x)$ centred at the site x and the rectangle (if

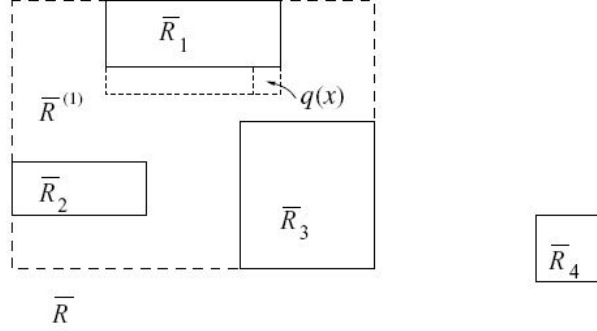


Figure 3.4:

any) among $\bar{R}_1, \dots, \bar{R}_k$ that intersects $q(x)$ along one of its edges; given the fact that the rectangles $\bar{R}_1, \dots, \bar{R}_k$ are mutually non-interacting, there is at most one among these rectangles, say $\bar{R}_1$, touching an edge of $q(x)$.

Let us now take the rectangular envelope $\bar{R}_1$ of $C^{(0)}$ and distinguish two cases, either the rectangle $\bar{R}_1$ is supercritical or not. (Notice that both $C^{(0)}$ and $\bar{R}_1$ may actually coincide with $q(x)$). See Figure 3.4. If $\bar{R}_1$ is supercritical, we decrease the energy of $\tilde{\eta}$ further by erasing all rectangles among $\bar{R}_1, \dots, \bar{R}_k$ that were not contributing to the set $C^{(0)}$ and consider the configuration yielded by the set $C^{(0)}$.

Suppose that $\bar{R}_1$ is supercritical because its larger side is $m = L - 1$ (m cannot be equal to L otherwise $\hat{\sigma}$ would have almost encircled Λ); since it is energetically favourable to add edges of length $L - 1 > l^*$, we see that the case with minimal energy corresponds to $l = l^* - 1$ so that

$$H(C^{(0)}) > H(\mathcal{P}), \quad \forall L \geq l^* + 3. \quad (3.21)$$

Notice that if we had chosen $L = l^* + 2$ we would have had the possibility

$$H(C^{(0)}) = H(\mathcal{P}).$$

On the other hand, it is easy to convince oneself that among the other cases, with $\bar{R}^{(1)}$ supercritical because it has minimal edge $l \geq l^*$, the one with minimal energy corresponds to $\bar{R}_1$ with edges $l^* - 1, l^*$ and $q(x)$ touching one of the sides of length l^* so that $C^{(0)} \in \mathcal{P}$. Indeed $\bar{R}_1$ must be of the form $R(l^* - 1, m)$ (or $R(m, l^* - 1)$) with $m \geq l^*$ and we know that contracting orthogonally to the edge $l^* - 1$, i.e. cutting a row or column of length $l^* - 1$, decreases the energy. This yields the bound (3.20) with the equality holding if and only if $C^{(0)} \in \mathcal{P}$.

Next, consider the case when $\bar{R}_1$ is subcritical. Take $\bar{R}_1$ and all rectangles $\bar{R}_2, \dots, \bar{R}_k$ (that were not used for $C^{(0)}$) and construct from them the set of chains $\{E_j^{(1)}\}_{j=1, \dots, n_1}$ of the first generation. A sequence $\{E_j^{(1)}\}_{j=1, \dots, n_1}$, $r = 1, \dots, s$ of sets of chains of following generations is obtained from it by iteration. Since the rectangles $\bar{R}_1, \dots, \bar{R}_k$ are mutually non-interacting, for every generation r we get a chain, say $E_1^{(r)}$, consisting of a rectangle $\bar{R}^{(r)}$ containing the site

x and certain subset of $\bar{R}_1, \dots, \bar{R}_k$. The remaining chains $E_j^{(r)}$, $j = 2, \dots$ contain each just one rectangle from those among $\bar{R}_1, \dots, \bar{R}_k$ that have not appeared in $E_p^{(r)}$, $p \leq r$, in the preceding steps. Clearly, there is only one chain in the last generation $E_1^{(s)} = \{\bar{R}^{(s)}\} \equiv \{\bar{R}\}$.

Let us now consider the last rectangle $\bar{R}^{(p)}$ among $\bar{R}^{(r)}$, $r = 1, \dots, s$ that is subcritical and take the chain $E_1^{(p)}$ with the rectangles in $E_1^{(r)} \setminus \bar{R}^{(p)}$ ordered in a particular way, say in lexicographic order of their upper left corner. Notice that, by hypothesis the rectangles in $E_1^{(r)} \setminus \bar{R}^{(p)}$ are non-interacting, so they form the chain $E_1^{(p)}$ together with $\bar{R}^{(p)}$ only because they interact directly with $\bar{R}^{(p)}$. Let us unite them, one by one in the given order, with the rectangle $\bar{R}^{(p)}$ until the circumscribed rectangle is supercritical. Cutting off the remaining rectangles from the chain $E_1^{(p)}$ we get the chain $\tilde{E}_1^{(p)} \subseteq E_1^{(p)}$. Let us use $\tilde{R}'$ to denote the last rectangle that was attached to form the chain $\tilde{E}_1^{(p)}$, and $\tilde{R}$ the circumscribed rectangle to the union of rectangles from $\tilde{E}_1^{(p)} \setminus \{\tilde{R}'\}$. Clearly, $\tilde{R}$ and $\tilde{R}'$ are subcritical interacting rectangles with a supercritical envelope R^* of their union. Then we have two possible situations.

Case (A). There exists a rectangle $R(l_1, l_2) =: Q^*$ with $l_1 = l_2 = l^*$ (first supercritical square), contained in R^* such that it intersects both rectangles $\tilde{R}$ and $\tilde{R}'$ in non-degenerated rectangles $\hat{R}$ and $\hat{R}'$, $\hat{R} = \tilde{R} \cap Q^*$ and $\hat{R}' = \tilde{R}' \cap Q^*$, and has non-empty intersection also with the intersection $\tilde{R} \cap \tilde{R}'$ (if it is non-empty).

Case (B). R^* has its larger side of length $l_1 \vee l_2 \in \{L-1, L\}$, i.e. R^* is encircling or almost encircling the torus; moreover the shorter side is $l_1 \wedge l_2 = l \in [1, l^* - 1]$. Now we observe that, given a rectangle $R(l_1, l_2)$ we decrease the energy if we contract it along a direction orthogonal to a side $l \leq l^* - 1$; moreover we decrease the energy if we expand it along a direction orthogonal to a side $l \geq l^*$. In other words if we erase from a rectangle a column or row adjacent to the interior from a side $l \leq l^* - 1$ or we add a column or row adjacent to the exterior to a side $l \geq l^*$, we decrease the energy.

Consider first case (A). Taking into account the above remark we further decrease the energy with the following transformation $\mathcal{M}$ that also further shrinks the corresponding configuration.

Let $\tilde{l}_1, \tilde{l}_2$ be the edges of $\tilde{R}$ and $\hat{l}_1, \hat{l}_2$ be the edges of $\hat{R} \equiv \tilde{R} \cap Q^*$.

We distinguish two cases.

- (1) If $m = \hat{l}_1 \vee \hat{l}_2 < l^*$ we just substitute $\tilde{R}$ with $\hat{R}$. We set $R := \mathcal{M}\tilde{R} \equiv \hat{R}$.
- (2) if $m \geq l^*$ we substitute $\tilde{R}$ with the rectangle $R := \mathcal{M}\tilde{R} = R(l, l^*)$ obtained as intersection of $\tilde{R}$ with the strip of thickness l^* containing Q^* orthogonal to the direction of the side of length $\geq l^*$ of $\tilde{R}$ (see Figure 3.5).

We act in a totally analogous way with $\tilde{R}'$ to get $R' := \mathcal{M}\tilde{R}'$. One has

$$H(\tilde{\eta}) \geq H(\tilde{R}) + H(\tilde{R}') \geq H(R) + H(R'), \quad (3.22)$$

where $H(R)$ denotes the energy of the configuration with plus in R and so on. To see this, it is enough to realize that the energy of $\tilde{\eta}$ is certainly higher than the

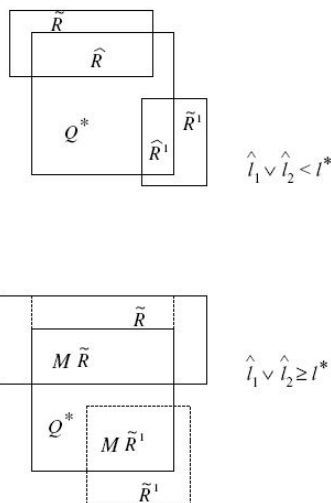


Figure 3.5:

energy of all among the rectangles $\bar{R}^{(1)}, \bar{R}_2, \dots, \bar{R}_k$ that were subsequently used in the construction of $\tilde{E}_1^{(p)} \setminus \{\tilde{R}'\}$ plus the energy associated with the rectangle $\tilde{R}'$ (notice that $\tilde{R}'$ does not intersect the remaining rectangles from the original set $\bar{R}_1, \dots, \bar{R}$ used to construct $\tilde{E}_1^{(p)}$ and it can only touch by its corners the set $C^{(0)}$). The first term can be subsequently bounded from below by $H(\tilde{R})$ and we get the last inequality in (3.22) by observing that R, R' are obtained from $\tilde{R}$ and $\tilde{R}'$ by applying the transformation $\mathcal{M}$; $\tilde{R}$ and $\tilde{R}'$ are subcritical and thus one gains energy by reducing them to R and R' via successive cuttings of rows or columns shorter than l^* .

Now, consider the case when both $R = \hat{R}$ and $\hat{R} = \hat{R}'$. We have

$$H(R) + H(R') > H(Q^*) + h(l^* - 1) \quad (3.23)$$

which implies (3.22). Indeed, if the rectangles R and R' intersect in more than one point, there is a surplus of at least two bonds in the sum of their boundaries yielding at least $2J > (l^* - 1)h$. If R and R' just touch in the corner, the boundary has the same number of bonds as in Q^* and there are at least l^* minus sites inside Q^* . If R and R' are interacting according to case (ii) from definition 3.12 of interacting rectangles, the number of unit edges is at least that in the configuration Q^* but, again, there are at least l^* minus inside the square Q^* ; thus in all analysed cases we get (3.23).

Still in case (A), when the transformation $\mathcal{M}$ does not coincide with the intersection with Q^* for both rectangles $\tilde{R}, \tilde{R}'$, there is at least one rectangle, between R, R' , say R , with one of its edges of length l^* and the other $l = l_1 \wedge l_2 \leq l^* - 1$. We further decrease the energy by expanding, if necessary, orthogonally to the large side and thus always taking $l = l^* - 1$. From this, using (3.22), since the energy of the other (subcritical) rectangle R' is always larger than or equal to the energy of a unit square that, in turn, is strictly larger than $2J - h$, we get

(3.20); indeed $2J - h$ represents the difference between η and the energy of an $l^* \times (l^* - 1)$ rectangle.

Let us now analyse case (B). In this case, with reasoning similar to that leading to (3.23) in case (A), we easily get

$$H(\tilde{\eta}) \geq H(\tilde{R}) + H(\tilde{R}') \geq H(R^*) + hl^*. \quad (3.24)$$

Since the minimal side length of R^* is $l < l^*$ and the maximal one is $m \geq l^* + 2$, we strictly decrease the energy by substituting $R(l^* - 1, l^*)$ for R^* , so that we get:

$$H(R^*) > H(R(l^* - 1, l^*)). \quad (3.25)$$

We conclude that

$$H(\tilde{\eta}) > H(P). \quad (3.26)$$

From (3.26) and (3.21) we deduce that when $L > l^* + 2$ the minimal saddles on ∂G and then the minimal saddles between $-\underline{1}$ and $+\underline{1}$ never correspond to the formation of a cluster encircling the torus.

Thus, we are left with the task of finding configurations in ∂G for which the energy equals the right-hand side in (3.20). Let us suppose that η satisfies the equality in (3.20). Then, necessarily, $\bar{R}^{(1)}$ in the construction above is supercritical. If it were not and other steps of the construction and filling of final chains followed, we would run into a contradiction since in every one of those steps the energy strictly decreases with, as the proof shows, the inequality (3.20) maintained. This excludes the possibility of having an equality for the starting configuration η . Similar reasoning also shows that $\eta = \hat{\eta}$. Hence, $C^{(0)}$ consists of $q(x)$ attached to a single rectangle and to get the equality in (3.20) it must be a $(l^* - 1) \times l^*$ rectangle (see Figure 3.4). Thus, the only possibility of achieving an equality in (3.20) is to take $\eta \in \mathcal{P}$ and we can conclude that

$$\min_{\{\sigma \in \partial G\}} H(\sigma) = H(P)$$

and

$$\min_{\{\sigma \in \partial G \setminus P\}} H(\sigma) = H(P) + h$$

which implies property (d) of G . This concludes the proof of the claim.

Now it is easy to conclude the proof of theorem 3.1. Indeed let $\mathcal{M}^{sub}$ denote the set of subcritical minima $\zeta \in \mathcal{X}_{nw}$, i.e. no rectangles in ζ (if any) encircle (or almost encircle) the torus and all the rectangles in ζ have minimal side length smaller than the critical value l^* . Suppose, for simplicity, that $\zeta \in \mathcal{M}^{sub}$ contains a unique subcritical rectangle. Let $B(\zeta)$ be the strict basin of attraction of ζ (see definition 2.15 in Chapter 2); we know, by lemma 3.14 that the set of minimal saddles in its boundary (see Chapter 2 after definition 2.11) is given by $U^-(\zeta)$. It follows from theorem 2.21 and proposition 2.22, applied to the cycle $B(\zeta)$ that for all $\varepsilon > 0$, within a time $e^{\beta(h(l-1)+\varepsilon)}$ our process, with a probability tending to one as $\beta \rightarrow \infty$, will escape from $B(\zeta) \cup \partial B(\zeta)$ through U^- . Moreover, looking at U^- , we deduce that it will enter into $B(\zeta')$ where ζ' is a rectangular configuration obtained from ζ by cutting one row or column of

minimal length. Indeed all downhill paths emerging from $U^- \equiv F(\partial B(\zeta))$ and going outside $B(\zeta)$, enter $B(\zeta')$ for one of the above specified ζ' . The general case of ζ containing several rectangles is analogous. In this way, by iterating the argument we conclude that for all $\zeta \in G$ and $\varepsilon > 0$,

$$P_\zeta(\tau_{-\underline{1}} < e^{\beta[(l^*-1)+\varepsilon]}; \tau_{-\underline{1}} < \tau_{\partial G}) \longrightarrow 1 \text{ as } \beta \rightarrow \infty. \quad (3.27)$$

Next, by applying theorem 2.22 (ii) and (iv) to the cycle $A_{-1} \subseteq G$ we know that for all $\varepsilon, \varepsilon' > 0$ and β sufficiently large:

$$P_{-\underline{1}}(\tau_P < e^{\beta(\Gamma+\varepsilon)} > e^{-\varepsilon'}). \quad (3.28)$$

So, by (3.27), (3.28), using recurrence as in theorem 2.22 in Chapter 2, we deduce that for all $\varepsilon > 0$, $\zeta \in G$,

$$P_\zeta(\tau_{\partial G} < e^{(\Gamma+\varepsilon)}) \longrightarrow 1 \text{ as } \beta \rightarrow \infty. \quad (3.29)$$

On the other hand, using (d) of claim 3.16 we know that

$$\Gamma' := \min_{\eta \in \partial G \subseteq P} H(\eta) - H(-\underline{1}) > \Gamma. \quad (3.30)$$

Combining (3.29), and (3.27), (3.30), with the simple consequence of stationarity of the Gibbs measure given by lemma 2.21 we get that, analogous to corollary 2.24, for all $\zeta \in G$,

$$P_\zeta(\sigma_{\tau_{\partial G}} \notin P) \longrightarrow 0 \text{ as } \beta \rightarrow \infty, \quad (3.31)$$

Using an argument like the one leading to the proof of proposition 2.9, we conclude that

$$P_\zeta(\tau_{\bar{P}} < e^{\beta(l^*-1)+\varepsilon}) \rightarrow 1 \text{ as } \beta \rightarrow \infty. \quad (3.32)$$

where $\bar{P}$ is the set of configurations obtained from P by flipping a minus spin adjacent both to the quasi-square and to the unit square protuberance; in other words the configurations in $\bar{P}$ are obtained from those in $\mathcal{R}(l^*-1, l^*)$ by attaching to one of the longer sides of the the quasi-square a stable 1×2 rectangular protuberance.

Starting from $\bar{P}$, which certainly belongs to the cycle $A_{+\underline{1}}$, by corollary 2.23, we deduce that for all $\varepsilon > 0$,

$$P_{\bar{P}}(\tau_{+\underline{1}} < e^{\beta(2J-h\varepsilon)}) \longrightarrow 1 \text{ as } \beta \rightarrow \infty, \quad (3.33)$$

since the maximal internal barrier $\Theta(A_{+\underline{1}})$ is seen immediately to be $2J - h$. Again by lemma 2.21, since $\Gamma = \min_{\sigma \in \partial G} H(\sigma) - H(-\underline{1})$, we have for all $\varepsilon > 0$,

$$P_{-\underline{1}}(\tau_{\partial G} < e^{\beta(\Gamma-\varepsilon)}) \longrightarrow 1 \text{ as } \beta \rightarrow \infty, \quad (3.34)$$

By (3.32) and (3.33) on the one hand, and (3.34) on the other hand, using that G is connected, contains $-\underline{1}$ but not $+\underline{1}$, so that any path $\omega : -\underline{1} \longrightarrow +\underline{1}$ has to cross its boundary, we conclude the proof of point (i) of theorem 3.5.

To prove point (ii) we note that the fact that P is a gate for the transition $-\underline{1} \longrightarrow +\underline{1}$ (consequence of claim 3.16) implies that with a probability tending to one as β tends to infinity, our process will visit P during the first excursion

between $-\underline{1}$ and $+\underline{1}$. Indeed a path not visiting $\mathcal{P}$ between $\theta_{-\underline{1},+\underline{1}}$ and $\tau_{+\underline{1}}$ has to cross ∂G at an energy strictly larger than $H(\mathcal{P})$:

$$P_{-\underline{1}}(\theta_{-\underline{1},\mathcal{P},+\underline{1}} > \tau_{+\underline{1}}) \leq P_{-\underline{1}}(\tau_{\partial G \setminus \mathcal{P}} < \tau_{+\underline{1}}). \quad (3.35)$$

Given any $\delta > 0$, we write:

$$P_{-\underline{1}}(\tau_{\partial G \setminus \mathcal{P}} < \tau_{+\underline{1}}) \leq P_{-\underline{1}}(\tau_{\partial G \setminus \mathcal{P}} < e^{\beta(\Gamma+\delta)}) + P_{-\underline{1}}(\tau_{+\underline{1}} > e^{\beta(\Gamma+\delta)}) \quad (3.36)$$

By point (i) of theorem 3.1 and lemma 2.20, choosing $\sigma < \min_{\sigma \in \partial G \setminus \mathcal{P}} H(\sigma) - H(-\underline{1}) - \Gamma$ we get point (ii). The proof of theorem 3.1 is concluded.

Remark 3.17. *We have already seen that $\mathcal{P}$, as a consequence of claim 3.16, is a gate for the transition $-\underline{1} \rightarrow +\underline{1}$. Moreover it also follows from point (c) of claim 3.16 that $\mathcal{P}$ is a minimal gate; indeed for all $\eta \in \mathcal{P}$ there is a path in $(-\underline{1} \rightarrow +\underline{1})_{\text{opt}}$ intersecting $S(-\underline{1}, +\underline{1})$ only in η . This also shows that $\mathcal{P} \equiv G(-\underline{1}, +\underline{1})$ (see definition 2.9). Indeed take any $\xi \in S(-\underline{1}, +\underline{1}) \setminus \mathcal{P}$; given any $\omega \in (-\underline{1} \rightarrow +\underline{1})_{\text{opt}}$ such that $\xi \in \omega \cap S(-\underline{1} \rightarrow +\underline{1})$, we know that it has to visit $\mathcal{P}$ but since, as already noticed, for all $\eta \in \mathcal{P}$ there exists $\omega' \in (-\underline{1} \rightarrow +\underline{1})_{\text{opt}}$ such that $\omega' \cap S(-\underline{1}, +\underline{1}) = \eta$, we deduce that ξ is unessential (see after definition 2.10 and by proposition 2.11), we conclude that $\xi \in S(-\underline{1}, +\underline{1}) \setminus G(-\underline{1}, +\underline{1})$ so that $G(-\underline{1}, +\underline{1}) \equiv \mathcal{P}$.*

We notice that the argument of the proof of theorem 3.5 and in particular claim 3.16 justifies the choice of $A_{-\underline{1}}$ as the basin of metastability. Indeed our process, with high probability for large β , will stay inside $A_{-\underline{1}}$ before performing a transition to $+\underline{1}$ through $\mathcal{P}$.

Finally it is immediate to show that with high probability for large β , our process visits $\mathcal{P}$ between $\theta_{-\underline{1},+\underline{1}}$ and $\tau_{+\underline{1}}$ only once. Let us now state a more detailed result concerning the tube of typical trajectories during the first excursion from $-\underline{1}$ to $+\underline{1}$.

We first introduce a *standard tube* (of rectangles) as a subset $\mathcal{T}$ of $(\mathcal{Z}_+)^2$ consisting of points corresponding either to small quasi-squares (with $l = l_1 \wedge l_2 < l^*$) or large rectangles (with $l = l_1 \wedge l_2 \geq l^*$):

$$\mathcal{T} = \mathcal{L}_1 \cup \mathcal{L}_2 \quad (3.37)$$

Here (see Figure 3.6)

$$\begin{aligned} \mathcal{L}_1 &= \{\bar{l} \equiv (l_1, l_2) \in (\mathcal{Z}_+)^2 : 1 \leq l_1 \wedge l_2 \leq l^* - 1, |l_1 - l_2| \leq 1\}, \\ \mathcal{L}_2 &= \{(l_1, l_2) \in (\mathcal{Z}_+)^2 : l^* \leq l_1 \wedge l_2 \leq L\}. \end{aligned} \quad (3.38)$$

We call a *standard sequence of rectangles* any sequence $\bar{l}^{(1)}, \dots, \bar{l}^{(2L_1)}, \bar{l}^{(i)} \in (\mathcal{Z}_+)^2$ such that

$$\{\bar{l}^{(i)}\}_{i=1, \dots, 2L-1} \in \mathcal{T}$$

$\bar{l}^{(1)} = (1, 1)$ and the sequence $\{\bar{l}^{(i)}\}_{i=1, \dots, 2L-1}$ is monotonous and consists of nearest neighbours in the sense

$$\bar{l}^{(i+1)} \equiv (l_1^{(i+1)}, l_2^{(i+1)}) = (l_1^{(i)}, l_2^{(i)}) + e,$$

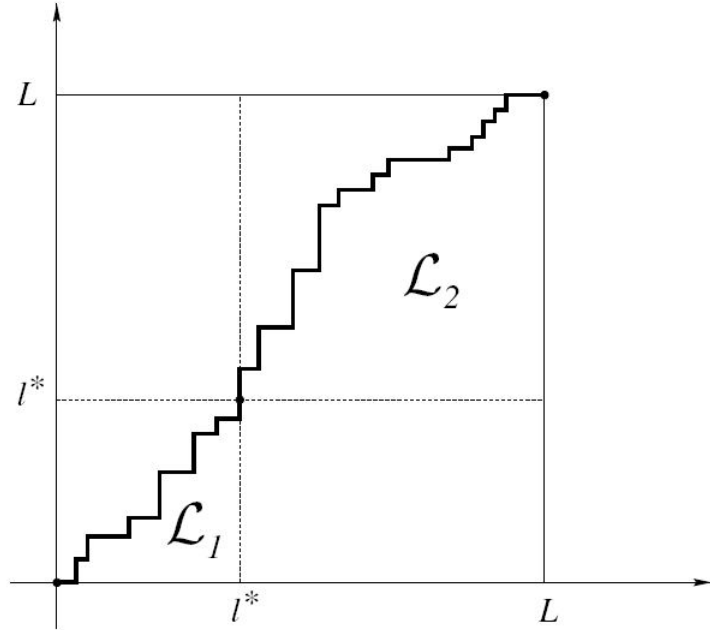


Figure 3.6:

where e is either $e_1 = (1, 0)$ or $e_2 = (0, 1)$. Let $\tau_0, \tau_1, \dots, \tau_\eta, \dots$ be random times after $\theta_{-\underline{1}, +\underline{1}}$ in which σ_t visits the set R of rectangular configurations (after a change):

$$\tau_0 = \theta_{-\underline{1}, +\underline{1}}$$

(see (3.8))

$$\tau_{n+1} = \min\{t > \tau_\eta : \sigma_t \in R \setminus \{\sigma_{\tau_\eta}\}\}, \quad n = 0, 1, 2, \dots \quad (3.39)$$

We say that σ_t is an ξ -standard path if

- (1) $\sigma_{\tau_0} = -\underline{1}$, $\{\sigma_{\tau_\eta}\}_{n=0,1,\dots}$ is a standard sequence of rectangles,
- (2) the random times τ_η satisfy the following conditions:
 - (a) $\tau_1 < e^{\varepsilon\beta}$, $\tau_2 - \tau_1 < e^{\varepsilon\beta}$, $\tau_3 - \tau_2 < e^{\varepsilon\beta}$,
 - (b) $\exp\{\beta(h(l-1) - \varepsilon)\} \leq \tau_n - \tau_{n-1} \leq \exp\{\beta(h(l-1) + \varepsilon)\}$, whenever $\sigma_{\tau_{n-1}} \in \mathcal{R}(l, l)$ for $2 \leq l < l^*$, or $\sigma_{\tau_{n-1}} \in \mathcal{R}(l, l+1)$ for $2 \leq l < l^*$,
 - (c) $\exp\{\beta(2J - h\varepsilon)\} \leq \tau_n - \tau_{n-1} \leq \exp\{\beta(2J - h + \varepsilon)\}$, whenever $\sigma_{\tau_{n-1}} \in \mathcal{R}(l_1, l_2)$ for $l_1 \wedge l_2 \geq l^*$, $l_1 \vee l_2 \leq L - 2$.

We use $\mathcal{T}_\varepsilon$ to denote the set of all ε -standard paths.

The results for the asymptotics of the first excursion from $-\underline{1}$ to $+\underline{1}$ are then summarized in the following theorem.

Theorem 3.18. *For all $\epsilon > 0$:*

$$\lim_{\beta \rightarrow \infty} P_{-\underline{1}}(\{\sigma_t\}_{t=1,2,\dots} \in \mathcal{T}_\epsilon) = 1. \quad (3.40)$$

Proof. Consider the cycles $A_{-\underline{1}}, A_{+\underline{1}}$ given as the maximal sets of configurations with energy smaller than $H(P)$ containing $-\underline{1}, +\underline{1}$, respectively.

Recall that $\mathcal{P}$ is a minimal gate coinciding with $G(-\underline{1}, +\underline{1})$. Suppose we condition to cross between $\theta_{-\underline{1}, +\underline{1}}$ and $\tau_{+\underline{1}}$ the minimal gate $\mathcal{P}$ in η ; it is seen immediately that there are two classes of configurations, say $\eta^{(-)}$ and $\eta^{(+)}$, with $\eta^{(-)}$ a singleton in $A_{-\underline{1}}$ and $\eta^{(+)}\mathcal{P} \subseteq A_{+\underline{1}}$, such that between $\theta_{-\underline{1}, +\underline{1}}$ and $\tau_{+\underline{1}}$ our process performs the path $\eta^{(-)}, \eta, \eta^{(+)}$. $\eta^{(-)}$ is the quasi-square obtained from η by removing the unit square protuberance, whereas $\eta^{(+)}$ is the set of configurations obtained from η by flipping a minus spin adjacent both to the quasi-square and to the unit square protuberance producing a stable 1×2 protuberance. Then, to find the tube of typical trajectories between $\theta_{-\underline{1}, +\underline{1}}$ and $\tau_{+\underline{1}}$, we have to find the typical tube of first exit from $A_{-\underline{1}}$ conditioning to $\sigma_{\tau_{\partial A_{-\underline{1}}}} = \eta$ and the tube of first descent to the bottom $+\underline{1}$ of the cycle $A_{+\underline{1}}$ starting from $\eta^{(+)}$; to this end, by applying theorems 2.29, we have only to find the standard cascades (see (2.44)) from $\eta^{(-)}$ in $A_{-\underline{1}}$ and from $\eta^{(+)}$ in $A_{+\underline{1}}$. The sequence of minimaxes necessary to determine the standard cascades is easily deduced by lemma 3.14. This concludes the proof of the theorem. $\square$

Notice that the case $l_1 \vee l_2 > L - 2$ has to be treated separately, in the obvious way.

3.5 Alternative method to determine $\Phi(-\underline{1}, +\underline{1})$

Let us now present, always for $L \geq l^* + 3$, another method to solve the main model-dependent variational problem, i.e. to determine the communication height $\Phi(-\underline{1}, +\underline{1})$ between $-\underline{1}$ and $+\underline{1}$. It is much simpler but it is specific to the standard stochastic Ising model since it exploits its peculiar properties. For n integer, $0 \leq n \leq |\Lambda|$, we introduce the set

$$\nu_n := \left\{ \sigma \in \mathcal{X} : \sum_{x \in \Lambda} \frac{\sigma(x+1)}{2} = n \right\} \quad (3.41)$$

namely ν_n is the set of configurations with a number of plus spins fixed at the value n . It is clear that, by continuity of the dynamics, every path going from $-\underline{1}$ to $+\underline{1}$ has to cross each one of the sets ν .

The *reference path* ω^R Let us now introduce a particular path $\omega^R : -\underline{1} \rightarrow +\underline{1}$ that we call a *reference path*. We set $\omega_n = \{\omega_n^R\}$ with $n = 0, \dots, |\Lambda|$, namely,

$$\omega_0^R = -\underline{1} \quad \omega_1^R = \{x_0\} \dots \quad \omega_{|\Lambda|}^R = +\underline{1} \quad (3.42)$$

where x_0 is a fixed site in $(\cdot)$, say the origin, and ω^R consists of a growing sequence of single clusters given by a quasi-square ($R(l, l)$ or $R(l-1, l)$) with a bar attached to one of its largest sides (here by bar we mean a rectangle $R(l, l')$ with

$l' \leq l$). These clusters are called standard polyominoes (for the two-dimensional case) in [2].

Thus ω^R hits every ν_n with $n = l^2$, $n \in \{1, \dots, |\Lambda| - 1\}$, in a square $R(l, l)$ and every ν_n with $n = l(l+1)$, $n \in \{1, \dots, |\Lambda| - 1\}$ in a quasi-square $R(l, l+1)$. The part of ω^R between $R(l, l+1)$ and $R(l+1, l+1)$ is as follows: first we add a unit square protuberance to one of the longest sides of $R(l, l+1)$; then we flip, successively, the minus spins adjacent to the exterior to $R(l, l+1)$ and to the growing bar, until we get $R(l+1, l+1)$. Similarly we go from $R(l, l)$ to $R(l, l+1)$. The order of the directions of growth of the standard polyominoes, as well as the sequence of growing bars attached to the quasi-square, may be picked arbitrarily but are fixed.

An easy computation shows that $\max_{\sigma \in \omega_R} H(\sigma) = H(\mathcal{P})$; we immediately get

$$\Phi(-\underline{1}, +\underline{1}) = H(S(-\underline{1}, +\underline{1})) \leq H(\mathcal{P}). \quad (3.43)$$

We observe that we can use ω^R as reference path, for a comparison, for both the transitions from ν_{l^2} to $\nu_{l(l+1)}$ and from $\nu_{l(l+1)}$ to $\nu_{(l+1)^2}$.

It is easy to solve the isoperimetric problem for $n = l^2$, $n = l(l+1)$, i.e. to find the configuration with minimal perimeter for a given number of plus spins. We get

$$F(\nu_{l^2}) = \mathcal{R}(l, l), \quad F(\nu_{l(l+1)}) = \mathcal{R}(l, l+1); \quad (3.44)$$

recall that by $F(Q)$ we denote the set of ground states in $Q \subseteq \mathcal{X}$ (see definition 2.2 in Chapter 2).

Indeed, let us first note that for any $n \in N$, given a number of up spins n , to minimize the energy, i.e. the total perimeter p , it is always convenient to collect the up spins into a single cluster without holes, in the following sense. Consider a configuration $\eta \in \{-\underline{1}, +\underline{1}\}^\Lambda$ containing at least two disjoint clusters C_1 and C_2 ; with a suitable translation of C_1 towards the other clusters we can join C_1 to the rest in such a way that the translated C_1 will have at least one unit edge of its boundary in common with the boundary of another cluster; then the total perimeter strictly decreases. In this way, by uniting the clusters of η we can always transform it into another configuration η_1 containing a single cluster and having strictly smaller energy. Moreover if in η_1 there are holes, namely minus spins surrounded by a circuit of pluses, by moving plus spins lying in some external corners where the number of n.n. plus spins is ≤ 2 to some internal hole with number of n.n. plus spins ≥ 2 , it is possible to construct a configuration η_2 without holes eventually by strictly decreasing the energy. Similarly, if η_2 is not monotonous, i.e. its perimeter is strictly larger than that of the circumscribed rectangle, it is always possible to transform η_2 into a configuration η_3 containing a single monotonous cluster by strictly decreasing the energy.

The energy of this configuration η_3 , when l_1, l_2 are the side lengths of the circumscribed rectangle, is $2J(l_1 + l_2)hn + H(-\underline{1})$. Thus, to minimize the energy in ν_n we are left to find $l_1, l_2 \in N$ minimizing $(l_1 + l_2)$ in the set $l_1 l_2 \geq n$, $1 \leq l_1, l_2 \leq n$. It is an easy exercise to prove that if n is of the form $n = l^2$,

$n = l(l+1)$, $l \in N$, this minimum is uniquely achieved for $(l_1, l_2) = (l, l)$, $(l_1, l_2) \in \{(l, l+1), (l+1, l)\}$, respectively, thus proving (3.44).

$$\Phi(\nu_{l^2}, \nu_{(l^2+1)}) = \Phi(\mathcal{R}(l, l), \nu_{(l^2+1)}) = H(Q_l),$$

$$\Phi(\nu_{l(l+1)}, \nu_{[(l+1)l+1]}) = \Phi(\mathcal{R}(l, l+1), \nu_{[(l+1)l+1]}) = H(P_l). \quad (3.45)$$

where Q_l is the set of clusters obtained from the squares in $\mathcal{R}(l, l)$ by adding a unit square protuberance to one of its sides; P_l is the set of clusters obtained from the quasi-squares in $\mathcal{R}(l, l+1)$ by adding a unit square protuberance to one of its longer sides. To prove (3.45) we first notice that in order to determine $\Phi(V_{l^2}, \nu_{(l^2+1)})$ we can restrict ourselves, in ν_{l^2} , to $\mathcal{R}(l, l)$, otherwise we would overpass the energy of the reference saddle given by ω^R . Indeed we have

$$\min_{\sigma \in \nu_{l^2} \setminus \mathcal{R}(l, l)} H(\sigma) - H(\mathcal{R}(l, l)) \geq 2J. \quad (3.46)$$

It is immediate to show, using comparison with ω^R , that $\Phi(v(l, l), \nu_{(l^2+1)}) \leq H(Q_l) = H(\mathcal{R}(l, l)) + 2J - h$; thus we have

$$\Phi(\nu_{l^2} \setminus \mathcal{R}(l, l), \nu_{(l^2+1)}) \geq \Phi(\mathcal{R}(l, l), \nu_{(l^2+1)}) + h. \quad (3.47)$$

The case of $\Phi(\nu_{l(l+1)}, \nu_{[(l+1)l+1]})$ is analogous; the proof of (3.45) is concluded. We have, in particular:

$$\Phi(\nu_{(l^*-1)l^*}, \nu_{[(l^*-1)l^*+1]}) = H_{(Pl^*-1)} \equiv H(P). \quad (3.48)$$

Since any path $\omega \in (-\underline{1} \rightarrow +\underline{1})_{opt}$ has to make the one-step transition between $\nu_{(l^*-1)l^*}$ and $\nu_{[(l^*-1)l^*+1]}$ we get from (3.48) that $\Phi(-\underline{1}, +\underline{1}) \geq H(P)$ which, together with (3.43), implies $\Phi(-\underline{1}, +\underline{1}) = H(P)$. This concludes the alternative computation of the communication height between $-\underline{1}$ and $+\underline{1}$ and, looking at ω^R , also concludes the proof that $\mathcal{P} \subseteq S(-\underline{1}, +\underline{1})$. (Notice that the above method does not prove that $\mathcal{P}$ is a gate.)

We remark that for $L = l^* + 1$ the global saddle is just the set of rectangles $\mathcal{R}(l^* - 1, l^*)$ whereas for $L = l^* + 2$ the global saddle (being also a minimal gate) is given by the set (containing $\mathcal{P}$) of clusters obtained by attaching a unit square protuberance to any of the edges of a rectangle in $\mathcal{R}(l^* - 1, l^*)$.

Chapter 4

Metastability behavior for Lattice Gas Model

4.1 The Van Der Waals-Maxwell theory

Metastability is a relevant phenomenon for thermodynamic systems close to a first order phase transition. Examples are supercooled vapours and liquids, supersaturated vapours and solutions, as well as ferromagnets in the part of the hysteresis loop where the magnetization is opposite to the external magnetic field. A metastable state occurs when some thermodynamic parameter such as the temperature, pressure or magnetic field is changed from a value giving rise to a stable state with a unique phase, say X , to one for which at least part of the system should be in some new equilibrium phase Y . Then, in particular experimental situations, instead of undergoing the phase transition, the system goes over continuously into a false equilibrium state with a unique phase X' , far from Y but actually close to the initial equilibrium phase X . It is this apparent equilibrium situation that is called a metastable state. Its properties are very similar to those of the stable equilibrium state; for example for a supersaturated vapor one can determine the pressure experimentally as a function of the temperature and the specific volume. We speak of the metastable branch of the isothermal curve.

The distinguishing feature of metastability is that, eventually, either via an external perturbation or via a spontaneous fluctuation, a nucleus of the new phase appears, starting an irreversible process which leads to the stable equilibrium state Y , where the phase transition has taken place.

Let us first illustrate metastability in more detail with the example of liquid vapour phase transition; subsequently we shall describe magnetic systems.

Consider an isothermal compression of a gas at a temperature T below its critical temperature T_c . (see Figure 4.1). Suppose we start with a specific volume v slightly larger than the value v_g corresponding to the condensation point at temperature T (the specific volume v is given by $v = V/N$, where V is the volume and N is the number of molecules). If our sample is reasonably free of

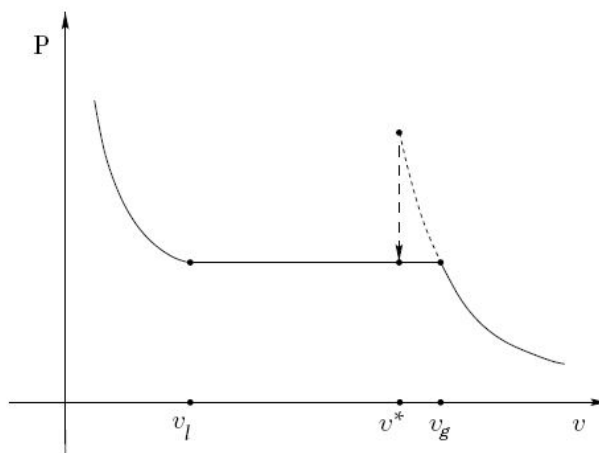


Figure 4.1:

impurities and if we proceed in the compression slowly by avoiding significant density gradients, we can obtain a pure gaseous phase, with $v < v_g$, commonly called a supersaturated vapour. It is observed experimentally that, by continuing in the isothermal compression, we end up with a value v^* of the specific volume for which the gas becomes unstable; then we start observing the appearance and growth of the new liquid phase until the segregation between liquid and gas is completed, and a fraction $\alpha = (1/v^* - 1/v_g)(1/v_l - 1/v_g)^{-1}$ of the fluid is finally in the liquid phase with specific volume v_l .

Now, in the final stable equilibrium, the liquid and gaseous phases are segregated and coexist at the saturated vapor pressure.

For $v \in (v^*, v_g)$ the properties of the (supersaturated) vapour are quite similar to those of the normal gas with $v > v_g$. Apparently we have an equilibrium pure gaseous phase. The main difference is that even a relatively small disturbance can induce the nucleation of the liquid phase. An impurity or any external perturbation inducing a localized density change can produce a nucleus of condensation around which the liquid phase starts growing by absorbing molecules from the surrounding supersaturated vapor. If v is very near to (but still larger than) v^* , even a spontaneous thermal fluctuation can be responsible for the formation of a condensation nucleus. In this last case we speak of homogeneous nucleation since these density fluctuations take place everywhere in the bulk. Again the final stable state corresponds to a fraction $\alpha = (1/v - 1/v_g)(1/v_l - 1/v_g)^{-1}$ of liquid coexisting with the saturated gas. This behavior is typical of a conservative evolution which preserves the number of molecules.

Another relevant example of phase transition giving rise to metastability phenomena is that which takes place for ferromagnetic systems at temperature T below the Curie point T_c . As we shall see, this case is naturally described in a non-conservative context. Figure 4.2 shows, for $T < T_c$, a typical graph of

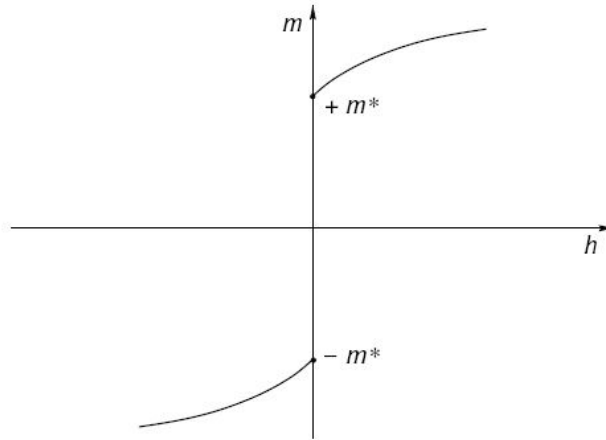


Figure 4.2:

magnetization m versus external magnetic field h for an ideal ferromagnet. We observe the phenomenon of spontaneous magnetization:

$$\lim_{h \rightarrow 0^+} m(h) > 0, \quad \text{and} \quad \lim_{h \rightarrow 0^-} m(h) < 0. \quad (4.1)$$

For $T > T_c$ there is a *paramagnetic* behavior:

$$\lim_{h \rightarrow 0} m(h) = 0. \quad (4.2)$$

The existence of a spontaneous magnetization can be interpreted as coexistence, for the same value of the magnetic field $h = 0$, of two different phases with opposite magnetization. What is observed for a real ferromagnet is the *hysteresis loop* shown in Figure 4.3. For $T < T_c$, suppose we change the value of the magnetic field from small negative to zero, and then to small positive values. Our magnet persists, apparently in equilibrium, in a state with magnetization opposite to the external magnetic field h . This situation corresponds to a metastable state since the true equilibrium state would have magnetization parallel to the field. We can continue increasing h up to a limiting value h^* , called the *coercive field*, at which we observe a decay to the stable state with positive magnetization. In a similar way we can cover the rest of the loop. The static and dynamic properties of the system along the metastable arc are similar to those we have already described in the case of fluids. The main difference here is that we do not have the global constraint that we had before, of fixed total number of molecules; now the corresponding quantity, i.e. the total number of up spins, is not at all fixed. From the point of view of equilibrium statistical mechanics the situation described for a fluid corresponds to the *canonical ensemble* whereas the situation for a magnet corresponds to the *grand canonical ensemble*.

The specific features that a theory of metastability have to explain are both static and dynamic in nature. We would like to find the equation of state of metastable states. For example in the case of liquidvapour phase transition we would like to determine the value of $v^* = v^*(T)$ and the arc of the isotherm

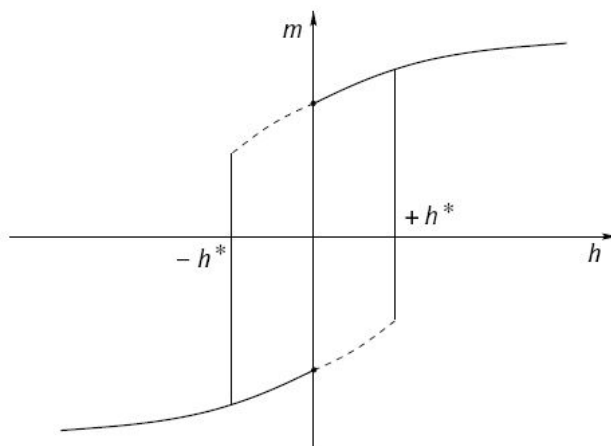


Figure 4.3:

describing the supersaturated vapor between v^* and v_g . On the other hand, the most relevant dynamical quantity is the lifetime of the metastable state. Its correct definition is also part of the problem. We expect the lifetime to become very small as v tends to v^* , whereas we expect that it tends to infinity as v goes to v_g .

A first possible explanation of metastability can be found in the framework of the classical van der Waals Maxwell theory.

The equation of state of real gases introduced by van der Waals is based on semiphenomenological grounds. His approach is neither purely thermodynamical nor is it based on a genuine microscopical point of view. The van der Waals equation of state for one mole of fluid is:

$$(P + \frac{a}{v^2})(v - b) = kT, \quad (4.3)$$

where P is the pressure, T is the absolute temperature, k is Boltzmanns constant and $a \geq 0$, $b \geq 0$ are parameters depending on the particular fluid.

This equation of state is simply obtained from the perfect gas law $Pv = kT$, by introducing the corrective terms a/v^2 and $-b$. The first term takes into account the intermolecular attraction, and the term $-b$ takes into account the intrinsic volume occupied by molecules, seen as extended instead of point-like objects.

For a more detailed treatment of the van der Waals equation we refer, for instance, to [13].

4.2 Isotropic dynamics

As in ref [32], the two typical examples of metastable states are (i) a supersaturated vapor and (ii) a magnetic system with magnetization opposite to the

external magnetic field. When describing these systems by lattice Ising-like models, it is natural to use occupation number variables $\eta(x) \in \{0, 1\}$ for the first case and spin variables $\sigma(x) \in \{-1, +1\}$ for the second case. Of course, given any particular model we can interchange the representation via the transformation $\eta(x) = (1 + \sigma(x))/2$. This trivial change of variables allows two different interpretations for the same model. For example, standard stochastic Ising models that we introduced in magnetic language can also be used to model the time evolution of a fluid. The corresponding dynamics is *non-conservative* in the sense that it does not preserve the number of particles. To describe a fluid it is much more natural to use a *conservative* dynamics.

Now discussing metastable behavior for a class of lattice gas models subject to stochastic dynamics that conserve the number of particles (in the spin representation the conserved quantity would be the magnetization).

We want, in particular, to analyze the Kawasaki dynamics, i.e. a family of Markov chains (in continuous or discrete time) that are reversible with respect to the Gibbs measure for the Ising Hamiltonian (3.1), whose elementary process, instead of being a single spin-flip, like in Glauber dynamics, consists of a double spin-flip, interchanging the values of spin of two neighboring sites. In lattice gas language this corresponds to a jump of a particle to an empty neighboring site. Let us now give some preliminary definitions. Let Λ_β be a large finite box centered at the origin with periodic boundary conditions. We consider simultaneously the two-dimensional case where $\Lambda_\beta \subseteq \mathbb{Z}^2$. The subscript β in Λ_β is to recall that the side length of Λ_β will depend on Λ_β . Indeed it will grow at a suitable exponential rate with β .

With each $x \in \Lambda_\beta$ we associate an occupation variable $\eta(x)$, taking the values 0 or 1, indicating absence or presence of a particle. A lattice gas configuration is denoted by $\eta \in \mathcal{X} = \{0, 1\}^{\Lambda_\beta}$. The equilibrium properties in a conservative context are described by a canonical Gibbs measure that we are going to define for the Ising lattice gas. Let Λ_β^* be the set of bonds Λ_β (equivalent to an ordered pairs of n.n. sites) in β ; we consider the interaction defined by the following canonical Hamiltonian:

$$H^{can}(\eta) = -U \sum_{(x,y) \in \Lambda_\beta^*} \eta(x)\eta(y) \quad (4.4)$$

i.e. there is a binding energy $-U < 0$ between neighboring occupied sites and no interaction otherwise. For $A \subseteq \Lambda_\beta$, we denote by $N_A(\eta)$ the number of particles in A of the configuration η :

$$N_A(\eta) = \sum_{x \in A} \eta(x). \quad (4.5)$$

We fix the number of particles in Λ_β at the value

$$N = e^{-\Delta\beta} |\Lambda_\beta|. \quad (4.6)$$

where $\Delta > 0$ is an activity parameter. This corresponds to a density equal to

$$\rho = \frac{1}{|\Lambda_\beta|} \sum_{x \in \Lambda_\beta} \eta(x) = e^{-\Delta\beta}. \quad (4.7)$$

we denote $\mathcal{V}_N$ the set of configurations with N particles:

$$\mathcal{V}_N = \{\eta \in \mathcal{X}_\beta : N_{\Lambda_\beta}(\eta) = N\}. \quad (4.8)$$

On $\mathcal{V}_N$ we define the *canonical Gibbs measure*

$$\nu_N(\eta) = \frac{\exp(-\beta H^{can}(\eta)) \mathbf{1}_{\nu_N(\eta)}}{Z_N^{can}}, \quad Z_N^{can} = \sum_{\eta \in \mathcal{V}_N} \exp(-\beta H^{can}(\eta)). \quad (4.9)$$

We see from (4.7) and (4.6) that in order to have particles at all we must pick $|\Lambda_\beta|$ at least exponentially large in β . This means that the regime where the volume is fixed, considered up to now in this chapter and in particular in the case of non-conservative Glauber dynamics, has no relevance here.

We define a stochastic dynamics, called Kawasaki dynamics, in terms of a continuous time Markov chain $(\eta_t)_{t \geq 0}$ with state space $\mathcal{V}_N$, and with generator L given by:

$$(Lf)(\eta) = \sum_{(x,y) \in \Lambda_\beta^*} c((x,y), \eta) [f(\eta^{(x,y)}) - f(\eta)], \quad (4.10)$$

where

$$\eta^{(x,y)}(z) = \begin{cases} \eta(z) & \text{if } z \neq x, y \\ \eta(x) & \text{if } z = y \\ \eta(y) & \text{if } z = x \end{cases} \quad (4.11)$$

and

$$c((x,y), \eta) = \exp[-\beta(H^{can}(\eta^{(x,y)}) - H^{can}(\eta))]_+ \quad (4.12)$$

Let us start with a heuristic discussion based on static grounds. Consider the lattice gas at low temperature at its condensation point. Let

$$\rho_l(\beta) = \frac{1 + m^*(\beta)}{2}, \quad \rho_g(\beta) = \frac{1 - m^*(\beta)}{2}, \quad (4.13)$$

denote the densities of the liquid and gas phases. Here $m^*(\beta)$ is the spontaneous magnetization in the spin language given by $m^*(\beta) = \lim_{h \rightarrow 0^+} m(\beta, h)$. Taking the Hamiltonian (4.1) where the ferromagnetic coupling constant is $J/2$ and the magnetic field is $h/2$, we have, in d dimensions,

$$m^*(\beta) = 1 - 2e^{-2dJ\beta}[1 + o(1)], \quad \text{so that } \rho_g(\beta) = e^{-dU\beta}[1 + o(1)], \quad \beta \rightarrow \infty \quad (4.14)$$

as follows easily from a perturbative argument, based on low temperature expansions, since the energy cost to invert the spin at the origin, with zero magnetic field, is $2dJ$ and $J = U/2$; thus we see that $e^{-dU\beta}$ can be identified as the leading term of the density of the saturated gas at the condensation point (in the sense that $\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \log \rho_g(\beta) = dU$).

When describing a pure gaseous phase outside the coexistence region ($\rho < \rho_g(\beta)$) we know that the canonical Gibbs measure is equivalent to the grand canonical Gibbs measure given by

$$\mu(\eta) = \frac{\exp(-\beta H(\eta))}{Z}, \quad Z = \sum_{\eta \in \mathcal{X}_\beta} \exp(-\beta H(\eta)) \quad (4.15)$$

where

$$H(\eta) = H^{can}(\eta) - \lambda N_{\Lambda_\beta}(\eta) \quad (4.16)$$

$\lambda \in \mathcal{R}$ is the chemical potential taking a suitable value, in order to fix the average grand canonical density at the value $\rho = e^{-\Delta\beta}$; at very low temperature we have to choose $\lambda = -\Delta + o(1)$ as follows again by simple perturbative arguments since for large β the gas is very rarefied and for a free gas the density ρ equals the fugacity $z = \exp(\beta\lambda)$. The magnetic field appearing in spin representation see (4.4) is $h = 2U + \lambda$; thus we find again that the chemical potential fixing the density ρ at the value $\rho_g(\beta)$ corresponds to $h = 0$.

Suppose that, starting from the condensation point, we increase the density slightly, but avoiding the appearance of droplets of the liquid phase. Then we get a supersaturated gas that can be described in terms of a *restricted ensemble* namely the grand canonical Gibbs measure restricted to a suitable subset of configuration space, for instance, where all sufficiently large clusters are suppressed. At low temperature this supersaturated gas will stay rarefied, so that its metastable state can be described as a pure gas phase with strong mixing properties.

We can suppose that, for the description of metastability, the canonical and grand canonical Gibbs measures are equivalent, provided they are suitably restricted as described above. Under these conditions let us make, in the limit of large β , a rough calculation of the probability, at the metastable equilibrium, of finding a cubic droplet of occupied sites centered at the origin. In two dimensions let us denote by $\mu^*(l \times l)$, the probability, under the restricted ensemble, of seeing a square droplet of side l centered at the origin; and in three dimensions let us denote by $\mu^*(m \times m \times m)$ the probability, under the restricted ensemble, of seeing a cubic droplet of side m centered at the origin. We have:

$$\mu^*(l \times l) \simeq \rho^{l^2} e^{2l(l-1)U\beta}, \quad (4.17)$$

since ρ is the probability of finding a particle at a given site and $-U$ is the binding energy between particles at neighboring sites. Substituting $\rho = e^{-\Delta\beta}$ we obtain

$$\mu^*(l \times l) \simeq e^{-\beta E_2(l)}, \quad (4.18)$$

where

$$E_2(l) = 2Ul - (2U - \Delta)l^2. \quad (4.19)$$

Let $2U > \Delta$. The maximum of $E_2(l)$ is at $l = U/(2U - \Delta)$. This means that if this ratio is non-integer, droplets with side length $l < l_c$ have a probability decreasing in l while droplets with side length $l \geq l_c$ have a probability increasing in l , where

$$l_c = \lceil \frac{U}{2U - \Delta} \rceil. \quad (4.20)$$

Then, in two dimensions, the choice $\Delta \in (U, 2U)$ corresponds to $l_c \in (1, \infty)$, i.e. to a non-trivial critical droplet size. Use $J = U/2$, $h = 2U + \lambda$, $\lambda = -\Delta$, to see that (4.20) is in agreement with (3.7).

The metastable behaviour for the non-conservative case in spin language occurs when $h \in (0, 2J)$. This corresponds precisely to $\Delta \in (U, 2U)$.

In physical terms, $\Delta \in (0, U)$ corresponds to the unstable gas, $\Delta = U$ to the instability threshold commonly called the spinodal point $\Delta \in (U, 2U)$ to the metastable gas, $\Delta = 2U$ to the condensation point, and $\Delta \in (2U, +\infty)$ to the stable gas.

Similarly, in three dimensions we get:

$$\mu^*(m \times m \times m) \simeq \rho^{m^3} e^{\beta[3Um^3 - 3Um^2]}. \quad (4.21)$$

Substituting $\rho = e^{-\Delta\beta}$, we obtain

$$\mu^*(m \times m \times m) \simeq e^{-\beta E_3(m)}. \quad (4.22)$$

with

$$E_3(m) = -(3U - \Delta)m^3 + 3Um^2. \quad (4.23)$$

Let $\Delta < 3U$. The maximum of $E_3(m)$ occurs at $m = 2U/(3U - \Delta)$. If this ratio is non-integer, then cubic droplets with side length $m < m_c$ have a probability decreasing in m , while cubic droplets with side length $m \geq m_c$ have a probability increasing in m , where

$$m_c = \lfloor \frac{2U}{3U - \Delta} \rfloor + 1. \quad (4.24)$$

The metastable regime in three dimensions is $\Delta \in (U, 3U)$ corresponding to $m_c \in (1, +\infty)$; the analogue in the non-conservative Glauber case is $h \in (0, 4J)$.

4.2.1 Dynamics in two dimensions

Let us now consider the metastable behavior from a dynamic point of view and see what happens locally. Let us first consider the two-dimensional case. We want to compare the probabilities of growing or shrinking for a square cluster of particles. The argument will be very rough. Suppose we pick a large finite box Λ , centered at the origin, and start with an $l \times l$ droplet inside Λ . Suppose that the effect on Λ of the gas in $\Lambda_\beta \setminus \Lambda$ (may be described in terms of the *creation* of new particles with rate $\rho = e^{-\Delta\beta}$ at sites on the interior boundary of Λ and the annihilation of particles with rate 1 at sites on the exterior boundary of Λ). So the cost of creating a new particle is Δ whereas the cost of annihilating a particle is zero.

In other words, suppose that inside Λ the Kawasaki dynamics may be described by a Metropolis algorithm with energy given by the (*local grand canonical Hamiltonian*):

$$H(\eta) = H^{can}(\eta) + \Delta N_\Lambda(\eta). \quad (4.25)$$

Then the energy barriers for adding respectively removing a row or column of length l are given in terms of the local saddles of H :

$$\text{Energy barrier for adding} = 2\Delta - U, \quad (4.26)$$

which corresponds to a configuration η obtained by creating two particles (cost of 2Δ) one of which is attached to the droplet (gain of $-U$); indeed it is immediate

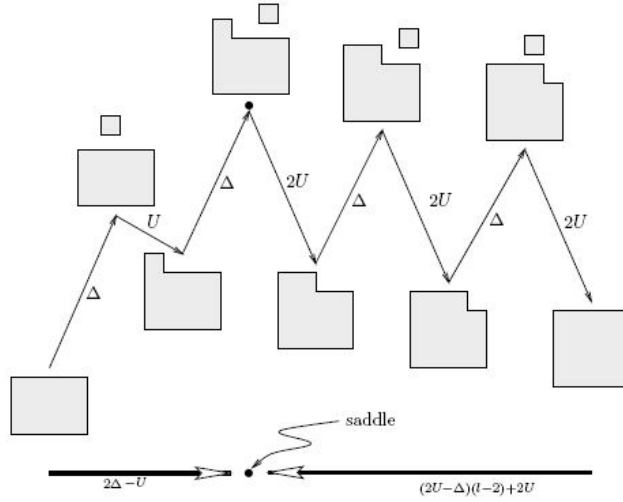


Figure 4.4:

to construct two declining paths (see Chapter 2) emerging from η and going respectively to the original rectangular droplet and to the rectangular droplet obtained by adding a row or column.

$$\text{Energy barrier for removing} = (2U - \Delta)(l - 2) + 2U, \quad (4.27)$$

which corresponds to a configuration η' obtained by the consecutive removal and annihilation of $l - 2$ corners from the original droplet at a cost $2U - \Delta$ per step, followed by a final removal without annihilation at a cost $2U \times \eta'$ is similar to η : indeed it can be obtained from the contracted rectangle $(l - 1) \times l$ by creating two particles one of which is attached to the rectangle; see (Figure 4.4). The balance of the two barriers indeed gives the critical size l_c in (4.20).

4.3 Local Kawasaki Dynamics

4.3.1 Definition of the Model

Let $\Lambda \subset \mathbb{Z}^2$ be a finite box centered at the origin that will be chosen large enough. Let $\partial^- \Lambda$ be the interior boundary of Λ and let $\Lambda_0 = \Lambda \setminus \partial^- \Lambda$ be the interior of Λ . With each $x \in \Lambda$ we associate an occupation variable $\eta(x)$, assuming values 0 or 1. A lattice configuration is denoted by $\eta \in \mathcal{X} = \{0, 1\}^\Lambda$. We often identify η with its support, i.e. the set of occupied sites in η .

Each configuration $\eta \in \mathcal{X}$ has an energy given by the following Hamiltonian:

$$H(\eta) = -U \sum_{(x,y) \in \Lambda^{*, -}} \eta(x)\eta(y) + \Delta \sum_{x \in \Lambda} \eta(x) \quad (4.28)$$

where

$$\Lambda^{*, -} = \{(x, y) : x, y \in \Lambda_0, |x - y| = 1\} \quad (4.29)$$

is the set of non-oriented bonds in Λ_0 . The interaction consists of a binding energy $-U < 0$ for each nearest-neighbor pair of particles in Λ_0 . In addition, there is an activation energy $\Delta > 0$ for each particle in Λ .

4.3.2 Kawasaki dynamics

We next define Kawasaki dynamics on Λ , with a boundary condition that mimicks the effect of an infinite gas reservoir outside Λ with density $\rho = e^{-\Delta\beta}$. Let $b = (x \rightarrow y)$ be an oriented bond, i.e. an ordered pair of nearest-neighbor sites, and define

$$\begin{aligned}\partial^* \Lambda^{out} &= \{b = (x \rightarrow y) : x \in \partial^- \Lambda, y \in \partial^+ \Lambda\} \\ \partial^* \Lambda^{in} &= \{b = (x \rightarrow y) : y \in \partial^- \Lambda, x \in \partial^+ \Lambda\} \\ \Lambda^{*,orie} &= \{b = (x \rightarrow y) : x, y \in \Lambda\}\end{aligned}\tag{4.30}$$

and put $\bar{\Lambda}^{*,orie} = \partial^* \Lambda^{out} \cup \partial^* \Lambda^{in} \cup \Lambda^{*,orie}$. Two configurations $\eta, \eta_0 \in \mathcal{X}$ with $\eta \neq \eta_0$ are said to be communicating states if there exists a bond $b \in \bar{\Lambda}^{*,orie}$ such that $\eta' = T_b \eta$, where $T_b \eta$ is the configuration obtained from η as follows:

For $b = (x \rightarrow y) \in \Lambda^{*,orie}$, $T_b \eta$ denotes the configuration obtained from η by interchanging particles along b :

$$T_b \eta(z) = \begin{cases} \eta(z) & \text{if } z \neq x, y \\ \eta(x) & \text{if } z = y \\ \eta(y) & \text{if } z = x \end{cases}\tag{4.31}$$

For $b = (x \rightarrow y) \in \partial^* \Lambda^{out}$ we set:

$$T_b \eta(z) = \begin{cases} \eta(z) & \text{if } z \neq x \\ 0 & \text{if } z = x \end{cases}\tag{4.32}$$

this describes the annihilation of particles along the border.

For $b = (x \rightarrow y) \in \partial^* \Lambda^{in}$ we set:

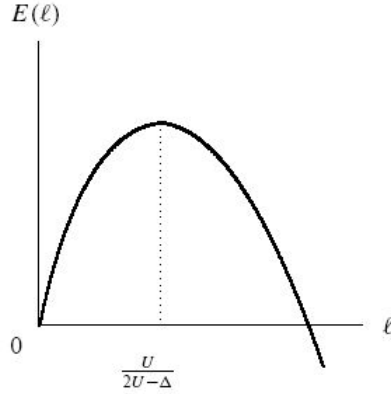
$$T_b \eta(z) = \begin{cases} \eta(z) & \text{if } z \neq y \\ 1 & \text{if } z = y \end{cases}\tag{4.33}$$

this describes the creation of particles along the border.

The Kawasaki dynamics is the discrete time Markov chain $(\eta_t)_{t \in \mathbb{N}}$ on state space $\mathcal{X}$ given by the following transition probabilities: for $\eta \neq \eta'$:

$$P(\eta, \eta') = \begin{cases} |\bar{\Lambda}^{*,orie}|^{-1} \exp[-\beta H(\eta) - H(\eta')]_+ & \text{if } \exists b \in \bar{\Lambda}^{*,orie} : \eta' = T_b \eta \\ 0 & \text{otherwise} \end{cases}\tag{4.34}$$

and $P(\eta, \eta) = 1 - \sum_{\eta' \neq \eta} P(\eta, \eta')$, where $[a]_+ = a \vee 0$. This is a standard Metropolis dynamics with an open boundary: along each bond touching $\partial^- \Lambda$ from the outside, particles are created with rate $\rho = e^{-\Delta\beta}$ and are annihilated with rate 1, while inside Λ_0 particles are conserved. Note that an exchange of occupation numbers inside the ring $\Lambda \setminus \Lambda_0$ does not involve any change in energy.

Figure 4.5: $l \mapsto E(l)$

4.3.3 Rough description of nucleation in two dimensions

In two dimensions, we will be interested in the *metastable regime*

$$\Delta \in (U, 2U), \quad \beta \rightarrow \infty. \quad (4.35)$$

In this regime, droplets tend to grow slowly: single particles attached to one side of a droplet typically detach before the arrival of a next particle (because $e^{U\beta} \ll e^{\Delta\beta}$), while bars of two or more particles typically do not detach (because $e^{U\beta} \ll e^{2U\beta}$).

As was pointed out in den Hollander, Olivieri, and Scoppola [28], section 4.2, the energy $E(l)$ of an $l \times l$ droplet in Λ_0 equals (recall (4.28) and see Fig. 4.5)

$$E(l) = -U[2l(l-1)] + \Delta l^2 = 2Ul - (2U - \Delta)l^2, \quad (4.36)$$

which is maximal at $l = U/(2U - \Delta)$:

The critical droplet size is therefore given by

$$l_c = \lceil \frac{U}{2U - \Delta} \rceil \quad (4.37)$$

($\lceil \cdot \rceil$ denotes the upper integer part), provided we assume that

$$\frac{U}{2U - \Delta} \notin \mathcal{N} \quad (4.38)$$

in order to avoid ties. Throughout the sequel we assume that (4.38) is in force. Thus, an $(l_c - 1) \times (l_c - 1)$ droplet is subcritical while an $l_c \times l_c$ droplet is supercritical. We need some definitions.

Definition 4.1. Suppose that the finite box $\Lambda \subset \mathbb{Z}^2$ is sufficiently large.

- (i) For $x \in \Lambda_0$, let $nn(x) = \{y \in \Lambda_0 : |y - x| = 1\}$ be the set of nearest neighbor sites of x in Λ_0 .

- (ii) A free particle in $\eta \in \mathcal{X}$ is a site $x \in \eta \cap \partial^- \Lambda$ or a site $x \in \eta \cap \Lambda$ such that $\sum_{y \in nn(x) \cap \Lambda_0} \eta(y) = 0$, i.e., a particle not in interaction with any other particle (remember from (4.2) that particles in the interior boundary $\partial^- \Lambda$ have no interaction with other particles).

We denote by η_{fp} the union of free particles in $\partial^- \Lambda$ and free particles in Λ_0 and by η_{cl} the clustered part of η

$$\eta_{cl} := \eta \cap \Lambda_0 \setminus \eta_{fp}. \quad (4.39)$$

Definition 4.2. (i) Throughout the sequel, we identify a configuration $\eta \in \mathcal{X}$ with its support, $\text{supp}(\eta) = \{x \in \Lambda : \eta(x) = 1\}$, and write $x \in \eta$ to indicate that η has a particle at x .

- (ii) The configuration space $\mathcal{X}$ can be partitioned as

$$\mathcal{X} = \bigcup_{n=0}^{|\Lambda|} \nu_n, \quad (4.40)$$

Where

$$\nu_n = \{\eta \in \mathcal{X} : |\eta| = n\} \quad (4.41)$$

is the set of configurations with n particles, called the n -manifold.

Each configuration can be decomposed into maximally connected components, called *clusters*. The following sets of configurations will determine the geometry of the critical droplet, as will become clear later on.

4.4 Results for Ising-Kawasaki Model

We study metastable behavior for a class of lattice gas models subject to stochastic dynamics that retains the locality particle size; local Kawasaki dynamics. In particular we study the transition time between $\underline{0}$ metastable states and $\underline{1}$ the stable states.

4.4.1 Critical droplets

Recall the discussion about the metastable regime in part 4.1. In particular in equations (4.16) and (4.17).

Definition 4.3. (a) Let Q denote the set of configurations having one cluster anywhere in Δ_0 consisting of an $(l_c - 1) \times l_c$ quasi-square with a single protuberance attached to one of its sides.

- (b) Let D denote the set of configurations that can be reached from some configuration in Q via a U -path, i.e.,

$$D = \{\eta' \in V_{nc} : \exists \eta \in Q : H(\eta) = H(\eta'), \Phi_{V_{nc}}(\eta, \eta') \leq H(\eta) + U\} \quad (4.42)$$

where $n_c = l_c(l_c - 1) + 1$ is the volume of the clusters in Q .

- (c) Let $C^* = D^{fp}$, where $(\cdot)^{fp}$ denotes addition of a free particle anywhere in Λ (see fig 4.6).

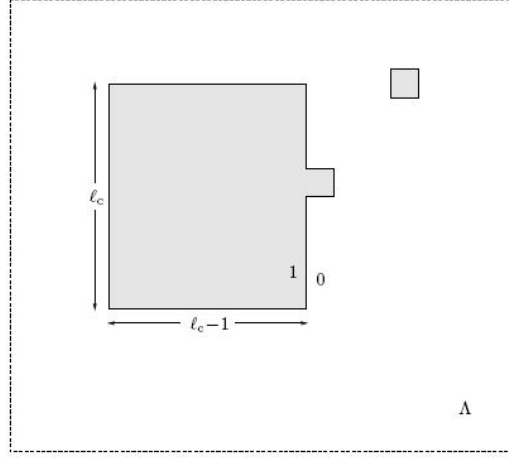


Figure 4.6: A canonical critical droplet: an element of $Q^{fp} \subseteq D^f p = C^*$

(d) Let

$$\begin{aligned}
 \Gamma_i^* &= H(C^*) = H(D^{fp}) = H(D) + \Lambda = H(Q) + \Lambda \\
 &= U[(l_c - 1)^2 + l_c(l_c - 2) + 1] + \Lambda[l_c(l_c - 1) + 2] \\
 &= 2U[l_c + 1] - (2U - \Delta)[l_c(l_c - 1) + 2]
 \end{aligned} \tag{4.43}$$

denote the energy of the configurations in C^* .

As we will see shortly, Q plays the role of the set of canonical protocritical droplets for the nucleation, $Q \subseteq D$ the set of protocritical droplets, and C^* the set of critical droplets. Think of D as the set of configurations the dynamics can reach after hitting Q before the creation of the next free particle in $\partial^- \Lambda$ (which takes a time $e^{U\beta} \ll e^{\Delta\beta}$). This particle moves the configuration into C^* and completes the formation of the critical droplet (= critical cluster + free particle) that triggers the nucleation. If subsequently the free particle moves to the critical cluster and attaches itself properly (i.e., in a corner), then the dynamics has moved over the hill and proceeds to fill Λ_0 .

Definition 4.4. Let

$$\begin{aligned}
 \underline{0} &= \{\eta \in \mathcal{X}, \eta(x) = 0 \ \forall x \in \Lambda\} \\
 \underline{1} &= \{\eta \in \mathcal{X}, \eta(x) = 1 \ \forall x \in \Lambda^-, \eta(x) = 0 \ \forall x \in \partial^- \Lambda\}
 \end{aligned} \tag{4.44}$$

denote the configurations where Λ is empty, respectively, Λ_0 is full and $\partial^- \Lambda$ is empty. We assume that Λ is so large that

$$H(\underline{1}) < H(\underline{0}) = 0 \tag{4.45}$$

In this case, $\underline{1}$ is the global minimum of H . The main result known about nucleation in two dimensions reads as follows.

Theorem 4.5. (den Hollander, Olivieri, and Scoppola)

(i) $\Phi(\underline{0}, \underline{1}) = \Gamma_i^*$ and $C^* \subseteq S(\underline{0}, \underline{1})$,

(ii) $\forall \delta > 0$,

$$\lim_{\beta \rightarrow \infty} P_{\underline{0}}(e^{(\Gamma_i^* - \delta)\beta} < \tau_{\underline{1}} < e^{(\Gamma_i^* + \delta)\beta}) = 1. \quad (4.46)$$

(iii)

$$\lim_{\beta \rightarrow \infty} P_{\underline{0}}(\tau_{C^*} < \tau_{\underline{1}} \mid \tau_{\underline{1}} < \tau_{\underline{0}}) = 1 \quad (4.47)$$

theorem 4.5 (i) identifies Γ_i^* as the communication height for the nucleation and C^* as a subset of the communication level set for the nucleation. theorem 4.3 (ii) identifies the nucleation time to exponential order in β , with exponent Γ_i^* .

Proof. Immediate. $\square$

theorem 4.5 (iii) states that C^* is a gate for the nucleation.

4.4.2 Sharp description of nucleation in two dimensions

Theorem 4.6. $D = \bar{D} \cup \tilde{D}$, where

(i) $\bar{D}$ is the set of configurations having one cluster anywhere in Δ_0 consisting of an $(l_c - 2) \times (l_c - 2)$ square with four bars of lengths $\bar{k}_i$, $i = 1, 2, 3, 4$, attached to its four sides satisfying

$$1 \leq \bar{k}_i \leq l_c - 1, \quad \sum_i \bar{k}_i = 3l_c - 3, \quad (4.48)$$

(ii) $\tilde{D}$ is the set of configurations having one cluster anywhere in Δ_0 consisting of an $(l_c - 3) \times (l_c - 1)$ rectangle with four bars of lengths $\tilde{k}_i$, $i = 1, 2, 3, 4$, attached to its four sides satisfying

$$1 \leq \tilde{k}_i \leq l_c - 1, \quad \sum_i \tilde{k}_i = 3l_c - 3. \quad (4.49)$$

Remark 4.7. In the first half of theorem 4.6, the four bars may be placed anywhere in the ring around the square, i.e., anywhere in the union of the two rows, the two columns and the four corners forming the outer layer of the square. A total of $3l_c - 3$ particles must be accommodated in this ring in such a way that each side of the ring, i.e., each row or column with its two adjacent corners, contains precisely one bar. Thus, a bar may include a corner of the ring provided the neighboring bar also includes this corner. Similarly for the second half of theorem 4.6. Compare definitions 4.1 (a) and 4.6. Write $Q = \bar{Q} \cup \tilde{Q}$, where

(i) $\bar{Q}$ are those configurations where the single particle is attached to one of the longest sides of the $(l_c - 1) \times l_c$ quasi-square.

(ii) $\tilde{Q}$ are those configurations where the single particle is attached to one of the smallest sides of the $(l_c - 1) \times l_c$ quasi-square.

Then $\bar{Q}$ consists of precisely those configurations in $\bar{D}$ where one $\bar{k}_i$ equals 1 and the others are maximal. Similarly, $\tilde{Q}$ consists of precisely those configurations in $\tilde{D}$ where one $\tilde{k}_i$ equals 1 and the others are maximal.

Recall the definitions of gate and saddle from (chapter 2).

Theorem 4.8. (i) $\mathcal{G}(\underline{0}, \underline{1}) \subset S(\underline{0}, \underline{1})$ and $C^* \subset S(\underline{0}, \underline{1})$.

(ii)

$$\lim_{\beta \rightarrow \infty} P_{\underline{0}}(\tau_Q < \tau_{C^*} < \tau_{\underline{1}} \mid \tau_{\underline{1}} < \tau_{\underline{0}}) = 1, \quad (4.50)$$

(ii)

$$\lim_{\beta \rightarrow \infty} P_{\underline{0}}(\eta_{\tau_{c^*-}} = \eta \mid \tau_{C^*} < \tau_{\underline{0}}) = \frac{1}{|D|}. \quad (4.51)$$

with τ_{c^*-} the time just prior to τ_{C^*} .

Proof. Immediate. $\square$

Theorem 4.8 (i) shows that $S(\underline{0}, \underline{1})$ has dead-ends and is larger than the set of critical droplets C^* . Theorem 4.8 (ii) says that Q is hit prior to C^* . Theorem 4.8(iii) says that the entrance distribution of C^* is uniform, i.e., the protocritical droplets in D , seen just prior to the creation of the free particle in $\partial^-\Lambda$, occur with equal probability. (Incidentally, the exit distribution is not uniform and turns out to be hard to compute.)

Theorem 4.9. There exists a constant $K = K(\Lambda, l_c)$ such that

$$E_{\underline{0}}(\tau_{\underline{1}}) = K e^{\Gamma_i^* \beta} [1 + o(1)], \quad \beta \rightarrow \infty, \quad (4.52)$$

Moreover

$$P_{\underline{0}}(\tau_{\underline{1}} > t E_{\underline{0}}(\tau_{\underline{1}})) = [1 + o(1)] e^{-t[1+o(1)]}. \quad (4.53)$$

Proof. Immediate. $\square$

Theorem 4.8 provides the sharp asymptotic for the nucleation time:

$$\lim_{\beta \rightarrow \infty} P_{\underline{0}}(\tau_{\underline{1}} > t K e^{\Gamma_i^* \beta}) = e^{-t} \quad t \geq 0. \quad (4.54)$$

The exponential law is typical for success only occurs after many unsuccessful attempts.

Theorem 4.10. As $\Lambda \rightarrow \mathbb{Z}^2$,

$$K(\Lambda, l_c) \sim \frac{1}{4\pi N(l_c)} \frac{\log|\Lambda|}{|\Lambda|} \quad (4.55)$$

($\sim$ means that the ratio of the left and the right side tends to 1) with

$$N(l_c) = \frac{1}{3}(l_c - 1)l_c^2(l_c + 1) \quad (4.56)$$

the cardinality of $D = D(\Lambda, l_c)$ modulo shifts.

Proof. Immediate. $\square$

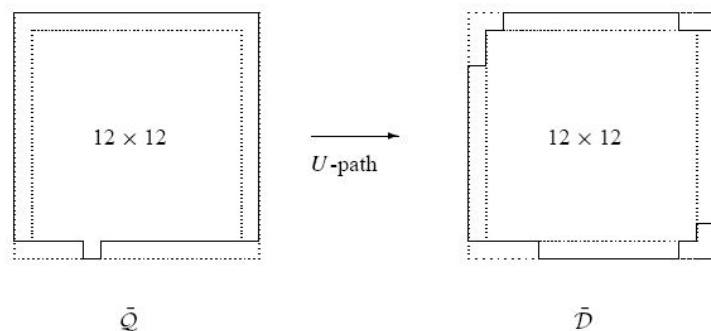


Figure 4.7: Configurations in $\bar{Q}$ and $\bar{D}$ for $l_c = 14$. A similar picture applies for $\tilde{Q}$ and $\tilde{D}$ with a 11×13 rectangle in the center.

4.5 Geometry in two dimensions

In this section we collect the key geometric facts that underlie our analysis. In section 4.5.1 we introduce some geometric definitions. In section 4.5.2 we prove theorem 4.11, which identifies the full geometry of the set of protocritical droplets. In section 4.5.2 we obtain the structure of the communication level set for the nucleation. In section 4.4.2 we prove two global geometric facts that will be needed in section 4.6.3.

4.5.1 Some geometric definitions

Definition 4.11. - A 1-protuberance in $\eta \in \mathcal{X}$ is a site $x \in \eta \cap \Lambda_0$ such that $y \in \sum_{nn(x)} \eta(y) = 1$.

- A corner in $\eta \in \mathcal{X}$ is a site $x \in \Lambda_0$ such that $y \in \sum_{nn(x)} \eta(y) \geq 2$. A corner in η can either be occupied or vacant.

Definition 4.12. Given a configuration $\eta \in \mathcal{X}$, consider the set $C(\eta) \subseteq \mathcal{R}^2$ defined as the union of the closed unit squares centered at the sites inside Λ_0 where η has a particle. The maximal connected components $C_1, \dots, C_m, m \in \mathbb{N}$, of $C(\eta)$ are called clusters of η (two unit squares touching only at the corners are not connected). There is a one-to-one correspondence between configurations $\eta \subseteq \Lambda_0$ and sets $C(\eta)$. A configuration $\eta \in \mathcal{X}$ is characterized by a set $C(\eta)$, depending only on $\eta \cap \Lambda_0$, plus possibly a set of particles in $\partial^- \Lambda$, namely, $\eta \cap \partial^- \Lambda$. Thus, we are actually identifying two different objects: a configuration $\eta \in \mathcal{X}$ and the pair $(C(\eta), \eta \cap \partial^- \Lambda)$.

Lemma 4.13. For $\eta \in \mathcal{X}$, let $|\eta|$ be the number of particles in η , $\gamma(\eta)$ the Euclidean boundary of $C(\eta)$, called the contour of η , and $|\gamma(\eta)|$ the length of $\gamma(\eta)$, i.e., the number of broken bonds in η . Then the energy associated with η is given by

$$H(\eta) = \frac{U}{2} |\gamma(\eta)| - (2U - \Delta) |\eta \cap \Lambda_0| + \Delta |\eta \cap \partial^- \Lambda|. \quad (4.57)$$

Proof. Immediate. $\square$

Definition 4.14. (i) A bar is a $1 \times k$ rectangle with $k \geq 1$. A bar is called a row or a column if it fills a side of a rectangle.

(ii) A corner of a rectangle is an intersection of two bars attached to the rectangle.

(iii) A quasi-square is an $l \times (l + \delta)$ rectangle with $l \geq 1$ and $\delta \in \{0, 1\}$. A square is a quasi-square with $\delta = 0$.

(iv) If η is a configuration with a single contour, then we denote by $CR(\eta)$ the rectangle circumscribing η , i.e., the smallest rectangle containing η .

(v) Given η such that $CR^-(\eta) \subseteq \eta$, we say that it is possible to move a particle from row $r_\alpha(\eta) \subseteq \partial^- CR(\eta)$ to row $r_{\alpha'}(\eta) \subseteq \partial^- CR(\eta)$ via corner $c_{\alpha\alpha'}(\eta) \subseteq \partial^- CR(\eta)$ if (see Figs 4.5 and 4.6)

$$|c_{\alpha,\alpha'}(\eta) \cap \eta| = 0, \quad |r_\alpha(\eta) \cap \eta| \geq 1, \quad 1 \leq |r_{\alpha'}(\eta) \cap \eta| \leq |r_{\alpha'}(\eta)|, \quad (4.58)$$

where $\alpha\alpha' \in \{ne, nw, se, sw\}$ with $n = \text{north}$, $s = \text{south}$, etc. By convention, corners are not part of rows. If equality holds in the last inequality, then we need to place the bar in the row opposite to $r_\alpha(\eta)$, say $r_{\alpha''}(\eta)$, a distance 1 away from $c_{\alpha\alpha'}(\eta)$ in order to be able to accommodate the shift of a bar in $r_{\alpha'}(\eta)$ that is necessary to accommodate the particle that moves around the corner.

4.5.2 Protocritical droplets: Proof of Theorem 4.6

The proof of theorem 4.4 will be given in two steps:

$$\begin{aligned} (i) \quad & \bar{D} \cup \tilde{D} \subseteq D \\ (ii) \quad & D \subseteq \bar{D} \cup \tilde{D} \end{aligned} \quad (4.59)$$

Proof. of (i). Recall the definition of U-path and the definitions of $\bar{Q}, \tilde{Q}$ and $\bar{D}, \tilde{D}$. To prove (i) we must show that for all $\eta \in \bar{D} \cup \tilde{D}$,

$$(i1) \quad H(\eta) = H(\bar{Q} \cup \tilde{Q})$$

$$(i2) \quad \exists \omega : \bar{Q} \cup \tilde{Q} \rightarrow \eta : \max_i H(\omega_i) \leq H(\bar{Q} \cup \tilde{Q}) + U, \quad |\omega_i| = n_c \quad \forall i. \quad (4.60)$$

$\square$

Proof. of (i1) Any $\eta \in \bar{D} \cup \tilde{D}$ has a single contour $\gamma(\eta)$ inside $\Lambda - 0$ of length $|\gamma(\eta)| = 4l_c$ and volume $|\eta \cap \Lambda_0| = l_c(l_c - 1) + 1 = n_c$, while $|\eta \cap \partial^- \Lambda| = 0$ (see Fig. 4.7). Thus, by (4.59), H is constant on $\bar{D} \cup \tilde{D}$. Since $\bar{Q} \cup \tilde{Q} \subseteq \bar{D} \cup \tilde{D}$, this completes the proof of (i1). $\square$

Proof. of (i2). Note that, because $\bar{Q}$ and $\tilde{Q}$ are connected via a U-path (disconnect the 1-protuberance and re-attach it to one of the neighboring sides of the $(l_c - 1) \times l_c$ quasi-square), we have

Figure 4.8: Translation of a bar on a side of a rectangle at cost U Figure 4.9: Motion of a particle around a corner of a rectangle at cost U .

$$D = \{\eta \in \mathcal{X} : \exists \text{U-path from } \bar{Q} \text{ to } \eta\} = \{\eta \in \mathcal{X} : \exists \text{U-path from } \tilde{Q} \text{ to } \eta\}. \quad (4.61)$$

First we prove that for any $\eta \in \bar{D}$ there exists an $\omega : \bar{Q} \rightarrow \eta$ such that $\max_i H(\omega_i) \leq H(\bar{Q}) + U$ and $|\omega_i| = n_c$ for all i . We start the path from some $\zeta \in \bar{Q}$. Then, recalling the labeling in theorem 4.6, we have

- $\bar{k}_1(\zeta) = 1$ contained in $r_e(\zeta)$;
- $\bar{k}_2(\zeta) = l_c - 2$ contained in $r_n(\zeta)$;
- $\bar{k}_3(\zeta) = \bar{k}_4(\zeta) = l_c - 1$ contained in $r_\omega(\zeta) \cup c_{n,\omega}(\zeta)$ and $r_s(\zeta) \cup c_{s,\omega}(\zeta)$, respectively.

Here, without loss of generality, we assume that the 1-protuberance is attached to $r_e(\zeta)$ and proceed anti-clockwise. Using the mechanism described in Figs. 4.8 and 9, we move $\bar{k}_2(\zeta) - \bar{k}_2(\eta)$ particles from $r_n(\zeta)$ to $r_e(\zeta)$, one by one. After that we move $\bar{k}_3(\zeta) - \bar{k}_3(\eta) + \bar{k}_4(\zeta) - \bar{k}_4(\eta)$ particles from $r_s(\zeta) \cup c_{sw}(\zeta)$ to $r_e(\zeta)$. Finally, we move $\bar{k}_3(\zeta) - \bar{k}_3(\eta)$ particles from $r_\omega(\zeta) \cup c_{nw}(\zeta)$ to $r_\omega(\zeta) \cup c_{sw}(\zeta)$. The result is a configuration $\eta \in \bar{D}$. Next we prove that for any $\eta \in \bar{D}$ there exists an $\omega : \bar{D} \rightarrow \eta$ such that $\max_i H(\omega_i) \leq H(\bar{Q}) + U$ and $|\omega_i \cap \Lambda| = n_c$ for all i . We start the path from some $\zeta \in \bar{D}$. We have

- $\tilde{k}_1(\zeta) = 1$ contained in $r_e(\zeta)$;
- $\tilde{k}_2(\zeta) = l_c - 2$ contained in $r_n(\zeta)$;
- $\tilde{k}_3(\zeta) = \tilde{k}_4(\zeta) = l_c - 1$ contained in $r_\omega(\zeta) \cup c_{n,\omega}(\zeta) \cup c_{s,\omega}(\zeta)$.

We move $\tilde{k}_2(\zeta) - \tilde{k}_2(\eta)$ particles from $r_n(\zeta)$ to $r_e(\zeta)$. After that we move $\tilde{k}_3(\zeta) - \tilde{k}_3(\eta) + \tilde{k}_4(\zeta) - \tilde{k}_4(\eta)$ particles from $r_s(\zeta) \cup c_{sw}(\zeta)$ to $r_e(\zeta)$. Finally, we move $\tilde{k}_3(\zeta) - \tilde{k}_3(\eta)$ particles from $r_\omega(\zeta) \cup c_{nw}(\zeta)$ to $r_s(\zeta) \cup c_{sw}(\zeta)$. The result is a configuration $\zeta \in \bar{D}$. This completes the proof of (i2). $\square$

Proof. of (ii) By (4.60), all configurations in $\bar{D} \cup \tilde{D}$ are connected via a U-path. Since $\bar{Q} \cup \tilde{Q} \subseteq D \cap (\bar{D} \cup \tilde{D})$, in order to prove (ii) it suffices to show that $\bar{D} \cup \tilde{D}$ cannot be exited via a U-path (recall (4.61)). $\square$

Call a path *clustering* if all the configurations in the path consist of a single cluster and no free particles. Below we will prove that for any $\eta \in \bar{D} \cup \tilde{D}$ and any η' connected to η by a clustering U-path,

$$\begin{aligned} (a) \quad CR(\eta') &= CR(\eta), \\ (b) \quad CR^-(\eta) &\subseteq \eta'. \end{aligned} \tag{4.62}$$

What (4.62) says is that neither $\bar{D}$ nor $\tilde{D}$ can be exited via a clustering U-path. From this in turn we deduce that for any $\eta \in \bar{D} \cup \tilde{D}$ and any η' connected to η by a U-path we must have that $\eta' \in \bar{D} \cup \tilde{D}$, which is what we want to prove. The argument for the latter goes as follows. Detaching a particle costs $2U$ unless the particle is a 1-protuberance, in which case the cost is U . The only configurations in $\bar{D} \cup \tilde{D}$ having a 1-protuberance are those in $\bar{Q} \cup \tilde{Q}$ (recall the remarks made below theorem 4.6). If we detach the 1-protuberance from a configuration in $\bar{Q} \cup \tilde{Q}$ at cost U , then we obtain an $(l_c - 1) \times l_c$ quasi-square plus a free particle. Since now only moves at zero cost are allowed, only the free particle can move. Since in a U-path the particle number is conserved, the only way to regain U and complete the U-path is to re-attach the free particle to the quasi-square, in which case we return to $\bar{Q} \cup \tilde{Q}$.

Remark 4.15. *Note that the motion of particles along the border a droplet may shift the droplet. Indeed, from any configuration in $\bar{Q} \cup \tilde{Q}$ the 1-protuberance may detach itself and re-attach itself to a different side of the quasi-square or rectangle (recall Fig. 4.7). Thus, the U-path may shift the protocritical droplet to anywhere in Λ_0 .*

Proof. of (a) Starting from any $\eta \in \mathcal{X}$ it is geometrically impossible to modify $CR(\eta)$ without detaching a particle. $\square$

Proof. of (b) Fix $\eta' \in \bar{D} \cup \tilde{D}$. The proof is done in two steps.

- 1 . Let us first consider clustering U-paths along which we do not move a particle from $CR^-(\eta)$. Along such paths we only encounter configurations in $\bar{D} \cup \tilde{D}$ or configurations obtained from $\bar{D} \cup \tilde{D}$ by breaking one of the bars in $\partial^- CR(\eta)$ into two pieces, at cost U (because there is no particle outside $CR(\eta)$ that can help to lower the cost). From the latter only moves at zero cost are possible, so no particle can be detached, and the only way to regain U and complete the U-path is to restore a bar.
- 2 . Let us next consider clustering U-paths along which we move a particle from a corner of $CR^-(\eta)$. This move costs $2U$, which exceeds U . The overshoot U must be regained by letting the particle slide next to a bar that is attached to a side of $CR^-(\eta)$ (see Fig. 4.5). Since there are never two bars attached to the same side, we can at most gain U . This is why it is not possible to move a particle from $CR^-(\eta)$ other than from a corner. From here only moves at zero cost are allowed. There are no 1-protuberances present anymore, because only the configurations in $\bar{Q} \cup \tilde{Q}$ have a 1-protuberance. Thus, no particle outside $CR^-(\eta)$ can move, except the one that just detached itself from $CR^-(\eta)$. This particle can move back, in which case we return to the same configuration. In fact, all possible moves at zero cost consist in moving the hole just created in

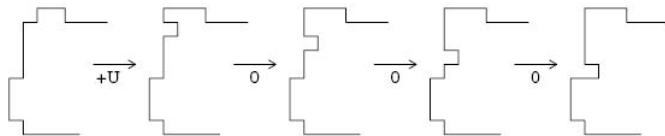
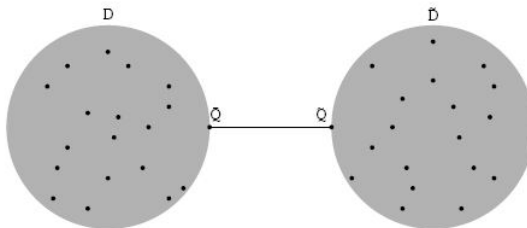


Figure 4.10: Creation and motion of the hole at cost 0

Figure 4.11: Dumb-bell shape of $D = \bar{D} \cup \tilde{D}$ for U-paths

$CR^-(\eta)$ along the side of $CR^-(\eta)$, until it reaches the height of the top of the bar attached to this side of $CR^-(\eta)$, after which it cannot advance anymore at zero cost (see Fig. 4.10). All these moves do not change the energy, except the one that returns the particle to its original position and regains U .

□

This proves our claim in (4.62), completes the proof of (ii) in (4.59), and hence of theorem 4.6.

We saw above that U-paths cannot exit $D = \bar{D} \cup \tilde{D}$, but can make a crossover between $\bar{D}$ and $\tilde{D}$. This crossover can, however, only occur between $\bar{Q}$ and $\tilde{D}$. A schematic picture of D therefore is:

4.6 Structure of the communication level set

4.6.1 Optimal paths

Most of this section is based on a line of argument in den Hollander, Nardi, Olivieri and Scoppola [28]. We repeat this argument here because it is vital for understanding the rest of the paper. We begin by giving a precise description of $\Phi(\underline{0} \rightarrow \underline{1})_{opt}$, the set of *optimal paths for the nucleation*.

Proposition 4.16. *den Hollander, Olivieri, and Scoppola [28], proposition 4.24*

$$(i) \quad \Phi(\underline{0} \rightarrow \underline{1}) = \Gamma_i^*.$$

$$(ii) \quad C^* \subseteq \Phi(\underline{0} \rightarrow \underline{1}).$$

Proof.

(i) We prove that $\Phi(\underline{0} \rightarrow \underline{1}) \geq \Gamma_i^*$ and $\Phi(\underline{0} \rightarrow \underline{1}) \leq \Gamma_i^*$. All we need to do is to construct a path that connects $\underline{0}$ and $\underline{1}$ without exceeding energy Γ_i^* . This is done in three steps. $\square$

1. We first show that the configurations in Q are connected to $\underline{0}$ by a path that stays below Γ_i^* .

Lemma 4.17. *For any $\eta^{1pr} \in Q$ there exists an $\omega : \eta^{1pr} \rightarrow \underline{0}$ such that $\max_{\varepsilon \in \omega} H(\varepsilon) < \Gamma_i^*$.*

Proof. Fix $\eta^{1pr} \in Q$. Note that, by (4.49), we have $H(\eta^{1pr}) = \Gamma_i^* - \Delta$. First, we detach the 1-protuberance from the $(l_c - 1) \times l_c$ quasi-square, which costs U and raises the energy to $\Gamma_i^* - \Delta + U (< \Gamma_i^*)$, move the particle to the boundary of the box, which costs nothing, and move it out of the box, which pays Δ . We are then left with a quasi-square of energy

$$\Gamma_i^* - 2\Delta + U \quad (4.63)$$

Second, we detach a particle from a corner of the quasi-square, which costs $2U$, and move it out of the box, which pays Δ . Thus, the energy increases by $2U - \Delta$ when detaching and removing a particle from a corner of the quasi-square. We repeat this operation another $l_c - 3$ times, each time picking particles from the bar on the same shortest side. To guarantee that we never reach energy Γ_i^* , we have the condition that

$$(2U - \Delta)k + 2U < 2\Delta - U \text{ for } 0 \leq k \leq l_c - 3, \quad (4.64)$$

or

$$3 \leq l_c < \frac{U}{2U + \Delta} + 1. \quad (4.65)$$

The second inequality holds by the definition of l_c in (4.37), the first inequality by our exclusion of $l_c = 2$. Third, detaching the last particle costs U instead of $2U$. To guarantee that we still do not reach energy Γ_i^* , we have the condition that

$$(2U - \Delta)(l_c - 2) + U < 2\Delta - U, \quad (4.66)$$

which is weaker than (4.70) because $2U - \Delta < U$. Removal of the last particle pays Δ , so that we arrive at energy

$$(\Gamma_i^* - 2\Delta + U) + (2U - \Delta)(l_c - 2) + (U - \Delta) = \Gamma_i^* - 2\Delta + (2U - \Delta)(l_c - 1), \quad (4.67)$$

which is strictly smaller than (4.63) by the second inequality in (4.65). Thus, removal of a row of length $l_c - 1$ from the $(l_c - 1) \times l_c$ quasi-square in $\eta^{1pr} \in Q$ lowers the energy (see Fig. 4.12). We now have a square of side length $l_c - 1$. It is obvious that we can remove further rows without encountering new conditions, until we reach $\underline{0}$. $\square$

2. For $\eta^{1pr} \in Q$, let η^{2pr} be the configuration obtained from η^{1pr} by attaching an extra particle next to the 1-protuberance, thereby forming a 2-protuberance. We next show that η^{2pr} is connected to $\underline{1}$ by a path that stays below Γ_i^* .

Lemma 4.18. *For any $\eta^{1pr} \in Q$ exists an $\omega \eta^{2pr} \rightarrow \underline{1}$ such that $\max_{\varepsilon \in \omega} H(\varepsilon) < \Gamma_i^*$*

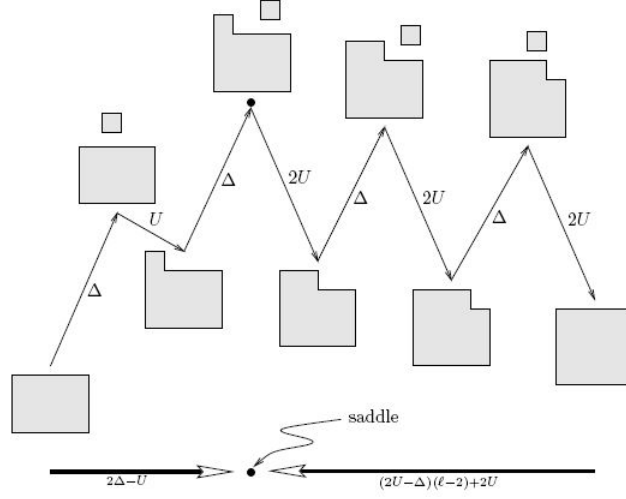


Figure 4.12: Cost of adding or removing a row of length 1.

Proof. Fix $\eta^{1pr} \in Q$. Note that $H(\eta^{2pr}) = \Gamma_i^* - 2U$. First, we create a particle, which costs Δ and raises the energy to $\Gamma_i^* - 2U + \Delta (< \Gamma_i^*)$, move it to the droplet, which costs nothing, and attach it next to the 2-protuberance, which pays $2U$, thereby forming a bar of length 3. This operation pays $2U - \Delta$. We can repeat this operation another $l_c - 3$ times until the row is filled. By that time we have a square of side length l_c and energy

$$\Gamma_i^* - 2U - (2U - \Delta)(l_c - 2). \quad (4.68)$$

Second, we create another particle and attach it anywhere to the square to form a new 1-protuberance. This operation costs $\Delta - U$. We must make sure that we can still create a particle without reaching energy Γ_i^* , which gives us the condition $\square$

$$(\Delta - U) + \Delta < 2U + (2U - \Delta)(l_c - 2), \quad (4.69)$$

$$l_c > \frac{U}{2U - \Delta} \quad (4.70)$$

which holds by the definition of l_c and the non-degeneracy hypothesis in (4.47). Third, we create another particle and attach it next to the new 1-protuberance. This brings us to energy

$$\Gamma_i^* - U - (2U - \Delta)l_c, \quad (4.71)$$

which is below the energy of η^{2pr} by (4.76). It is obvious that we can add further rows without encountering new conditions, until we reach 1.

3. We can now conclude the proof of $\Phi(0, 1) \leq \Gamma_i^*$ by constructing a bridge between η^{1pr} and η^{2pr} that does not exceed Γ_i^* . Namely, create a particle at the boundary, which costs Δ and raises the energy to Γ_i^* , move it to the droplet, which costs nothing, and place it next to the 1-protuberance, which pays $2U$.

The desired path $\omega(\underline{0} \rightarrow \underline{1})$ is realized by tracing the path in lemma 4.17 in the reverse direction, back from $\underline{0}$ to η^{1pr} , going over the bridge from η^{1pr} to η^{2pr} , and then following the path in lemma 4.18 from η^{2pr} to $\underline{1}$. This ω will be called the *reference path through η for the nucleation*.

$\Phi(\underline{0}, \underline{1}) \geq \Gamma_i^*$: The proof comes in three steps.

1. The first crucial ingredient in the proof is the following observation:

Lemma 4.19. *Any $\omega \in (\underline{0} \rightarrow \underline{1})_{opt}$ must pass through a configuration consisting of a single $(l_c - 1) \times l_c$ quasi-square somewhere in Λ_0 .*

Proof. Any path $\omega : \underline{0} \rightarrow \underline{1}$ must cross the set $\mathcal{V}_{l_c(l_c-1)}$. As shown in Alonso and in [2], theorem 2.6, in $\mathcal{V}_{l_c(l_c-1)}$ the unique (modulo translations and rotations) configuration of minimal energy is the $\mathcal{V}_{l_c(l_c-1)}$ quasi-square, which we denote by η and which has energy

$$H(\eta) = \Gamma_i^* - 2\Delta + U. \quad (4.72)$$

All other configurations in $\mathcal{V}_{l_c(l_c-1)}$ have energy at least $\Gamma_i^* - 2\Delta + 2U$. To increase the particle number starting from any such configuration, we must create a particle at cost Δ . But the resulting configuration would have energy $\Gamma_i^* - 2\Delta + U (> \Gamma_i^*)$ and thus would lead to a path exceeding energy Γ_i^* . $\square$

2. The second crucial ingredient in the proof is the following observation:

Lemma 4.20. *Any $\omega : (\underline{0} \rightarrow \underline{1})_{opt}$ must pass through Q .*

Proof. Follow the path until it hits the set $\mathcal{V}_{l_c(l_c-1)}$. According to lemma 4.11, the configuration in this set must be an $l_c(l_c - 1)$ quasi-square. Since we need not consider any paths that return to the set $\mathcal{V}_{l_c(l_c-1)}$ afterwards, a first step beyond the quasi-square must be the creation of a new particle. This brings us to energy

$$\Gamma_i^* - 2\Delta + U. \quad (4.73)$$

Before any new particle is created, we must lower the energy by at least U . The obviously only possible way to do this is to move the particle to the quasi-square and attach it to one of its sides, which reduces the energy to

$$\Gamma_i^* - \Delta. \quad (4.74)$$

and gives us a configuration in Q . $\square$

3. It now suffices to show that to reach $\underline{1}$ from Q we must reach energy Γ_i^* . This goes as follows. Starting from Q , it is impossible to reduce the energy without lowering the particle number. Indeed, this follows from [2], theorem 2.6, which asserts that the minimal energy in $\mathcal{V}_{l_c(l_c-1)+1}$ is realized (although not uniquely) by the configurations in Q . Since any further move to increase the particle number involves the creation of a new particle, the energy must reach Γ_i^* . This completes the proof of proposition 4.16 (i).

(ii) Our final observation is the following:

Lemma 4.21. *The set of configurations in $\mathcal{V}_{l_c(l_c-1)+1}$ that can be reached from $\underline{0}$ by a path that stays below Γ_i^* , and for which it is possible to add a particle without exceeding Γ_i^* coincides with the set D already defined.*

Proof. From step 2 above it is clear that the definition of D precisely assures that the assertion holds true. Indeed, by lemma 4.20, any $\omega : (\underline{0} \rightarrow \underline{1})_{opt}$ crosses $\mathcal{V}_{l_c(l_c-1)+1}$ in Q . Once it is in Q , before the arrival of the next particle, which costs Δ , it can reach all configurations that have the same energy, the same particle number, and can be reached at cost $\leq U < \Delta$. $\square$

By adding a particle to a configuration in D we arrive in $C^* = D^{fp}$, the set defined in definition 4.3 (c). This completes the proof of proposition 4.8 (ii).

We conclude the following:

Proposition 4.22. *Any $\omega : (\underline{0} \rightarrow \underline{1})_{opt}$ passes first through Q , then possibly through $D \setminus Q$, and finally through C^* .*

Proof. Combine lemmas 4.20, 4.21, and proposition 4.8 (i). $\square$

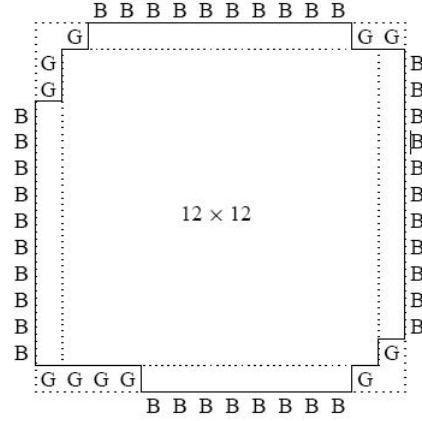
4.6.2 Motion on C^*

Proposition 4.23. (i) *Starting from $C^* \setminus Q^{fp}$, the only transitions that do not raise the energy are motions of the free particle, as long as the free particle is at lattice distance ≥ 3 from the protocritical droplet.*

(ii) *Starting from Q^{fp} , the only transitions that do not raise the energy are motions of the free particle and motions of the 1-protuberance along the side of the quasi-square where it is attached, as long as the free particle is at lattice distance ≥ 3 from the protocritical droplet. When the lattice distance is 2, either the free particle can be attached to the protocritical droplet or the 1-protuberance can be detached from the protocritical droplet and attached to the free particle, to form a quasi-square plus a dimer. From the latter configuration the only transition that does not raise the energy is the reverse move.*

(iii) *Starting from C^* , the only configurations that can be reached by a path that lowers the energy and does not decrease the particle number are those where the free particle is attached to the protocritical droplet.*

Proof. Obvious. The restriction in (i) that the free particle must be at lattice distance ≥ 3 from the protocritical droplet is needed for the following reason: If the protocritical droplet is a configuration in $D \setminus Q$ and the free particle sits at lattice distance 2 from a corner of a bar, diagonally opposite the particle that sits in the corner of the bar, then at zero cost this particle may detach itself from the bar and slide inbetween the quasi-square and the free particle. For (iii) note the following: if we start from the configuration described above and slide the remaining particles in the bar one by one, all at zero cost except the last one, which pays U , then we reach a configuration where the free particle is attached to the protocritical droplet with the bar shifted. $\square$

Figure 4.13: Good sites (G) and bad sites (B) for $l_c = 14$.

For $\eta \in C^*$, we write $\eta = (\hat{\eta}, x)$ with $\hat{\eta} \in D$ the protocritical droplet and $x \in \Lambda$ the position of the free particle. Let us denote the configurations that can be reached from $\eta = (\hat{\eta}, x)$ according to proposition 4.23 (iii) by (see Fig. 4.13)

- $C^G(\hat{\eta})$ if the particle is attached in $\partial^- CR(\hat{\eta})$.
- $C^B(\hat{\eta})$ if the particle is attached in $\partial^+ CR(\hat{\eta})$.

Let

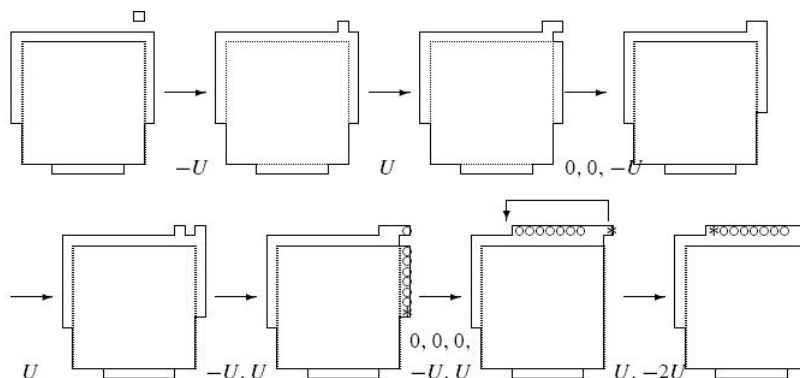
$$C^G = \cup_{\hat{\eta} \in D} C^G(\hat{\eta}), \quad C^B = \cup_{\hat{\eta} \in D} C^B(\hat{\eta}) \quad (4.75)$$

The next proposition shows that when we reach C^G we have made it "over the hill", while when we reach C^B we have not.

Proposition 4.24. (i) If $\eta \in C^G$, then there exists an $\omega : \eta \rightarrow \underline{1}$ such that $\max_{\varepsilon \in \omega} H(\varepsilon) < \Gamma_i^*$.

(ii) If $\eta \in C^B$, then there are no $\omega : \eta \rightarrow \underline{0}$ or $\omega : \eta \rightarrow \underline{1}$ such that $\max_{\varepsilon \in \omega} H(\varepsilon) < \Gamma_i^*$.

Proof. (i) If $\eta \in C^G$, then its energy is either $\Gamma_i^* - 2U$ or $\Gamma_i^* - U$, depending on whether the particle was attached in a corner or as a 1-protuberance. In the latter case we can move the particle at no cost into a corner and gain an extra $-U$. After that it is possible to create a new particle and re-attach it, which leads to energy $\Gamma_i^* - 2U - (2U - \Delta)$. We can continue in this way, filling up all rows in $\partial^- CR(\eta)$, until we reach either an $l_c \times l_c$ square or an $(l_c - 1) \times (l_c + 1)$ rectangle, depending on whether arose from $\hat{D}$ or $\bar{D}$ (recall Fig. 4.5). In the first case we can proceed along the reference path for the nucleation constructed in the proof of proposition 4.16. In the latter case, however, we can connect to this reference path as follows. The energy of the $(l_c - 1) \times (l_c + 1)$ rectangle is $\Gamma_i^* - 2U - (2U - \Delta)(l_c - 3)$. This is lower than $\Gamma_i^* - \Delta$, because $l_c \geq 3$. Create a particle, which costs Δ , and attach it to one of the longest sides of the rectangle, which pays U . Now slide particles along the corner of the rectangle, following the mechanism described in Figs. 4.9 and 10, until an $l_c \times l_c$ square is reached.

Figure 4.14: An example of a path from C^B to $\underline{1}$.

This costs U and keeps the energy below Γ_i^* . From there again proceed along the reference path for the nucleation.

If $\eta \in C^B$, then $H(\eta) = \Gamma_i^* - U$, so as long as the energy stays below Γ_i^* it is impossible to create a new particle before further lowering the energy. But there are no moves available to lower the energy. The only moves available are those where the particle that was last attached is moving along the side or is detached again, which brings us back to C^* , or those starting a motion of particles along the border of the droplet (as in Fig. 4.9), which may or may not bring us back to C^* . In both cases the cost is U and the energy returns to Γ_i^* . $\square$

An example of a path from C^B to $\underline{1}$ that does not return to C^* is obtained as follows (see Fig. 4.14). Suppose that $\hat{\eta} \in D$ is such that one bar completes one side of $\partial^- CR(\eta)$, and suppose that the free particle attaches itself on top of that bar, forming a 1-protuberance. Then the energy is $\Gamma_i^* - U$. Slide this bar to the end of the side it is attached to (at cost and gain U) and slide the two bars on the neighboring sides to the end as well (at cost and gain U). Then the energy is again $\Gamma_i^* - U$. Now move the shorter bar on top of the longer bar via a motion as in Fig. 4.9. When the last particle of the bar is moved, it can be detached (at cost U) and re-attached (at gain $2U$). Then the energy is $\Gamma_i^* - 2U$. Now create a free particle (at cost Δ), move it to the droplet (at cost 0), and attach it in a corner of the droplet (at gain $2U$). Continue downhill in this way, adding on successive rows as in the reference path that was used above, until $\underline{1}$ is reached.

proposition 4.24 (ii) shows that the configurations in C^B are wells, i.e., their energy is $< \Gamma_i^*$, but to move to either $\underline{0}$ or $\underline{1}$ the energy must return to Γ_i^* . The configurations of the form "quasi-square plus dimer" described in (ii) in the proof of proposition 4.21 are elements of $S(\underline{0}, \underline{1})$ but not of C^* . Indeed, the only possible move at zero cost is the one where the free particle jumps back to the quasi-square. Thus, we see that

- C^* is a union of plateaus, index by $\hat{\eta} \in D$; each plateau consists of a protocritical droplet $\hat{\eta}$ and a collection of positions of the free particle,

indexed by $\Lambda \setminus (\hat{\eta} \cup \partial^+ \hat{\eta})$; each plateau has *wells* and *dead-ends* when the free particle is close to the protocritical droplet.

This property is special for Kawasaki dynamics. We will not attempt to describe the wells and dead-ends in full detail. For our sharp asymptotics of the average nucleation time we will not need this detail.

4.6.3 Graph structure of the energy landscape

Let us summarize what we have shown so far:

Proposition 4.25. *View $\mathcal{X}$ as a graph whose vertices are configurations and whose edges connect communicating configurations. Let*

- $\mathcal{X}^*$ be the subgraph of $\mathcal{X}$ obtained by removing all vertices η with $H(\eta) > \Gamma_i^*$ and all edges incident to these vertices;
- $\mathcal{X}^{**}$ be the subgraph of $\mathcal{X}^*$ obtained by removing all vertices η with $H(\eta) = \Gamma_i^*$ and all edges incident to these vertices;
- $\mathcal{X}_{\underline{0}}$ and $\mathcal{X}_{\underline{1}}$ be the connected components of $\mathcal{X}^{**}$ containing $\underline{0}$ and $\underline{1}$, respectively.

Then

- (i) $\mathcal{X}_{\underline{0}} \neq \mathcal{X}_{\underline{1}}$, and so $\mathcal{X}_{\underline{0}}$ and $\mathcal{X}_{\underline{1}}$ are disconnected in $\mathcal{X}^{**}$.
- (ii) $D \subseteq \mathcal{X}_{\underline{0}}$, $C^G \subseteq \mathcal{X}_{\underline{1}}$, $C^B \subseteq \mathcal{X}^{**} \setminus (\mathcal{X}_{\underline{0}} \cup \mathcal{X}_{\underline{1}})$.

4.6.4 Two global geometric facts

In sections 4.6.2 and 4.6.3 we have analysed the geometry of the configurations on and incident to C^* that are relevant for the nucleation. This will be sufficient for the computation of the average nucleation time. To make full use of the results of Bovier, Eckhoff, Gaynard, and Klein [12], we must establish two further facts, both concerning the global geometry of the energy landscape.

Proposition 4.18 below shows that there are no valleys in the energy landscape whose depth equals or exceeds the communication height between $\underline{0}, \underline{1}$.

Proposition 4.26. *For all $\eta \in \mathcal{X} \setminus \{\underline{0}, \underline{1}\}$*

$$\Phi(\eta, \{\underline{0}, \underline{1}\}) - H(\eta) < \Gamma_i^* = \Phi(\underline{0}, \underline{1}) \quad (4.76)$$

Proof. This is the analogue of proposition 4.18 in den Hollander, Nardi, Olivieri, and Scoppola [28] for three dimensions. The proof can be carried over to two dimensions verbatim. $\square$

Proposition 4.27 below shows that $\underline{0}$ is a proper metastable configuration because it lies at the bottom of its valley.

Proposition 4.27. *If $\eta \in \mathcal{X} \setminus \underline{0}$ is such that*

$$\Phi(\eta, \underline{0}) \leq \Phi(\eta, \underline{1}), \quad (4.77)$$

then

$$H(\eta) > 0.$$

Proof. Recall that $n_c = l_c(l_c - 1) + 1$. Define

$$\mathcal{V}_{\leq n_c} = \cup_{0 \leq n \leq n_c} \mathcal{V}_n \quad , \quad \mathcal{V}_{> n_c} = \mathcal{X} \setminus \mathcal{V}_{\leq n_c}. \quad (4.78)$$

First, we claim that if η satisfies (4.77) and $H(\eta) \leq 0$, then $\eta \in \mathcal{V}_{\leq n_c}$. Indeed, since $\Phi(\eta, \{\underline{0}, \underline{1}\}) = \Phi(\eta, \underline{0}) \wedge \Phi(\eta, \underline{1})$, it follows from (4.77), and (4.78) that $\Phi(\eta, \underline{0}) < \Gamma_i^* + H(\eta)$. So, if $H(\eta) \leq 0$, then $\Phi(\eta, \underline{0}) < \Gamma_i^*$. But in the proof of proposition 4.16 (i), we have shown that $\Phi(\eta, \underline{0}) \geq \Gamma_i^*$ for all $\eta \in \mathcal{V}_{> n_c}$ (n_c is the volume of the clusters in D).

Second, we claim that $\underline{0}$ is the only configuration in $\mathcal{V}_{\leq n_c}$ with zero energy, while all other configurations have strictly positive energy. Indeed, inserting the isoperimetric inequality

$$|\eta \cap \Lambda_0| \leq \left(\frac{\gamma(\eta)}{4} \right)^2 \quad \forall \eta \neq \mathcal{X} \setminus \underline{0} \quad (4.79)$$

into (4.57), we get

$$\begin{aligned} H(\eta) &\geq \frac{U}{2} |\gamma(\eta)| - (2U - \Delta) |\eta \cap \Lambda_0| \\ &\geq \frac{U}{2} 4 \sqrt{|\eta \cap \Lambda_0|} - (2U - \Delta) |\eta \cap \Lambda_0| \\ &= (2U - \Delta) \sqrt{|\eta \cap \Lambda_0|} \left(2 \frac{U}{2U - \Delta} - (|\eta \cap \Lambda_0|)^{\frac{1}{2}} \right) \\ &> (2U - \Delta) \sqrt{|\eta \cap \Lambda_0|} (2(l_c - 1) - (l_c(l_c - 1) + 1)^{\frac{1}{2}}) \\ &> (2U - \Delta) \sqrt{|\eta \cap \Lambda_0|} (l_c - 1) > 0. \end{aligned} \quad (4.80)$$

□

Chapter 5

Metastability for lattice gas model under Kawasaki dynamics: Weak Anisotropy

In this chapter we discuss results of [48] where the authors analyze metastability and nucleation in the context of a local version of the Kawasaki dynamics for the two-dimensional anisotropic Ising lattice gas at very low temperature. Let $\Lambda \subset \mathbb{Z}^2$ be a sufficiently large finite box. Particles perform simple exclusion on Λ , but when they occupy neighboring sites they feel a binding energy $-U_1 < 0$ in the horizontal direction and $-U_2 < 0$ in the vertical direction; we assume $U_1 \geq U_2$, and condition of weak anisotropy, i.e., $0 < \epsilon \ll U_2$ and $U_2 < U_1 < 2U_2 - 2\epsilon$. Along each bond touching the boundary of Λ from the outside, particles are created with rate $\rho = e^{-\Delta\beta}$ and are annihilated with rate 1, where β is the inverse temperature and $\Delta > 0$ is an activity parameter. Thus, the boundary of Λ plays the role of an infinite gas reservoir with density ρ . We take $\Delta \in (U_1, U_1 + U_2)$ where the totally empty (full) configuration can be naturally associated to metastability (stability). The authors assuming weak anisotropy investigate how the transition from empty to full takes place under the dynamics. In particular, the authors identify the size and some characteristics of the shape of the critical droplet and the time of its creation in the limit as $\beta \rightarrow \infty$. In both case the authors find that Wulff shape is not relevant for the nucleation pattern.

5.1 Definition of the Model and Main Result

Let $\Lambda \subset \mathbb{Z}^2$ be a finite box centered at the origin that will be chosen large enough. Let $\partial^-\Lambda$ be the interior boundary of Λ and let $\Lambda_0 = \Lambda \setminus \partial^-\Lambda$ be the interior of Λ . With each $x \in \Lambda$ we associate an occupation variable $\eta(x)$, assuming values 0 or 1. A lattice configuration is denoted by $\eta \in \mathcal{X} = \{0, 1\}^\Lambda$.

We often identify η with its support, i.e. the set of occupied sites in η .

Each configuration $\eta \in \mathcal{X}$ has an energy given by the following Hamiltonian:

$$H(\eta) = -U_1 \sum_{(x,y) \in \Lambda_{0,h}^*} \eta(x)\eta(y) - U_2 \sum_{(x,y) \in \Lambda_{0,v}^*} \eta(x)\eta(y) + \Delta \sum_{x \in \Lambda} \eta(x) \quad (5.1)$$

where $\Lambda_{0,h}^*$ (resp. $\Lambda_{0,v}^*$) is the set of the horizontal (vertical) un-oriented bonds joining n.n. points in Λ_0 . Thus the interaction is acting only inside Λ_0 ; the binding energy associated to a horizontal (vertical) bond is $-U_1 < 0$ ($-U_2 < 0$). We can suppose without loss of generality that $U_1 \geq U_2$. (Note that $H - \Delta \sum_{x \in \partial^- \Lambda} \eta(x)$ can be viewed as the Hamiltonian, in lattice gas variables, for an Ising system enclosed in Λ_0 , with 0 boundary conditions.) See the local Kawasaki dynamics in chapter 4 (Kawasaki Dynamics).

5.1.1 Clusters, projections, and vacancies

Next we introduce a geometric description of the configurations in terms of contours. Recall the definitions 4.11 and 4.39.

Given a configuration $\eta \in \mathcal{X}$, consider the set $C(\eta_{cl}) \subset R^2$ defined as the union of the 1×1 closed squares centered at the occupied sites of η_{cl} in Λ_0 . The maximal connected components $C_1, \dots, C_m$ ($m \in N$) of $C(\eta_{cl})$ are called clusters of η . There is a one-to-one correspondence between configurations $\eta_{cl} \subset \Lambda_0$ and sets $C(\eta_{cl})$. A configuration $\eta \in \mathcal{X}$ is characterized by a set $C(\eta_{cl})$, depending only on $\eta \cap \Lambda_0$, plus possibly a set of free particles in $\partial^- \Lambda$ and in Λ_0 . We are actually identifying three different objects: $\eta \in \mathcal{X}$, its support ($\text{supp}(\eta) \subset \Lambda$), and the pair $(C(\eta_{cl}), \eta_{fp})$; we write $x \in \mathcal{X}$ to indicate that η has a particle at $x \in \Lambda$.

For $\eta \in \mathcal{X}$, let $|\eta|$ be the number of particles in η , $\gamma(\eta)$ the Euclidean boundary of $C(\eta_{cl})$, $\gamma(\eta) = \partial C(\eta_{cl})$; we denote by $g_1(\eta)$ ($g_2(\eta)$) one half of the horizontal (vertical) length of $\gamma(\eta)$, i.e., one half of the number of horizontal (vertical) broken bonds in η_{cl} . Then the energy associated with η is given by

$$H(\eta) = -(U_1 + U_2 - \Delta)|\eta_{cl}| + U_1 g_2(\eta) + U_2 g_1(\eta) + \Delta |\eta_{fp}|. \quad (5.2)$$

The maximal connected components of $\partial C(\eta_{cl})$ are called *contours* of η .

Let $p_1(\eta)$ and $p_2(\eta)$ be the total lengths of horizontal and vertical projections of $C(\eta_{cl})$, respectively. More precisely let $r_{j,1} = \{x \in \mathcal{Z}_2 : (x)_1 = j\}$ be the j th column and $r_{j,2} = \{x \in \mathcal{Z}_2 : (x)_2 = j\}$ be the j th row, where $(x)_1$ or $(x)_2$ denote the first or second component of x . We say that a line $r_{j,1}$ ($r_{j,2}$) is active if $r_{j,1} \cap C(\eta_{cl}) \neq \emptyset$ ($r_{j,2} \cap C(\eta_{cl}) \neq \emptyset$).

$$\pi_1(\eta) = \{j \in \mathcal{Z} : r_{j,1} \cap C(\eta_{cl}) \neq \emptyset\} \quad (5.3)$$

and $p_1(\eta) := |\pi_1(\eta)|$. In a similar way we define the vertical projection $\pi_2(\eta)$ and $p_2(\eta)$. We also call $\pi_1(\eta)$ and $\pi_2(\eta)$ the horizontal and vertical shadows of η_{cl} , respectively.

Note that $g_1, g_2, \pi_1, \pi_2, p_1, p_2$ are actually depending on η only through η_{cl} , even though, for notational convenience, we omit the subscript cl in their functional dependence.

Note that η_{cl} is not necessarily a connected set and so both the horizontal and vertical projections $\pi_1(\eta)$, $\pi_2(\eta)$ are not in general connected. We have obviously:

$$g'_i(\eta) := g_i(\eta) - p_i(\eta) \geq 0. \quad (5.4)$$

A single cluster C is called monotonic if $g_i(C) = p_i(C)$ for $i = 1, 2$, i.e., g_1 and g_2 equal, respectively, the horizontal and vertical side lengths of the rectangle $R(C)$ circumscribed to the unique cluster C . More generally, we call monotonic a configuration such that $g_i(\eta) = p_i(\eta)$ for $i = 1, 2$.

We write

$$\begin{aligned} s(\eta) &:= p_1(\eta) + p_2(\eta), \\ v(\eta) &:= p_1(\eta)p_2(\eta) - |\eta_{cl}|, \\ n(\eta) &= |\eta_{fp}|. \end{aligned} \quad (5.5)$$

Note that $s(\eta)$ coincides with the semi-perimeter if η is a configuration with a single monotonic cluster. It is immediate to show that $v(\eta)$ is a non-negative integer and that it is equal to zero if η_{cl} has a unique rectangular cluster with semi-perimeter $s(\eta)$; it represents the number of vacancies in η . Define:

$$P_1(\eta) = \cup_{j \in \pi_1(\eta)} r_{j,1} \quad , \quad P_2(\eta) = \cup_{j \in \pi_2(\eta)} r_{j,2} \quad (5.6)$$

the minimal unions of columns and rows, respectively, in $\mathbb{Z}^2$ containing η_{cl} . By definition we have

$$\eta_{cl} \subseteq P_1(\eta) \cap P_2(\eta) \quad (5.7)$$

where $P_1(\eta) \cap P_2(\eta)$ is, in general, the union of rectangles such that $|P_1(\eta) \cap P_2(\eta)| = p_1(\eta)p_2(\eta)$. The vacancies of are the sites in $P_1(\eta) \cap P_2(\eta) \setminus \eta_{cl}$.

Given a non-empty set $A \in \mathcal{X}$, define

$$\partial A = \{(\bar{\eta}, \eta) > 0, \bar{\eta} \in \partial^- A, \eta \in \partial^+ A, \text{ with } P(\bar{\eta}, \eta) > 0\} \quad (5.8)$$

that is the set of moves exiting from A . (Recall the definition 2.1 of *exterior and interior boundary*).

We define

$$H_{min}(\partial A) := \min_{(\bar{\eta}, \eta) \in \partial A} [H(\bar{\eta}) \vee H(\eta)] \quad (5.9)$$

and we denote by $(\partial A)_{min}$ min the subset of (∂A) where this minimum is realized:

$$(\partial A)_{min} := \{(\bar{\eta}, \eta) \in \partial A : [H(\bar{\eta}) \vee H(\eta)] = H_{min}(\partial A)\} \quad (5.10)$$

5.1.2 Standard and Domino Rectangles

We denote by $\mathcal{R}(l_1, l_2)$ the set of configurations whose single contour is a rectangle $R(l_1, l_2)$, with $l_1, l_2 \in N$. For any $\eta, \eta' \in \mathcal{R}(l_1, l_2)$ we have immediately

$$H(\eta) = H(\eta') = H(R(l_1, l_2)) = U_1 l_2 + U_2 l_1 - \epsilon l_1 l_2 \quad (5.11)$$

where

$$\epsilon := U_1 + U_2 - \Delta \quad (5.12)$$

A configuration η is *s-minimal* if it minimizes the energy in ν_s , i.e., if it belongs to $F(\nu_s)$

Let

$$\bar{l} = \lceil \frac{U_1 - U_2}{U_1 + U_2 - \Delta} \rceil, \quad (5.13)$$

where $\lceil \cdot \rceil$ denotes the integer part plus 1. For $x \in \mathcal{Z}$, $n \in \mathcal{N}$ we denote as $[x]_n$ the class $x \bmod n$ in $\mathcal{Z}_n$.

(i) Standard Rectangles.

For any $s > \bar{l} + 2$, if s has the same parity as $\bar{l}$ i.e., $[s - \bar{l}]_2 = [0]_2$, then we define the set of 0-standard rectangles as $R^{0-st}(s) = R(l_1(s), l_2(s))$ with $l_1(s) - l_2(s) = \bar{l}$, i.e., the set of rectangles with sides

$$l_1(s) = \frac{s + \bar{l}}{2}, \quad l_2(s) = \frac{s - \bar{l}}{2}, \quad [s - \bar{l}]_2 = [0]_2 \quad (5.14)$$

If s has the same parity as $\bar{l} - 1$ i.e., $[s - \bar{l}]_2 = [1]_2$, we define the set of 1-standard rectangles as $R^{1-st}(s) = R(l_1(s), l_2(s))$ with $l_1(s) - l_2(s) = \bar{l} - 1$, i.e., the rectangles with side length

$$l_1(s) = \frac{s + \bar{l} - 1}{2}, \quad l_2(s) = \frac{s - \bar{l} + 1}{2}, \quad [s - \bar{l}]_2 = [1]_2 \quad (5.15)$$

and for this value of s we call quasi standard and denote by $R^{q-st}(s)$, the rectangles.

We set

$$R^{st}(s) = \begin{cases} R^{0-st}(s) & \text{if } [s - \bar{l}]_2 = [0]_2 \\ R^{1-st}(s) & \text{if } [s - \bar{l}]_2 = [1]_2 \end{cases} \quad (5.16)$$

(ii) Domino and quasi domino rectangles.

Let $2 \leq l_2 \leq \bar{l}$. A rectangle $R(l_1, l_2)$ with $l_1 = 2l_2$ is called 0-domino whereas one with $l_1 = 2l_2 - 3$ is called 0quasi-domino. In both cases $s = l_1 + l_2$ is such that $[s]_3 = [0]_3$. We denote by $R^{0-dom}(s)$, ($R^{0q-dom}(s)$) the set of 0-domino rectangles (0-quasi-domino rectangles) with semi-perimeter s .

Similarly a rectangle $R(l_1, l_2)$ with $l_1 = 2l_2 - 2$ is called 1-domino and one with $l_1 = 2l_2 + 1$ called 1quasi-domino. In both cases the semi-perimeter s is such that $[s]_3 = [1]_3$. The sets of these rectangles are denoted by $R^{1-dom}(s)$ and $R^{1q-dom}(s)$, respectively.

A rectangle $R(l_1, l_2)$ with $l_1 = 2l_2 - 1$ is called 2-domino. In this case $[s]_3 = [2]_3$, and the set of these rectangles is denoted by $R^{2-dom}(s)$.

As it will be clear in section 5.2; we do not need to introduce 2quasi-domino rectangles (see Fig. 5.7). Note that for each $s \in [4, 3l]$ there exists n -domino rectangles with n such that $[s]_3 = [n]_3$. If s is such that $n = 1, 0$ then there exists also a n -quasi-domino rectangle.

5.1.3 Main Results for transition time

Let

$$\underline{0} = \{\eta \in \mathcal{X} : \eta(x) = 0 \ \forall x \in \Lambda\} \quad (5.17)$$

be the configuration with Λ empty and

$$\underline{1} = \{\eta \in \mathcal{X} : \eta(x) = 1 \ \forall x \in \Lambda_0, \ \eta(x) = 0 \ \forall x \in \Lambda \setminus \Lambda_0\} \quad (5.18)$$

be the configuration with Λ_0 full and $\Lambda \setminus \Lambda_0$ empty.

$$\begin{aligned} \Gamma_{wa} &:= \Phi(\underline{1}, \underline{0}) - H(\underline{0}) = H(\mathcal{P}_{wa}) - H(\underline{0}) = \\ U_1 l_2^* + U_2 (l_1^* - 1) - (U_1 + U_2 - \Delta) l_2^* (l_1^* - 1) + 2\Delta - U_1 \end{aligned} \quad (5.19)$$

Recall the definition of transition time $\tau_{\underline{1}}$ from chapter 3.

Weak Anisotropy conditions

As discussed heuristically in section 5.2, the behavior of the model strongly depends on the different values of the parameters. In this chapter we will consider the case of weak anisotropy. We will assume:

$$0 < \epsilon \ll U_2 \text{ and } U_2 < U_1 < 2U_2 - 2\epsilon \quad (5.20)$$

where $\ll$ means sufficiently smaller; for instance $\epsilon \leq U_2/100$ is enough. Note that this is not a significant restriction since the case of large values of the critical sizes l_1^* , l_2^* is the relevant case from a physical point of view. The isotropic case $U_1 = U_2$ has been already treated in refs. [32], [36] and chapter 4.

The main results about the asymptotic of the tunneling time and the gate to stability are contained in the following:

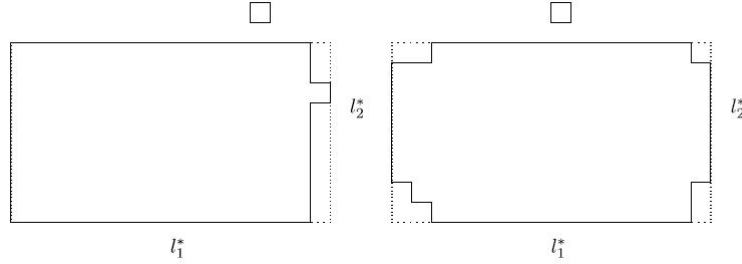
Theorem 5.1. (*Nardi, Olivieri, and Scoppola*). *Let U_1, U_2, Δ be such that $U_2/(U_1 + U_2 - \Delta)$ is not integer and (5.20) holds. Let Λ be a box with side $L + 2$. For L sufficiently large and for any $\delta > 0$,*

$$\lim_{\beta \rightarrow \infty} P_{\underline{0}}(e^{\beta(\Gamma_{wa} - \delta)} \leq \tau_{\underline{1}} \leq e^{\beta(\Gamma_{wa} + \delta)}) = 1 \quad (5.21)$$

$$\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \log E_{\underline{0}} \tau_{\underline{1}} = \Gamma_{wa}, \quad (5.22)$$

and moreover if we define $T_\beta := \inf\{n \geq 1 : P_{\underline{0}}(\tau_{\underline{1}} \leq n) \geq 1 - e^{-1}\}$ then,

$$\lim_{\beta \rightarrow \infty} P_{\underline{0}}(\tau_{\underline{1}} > tT_\beta) = e^{-t} \quad (5.23)$$

Figure 5.1: Configurations in $\mathcal{P}_{wa}$

and

$$\lim_{\beta \rightarrow \infty} \frac{E_0(\tau_1)}{T_\beta} = 1. \quad (5.24)$$

Theorem 5.1, and equation(5.21): For $\beta \rightarrow \infty$ the nucleation time from $\underline{0}$ to $\underline{1}$ behaves asymptotically, in probability, as $\Gamma_{wa}\beta + o(\beta)$.

Theorem 5.1, equations (5.22) and (5.23) : The nucleation time from $\underline{0}$ to $\underline{1}$ has mean value asymptotically given, for large β , by $e^{\Gamma_{wa}\beta}$ and its distribution, after a suitable re scaling, is asymptotically exponential.

5.1.4 Main Results for the Gate

We write

$$l_1^* = \lceil \frac{U_1}{U_1 + U_2 - \Delta} \rceil, l_2^* = \lceil \frac{U_2}{U_1 + U_2 - \Delta} \rceil \quad (5.25)$$

$$s^* = l_1^* + l_2^* - 1, \quad (5.26)$$

and

$$\mathcal{P}_{wa} := \{ \eta : n(\eta) = 1, v(\eta) = l_2(s^*) - 1, \eta_{cl} \text{ is connected} \\ \text{circumscribed rectangle in } R(l_1(s^*) + 1, l_2(s^*)) \} \quad (5.27)$$

with $l_i(s)$, $i = 1, 2$ defined as in (5.25) (recall (5.13)). See Fig. 5.1 for an example of configuration in $\mathcal{P}_{wa}$. From (5.50), it follows that $H(\eta)$ is constant on $\mathcal{P}_{wa}$.

Theorem 5.2. (Nardi, Olivieri, and Scoppola). *Let U_1, U_2, Δ be such that $U_2/(U_1 + U_2 - \Delta)$ is not integer and (5.20) holds. Let Λ be a box with side $L + 2$. For L sufficiently large,*

$$\lim_{\beta \rightarrow \infty} P_{\underline{0}}(\theta_{\underline{0}, \underline{1}} < \theta_{\underline{0}, \mathcal{P}_{wa}, \underline{1}} < \tau_{\underline{1}}) = 1. \quad (5.28)$$

Theorem 5.2: The set $\mathcal{P}_{wa}$ is a gate for the nucleation: all paths from the metastable state $\underline{0}$ to the stable state $\underline{1}$ pass through this set with a probability tending to 1 as $\beta \rightarrow \infty$. Note that we do not establish in this theorem the minimality of the gate $\mathcal{P}_{wa}$ (see definition above), which would involve a much more detailed analysis.

Theorem 5.3. (Nardi, Olivieri, and Scoppola). *Let U_1, U_2, Δ be such that $U_2/(U_1 + U_2 - \Delta)$ is not integer and (5.20) holds. Let Λ be a box with side $L + 2$ and let $\mathcal{R}^{\leq(l_1, l_2)} \mathcal{R}^{\geq(l_1, l_2)}$ be the set of configurations whose single contour is a rectangle contained in (containing) a rectangle with sides l_1, l_2 . Then, for L sufficiently large,*

$$\begin{aligned} \text{if } \eta \in \mathcal{R}^{\leq(l_1^* - 1, l_2^* - 1)} &\implies \lim_{\beta \rightarrow \infty} P_\eta(\tau_{\underline{0}} < \tau_{\underline{1}}) = 1, \\ \text{if } \eta \in \mathcal{R}^{\geq(l_1^*, l_2^*)} &\implies \lim_{\beta \rightarrow \infty} P_\eta(\tau_{\underline{1}} < \tau_{\underline{0}}) = 1. \end{aligned} \quad (5.29)$$

Theorem 5.3: l_1^* and l_2^* are the critical sizes, i.e., sub-critical rectangles shrink to $\underline{0}$, super-critical rectangles grow to $\underline{1}$.

5.2 Heuristics

5.2.1 Metastability: Static Heuristics

We will consider the regime

$$\Delta \in (U_1, U_1 + U_2), \quad \beta \rightarrow \infty, \quad (5.30)$$

which corresponds to a metastable behavior. This is the analogue of the non-conservative case discussed in [40]. In the grand-canonical Gibbs measure the configuration can be represented in terms of spin variables. Indeed, after we make the substitution $\eta(x) = (1 + \sigma(x))/2$ in (5.1), where $\sigma(x) \in \{1, +1\}$ is the spin variable, we can write

$$\begin{aligned} H^{spin}(\sigma) &= -U_1 \sum_{(x,y) \in \Lambda_{0,h}^*} \frac{1 + \sigma(x)}{2} \frac{1 + \sigma(y)}{2} \\ &\quad - U_2 \sum_{(x,y) \in \Lambda_{0,v}^*} \frac{1 + \sigma(x)}{2} \frac{1 + \sigma(y)}{2} - \Delta \sum_{(x,y) \in \Lambda_0} \frac{1 + \sigma(x)}{2} \\ &= -\frac{U_1}{4} \sum_{(x,y) \in \Lambda_{0,h}^*} \sigma(x)\sigma(y) - \frac{U_2}{4} \sum_{(x,y) \in \Lambda_{0,v}^*} \sigma(x)\sigma(y) \\ &\quad - \left(\frac{U_1 + U_2 - \Delta}{2} \right) \sum_{(x,y) \in \Lambda_0} \sigma(x) + c_1 \end{aligned} \quad (5.31)$$

where c_1 is a constant. Then we have a spin Hamiltonian for anisotropic Ising model (see [40]) with pair interaction $J_1 = U_1/2$, $J_2 = U_2/2$ and magnetic field $h = U_1 + U_2 - \Delta$.

The metastable behavior for the non-conservative case in the spin language occurs when $h \in (0, J_1 + J_2)$, this corresponds to $\Delta \in ((U_1 + U_2)/2, U_1 + U_2)$. The magnetic field vanishes when $\Delta = U_1 + U_2$, which corresponds to the condensation point of the lattice gas. Indeed at this point the density of liquid and gas phase are

$$\rho_1(\beta) = \frac{1 + m^*(\beta)}{2} \quad \rho_g(\beta) = \frac{1 - m^*(\beta)}{2} \quad (5.32)$$

where $m^*(\beta)$ is the spontaneous magnetization. A perturbative argument based on low-temperature expansion, shows that

$$1 - m^*(\beta) = 2e^{-2(J_1+J_2)\beta}(1 + o(1)), \text{ as } \beta \rightarrow \infty \quad (5.33)$$

Indeed $2(J_1 + J_2)$ represents the formation energy of a unit square droplet for $h = 0$. This, via the identification $J_1 = U_1/2$, $J_2 = U_2/2$, shows that

$$\rho_g(\beta) = e^{-(U_1+U_2)\beta}[1 + o(1)] \text{ as } \beta \rightarrow \infty \quad (5.34)$$

This can be identified as the density of the saturated vapor (in the sense of logarithmic equivalence in β). Suppose that we slightly increase the density, avoiding however the appearance of liquid droplets. We can describe this situation by means of the so-called restricted ensemble (see [28]), namely, the gran-canonical Gibbs measure restricted to a suitable subset of configurations, for instance, where all sufficiently large clusters are suppressed. At low temperature this supersaturated vapor will stay rarefied, so it can be described as pure gas phase with strong mixing properties.

Let us make a rough calculation of the probability to see an $l_1 \times l_2$ droplet of occupied sites centered at the origin. Under restricted ensemble, which we denote by μ^* , we have

$$\mu^*(l_1 \times l_2 \text{droplet}) \simeq \rho^{l_1 l_2} e^{(-U_1+U_2)\beta l_1 l_2 - \beta U_1 l_2 - \beta U_2 l_1} \quad (5.35)$$

since ρ is close to the probability to find a particle at a given site and U_1 (resp. U_2) is the binding energy between particles at the neighboring horizontal (resp. vertical) sites. Writing $\rho = e^{-\Delta\beta}$ we obtain

$$\mu^*(l_1 \times l_2 \text{droplet}) \simeq e^{-\beta[(\Delta - U_1 - U_2)l_1 l_2 + U_1 l_2 + U_2 l_1]} \quad (5.36)$$

where the exponent has a saddle point at

$$l_1 = \frac{U_1}{U_1 + U_2 - \Delta}, \quad l_2 = \frac{U_2}{U_1 + U_2 - \Delta}, \quad (5.37)$$

This means that droplets with side length $l_1 < l_1^*$ and $l_2 < l_2^*$ have a probability that decreases in l_1, l_2 and droplets with side length $(l_1, l_2) \geq (l_1^*, l_2^*)$ a probability that increases in l_1, l_2 . This would leave to the conclusion that l_1^*, l_2^* are the side length of the critical droplet; this is known to be false under Glauber dynamics (see [40]). This shows how naive is a pure static argumentation. Indeed the dynamical mechanism for the transition between rectangular droplets have an influence in establishing the tendency to grow or shrink of the clusters.

The choice $\Delta \in (U_1, U_1 + U_2)$ corresponds to $(l_1^*, l_2^*) \in (1, \infty) \times (1, \infty)$, i.e. to a non-trivial critical droplet size. In physical terms, $\Delta \in (0, U_1)$ represents the unstable gas, $\Delta \in (U_1, U_1 + U_2)$ the metastable gas, $\Delta = U_1 + U_2$ the condensation point, and $\Delta \in (U_1 + U_2, \infty)$ the stable gas. The most interesting part of the metastable regime is $0 < \epsilon \ll U_2$ with $\epsilon = U_1 + U_2 - \Delta$, which corresponds to both l_1^* and l_2^* very large.

5.2.2 Dynamic Heuristics

What follows is a heuristic discussion aimed to characterize the nucleation pattern. As we said in section 5.1 the locally conservative character of our dynamics makes difficult to determine, on rigorous grounds, the tube of typical trajectories realizing the transition from metastability to stability. However, we think that our heuristic arguments are quite convincing but, for a full proof, some more effort is needed.

Key transitions

We start with a coarse graining description: we will restrict ourselves to determine the sequence of rectangles visited by typical trajectories. This is justified since, starting from any configuration, the process will relatively fast go to a rectangle and subsequently it will stay for a long period inside a cycle that plays the role of a generalized basin of attraction of this rectangle. The full tube should also specify the proper interpolation between contiguous rectangles. Heuristic discussion will also include some information about these interpolations.

By the continuity properties of the dynamics it is reasonable to expect that only transitions between neighboring rectangles have to be taken into consideration.

More precisely, starting from a configuration $\eta \in R(l_1, l_2)$, with $l_1, l_2 \geq 2$, the possible successive rectangles in the tube have to belong to one of the following classes: $R(l_1 + 1, l_2)$, $R(l_1, l_2 + 1)$, $R(l_1 - 1, l_2)$, $R(l_1, l_2 - 1)$, $R(l_1 - 1, l_2 + 1)$, and $R(l_1 + 1, l_2 - 1)$. So we shall consider the following transitions:

From $R(l_1, l_2)$ to $R(l_1, l_2 + 1)$, corresponding to vertical growth, that will be denominated *add row* and symbolically denoted by the arrow $\uparrow$ pointing north direction;

From $R(l_1, l_2)$ to $R(l_1 + 1, l_2)$, corresponding to horizontal growth, that will be denominated *add column* and denoted by the arrow $\rightarrow$ pointing east;

From $R(l_1, l_2)$ to $R(l_1, l_2 - 1)$, corresponding to vertical contraction, that will be denominated *remove row* and denoted by the arrow $\downarrow$ pointing south;

From $R(l_1, l_2)$ to $R(l_1 - 1, l_2)$, corresponding to horizontal contraction, that will be denominated *remove column* and denoted by the arrow $\leftarrow$ pointing west;

From $R(l_1, l_2)$ to $R(l_1 - 1, l_2 + 1)$, corresponding to a readjustment of the edges, making higher and narrower the rectangle by removing a column and simultaneously adding a row. It will be denominated *column to row* and denoted by the arrow $\nwarrow$ pointing northwest;

From $R(l_1, l_2)$ to $R(l_1 + 1, l_2 - 1)$, corresponding to a readjustment opposite to the previous one. It will be denominated *row to column* and denoted by the arrow $\searrow$ pointing southeast.

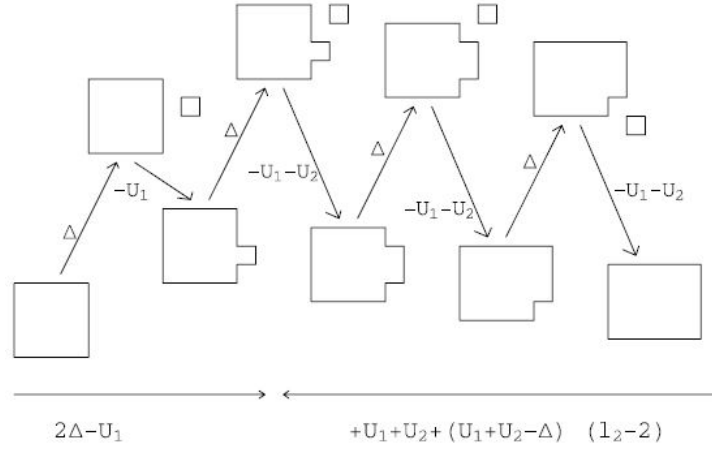


Figure 5.2: The procedure to grow a column

The transition from $R(l_1, l_2)$ to $R(l_1 - 1, l_2 - 1)$ and $R(l_1 + 1, l_2 + 1)$ are not considered as elementary since, as it can be easily seen, a suitable combination of two of the above transitions takes place with larger probability.

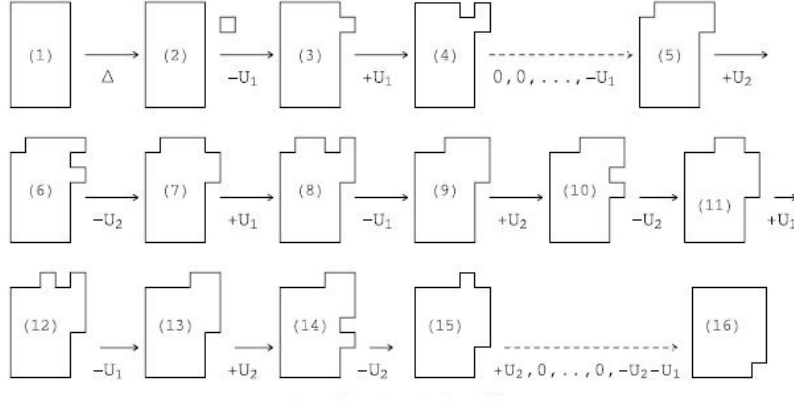
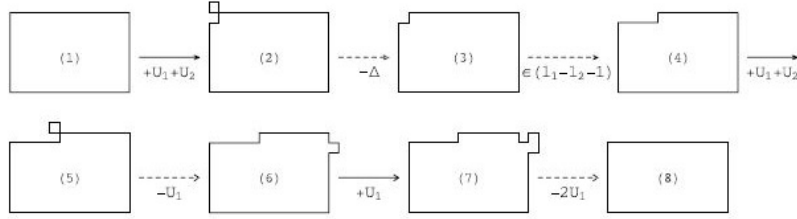
At first sight the optimal interpolation paths realizing the above transitions between contiguous rectangles are the ones depicted in Figs. 5.2-4. Let us call $\Omega^{(1)}$ the set of paths as the one depicted in Fig. 5.2. They are the natural candidates to realize, in an optimal way, the transition $\uparrow$. For the transition $\rightarrow$ we have an analogous set of paths that we call $\Omega^{(1)}$.

Let us call B the time-reversal operator acting on finite paths; we have for $\omega = \omega_1, \dots, \omega_T$

$$B\omega = \omega', \text{ with } \omega'_i = \omega_{T+1-i}, \quad i = 1, \dots, T \quad (5.38)$$

For the transition $\downarrow$ we choose the set of paths $\Omega^{(3)}$ obtained by time reversal from the paths, analogous to the ones in $\Omega^{(1)}$, that realize the transition $R(l_1 - 1, l_2)$ to $R(l_1, l_2)$.

Similarly, for the transition $\leftarrow$ we use the set of paths $\Omega^{(4)}$ obtained by time-reversal from the paths, analogous to the ones in $\Omega^{(3)}$, that realize the transition $R(l_1, l_2 - 1)$ to $R(l_1, l_2)$. The set of paths that we consider as the optimal interpolation for the transition from $R(l_1, l_2)$ to $R(l_1 - 1, l_2 + 1)$ in the two cases $l_1 < l_2$, $l_1 \geq l_2$, are called $\Omega^{(5)}$ and $\bar{\Omega}^{(5)}$, respectively. A path in $\bar{\Omega}^{(5)}$ is represented in Fig. 5.3. where each arrow corresponds to a move and the quantities under the arrows represent the corresponding energy barriers ΔH . Dotted arrows indicate sequences of moves. The maximal energy along the path is reached in the configuration (2). A path in $\Omega^{(5)}$ is represented in Fig. 5.4 where to simplify we indicate under the dotted arrows the sum of the corresponding ΔH . Along this path the maximal energy is reached in configuration (5). In a similar way we define the optimal interpolation paths $\Omega^{(7)}$ and $\bar{\Omega}^{(7)}$ for the transition from $R(l_1, l_2)$ to $R(l_1 + 1, l_2 - 1)$. We call canonical the paths in the above sets.

Figure 5.3: A path in $\Omega^{(5)}$.Figure 5.4: A path in $\bar{\Omega}^{(5)}$.

Given (l_1, l_2) , to determine the most probable transition between $R(l_1, l_2)$ and one of the previous six contiguous rectangles, we will use the criterion of the smallest energy barrier, defined as the difference between the communication height and $H(R(l_1, l_2))$. We call *energy barrier from η to η'* along the path $= (\omega_1 = \eta, \dots, \omega_n = \eta')$ the difference between the maximal height reached along this path and $H(\eta)$. We compute the energy barriers along the canonical paths and we use them to estimate the true energy barriers. We denote by $\Delta H(\text{add row})$ the energy barrier along the paths in $\Omega^{(1)}$; similarly for the other transitions.

From Figs. 5.2-4 via easy computations, we get:

$$\Delta H(\text{add row}) = 2\Delta - U_2$$

$$\Delta H(\text{add column}) = 2\Delta - U_1$$

$$\Delta H(\text{remove row}) = \epsilon(l_1 - 2) + U_1 + U_2$$

$$\Delta H(\text{remove column}) = \epsilon(l_2 - 2) + U_1 + U_2$$

$$\Delta H(\text{row to column}) = \Delta \text{ if } l_1 < l_2$$

$$\begin{aligned}
\Delta H(\text{row to column}) &= \epsilon(l_1 - l_2) + U_1 + U_2 \text{ if } l_1 \geq l_2 \\
\Delta H(\text{column to row}) &= \Delta - U_2 + U_1 \text{ if } l_1 < l_2 \\
\Delta H(\text{column to row}) &= \Delta - U_2 + U_1 + \epsilon(l_2 - l_1 + 1) \text{ if } l_1 \geq l_2 \quad (5.39)
\end{aligned}$$

These estimated energy barriers are, of course, larger than or equal to the true ones; the equality does not hold in general, since the above canonical paths sometimes happen to be non-optimal. For example, a deeper analysis leads to the conclusion that to add a row, instead of using a path in $\bar{\Omega}^{(1)}$, it is more convenient to compose $\Omega^{(2)}$ and $\Omega^{(5)}$, resp. $\bar{\Omega}^{(5)}$, when $l_1 < l_2$, resp. $l_1 \geq l_2$.

Let us now make a comparison between the estimated energy barriers appearing in equation (5.39). For $l_1 \leq l_2$, we can easily check that $\Delta H(\text{row to column}) \leq U_1 + U_2 = \Delta + \epsilon$ is the smallest estimated energy barrier. So in the sequel we will consider only the case $l_1 > l_2$.

$U_1 < 2U_2 - \epsilon$, that we refer to as *weak anisotropy*, where, since for $l_1 > l_2$ we have:

$$\begin{aligned}
\Delta - U_2 + U_1 &< 2\Delta - U_1 < 2\Delta - U_2 \text{ and} \\
U_1 + U_2 + \Delta(l_2 - 2) &< U_1 + U_2 + \Delta(l_1 - 2), \quad (5.40)
\end{aligned}$$

we have only to compare $\Delta H(\text{column to row})$, $\Delta H(\text{remove column})$, and $\Delta H(\text{row to column})$. We have

$$\Delta H(\text{remove column}) < \Delta H(\text{column to row}) \iff l_2 \leq \bar{l}, \quad (5.41)$$

$$\Delta H(\text{remove column}) \leq \Delta H(\text{row to column}) \iff 2l_2 - 2 \leq l_1, \quad (5.42)$$

$$\Delta H(\text{row to column}) < \Delta H(\text{column to row}) \iff l_1 - l_2 \leq \bar{l} - 2, \quad (5.43)$$

Using the previous comparisons we partition the $R(l_1, l_2)$ rectangles into four sets A, B, C, D : in the set $A = \{l_2 \leq \bar{l}, l_1 > 2l_2 - 2\}$ the minimal estimated energy barrier is $\Delta H(\text{remove column})$;

In the set $B = \{l_2 > \bar{l}, l_1 > l_2 + \bar{l} - 2\} \cup \{l_1 \leq l_2\}$ the minimal estimated energy barrier is $\Delta H(\text{column to row})$;

In the set $C = \{l_1 \leq l_2 + \bar{l} - 2, l_1 < 2l_2 - 2\}$ the minimal estimated energy barrier is $\Delta H(\text{row to column})$.

In the set $D = \{l_2 \leq \bar{l}, l_1 = 2l_2 - 2\}$ we have degeneracy of the minimal estimated energy barrier: $\Delta H(\text{remove column}) = \Delta H(\text{row to column})$.

We represent $R(l_1, l_2)$ as points in $\mathcal{Z}^2$ of coordinates l_1, l_2 (representing, respectively, the horizontal and vertical edges). Emerging from any representative point, we plot the arrows corresponding to transitions with minimal ΔH between $R(l_1, l_2)$ and contiguous rectangles. In Fig. 5.5 we draw this system of arrows. Note that the multiplicity of the arrows emerging from a point, corresponding to degeneracy of the minimal ΔH , takes place only in the set D. In the figure the southeastnorthwest arrows $\nearrow \searrow$ represent the superposition of

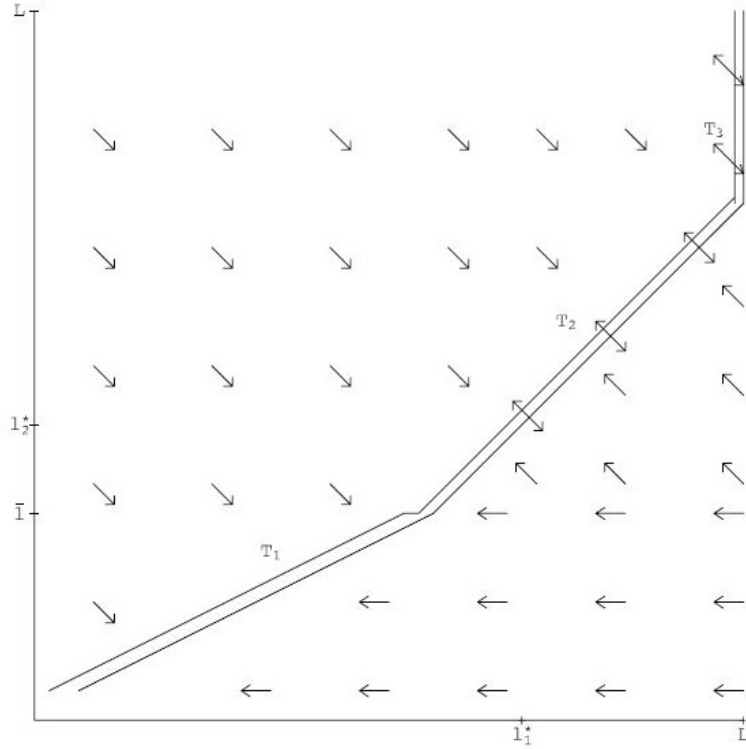


Figure 5.5: Weak anisotropy: minimal transitions and tube of typical trajectories.

two arrows $\searrow$ and $\swarrow$.

In the weak anisotropic case, from Fig. 5.5, it is evident that in the plane (l_1, l_2) there is a region T , represented in the figure, which is attractive in the sense that if we follow the oriented paths given by the sequences of arrows emerging from every point outside T we end up inside T . The region T consists of three parts: $T_1 = \{(l_1, l_2) : l_2 \leq \bar{l} \text{ and } 2l_2 - 3 \leq l_1 \leq 2l_2 - 1\}$ containing domino shape rectangles, $T_2 = \{(l_1, l_2) : l_2 > \bar{l} \text{ and } l_2 + \bar{l} - 1 \leq l_1 \leq l_2 + \bar{l}\}$ containing standard rectangles (see section 5.1.2) and $T_3 = \{(l_1, l_2) : l_1 = L \text{ and } l_2 \geq L - \bar{l}\}$.

Let us now consider the arrows inside the region T . From each $\eta \in T_1$, with $l_1 = 2l_2 - 2$, as a consequence of the degeneracy $\Delta H(\text{remove column}) = \Delta H(\text{row to column})$, we have two exiting arrows, one pointing to $\eta' \in R(l_1 - 1, l_2)$ and the other pointing to $\eta'' \in R(l_1 + 1, l_2 - 1)$. Subsequently, starting from η' the minimal estimated ΔH is unique and it corresponds to an arrow pointing to $R(l_1, l_2 - 1)$; analogously starting from η'' the minimal ΔH is unique and it corresponds to a arrow also pointing to $R(l_1, l_2 - 1)$ (see Fig. 5.6).

In T_2 , for each value of the semi-perimeter s , there are pairs of configurations (η, η') such that the minimal among the estimated energy barriers starting from η corresponds to the transition from η to η' and conversely the

minimal estimated energy barrier from η' corresponds to the transition from η' to η . So inside T_2 there are pairs of arrows forming two-states loops that we represent as $\nwarrow \searrow$. This suggests that in T_2 a more detailed study is necessary, based on the analysis of suitable cycles containing the above described loops. These cycles represent a sort of generalized basin of attraction of the standard rectangles contained in the loops: they are the maximal cycles containing a unique standard rectangle. We do not develop in this paper the analysis of these cycles since their structure is quite complicated and they are very big especially close to the critical size (l_1^*, l_2^*) . These cycles contain, among others, rectangular configurations and in each cycle all the rectangular configurations have the same semi perimeter s , i.e., belong to the same manifold ν_s . We just make a guess on the transitions leaving these cycles through the points of minimal energy in their boundary; we draw in our picture the arrows between rectangular configurations corresponding to these most probable exits. It turns out that these arrows are horizontal pointing east if $l_2 \geq l_2^*$ and pointing west if $l_2 < l_2^*$ (see Fig. 5.6).

In both cases these horizontal arrows point to configurations which are again in the set T , so that we can iterate the argument to analyze all the arrows in T . Thus we associate to the loops $\nwarrow \searrow$ in the picture cycles containing rectangles in ν_s and transitions given by the horizontal arrows. In T_3 we can argue like in T_2 (see Fig 5.6).

It is natural at this point to distinguish two parts in the set T : the sub critical part T_{sub} corresponding to T_1 plus the part of T_2 with horizontal arrows pointing west, i.e., with $l_2 < l_2^*$ and the super critical part T_{sup} , corresponding to the configurations in T_2 with horizontal arrows pointing east, i.e., with $l_2 \geq l_2^*$ and T_3 .

Let us now summarize our heuristic discussion in the weakly anisotropic case. We expect that every rectangle outside T is attracted by T ; the configurations in T_{sub} are sub critical in the sense that they tend to shrink along T following standard or domino shape, depending on l_2 ; configurations in T_{sup} are super critical in the sense that they tend to grow following standard shapes in T_2 and a sequences of rectangles with bases $L - 1$ or L in T_3 . Moreover to every loop of arrows in T_2 we associate a permanence set containing rectangles in a given manifold ν_s . This heuristical discussion provides a description of the tube of typical nucleating path. Suppose first to consider the typical paths going from the maximal sub critical rectangle to $\emptyset$. From the discussion on the sub critical part of T_2 we have that the sequence of cycles corresponding to the loops $\nwarrow \searrow$, connected by the horizontal arrows pointing west define a coarse grained cycle path corresponding to the first part of the tube of typical trajectories going to $\emptyset$. Looking at T_1 we see that there are no loops there; we can associate to each rectangular configuration η in T_1 the maximal cycle containing η and not containing other rectangular configurations. By using the arrows of the figure we obtain, in this way, a coarse grained cycle path corresponding to the domino part of the tube. The coarse graining of these cycle paths can be resolved by introducing a suitable interpolation between rectangular configurations corresponding to each arrow in the picture, obtaining, in this way a family of true cycle paths, T_{sub} , describing the tube of typical paths going from the maximal

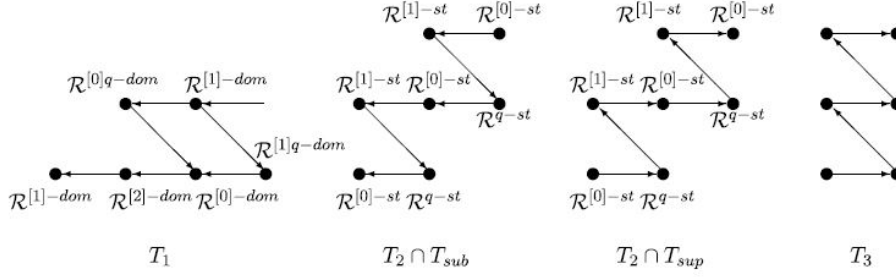


Figure 5.6: Minimal trajectories inside T_1 , T_2 with $l_2 < l_2^*$, T_2 with $l_2 \geq l_2^*$, and T_3 .

sub critical rectangle to $\underline{0}$.

A similar discussion can be applied to the study of the tube of typical paths going from the minimal super critical rectangle to $\underline{1}$ obtaining in the same way the family of cycle paths T_{sup} .

The tube of the typical nucleating paths describing the first excursion from $\underline{0}$ to $\underline{1}$, can be obtained by applying general arguments based on reversibility and by providing a suitable interpolation between the maximal sub critical rectangle and the minimal super critical one. More precisely to obtain the typical tube from $\underline{0}$ to $\underline{1}$ we apply the time reversal operator B (see (5.38)), to the tube T_{sub} and we join it to T_{sup} by means of this interpolation. These interpolations between rectangular configurations can be obtained by using the reference path ω^* described in section 5.3.2; ω^* can be considered as a representative of typical nucleation path.

Some aspects of the behavior that we have heuristically described are rigorously discussed in this paper; in particular we determine a gate $\mathcal{P}_{wa}$ for the transition between $\underline{0}$ and $\underline{1}$ (see theorem 5.2) and we give a sufficient condition to discriminate sub critical and super critical standard rectangles (see theorem 5.3).

5.3 Proof of the Theorems for the Transition time

The proofs of theorems 5.1, and 5.2 are based on the following results proved in [43] on the asymptotic of tunneling time and on the gates in the general setup of reversible Markov chains.

The following theorems are presented in chapter 2 as theorem 2.43, theorem 2.46, theorem 2.47, and theorem 2.49. We restate them here for convenience.

Theorem 5.4. *Let $\eta_0 \in \mathcal{X}^m$ and let $\bar{\Gamma}$ be the stability level of the metastable state η_0 , i.e., $\bar{\Gamma} := V_{\eta_0}$. Then, for any $\delta > 0$, there exist β_0 and $K > 0$ such*

that for any $\beta > \beta_0$

$$P_{\eta_0}(\tau_{\mathcal{X}^s} < e^{\beta(\bar{\Gamma}-\delta)}) < e^{-K\beta} \quad (5.44)$$

Moreover

$$\lim_{\beta \rightarrow \infty} \ln P_{\eta_0}(\tau_{\mathcal{X}^s} > e^{\beta(\bar{\Gamma}+\delta)}) = -\infty \quad (5.45)$$

i.e., this last probability is super-exponentially small in β .

Theorem 5.5. With η_0 and $\bar{\Gamma}$ as in the hypothesis of theorem 5.4, we have:

$$\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \log E_{\eta_0} \tau_{\mathcal{X}^s} = \bar{\Gamma}. \quad (5.46)$$

Moreover, if η_0 is the unique metastable state, $\eta_0 = \mathcal{X}^m$, and if we define $T_\beta := \inf\{n \geq 1 : P_{\eta_0}(\tau_{\mathcal{X}^s} \leq n) \geq 1 - e^{-1}\}$ then, for any $\delta > 0$,

$$\lim_{\beta \rightarrow \infty} \ln P_{\eta_0}(\tau_{\mathcal{X}^s} > tT_\beta) = e^{-t} \quad (5.47)$$

and

$$\lim_{\beta \rightarrow \infty} \frac{E_{\eta_0}(\tau_{\mathcal{X}^s})}{T_\beta} = 1 \quad (5.48)$$

Theorem 5.6. For any pair of states η, ε , for any gate $W = W(\eta, \varepsilon) \subseteq S(\eta, \varepsilon)$ for the transition $\eta \rightarrow \varepsilon$, there exists $c > 0$ such that

$$P_\eta(\tau_W > \tau_\varepsilon) \leq e^{-\beta c} \quad (5.49)$$

for sufficiently large β .

Theorems 5.1 and 5.2 are an immediate consequence of these results if we prove the following:

- (a) $H(\mathcal{P}_{wa}) =: \Gamma = \Phi(\underline{0}, \underline{1})$,
- (b) there exists $\Gamma_0 < \Gamma_{wa}$ such that $\mathcal{X}_{\Gamma_0} \subseteq \{\underline{0}, \underline{1}\}$,
- (c) $\mathcal{P}_{wa}$ is a gate for the transition $\underline{0} \rightarrow \underline{1}$.

Point (a) means that we are able to compute explicitly the communication height between $\underline{0}$ and $\underline{1}$.

Point (b) means that each configuration $\eta \notin \{\underline{0}, \underline{1}\}$ is Γ_0 -reducible i.e., we can find a configuration with smaller energy, $\eta' \in \psi_\eta$, with $\Phi(\eta, \eta') \leq H(\eta) + \Gamma_0$. In other words, there are no too deep wells in the energy landscape, no deeper than the well with bottom $\underline{0}$. We will call *reduction* this step of the proof.

To prove (a) and (c) the general strategy is to find a suitable set of states $\mathcal{B}_{wa}$ containing $\underline{0}$ and not containing $\underline{1}$ so that $\partial\mathcal{B}_{wa}$ has to be crossed by every path going from $\underline{0}$ to $\underline{1}$ (see section 5.3.3). Moreover we find a reference path $\omega^* : \underline{0} \rightarrow \underline{1}$ (see section 5.3.2) such that the maximum of the energy in ω^* is reached when crossing $\partial\mathcal{B}_{wa}$ and this maximal energy in ω^* is equal to $H_{\min}(\partial\mathcal{B}_{wa})$. As shown in section 5.3.4, these two ingredients are sufficient to

determine the communication height $(\underline{0}, \underline{1})$. Moreover by characterizing geometrically the moves producing the crossing of $\partial\mathcal{B}_{wa}$, we will obtain the gate for the transition $\underline{0} \rightarrow \underline{1}$.

In section 5.4.1, we will prove point (b) and we will also easily show that (a) and (b) imply that $\bar{\Gamma} := V_{\underline{0}} = (\underline{0}, \underline{1}) = \Gamma_{wa}$ and $\underline{0} = \mathcal{X}^m$ and $\underline{1} = \mathcal{X}^s$, if the side L of the volume Λ is large enough. Theorems 5.1, and 5.2 are therefore immediate consequences of theorem 5.4, theorem 5.5, and theorem 5.6.

In section 5.3.1 we prove a preliminary result on configurations of minimal energy at given s . The proof of theorem 5.3 is obtained in section 5.4.2.

5.3.1 Configurations of Minimal Energy at s Fixed

Lemma 5.7. *For any configuration η :*

$$H(\eta) = H(R(p_1(\eta), p_2(\eta))) + \epsilon v(\eta) + U_1 g'_2(\eta) + U_2 g'_1(\eta) + n(\eta)\Delta \quad (5.50)$$

Proof.

$$\begin{aligned} H(\eta) &= -U_1 \sum_{(x,y) \in \Lambda_1^*} \eta(x)\eta(y) - U_2 \sum_{(x,y) \in \Lambda_2^*} \eta(x)\eta(y) + \Delta \sum_{(x,y) \in \Lambda} \eta(x) \\ &= -(U_1 + U_2) \sum_{x \in \Lambda} \eta_{cl}(x) + U_1 g_2(\eta) + U_2 g_1(\eta) \\ &\quad + \Delta \sum_{x \in \Lambda} \eta_{cl}(x) + \Delta(\eta) \end{aligned} \quad (5.51)$$

by definition of $g'_1(\eta)$, $g'_2(\eta)$ this last expression is given by

$$\begin{aligned} &U_1(p_2(\eta) + g'_2(\eta)) + U_2(p_1(\eta) + g'_1(\eta)) - \epsilon|\eta_{cl}| + \Delta n(\eta) \\ &= H(R(p_1(\eta), p_2(\eta))) + \epsilon(p_1(\eta)p_2(\eta) - |\eta_{cl}|) \\ &\quad + U_1 g'_2(\eta) + U_2 g'_1(\eta) + n(\eta)\Delta \end{aligned} \quad (5.52)$$

□

We will denote by $p_{min}(\eta)$ the minimum between $p_1(\eta)$ and $p_2(\eta)$. The main property of standard rectangles is summarized by the following proposition.

Proposition 5.8. (a) *For all $s > \bar{l} + 2$ a configuration is s -minimal, i.e., it is a configuration of minimal energy in ν_s , if and only if it is a standard rectangle in $R^{st}(s)$:*

$$F(\nu_s) = R^{st}(s). \quad (5.53)$$

(b) *For all $s > \bar{l} + 2$, the configuration of minimal energy in the set*

$$A(s) := \{\eta \in \nu_s : v(\eta) \geq p_{min}(\eta) - 1\} \quad (5.54)$$

are the following

$$F(A(s)) = \{\eta \in \nu_s : v(\eta) = l_2(s-1) - 1, n(\eta) = g'_1(\eta) = g'_2(\eta) = 0\}$$

connected, with circumscribed rectangle in

$$R(l_1(s-1) + 1, l_2(s-1))\} \quad (5.55)$$

and consequently we have

$$H(F(A(s))) = H(R^{st}(s-1)) + \Delta - U_1. \quad (5.56)$$

Proof. To prove (a) we have first to prove that a configuration of minimal energy in V_s is a single rectangle without free particles; this part of the proof clearly does not require the condition $s > \bar{l} + 2$. Indeed by (5.50), since for any η the quantities $v(\eta)$, $g'_1(\eta)$, $g'_2(\eta)$, $n(\eta)$ are non-negative integers, we have that $H(\eta) \geq H(R(p_1(\eta), p_2(\eta)))$, where the identity holds only if $v(\eta) = g'_1(\eta) = g'_2(\eta) = n(\eta) = 0$. On the other side, $v(\eta) = g'_1(\eta) = g'_2(\eta) = n(\eta) = 0$ implies that η is a unique connected cluster since otherwise, either $g'_1(\eta) + g'_2(\eta) > 0$ or $(\eta) \geq p_1(\eta) \vee p_2(\eta)$. Indeed if we can decouple η into two disconnected components $\eta = \eta_0 \cup (\eta \setminus \eta_0)$ with $g_1(\eta) + g_2(\eta) = 0$, then we have that $P_1(\eta_0) \cap P_2(\eta \setminus \eta_0)$ and $P_2(\eta_0) \cap P_1(\eta \setminus \eta_0)$ are vacancies of η , so that the number of vacancies $v(\eta)$ can be estimated by

$$v(\eta) \geq |P_1(\eta_0) \cap P_2(\eta \setminus \eta_0)| + |P_2(\eta_0) \cap P_1(\eta \setminus \eta_0)| \geq p_1(\eta) \vee p_2(\eta). \quad (5.57)$$

Now if η is a unique connected cluster, since $v(\eta) = 0$, it must coincide with its circumscribed rectangle $R(p_1(\eta), p_2(\eta))$. In conclusion we have proved that $v(\eta) = g_1(\eta) = g_2(\eta) = n(\eta) = 0$ if and only if η is a unique rectangle without free particles.

We have to prove now that, to minimize the energy, the rectangular configuration must be a standard rectangle. We will write the energy of a rectangle (see (5.11)) as sum of two functions $H_1(s)$ and $H_2(d)$, where $s = l_1 + l_2$ and $d = l_1 - l_2$. So, if we substitute in (5.11) $l_1 = (s+d)/2$, $l_2 = (s-d)/2$, we have

$$H(R(l_1, l_2)) = H_1(s) + H_2(d) := [(U_1 + U_2)\frac{s}{2} - \frac{\epsilon^2}{4}] + [(U_2 - U_1)\frac{d}{2} + \frac{\epsilon}{4}d^2]. \quad (5.58)$$

Since we have to minimize the energy when s is constant we can neglect $H_1(s)$ and minimize the function $H_2(d)$. Indeed, since the difference and the sum of two integers belong to the same parity class, we have:

$$\min_{l_1, l_2 \geq 1, l_1, l_2 \in \mathcal{N}, l_1 + l_2 = s} H(R(l_1, l_2)) = H_1(s) + \min_{d \in \mathcal{Z}, |d| \leq s-2, [d]_2 = [s]_2} H_2(d). \quad (5.59)$$

As a function on $\mathcal{R}$, $H_2(d)$ has its minimum in $d_0 = (U_1 - U_2)/\epsilon$, $\bar{l} - 1 < d_0 < \bar{l}$. Moreover, its graph is a parabola symmetric w.r.t. the axis $x = d_0$, so $H_2(d) : \mathcal{N} \rightarrow \mathcal{R}$ has minimum in $d \in \{\bar{l} - 1, \bar{l}\}$ (see (5.13)). For any value of $s > \bar{l} + 2$ only one of these two values of d is acceptable, the one that has the same parity as s .

For any value of $s > \bar{l} + 2$ with $[s]_2 = [\bar{l}]_2$ we have $d = \bar{l}$ so that

$$F(V_s) = R\left(\frac{s + \bar{l}}{2}, \frac{s - \bar{l}}{2}\right) \quad (5.60)$$

and we note that $R(\frac{s + \bar{l}}{2}, \frac{s - \bar{l}}{2}) = R^{0-st}(s)$.

In the other case, for any $s > \bar{l} + 2$ with $[s]_2 \neq [\bar{l}]_2$ we have $d = \bar{l} - 1$ so that

$$F(V_s) = R\left(\frac{s + \bar{l} - 1}{2}, \frac{s - \bar{l} + 1}{2}\right) \quad (5.61)$$

we note that $R\left(\frac{s + \bar{l} - 1}{2}, \frac{s - \bar{l} + 1}{2}\right) = R^{1-st}(s)$.

This concludes the proof of part (a).

To prove (b) we first prove that a configuration of minimal energy in $A(s + 1)$ is a single connected and monotonic cluster without free particles with circumscribed rectangle $R(l_1, l_2)$ with $l_1 = p_1(\eta)$ and $l_2 = p_2(\eta)$ and $l_1 + l_2 = s + 1$ and with a number of vacancies $v(\eta) = p_{\min}(\eta) - 1$. Also in this case, this part of the proof clearly does not require the condition $s > \bar{l} + 2$. Indeed by (5.44), since for any the quantities $g'_1(\eta), g'_2(\eta), n(\eta)$ are non-negative integers and $v(\eta) \geq p_{\min}(\eta) - 1$, we have that $H(\eta) \geq H(R(p_1(\eta), p_2(\eta))) + \epsilon(p_{\min}(\eta) - 1)$, where the identity holds only if $g'_1(\eta) = g'_2(\eta) = n(\eta)$ and $v(\eta) = p_{\min}(\eta) - 1$.

But in the case $g'_1 = g'_2 = n(\eta) = 0$ and $v(\eta) = p_{\min}(\eta) - 1$, the configuration η is a single connected and monotonic cluster without free particles with circumscribed rectangle $R(l_1, l_2)$ with $l_1 = p_1(\eta)$ and $l_2 = p_2(\eta)$ and with a number of vacancies $v(\eta) = l_1 \wedge l_2 - 1$. Indeed, as shown in the proof of point (a), if η is not a unique connected cluster, either $g'_1 + g'_2 > 0$ or $v(\eta) \geq p_1(\eta) \vee p_2(\eta)$.

We have now to find the values of the projections l_1 and l_2 minimizing the energy in $A(s + 1)$. If η is such that $l_1 < l_2$ then η cannot minimize the energy in $A(s + 1)$. Indeed we have

$$\begin{aligned} H(\eta) &\geq U_1 l_2 + U_2 l_1 - \epsilon l_1 l_2 + \epsilon(l_1 - 1) \\ &> U_1 l_1 + U_2 l_2 - \epsilon l_1 l_2 + \epsilon(l_1 - 1) = H(\eta'), \end{aligned} \quad (5.62)$$

where η' is a configuration given by a rectangle with horizontal side of length $l_2 - 1$, and vertical side l_1 plus a protuberance on the vertical side, so that $p_1(\eta') + p_2(\eta') = s + 1$ and $v(\eta') = p_{\min}(\eta') - 1$.

If η is such that $l_1 \geq l_2$ then

$$H(\eta) \geq U_1 l_2 + U_2 l_1 - \epsilon(l_1 l_2 - l_2 + 1) =: \bar{H}(l_1, l_2). \quad (5.63)$$

so that

$$\min_{\eta \in A(s+1)} H(\eta) \geq \min_{l_1 + l_2 = s+1, l_1 \geq l_2 \geq 1} \bar{H}(l_1, l_2). \quad (5.64)$$

Defining the new variables $s + 1 = l_1 + l_2$ and $d = l_1 - l_2$ if we note that

$$\bar{H}(l_1, l_2) = H'_1(s + 1) + H'_2(d), \quad (5.65)$$

where

$$H'_1(s + 1) = \frac{\epsilon}{4}(s + 1)^2 + \frac{1}{2}(U_1 + U_2 + \epsilon)(s + 1) + \epsilon, \quad (5.66)$$

$$H'_2(d) = \frac{\epsilon}{4}d^2 - \frac{1}{2}(U_1 - U_2 + \epsilon)d \quad (5.67)$$

it is sufficient to find the value of d minimizing $H'_2(d)$, since

$$\min_{l_1+l_2=s+1, l_1 \geq l_2 \geq 1} \bar{H}(l_1, l_2) = H'_1(s+1) + \min_{d: [d]_2 = [s+1]_2, 0 < d \leq s-1} H'_2(d), \quad (5.68)$$

As a function on $\mathcal{R}$, $H'_2(d)$ has its minimum in $d_0 + 1 = ((U_1 - U_2)/\epsilon) + 1$. Moreover, its graph is a parabola symmetric w.r.t. the axis $x = d_0 + 1$, so $H'_2(d) : \mathcal{N} \rightarrow \mathcal{R}$ has minimum in $d = \bar{l}$ or in $d = \bar{l} + 1$. For any value of $s > \bar{l} + 2$ only one of these two values of d is acceptable, the one that has the same parity as $s + 1$.

So for any s with $[s]_2 = [\bar{l}]_2$ we have that the minimum is obtained for $d = \bar{l} + 1$, corresponding to the values $l_1 = (s + 1 + \bar{l} + 1)/2$ and $l_2 = (s + 1 - \bar{l} - 1)/2$. Note that $l_1 = ((s + l)/2) + 1 = l_1(s) + 1$ and $l_2 = (s - \bar{l})/2 = l_2(s)$. Equation (5.68) becomes

$$\begin{aligned} \min_{l_1+l_2=s+1, l_1 \geq l_2 \geq 1} \bar{H}(l_1, l_2) &= H(R(\frac{s+1+\bar{l}+1}{2}, \frac{s+1-\bar{l}-1}{2})) + \epsilon(\frac{s+1-\bar{l}-1}{2} - 1) \\ &= U_1(\frac{s-\bar{l}}{2}) + U_2(\frac{s+\bar{l}}{2}) + U_2 - \epsilon[(\frac{s-\bar{l}}{2})(\frac{s+\bar{l}}{2})] - \epsilon \\ &= H(R^{0-st}(s)) + U_2 + \epsilon = H(R^{0-st}(s)) + \Delta - U_1. \end{aligned} \quad (5.69)$$

And for any s with $[s]_2 \neq [\bar{l}]_2$ we have that the minimum is obtained for $d = \bar{l} + 1$, corresponding to the values $l_1 = (s + 1 + \bar{l})/2$ and $l_2 = (s + 1 - \bar{l})/2$. Note that $l_1 = ((s + l - 1)/2) + 1 = l_1(s) + 1$ and $l_2 = (s - \bar{l} + 1)/2 = l_2(s)$. Equation (5.68) becomes

$$\begin{aligned} \min_{l_1+l_2=s+1, l_1 \geq l_2 \geq 1} \bar{H}(l_1, l_2) &= H(R(\frac{s+1+\bar{l}}{2}, \frac{s+1-\bar{l}}{2})) + \epsilon(\frac{s+1-\bar{l}}{2} - 1) \\ &= U_1(\frac{s+1-\bar{l}}{2}) + U_2(\frac{s-1+\bar{l}}{2}) + U_2 - \epsilon[(\frac{s+1-\bar{l}}{2})(\frac{s-1+\bar{l}}{2})] - \epsilon \\ &= H(R^{1-st}(s)) + \Delta - U_1 \end{aligned} \quad (5.70)$$

that ends the proof of part (b). $\square$

5.3.2 Reference Path

We construct now a particular reference path $\omega^* : \underline{0} \rightarrow \underline{1}$ (see proof of theorems 5.1 and 5.2). It will be given by a particular sequence of growing domino and standard rectangles, such that the maximum of the energy on ω^* , $\{arg \max_{\omega^*} H\}$, is reached on particular configurations given by a rectangle $R(l_1^* - 1, l_2^*)$ with a protuberance on the shorter side and a free particle. We will prove in section 5.3.4 that $\omega^* \in (\underline{0} \rightarrow \underline{1})_{opt}$ so that $\{arg \max_{\omega^*} H\} \in S(\underline{0} \rightarrow \underline{1})$.

We want to recall here that in this paper we get only a partial solution to the problem of the determination of the tube of typical paths, i.e., the set of paths followed by the process with high probability during the transition from $\underline{0}$ to $\underline{1}$. It is easy to prove that a typical path is in the set $(\underline{0} \rightarrow \underline{1})_{opt}$. Note that

this set is much larger than the tube of typical paths; we have a lot of freedom in the construction of the reference path, especially far from its maximal energy value. However, we conjecture that the path ω^* , that we are going to construct, is not only optimal but also it suggests the structure of the tube of typical paths.

The idea of the construction of ω^* is the following: we first construct a skeleton path $\{\bar{\omega}_s\}_{s=2}^{2L}$ given by a sequence of rectangles with semi-perimeter s . For $s \leq 3\bar{l}$ these are domino rectangles (of type 0, 1, or 2) and for $s \geq 3\bar{l}$ these are standard rectangles (of types 0 or 1). Obviously $\bar{\omega}_s$ is not a path in the sense that the transition from $\bar{\omega}_s$ to $\bar{\omega}_{s+1}$ can not be given in a single step of the dynamics, since $\bar{\omega}_s$ and $\bar{\omega}_{s+1}$ are rectangles. Thus to obtain a path we have to interpolate each transition of the skeleton path $\bar{\omega}$. This is done in two different steps. We first introduce between $\bar{\omega}_s$ and $\bar{\omega}_{s+1}$ a sequence of configurations $\bar{\omega}_{s,1}, \dots, \bar{\omega}_{s,i_s}$, is given by $\bar{\omega}_s$ plus a growing row or column; again these configurations are given by a single increasing droplet. This step is non-trivial since, as explained in more detail later on, there are cases in which to grow a row we first grow a column and then we move this column to a new row with a motion along the border of the droplet. Indeed it turns out that this is more convenient from an energetic point of view and this strategy is crucial near the exit from B (see proof of theorems 5.1 and 5.2). The last interpolation, to obtain from the sequence of configurations $\bar{\omega}_{s,i}$ a path ω^* , i.e., with $P(\omega_j^*, \omega_{j+1}^*) > 0$, consists in inserting between every couple of consecutive configurations in $\bar{\omega}$ for which the cluster is increased by one particle, a sequence of configurations with a new particle initially created at the boundary of the box and then brought to the correct site with a sequence of consecutive moves of this free particle.

Skeleton: $\bar{\omega}$

Let us construct a sequence of rectangular configurations $\bar{\omega} = \{\bar{\omega}_s\}$ with $s = 0, \dots, 2L$, namely,

$$\bar{\omega}_1 = \emptyset, \quad \bar{\omega}_2 = \{x_0\}, \dots, \quad \bar{\omega}_{2L} = F(\mathcal{X}) \in \underline{1} \quad (5.71)$$

Step a. For any $s \leq 3\bar{l}$, $\{\bar{\omega}_s\}$ is a growing sequence of domino rectangles, depending on the value of s . Indeed, if $[s]_3 = [0]_3$ in $\mathcal{Z}_3$, i.e., $s = 3l_2$ for some $l_2 \leq \bar{l}$, we have $\bar{\omega}_s \in R(2l_2, l_2)$ is a 0-domino rectangle; if $[s]_3 = [1]_3$ in $\mathcal{Z}_3$, i.e., $s = 3l_2 - 2$ for some l_2 , we have $\bar{\omega}_s \in R(2l_2 - 2, l_2)$ is a 1-domino rectangle; if $[s]_3 = [2]_3$ in $\mathcal{Z}_3$, i.e., $s = 3l_2 - 1$ for some l_2 , we have $\bar{\omega}_s \in R(2l_2 - 1, l_2)$ is a 2-domino rectangle.

Step b. For $3\bar{l} \leq s \leq 2L - \bar{l}$, $\{\bar{\omega}_s\}$ is a growing sequence of standard rectangles if $[s - \bar{l}]_2 = [0]_2$ in $\mathcal{Z}_2$, i.e., $s = 2l_2 + \bar{l}$ for some $l_2 \geq \bar{l}$, we have $\bar{\omega}_s \in R(l_2 + \bar{l}, l_2)$ is a 0-standard rectangle; if $[s - \bar{l}]_2 = [1]_2$ in $\mathcal{Z}_2$, i.e., $s = 2l_2 + \bar{l} - 1$ for some $l_2 \geq \bar{l}$, we have $\bar{\omega}_s \in R(l_2 + \bar{l} - 1, l_2)$ is a 1-standard rectangle. Note that if $l_2 = \bar{l}$ the 2-domino and 1-standard shape coincide.

Step c. For $s \geq 2L - \bar{l}$, $\{\bar{\omega}_s\} \in R(L, s - L)$.

First interpolation: $\tilde{\omega}$.

Given a choice for $\bar{\omega}_s$, we can construct the path $\tilde{\omega}_{s,i}$ such that $\tilde{\omega}_{s,0} = \bar{\omega}_s$

and insert between each pair $(\tilde{\omega}_s, \tilde{\omega}_{s+1})$, $\forall s$ a sequence of configurations $\tilde{\omega}_{s,i}$ for $i = 0, 1, \dots, i_s$.

Step a.1 If $s \leq 3\bar{l}$ and $[s]_3 = [1]_3$ add a vertical column as in Fig. 5.2 passing from $\tilde{\omega}_{s,0} \in R(2l_2, l_2 + 1)$ to the 2-domino rectangle $\tilde{\omega}_{s,i_s} \in R(2l_2 + 1, l_2 + 1)$. More precisely $\tilde{\omega}_{s,1}$ is the configuration obtained creating a particle on the column (as in Fig. 5.2). We repeat this step for other $l_2 - 1$ particles that are created in the same column, so the configuration $\tilde{\omega}_{s,i_s} \in R(2l_2 + 1, l_2 + 1)$ is a 2-domino rectangle.

step a.2 If $s \leq 3\bar{l}$ and $[s]_3 = [2]_3$ add a vertical column as in Fig. 5.2 passing from $\tilde{\omega}_{s,0} \in R(2l_2 - 1, l_2)$ to $\tilde{\omega}_{s,i_s} \in R(2l_2, l_2)$ that is a 0-domino rectangle.

Step a.3 If $s \leq 3\bar{l}$ and $[s]_3 = [0]_3$ add a vertical column as in Fig. 5.2 passing from $\tilde{\omega}_{s,0} \in R(2l_2, l_2)$ to the quasi-domino rectangle $\tilde{\omega}_{s,l_2} \in R(2l_2 + 1, l_2)$ as described in the previous case a.1. Then use the path described in Fig. 5.4 to define the path from $\tilde{\omega}_{s,l_2} \in R(2l_2 + 1, l_2)$ to $\tilde{\omega}_{s,i_s} \in R(2l_2, l_2 + 1)$ that is a 1-domino rectangle.

Step b.1 If $3\bar{l} \leq s \leq 2L - \bar{l}$ and $[s - \bar{l}]_2 = [1]_2$ we have $\tilde{\omega}_s \in R(l_2 + \bar{l} - 1, l_2)$ for some value of l_2 , add a vertical column as in Fig. 5.2 to obtain $\tilde{\omega}_{s,i_s} \in R(l_2 + \bar{l}, l_2)$ that is a 0-standard rectangle in the same way as described in step a.1.

Step b.2 If $3\bar{l} \leq s \leq 2L - \bar{l}$ and $[s - \bar{l}]_2 = [0]_2$ we have $\tilde{\omega}_s \in R(l_2 + \bar{l}, l_2)$, add a vertical column as in Fig. 5.2 to obtain $\tilde{\omega}_{s,l_2} \in R(l_2 + \bar{l} + 1, l_2)$ a quasi-standard rectangle. Then we pass from $\tilde{\omega}_{s,l_2} \in R(l_2 + \bar{l} + 1, l_2)$ to $\tilde{\omega}_{s,i_s} \in R(l_2 + \bar{l}, l_2 + 1)$ that is a 1-standard rectangle using the path described in Fig. 5.4, in the same way as in step a.3.

Step c.1 Use first the path given by the time-reversal of the one represented in Fig. 5.4 to define a first interpolation between $R(L, s - L) = \tilde{\omega}_s$ and $R(L - 1, s - L + 1)$, and then use the path described in Fig. 5.2 to add a column to $R(L - 1, s - L + 1)$ in order to reach $R(L, s - L + 1) = \tilde{\omega}_{s+1}$.

Second interpolation: ω^* .

For any pair of configurations $(\tilde{\omega}_{s,i}, \tilde{\omega}_{s,i+1})$ such that $|\tilde{\omega}_{s,i}| < |\tilde{\omega}_{s,i+1}|$, by construction of the path $\tilde{\omega}_{s,i}$ the particles are created along the external boundary of the clusters. So there exists $x_1, \dots, x_{j_i}$ a connected chain of nearest neighbor empty sites of $\tilde{\omega}_{s,i}$ such that $x_1 \in \partial^- \Delta$ and x_{j_i} is the site where is located the additional particle in $\tilde{\omega}_{s,i+1}$.

Define the following:

$$\omega_{s,i,0}^* = \tilde{\omega}_{s,i}, \quad \omega_{s,i,j_i}^* = \tilde{\omega}_{s,i+1}, \quad \forall s = 0, \dots, 2(L + 2) \quad (5.72)$$

Insert between each pair $(\tilde{\omega}_{s,i}, \tilde{\omega}_{s,i+1})$, a sequence of configurations $\omega_{s,i,j}^*$, for $j = 1, \dots, j_i - 1$, where the free particle is moving from $x_1 \in \partial^- \Delta$ to the cluster until it reaches the position x_{j_i} .

Otherwise for any pair of configurations $(\tilde{\omega}_i, \tilde{\omega}_{i+1})$ such that $|\tilde{\omega}_i| = |\tilde{\omega}_{i+1}|$,

we define $\omega_{s,i,0}^* = \tilde{\omega}_{s,i}$; $\omega_{s,i+1,0}^* = \tilde{\omega}_{s,i+1}$. This conclude the definition of the reference path.

We want now to describe in more details the reference path $\omega_{s,i,j}^*$ near the critical value $s^* = l_1^* + l_2^* - 1$.

Proposition 5.9. *If the hypothesis (5.20) holds, we have:*

(i) *In the reference path ω^* the standard regime starts before s^* :*

$$s^* > 3\bar{l}. \quad (5.73)$$

(ii) *The standard rectangle with semi-perimeter s^* has sides:*

$$l_1(s^*) = l_1^*, \quad l_2(s^*) = l_2^* - 1, \quad \text{if } [s^* - \bar{l}]_2 = [0]_2, \quad (5.74)$$

$$l_1(s^*) = l_1^* - 1, \quad l_2(s^*) = l_2^*, \quad \text{if } [s^* - \bar{l}]_2 = [1]_2. \quad (5.75)$$

(iii) *The standard rectangle with semi-perimeter $s^* + 1$ has sides $l_1(s^* + 1) = l_1^*$ and $l_2(s^* + 1) = l_2^*$.*

(iv) *The standard rectangle with semi-perimeter $s^* - 1$ has sides $l_1(s^* - 1) = l_1^* - 1$ and $l_2(s^* - 1) = l_2^* - 1$.*

(v) *The standard rectangle of maximal energy is in $R^{st}(s^*)$:*

$$\arg \max_{\cup_{s > \bar{l}+2} R^{st}(s)} H = R^{st}(s^*). \quad (5.76)$$

We note that, by using point (ii) of the previous proposition 5.9, the circumscribed rectangle to the configurations in $\mathcal{P}_{wa}$, i.e., the rectangle with sides $l_1(s^*) + 1$, $l_2(s^*)$, is standard only in the case $[s^* - \bar{l}]_2 = [1]_2$. In the other case, $[s^* - \bar{l}]_2 = [0]_2$, the circumscribed rectangle is quasi-standard. The main property of the path ω^* is the following proposition.

Proof. Let $(\frac{U_1}{\epsilon}) =: \lfloor \frac{U_1}{\epsilon} \rfloor + \delta_1$ and $(\frac{U_2}{\epsilon}) =: \lfloor \frac{U_2}{\epsilon} \rfloor + \delta_2$. Form (5.25), we can write

$$l_1^* = \frac{U_1}{\epsilon} + 1 - \delta_1 \quad \text{and} \quad l_2^* = \frac{U_2}{\epsilon} + 1 - \delta_2. \quad (5.77)$$

Even case. If $0 < \delta_2 \leq \delta_1 < 1$:

$$\begin{aligned} \bar{l} &= \lfloor \frac{U_1}{\epsilon} - \frac{U_2}{\epsilon} \rfloor + 1 = \lfloor \frac{U_1}{\epsilon} \rfloor - \lfloor \frac{U_2}{\epsilon} \rfloor + \lfloor \delta_1 - \delta_2 \rfloor + 1 \\ &= l_1^* - l_2^* + 1 \Rightarrow [s^* - \bar{l}]_2 = [0]_2. \end{aligned} \quad (5.78)$$

Odd case. If $0 < \delta_1 < \delta_2 < 1$:

$$\begin{aligned} \bar{l} &= \lfloor \frac{U_1}{\epsilon} - \frac{U_2}{\epsilon} + 1 \rfloor = \lfloor \frac{U_1}{\epsilon} \rfloor - \lfloor \frac{U_2}{\epsilon} \rfloor + \lfloor \delta_1 - \delta_2 + 1 \rfloor \\ &= l_1^* - l_2^* \Rightarrow [s^* - \bar{l}]_2 = [1]_2. \end{aligned} \quad (5.79)$$

Let us prove (i); by (5.20) we have:

$$2l_2^* - l_1^* = 2\frac{U_2}{\epsilon} + 2 - 2\delta - \frac{U_1}{\epsilon} + \delta_1 \geq 3 - 2\delta_2 + \delta_1 \quad (5.80)$$

In the even case $[s^* - \bar{l}]_2 = [0]_2$ we have:

$$\begin{aligned} s^* - 3\bar{l} &= l_1^* + l_2^* - 1 - 3l_1^* + 3l_2^* - 3 = 2(2l_2^* - l_1^*) - 4 \\ &\geq 2(3 - 2\delta_2 + \delta_1) - 4 \geq 2(3 - \delta_2) > 0. \end{aligned} \quad (5.81)$$

In the odd case $[s^* - \bar{l}]_2 = [1]_2$ we have:

$$\begin{aligned} s^* - 3\bar{l} &= l_1^* + l_2^* - 1 - 3l_1^* + 3l_2^* = 2(2l_2^* - l_1^*) - 1 \\ &\geq 2(3 - 2\delta_2 + \delta_1) - 1 > 0. \end{aligned} \quad (5.82)$$

The proof of (ii), (iii), and (iv) is an immediate consequence of the definitions of standard rectangles.

Indeed in the even case we have:

$$l_1(s^*) = \frac{s^* + \bar{l}}{2} = l_1^*, \quad l_2(s^*) = \frac{s^* + \bar{l}}{2} = l_2^* - 1, \quad (5.83)$$

$$l_1(s^* + 1) = \frac{s^* + 1 + \bar{l} - 1}{2} = l_1^*, \quad l_2(s^* + 1) = \frac{s^* + 1 - \bar{l} + 1}{2} = l_2^*, \quad (5.84)$$

$$l_1(s^* - 1) = \frac{s^* - 1 + \bar{l} - 1}{2} = l_1^* - 1, \quad l_2(s^* - 1) = \frac{s^* - 1 - \bar{l} + 1}{2} = l_2^* - 1, \quad (5.85)$$

In odd case we have:

$$l_1(s^*) = \frac{s^* + \bar{l} - 1}{2} = l_1^* - 1, \quad l_2(s^*) = \frac{s^* - \bar{l} + 1}{2} = l_2^*, \quad (5.86)$$

$$l_1(s^* + 1) = \frac{s^* + 1 + \bar{l}}{2} = l_1^*, \quad l_2(s^* + 1) = \frac{s^* + 1 - \bar{l}}{2} = l_2^*, \quad (5.87)$$

$$l_1(s^* - 1) = \frac{s^* + \bar{l} - 1}{2} = l_1^* - 1, \quad l_2(s^* - 1) = \frac{s^* - \bar{l} - 1}{2} = l_2^* - 1, \quad (5.88)$$

To prove (v), by recalling (5.58), since $l_1(s) - l_2(s) = \bar{l}$ in case $[s^* - \bar{l}]_2 = [0]_2$ and $l_1(s) - l_2(s) = \bar{l} - 1$ in case $[s^* - \bar{l}]_2 = [1]_2$, we have:

$$\begin{aligned} H(R^{0-st}(s)) &= H(R(\frac{s^* + \bar{l}}{2}, \frac{s^* - \bar{l}}{2})) = H_1(s) + H_2(\bar{l}) \\ &= \frac{U_1 + U_2}{2}s - \frac{\epsilon}{4}s^2 + \frac{U_1 - U_2}{2}\bar{l} + \frac{\epsilon}{4}\bar{l}^2 \quad \text{for } [s - \bar{l}]_2 = [0]_2, \end{aligned} \quad (5.89)$$

$$\begin{aligned} H(R^{1-st}(s)) &= H(R(\frac{s^* + \bar{l} - 1}{2}, \frac{s^* - \bar{l} + 1}{2})) = H_1(s) + H_2(\bar{l} - 1) \\ &= \frac{U_1 + U_2}{2}s - \frac{\epsilon}{4}s^2 + \frac{U_1 - U_2}{2}(\bar{l} - 1) + \frac{\epsilon}{4}(\bar{l} - 1)^2 \quad \text{for } [s - \bar{l}]_2 = [1]_2, \end{aligned} \quad (5.90)$$

By maximizing the function $H_1(s) = ((U_1 + U_2)/2)s - (\epsilon/4)s^2$ in $\mathcal{R}$ we obtain the maximum in $s_0 = ((U_1 + U_2)/\epsilon) = l_1^* + l_2^* - 2 + \delta_1 + \delta_2$; moreover, $H_1(s)$ is a

parabola symmetric w.r.t. the axis $x = s_0$. We can conclude that the maximal energy of standard rectangles, 0 or 1-standard, for s integer, is obtained for $s \in \{s^* - 1, s^*, s^* + 1\}$. By a direct comparison we can conclude that this maximal energy is obtained for $s = s^*$. Indeed in case $[s^* - \bar{l}]_2 = [0]_2$ by proposition points (ii), (iii), and (iv) we have $R^{st}(s^*) = R(l_1^*, l_2^* - 1)$, $R^{st}(s^* - 1) = R(l_1^* - 1, l_2^* - 1)$ and $R^{st}(s^* + 1) = R(l_1^*, l_2^*)$ so that

$$H(R^{st}(s^*)) - H(R^{st}(s^* - 1)) = U_2 - \epsilon(l_2^* - 1) = \epsilon\delta_2 > 0, \quad (5.91)$$

$$H(R^{st}(s^*)) - H(R^{st}(s^* + 1)) = -U_1 - \epsilon l_1^* = \epsilon(1 - \delta_1) > 0, \quad (5.92)$$

In case $[s^* - \bar{l}]_2 = [1]_2$ we have $R^{st}(s^*) = R(l_1^* - 1, l_2^*)$, $R^{st}(s^* - 1) = R(l_1^* - 1, l_2^* - 1)$ and $R^{st}(s^* + 1) = R(l_2^*, l_2^*)$ so that:

$$H(R^{st}(s^*)) - H(R^{st}(s^* - 1)) = U_1 - \epsilon(l_1^* - 1)\epsilon\delta_1 > 0, \quad (5.93)$$

$$H(R^{st}(s^*)) - H(R^{st}(s^* + 1)) = -U_2 - \epsilon l_2^* = \epsilon(1 - \delta_2) > 0. \quad (5.94)$$

□

We note that, by using point (ii) of the previous proposition 5.9, the circumscribed rectangle to the configurations in $\mathcal{P}_{wa}$, i.e., the rectangle with sides $l_1(s^*) + 1, l_2(s^*)$, is standard only in the case $[s^* - \bar{l}]_2 = [1]_2$. In the other case, $[s^* - \bar{l}]_2 = [0]_2$, the circumscribed rectangle is quasi-standard.

The main property of the path ω^* is the following proposition.

Proposition 5.10. *If $U_2 < U_1 < 2U_2 - 2\epsilon$, $\epsilon = U_1 + U_2 - \Delta$ is sufficiently small and L large enough, we have that*

$$\{\arg \max_{\omega^*}\} H = \omega^* \cap \mathcal{P}_{wa}. \quad (5.95)$$

Proof. Let us consider the skeleton path $\{\bar{\omega}_s\}_{s=0, \dots, 2(L+2)}$, and let $\omega^*(\bar{\omega}_s, \bar{\omega}_{s+1})$ be the part of ω^* between $\bar{\omega}_s$ and $\bar{\omega}_{s+1}$, i.e., the interpolation of one step of the skeleton path. Defining

$$g(s) := \max_{\eta \in \omega^*(\bar{\omega}_s, \bar{\omega}_{s+1})} H(\eta) \quad (5.96)$$

We have:

$$\max_{\eta \in \omega^*} H(\eta) = \max_{s=0, \dots, 2(L+2)} g(s) \quad (5.97)$$

By the definition of ω^* we have that the function $g(s)$ takes the following values:

$$g(s) = \begin{cases} H(\bar{\omega}_s) + 2\Delta - U_1 & \text{if } s \leq 3\bar{l} \text{ and } [s]_3 \neq [0]_3 \text{ or } s > 3\bar{l} \\ H(\bar{\omega}_s) - \epsilon \frac{s}{3} + \Delta + U_1 & \text{if } s \leq 3\bar{l} \text{ and } [s]_3 = [0]_3. \end{cases} \quad (5.98)$$

Indeed for the values of s corresponding to steps a.1, a.2, and b.1 of the definition of the reference path, we can immediately verify that $g(s) = H(\bar{\omega}_s) + 2\Delta - U_1$. Steps a.3 and b.2 are more complicated since the reference path visits the quasi-domino and the quasi-standard configurations, respectively. In these cases we can easily verify the following:

If $s \leq 3\bar{l}$ and $[s]_3 = [0]_3$ then the path described in a.3 has a first part going

from $\bar{\omega}_s$ to $R^{q-\text{dom}}(s+1)$ reaching its maximal energy at $H(\bar{\omega}_s) + 2\Delta - U_1$. The second part of the path in a.3 goes from $Rq-\text{dom}(s+1)$ to $\bar{\omega}_{s+1} \in R^{\text{dom}}(s+1)$ with a maximal energy at $H(R^{q-\text{dom}}(s+1)) + \Delta + U_1 - U_2 = H(\bar{\omega}_s) + U_2 - \epsilon(s/3) + \Delta + U_1 - U_2$. We have:

$$\max\{H(\bar{\omega}_s) + 2\Delta - U_1, H(\bar{\omega}_s) - \epsilon \frac{s}{3} + \Delta + U_1\} = H(\bar{\omega}_s) - \epsilon \frac{s}{3} + \Delta + U_1. \quad (5.99)$$

In a similar way, for the standard regime, $s > 3\bar{l}$, if $[s - \bar{l}]_2 = [0]_2$ step b.2 gives:

$$\max\{H(\bar{\omega}_s) + 2\Delta - U_1, H(\bar{\omega}_s) - \epsilon \frac{s - \bar{l}}{3} + \Delta + U_1 - U_2\} = H(\bar{\omega}_s) + 2\Delta - U_1. \quad (5.100)$$

which completes the proof of (5.98). $\square$

We want now to evaluate the maximal value of $g(s)$ in the domino regime, i.e., for $s \leq 3\bar{l}$. The energy of domino configurations is an increasing function of s , for $s \leq 3\bar{l}$. More precisely the three functions:

$$\begin{aligned} h^{(0-\text{dom})}(n) &:= H(R^{0-\text{dom}}(3n)) = (U_1 + 2U_2)n - 2\epsilon n^2, \quad n = 0, \dots, \bar{l}, \\ h^{(1-\text{dom})}(n) &:= H(R^{1-\text{dom}}(3n+1)) = U_1(n+1) + 2U_2n - 2\epsilon n(n+1) \\ &\quad + 2U_2n - 2\epsilon n(n+1), \quad n = 0, \dots, \bar{l}-1, \\ h^{(2-\text{dom})}(n) &:= H(R^{2-\text{dom}}(3n+2)) = U_1(n+1) + U_2(2n+1) \\ &\quad - \epsilon(n+1)(2n+1), \quad n = 0, \dots, \bar{l}-1 \end{aligned} \quad (5.101)$$

are increasing functions of n . This implies that:

$$\begin{aligned} \max_{s \leq 3\bar{l}} g(s) &= \max\{H(\bar{\omega}_{3\bar{l}-2}) + 2\Delta - U_1, H(\bar{\omega}_{3\bar{l}-1}) + 2\Delta - U_1 \\ &\quad H(\bar{\omega}_{3\bar{l}}) + U_2 - \epsilon\bar{l} + \Delta + U_1 - U_2\} \end{aligned} \quad (5.102)$$

and by a direct comparison we obtain immediately

$$\max_{s \leq 3\bar{l}} g(s) = H(\bar{\omega}_{3\bar{l}}) - \epsilon\bar{l} + \Delta + U_1. \quad (5.103)$$

By proposition 5.9 (v), we have that in the standard regime, $s > 3\bar{l}$ the maximum value of $g(s)$ is obtained in s^* . To conclude the proof of the proposition we have to compare the maximal values of $g(s)$ in domino and standard regimes, since the energy of the configurations in T_3 can be made arbitrary small by choosing L large enough.

$$\begin{aligned} \max_{s=0, \dots, 2(L+2)} g(s) &= \max\{\max_{s \leq 3\bar{l}} g(s), \max_{s=3\bar{l}+1, \dots, 2(L+2)} g(s)\} \\ &= \max\{H(\bar{\omega}_{3\bar{l}}) - \epsilon\bar{l} + \Delta + U_1, H(\bar{\omega}_{s^*}) + 2\Delta - U_1\} \\ &= H(\bar{\omega}_{s^*}) + 2\Delta - U_1. \end{aligned} \quad (5.104)$$

Indeed, if we define $\bar{\delta} \in (0, 1)$ by means of the equality $\bar{l} = ((U_1 - U_2)/\epsilon) + 1 - \bar{\delta}$ we have immediately:

$$H(\omega_{3\bar{l}}) - \epsilon\bar{l} + \Delta + U_1 = H(\omega_{3\bar{l}}) + 2\Delta - U_1 + \epsilon\bar{\delta}. \quad (5.105)$$

On the other hand, by proposition (5.9) (i) we have $s^* > 3\bar{l}$ so that $H(\omega_{s^*}) \geq H(R^{st}(3\bar{l} + 1))$. By noting that $\omega_{3\bar{l}} \in R^{st}(3\bar{l})$ we have immediately that $U_1 < 2U_2 - 2\epsilon$ implies:

$$H(R^{st}(3\bar{l} + 1)) - H(R^{st}(3\bar{l})) = 2U_2 - U_1 - 2\epsilon + 2\epsilon\bar{\delta} > \epsilon\bar{\delta} \quad (5.106)$$

so that

$$H(\omega_{s^*}) \geq H(R^{st}(3\bar{l} + 1)) > H(R^{st}(3\bar{l})) + \epsilon\bar{\delta} \quad (5.107)$$

and the proof of (5.104) is completed.

By the definition of ω^* it is immediate to show that the configurations where this maximum value of energy is obtained, are the configurations in $\omega^* \cap \mathcal{P}_{wa}$.

5.3.3 The Exit from the Set

We define:

$$\begin{aligned} \mathcal{B}_{wa} &:= \{\eta : s(\eta) \leq s^*, \text{ or} \\ s(\eta) &= s^* + 1 \text{ and } v(\eta) \geq p_{min}(\eta) - 1, \text{ or} \\ s(\eta) &= s^* + 2 \text{ and } v(\eta) \geq s^* + p_{min}(\eta) - 2\} \end{aligned} \quad (5.108)$$

where s^* is defined in (5.26) and $p_{min}(\eta) = p_1(\eta) \wedge p_2(\eta)$. The main result of this section is given by the following proposition.

Proposition 5.11. *For $H_{min}(\partial\mathcal{B}_{wa})$ as chapter 2, $(\partial\mathcal{B}_{wa})_{min}$, Γ_{wa} as in (5.19) and $\mathcal{P}_{wa}$ as in (5.27), we have:*

$$H_{min}(\partial\mathcal{B}_{wa}) = \Gamma_{wa} \quad (5.109)$$

moreover

$$\text{if } (\bar{\eta}, \eta) \in (\partial\mathcal{B}_{wa})_{min}, \text{ then } H(\bar{\eta}) \geq H(\eta) \text{ and } \bar{\eta} \in \mathcal{P}_{wa} \quad (5.110)$$

In order to prove this proposition and in particular, in order to analyze the exiting move from $\mathcal{B}_{wa}$, we prove a preliminary result on single moves.

Let $(\bar{\eta}, \eta)$ be a move, i.e., $P(\bar{\eta}, \eta) > 0$, we define

$$\Delta(s) := s(\eta) - s(\bar{\eta}). \quad (5.111)$$

Lemma 5.12. *Let $p_{min}(\eta) \geq 4$, we have*

- (i) $|\Delta(s)| \leq 5$
- (ii) if $|\Delta(s)| = 1$ then $v(\eta) \geq p_{min}(\eta) - 3$,
if $|\Delta(s)| = 2$ then $n(\bar{\eta}) \geq 1$ and $v(\eta) \geq 2p_{min} - 5$,
if $|\Delta(s)| = 3$ then $n(\bar{\eta}) \geq 2$ and $v(\eta) \geq 3p_{min} - 6$,
if $|\Delta(s)| = 4$ then $n(\bar{\eta}) \geq 3$ and $v(\eta) \geq 4p_{min} - 7$
if $|\Delta(s)| = 5$ then $n(\bar{\eta}) \geq 4$ and $v(\eta) \geq 5p_{min} - 8$
- (iii) if $|\Delta(s)| = 1$ and $v(\eta) < p_{min} - 1$, then $n(\bar{\eta}) \geq 2$.

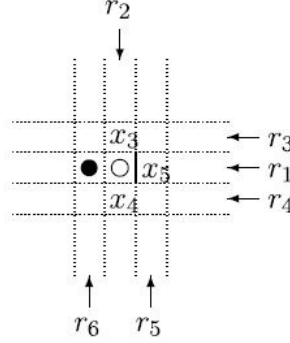


Figure 5.7:

Proof. We say that a line r (column or row in $\mathbb{Z}^2$) becomes active in the move from $\bar{\eta}$ to η if it was not active in $\bar{\eta}$ (i.e., $r \cap \bar{\eta}_{cl} = \emptyset$. and it is active in η , $\eta_{cl} \cap r \neq \emptyset$). In a single move at most five lines can become active: these are the row and the column containing the new position of the moved particle, (we will call these lines r_1 and r_2 , where r_1 is the line of the move, and r_2 is the line orthogonal to it), and the three lines through the three nearest neighbor sites x_3 , x_4 , and x_5 of the particle after the move, excluding the site that it occupied in $\bar{\eta}$ (lines r_3 , r_4 , and r_5) (see Fig. 5.8).

Lines r_3 , r_4 , and r_5 become active only if in the corresponding sites x_3 , x_4 , and x_5 , there was a free particle in $\bar{\eta}$, and the line r_1 , corresponding to the move, becomes active only if the moving particle was free before the move, otherwise it was already present in $\bar{\eta}$. Each line of types 3, 4, and 5 becoming active, brings in the new configuration at least $p_{min}(\eta) - 1$ vacancies; indeed $|r_i \cap \eta_{cl}| = 1$ for $i = 3, 4, 5$ since $r_i \cap \bar{\eta}_{cl} = \emptyset$; the line r_1 brings at least $p_{min}(\eta) - 2$ vacancies, and the line r_2 brings at least $p_{min}(\eta) - 3$ vacancies. Points (i) and (ii) immediately follow from this. To prove (iii) suppose first that $\Delta s = 1$ with $k \geq 2$ activated lines and k_1 deactivated lines (i.e., lines which were active in $\bar{\eta}$ and that are not active in η). Since $k \geq 2$ activated lines bring at least $2p_{min}(\eta) - 5$ vacancies, and $p_{min}(\eta) \geq 4$ in this case $v(\eta) \geq 2p_{min}(\eta) - 5 \geq p_{min}(\eta) - 1$. So the only possibility to have $\Delta s = 1$ and $v(\eta) < p_{min}(\eta) - 1$ is when there is only one line activated by the move and no deactivated lines, and this activated line is r_1 or r_2 . If the activated line is r_1 and if it brings only $p_{min}(\eta) - 2$ vacancies this means that in this line, in $\bar{\eta}$ there are two free particles, one of which is the moving particle. If the activated line is r_2 , it brings $p_{min}(\eta) - 3$ vacancies only if it contains 2 free particle before the move in the sites x_3 and x_4 (see Fig. 5.7); it bring $p_{min}(\eta) - 2$ vacancies if it contain a free particle in sites x_3 or x_4 before the move. If the moving particle is free in $\bar{\eta}$, we have $n(\bar{\eta}) \geq 2$, if the moving particle is not free in $\bar{\eta}$, then line r_6 (see Fig. 5.7) was active in $\bar{\eta}$ and it is continue to be active in η . Due to the fact that r_2 is the unique line that become active, the line orthogonal to r_2 through this free particle (i.e., lines 3 or 4, say r_3 for concreteness) must be active in $\bar{\eta}$ and remains active in η . So we can conclude that there is an additional vacancy in η in the site $r_6 \cap r_3$, this implies that in this case $v(\eta) \geq p_{min}(\eta) - 2 + 1$. Point (iii) is thus proved. $\square$

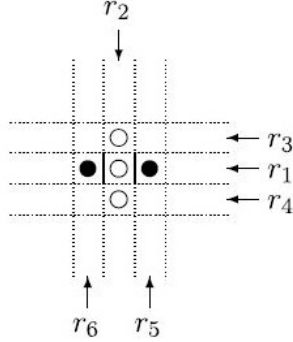


Figure 5.8:

Remark 5.13. We note that if $n(\bar{\eta}) = 0$ the unique line that can become active is r_2 and in this case in $\bar{\eta}$ sites x_3 and x_4 are empty and $x_5 \in \bar{\eta}_{cl}$, where $x_5 \in r_1$ (see Figs. 5.7 and 5.8), so that $\bar{\eta}$ is not monotonic ($g'_1(\bar{\eta}) + g'_2(\bar{\eta}) \geq 1$) in this case.

Proof. of the main proposition 5.11. Let $(\bar{\eta}, \eta) \in \partial B$ be the exiting move from $\mathcal{B}_{wa}$ and Δs be its corresponding variation of s . If $p_{min}(\eta) \leq 3$, for $\epsilon \leq U_2$, from explicit computations it follows:

$$H(\eta) > \Gamma_{wa}. \quad (5.112)$$

Suppose from now on $p_{min}(\eta) \geq 4$.

By using lemma 5.12, we can distinguish seven different cases corresponding to $\Delta s = -1, 0, 1, 2, 3, 4, 5$, since, by definition, the only possibility to leave $\mathcal{B}_{wa}$ with $\Delta s < 0$ is with $s(\bar{\eta}) = s^* + 2$ and $\Delta s = -1$.

Case -1. We will prove that if $\Delta s = -1$ and $(\bar{\eta}, \eta) \in \partial \mathcal{B}_{wa}$ then $H(\bar{\eta}) \vee H(\eta) > \Gamma_{wa}$. Since $s(\bar{\eta}) = s^* + 2$ we have that $H(\bar{\eta}) \leq \Gamma_{wa}$ only if $n(\bar{\eta}) = 0$, $g'_1(\bar{\eta}) + g'_2(\bar{\eta}) = 0$ and $p_{min}(\bar{\eta}) > 3$. Indeed, for $p_{min}(\bar{\eta}) \geq 4$ we have:

$$\begin{aligned} H(\bar{\eta}) &\geq H(R^{st}(s^* + 2)) + \epsilon(s^* + p_{min}(\bar{\eta}) - 2) \\ &= H(R^{st}(s^*)) + [H(R^{st}(s^* + 2)) - H(R^{st}(s^*))] + \epsilon(s^* + p_{min}(\bar{\eta}) - 2) \\ &= H(R^{st}(s^*)) + U_1 + U_2 + \epsilon(p_{min}(\bar{\eta}) - 3) \\ &\geq H(R^{st}(s^*)) + U_1 + U_2. \end{aligned} \quad (5.113)$$

So if we add at least U_2 coming from $g'_1(\bar{\eta}) + g'_2(\bar{\eta}) \geq 1$ or $n(\bar{\eta}) \geq 1$ we have $H(\bar{\eta}) \geq H(R^{st}(s^*)) + U_1 + 2U_2 > \Gamma_{wa}$. In the case $s(\bar{\eta}) = s^* + 2$ with $n(\bar{\eta}) = 0$ and $g'_1(\bar{\eta}) + g'_2(\bar{\eta}) = 0$, it is impossible to leave $\mathcal{B}_{wa}$. Indeed, by remark 5.13 it is impossible to activate lines and so $\Delta s = -1$ is obtained by a unique line becoming inactive. So we have $\Delta v := v(\eta) - v(\bar{\eta}) \geq -p_{max}(\bar{\eta})$. By using the obvious relation: $p_{max}(\bar{\eta}) = s^* + 2 - p_{min}(\bar{\eta})$ we obtain

$$v(\eta) \geq s^* + p_{min}(\bar{\eta}) - 2 - p_{max}(\bar{\eta}) = 2p_{min}(\bar{\eta}) - 4 \geq p_{min}(\bar{\eta}) - 1 \geq p_{min}(\eta) - 1 \quad (5.114)$$

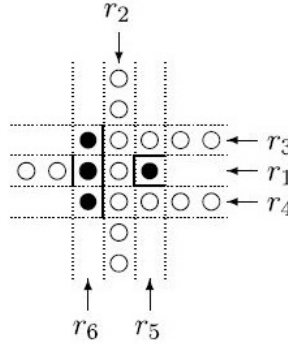


Figure 5.9:

and so $\eta \in \mathcal{B}_{wa}$ against $(\bar{\eta}, \eta) \in \partial \mathcal{B}_{wa}$.

Case 0. This is the case of the minimal exit from $\mathcal{B}_{wa}$. We have to distinguish two cases, indeed if $\Delta s = 0$, then $(\bar{\eta}, \eta) \in \partial \mathcal{B}_{wa}$ only if

- (a) $s(\bar{\eta}) = s^* + 1$ and $\Delta v \leq -1$,
- (b) $s(\bar{\eta}) = s^* + 2$ and $\Delta v \leq -1$.

Since the number of vacancies can decrease only if either $p_1(\eta) - p_1(\bar{\eta}) = p_2(\bar{\eta}) - p_2(\eta) \neq 0$ or $p_1(\eta) - p_1(\bar{\eta}) = p_2(\bar{\eta}) - p_2(\eta) = 0$ but $|\eta_{cl}| - |\bar{\eta}_{cl}| > 0$ that implies that in both case (a) and (b) we have

- (i) either $n(\bar{\eta}) \geq 1$ or
- (ii) $n(\bar{\eta}) = 0$ and, by remark 5.13, $g'_1(\bar{\eta}) + g'_2(\bar{\eta}) \geq 1$ and r_2 become active bringing at least $p_{min}(\eta) - 1$ vacancies in η .

Case (a-i) contains the minimal exit from $\mathcal{B}_{wa}$. Indeed by proposition (5.8) we have $H(\bar{\eta}) \geq \Gamma_{wa}$. Moreover if $\bar{\eta} \in P$ with $s(\bar{\eta}) = s^* + 1$, $n(\bar{\eta}) \geq 1$ and $v(\eta) \geq p_{min} - 1$ we have that $H(\bar{\eta}) > \Gamma_{wa}$ (see proposition 5.8).

Case (a) is compatible only with case (i) because in case (a-ii) $v(\eta) \geq p_{min}(\eta) - 1$ and $s(\eta) = s(\bar{\eta}) = s^* + 1$ implies $\eta \in \mathcal{B}_{wa}$ against $(\bar{\eta}, \eta) \in \partial \mathcal{B}_{wa}$. Cases (b-i) and (b-ii) can be treated as in point -1.

Case 1. Let $\Delta s = 1$, first suppose $s(\bar{\eta}) = s^*$; if $\eta \notin \mathcal{B}_{wa}$ then $v(\eta) < p_{min}(\eta) - 1$, indeed by lemma 5.12, (iii) we have $n(\bar{\eta}) \geq 2$ and by proposition 5.8 we can conclude

$$H(\bar{\eta}) \geq 2\Delta + H(R^{st}(s^*)) > \Gamma_{wa}. \quad (5.115)$$

So we have only to consider the cases:

- (a) $s(\bar{\eta}) = s^* + 1$,
- (b) $s(\bar{\eta}) = s^* + 2$,

Again we consider two possibilities

- (i) either $n(\bar{\eta}) \geq 1$ or
- (ii) $n(\bar{\eta}) = 0$ and, by remark 5.13, $g'_1(\bar{\eta}) + g'_2(\bar{\eta}) \geq 1$ and r_2 become active bringing at least $p_{min}(\eta) - 1$ vacancies in η .

In case (a-i), by proposition 5.8 we can conclude as in case (0.a-i)

In case (b-i) and (b-ii) we have immediately $H(\bar{\eta}) > \Gamma_{wa}$ as obtained in point -1 (see (5.113))

We have only to discuss the case (a-ii). In this case the only line that can become active is r_2 and the configuration $\bar{\eta}_{cl}$ is not connected. This also implies that there are no deactivating lines during the move. In this case we have to consider separately the case in which the move is horizontal or vertical.

- (h) Suppose first that the move is horizontal, i.e., r_1 is an horizontal line (see Fig. 5.8). In this case we have $g'_2(\bar{\eta}) \geq 1$ and so by proposition 5.8, case b):

$$H(\bar{\eta}) \geq H(R^{st}(s^*)) + \Delta - U_1 + U_1. \quad (5.116)$$

Moreover if $g'_2(\bar{\eta}) \geq 2$ and or $g'_2(\bar{\eta}) \geq 1$ we have immediately $H(\bar{\eta}) > \Gamma_{wa}$. If $g'_2 = 1$ and $g'_1 = 0$, we have to consider the following cases:

- If the moving particle has in $\bar{\eta}$ at least one vertical and one horizontal bond connecting it to other particles, then $\Delta H \geq U_2$ and so $H(\eta) > \Gamma_{wa}$.
- If the moving particle has in $\bar{\eta}$ two vertical bonds connecting it to other particles (see Fig. 5.9), then $v(\bar{\eta}) \geq p_1(\bar{\eta}) + p_2(\bar{\eta}) - 2$ since, by the hypothesis $g'_2(\bar{\eta}) = 1$ $g'_1(\bar{\eta}) = 0$, in the lines r_1, r_3 we have over all at least $p_1(\bar{\eta}) - 1$ vacancies. As shown in (5.109) this implies $H(\bar{\eta}) > \Gamma_{wa}$.
- If the moving particle has in $\bar{\eta}$ only one horizontal bond connecting it to other particles, then we can conclude that the line r_6 becomes inactive in the move, against $\Delta s = 1$.
- If the moving particle has in $\bar{\eta}$ only a vertical bond connecting it to other particles (see Fig. 5.10) as before, then we have $v(\bar{\eta}) \geq p_1(\bar{\eta}) + p_2(\bar{\eta}) - 2$. As shown in (5.117) this implies $H(\bar{\eta}) > \Gamma_{wa}$.

The proof is completed in this horizontal case once we show that a configuration $\bar{\eta}$ with: $s(\bar{\eta}) = s^* + 1$, $n(\bar{\eta}) = 0$, $g'_2(\bar{\eta}) = 1$ and $v(\bar{\eta}) \geq p_1(\bar{\eta}) + p_2(\bar{\eta}) - 2$ has $H(\bar{\eta}) > \Gamma_{wa}$. Indeed we have:

$$\begin{aligned} H(\bar{\eta}) &\geq H(R^{st}(s^* + 1)) + \epsilon(s^* - 1) + U_1 \\ &> H(R^{st}(s^* + 1)) + \epsilon(l_2^* - 1) + \Delta \geq \Gamma_{wa}. \end{aligned} \quad (5.117)$$

- (v) Suppose now that the move is vertical (see Fig. 5.11). In this case we have $g'_1(\bar{\eta}) \geq 1$ and so by proposition (5.8).

$$H(\bar{\eta}) \geq H(R^{st}(s^*)) + \Delta - U_1 + U_2. \quad (5.118)$$

We have to consider the following cases:

- If the moving particle has in $\bar{\eta}$ at least one vertical and one horizontal bond connecting it to other particles, then $\Delta H \geq U_1$ so that $H(\eta) > \Gamma_{wa}$.

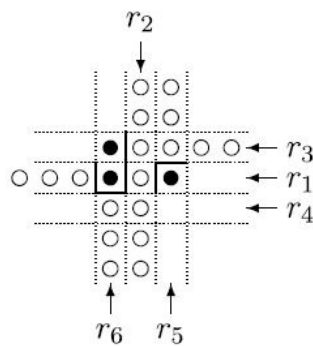


Figure 5.10:

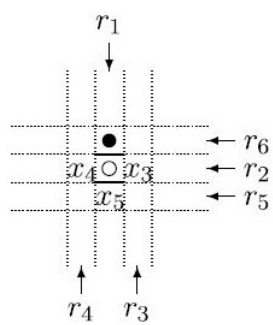


Figure 5.11:

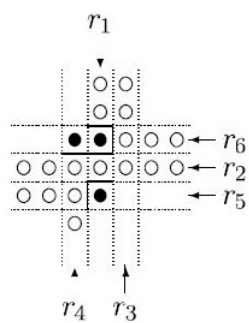


Figure 5.12:

- If the moving particle has in $\bar{\eta}$ at least two horizontal bonds connecting it to other particles, then $\Delta H = -U_2 + 2U_1$ so that $H(\eta) > \Gamma_{wa}$.
- If the moving particle has in $\bar{\eta}$ only one vertical bond connecting it to other particles, then we can conclude that the line r_6 becomes inactive in the move, against $\Delta s = 1$.
- If the moving particle has in $\bar{\eta}$ only one horizontal bond connecting it to other particles, then $\Delta H = U_1 - U_2$. If $g'_1(\bar{\eta}) = 1$ then $H(\eta) > \Gamma_{wa}$ since $v(\bar{\eta}) \geq p_1(\bar{\eta}) + p_2(\bar{\eta}) - 2$ (see Fig 5.12).

If $g'_1(\bar{\eta}) > 1$ then again we have $H(\eta) > \Gamma_{wa}$. The proof is completed in this vertical case if we prove that a configuration $\bar{\eta}$ with: $s(\bar{\eta}) = s^* + 1$, $n(\bar{\eta}) = 0$, $g'_1(\bar{\eta}) = 1$ and $v(\bar{\eta}) \geq p_1(\bar{\eta}) + p_2(\bar{\eta}) - 2$ has $H(\bar{\eta}) > \Gamma_{wa} - U_1 + U_2$, that is $H(\eta) > \Gamma_{wa}$. This computation is exactly the same as in the horizontal case (see equation (5.117)).

Case 2. If $\Delta s = 2$, $(\bar{\eta}, \eta) \in \partial \mathcal{B}_{wa}$ only if $s(\bar{\eta}) \geq s^*$, and by lemma 5.12 we know that $n(\bar{\eta}) \geq 1$. If $s(\bar{\eta}) = s^* + 1$ and $n(\bar{\eta}) = 1$ we can conclude as in case (0.a-i). If $s(\bar{\eta}) = s^* + 2$ since $n(\bar{\eta}) \geq 1$ we have immediately $H(\bar{\eta}) > \Gamma_{wa}$ (see equation (5.113)).

If $s(\bar{\eta}) = s^*$ and $n(\bar{\eta}) \geq 2$ then we have $H(\bar{\eta}) \geq 2\Delta + H(R^{st}(s^*)) > \Gamma_{wa}$. So we are left with the case: $s(\bar{\eta}) = s^*$ and $n(\bar{\eta}) = 1$.

If the unique free particle is the moving particle we can not have $\Delta s = 2$. Indeed r_3 , r_4 , and r_5 can not be activated and, in order to have $\Delta s = 2$, r_1 and r_2 have to become active. This implies that the sites x_3 , x_4 , and x_5 must be empty, but then $\Delta s = 0$.

If $g'_1(\bar{\eta}) + g'_2(\bar{\eta}) \geq 1$ we have

$$H(\bar{\eta}) \geq \Delta + H(R^{st}(s^*)) + U_2 > \Gamma_{wa} \quad (5.119)$$

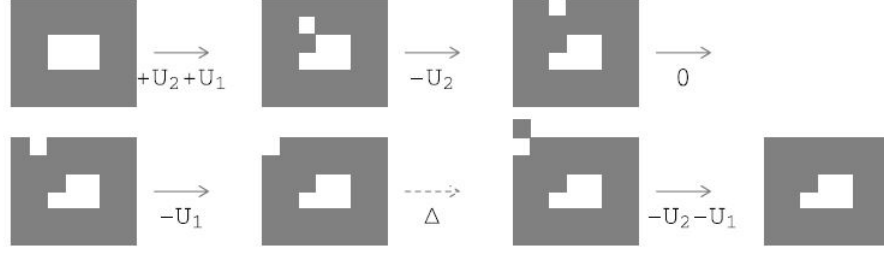
since $\Delta + U_2 > 2\Delta - U_1$. So we have to consider only the case $s(\bar{\eta}) = s^*$, $n(\bar{\eta}) = 1$, $g'_1(\bar{\eta}) = g'_2(\bar{\eta}) = 0$.

We distinguish two cases:

- (a) the free particle is in site x_i , with i equal 3 or 4 the lines that become active are r_2 and r_i . Due to $g'_1(\bar{\eta}) = g'_2(\bar{\eta}) = 0$ the site x_5 is empty, and the site $\{x_3, x_4\} \setminus \{x_i\}$ is empty.
- (b) the free particle is in site x_5 the lines that become active are r_2 and r_5 and the sites x_3 and x_4 are empty

In both cases if the moving particle has in $\bar{\eta}$ at least one vertical and one horizontal bond connecting it to other particles, then $\Delta H \geq U_2$ and so $H(\eta) \geq H(\bar{\eta}) + U_2 \geq H(R^{st}(s^*)) + \Delta + U_2 > \Gamma_{wa}$.

If the moving particle has in $\bar{\eta}$ either two bonds orthogonal to the move, or only one vertical or only one horizontal bond connecting it to other particles,

Figure 5.13: $(U_1 + U_2)$ -reduction of a rectangle with a hole

then it is impossible to leave $\mathcal{B}_{wa}$. Indeed in this case there exists a line r ($r = r_1$ or $r = r_6$) such that its intersection with $\bar{\eta}$ is only the moving particle. If $r = r_6$ then this line become inactive after the move against $\Delta s = 2$. If $r = r_1$ then the number of vacancies in η are at least the vacancies induced by the two activating lines and r_1 . This means that in case (a) r_i and r_2 becomes active

$$|r_1 \cap \eta_{cl}| = 1, \quad |r_2 \cap \eta_{cl}| = 2, \quad |r_i \cap \eta_{cl}| = 1, \quad (5.120)$$

so that

$$v(\eta) \geq p_1 - 1 + p_2 - 2 + p_{min}(\eta) - 1 = s(\eta) + p_{min}(\eta) - 4 = s^* + p_{min}(\eta) - 2. \quad (5.121)$$

In case (b) lines r_5 and r_2 become active and

$$|r_1 \cap \eta_{cl}| = 2, \quad |r_2 \cap \eta_{cl}| = 1, \quad |r_5 \cap \eta_{cl}| = 1, \quad (5.122)$$

and so $\eta \in B$ against $(\bar{\eta}, \eta) \in \partial \mathcal{B}_{wa}$.

Case 3. If $\Delta s = 3$, $(\bar{\eta}, \eta) \in \partial \mathcal{B}_{wa}$ only if $s(\bar{\eta}) \geq s^* - 1$, and by lemma 5.12 we know that $n(\bar{\eta}) \geq 2$. Therefore, we have

$$H(\bar{\eta}) \geq 2\Delta + H(R^{st}(s^* - 1)) > \Gamma_{wa} \quad (5.123)$$

since $H(R^{st}(s^* + 1)) - H(R^{st}(s^* - 1)) = U_1 + U_2 - \epsilon(s^* + 1)$ and so $2\Delta + H(R^{st}(s^* - 1)) = 2\Delta + H(R^{st}(s^* + 1)) - U_1 - U_2 + \epsilon(s^* + 1) > H(R^{st}(s^* + 1)) + \epsilon(l_2^* - 1) + \Delta = \Gamma_{wa}$.

Case 4. If $\Delta s = 4$, $(\bar{\eta}, \eta) \in \partial \mathcal{B}_{wa}$ only if $s(\bar{\eta}) \geq s^* - 2$, and by lemma 5.12 we know that $n(\bar{\eta}) \geq 3$. Therefore, we have $H(\bar{\eta}) \geq 3\Delta + H(R^{st}(s^* - 2)) > \Gamma_{wa}$ as before.

Case 5. If $\Delta s = 5$, $(\bar{\eta}, \eta) \in \partial \mathcal{B}_{wa}$ only if $s(\bar{\eta}) \geq s^* - 3$, and by lemma 5.12 we know that $n(\bar{\eta}) \geq 4$. Therefore, we have $H(\bar{\eta}) \geq 4\Delta + H(R^{st}(s^* - 3)) > \Gamma_{wa}$ as before.

□

5.3.4 Communication Height and Gate

By definition of communication height $\Phi(\underline{0}, \underline{1})$, by proposition 5.10 we have immediately:

$$\Phi(\underline{0}, \underline{1}) := \max_i H(\omega_i^*) = H(\mathcal{P}_{wa}) = \Gamma_{wa}, \quad (5.124)$$

where $\mathcal{P}_{wa}$ and Γ_{wa} are defined in (5.19) and (5.27), respectively. On the other side, since every path going from $\underline{0}$ to $\underline{1}$ has to leave $\mathcal{B}_{wa}$, we have by proposition 5.11 that

$$\Phi(\underline{0}, \underline{1}) := \min_{\omega: \underline{0} \rightarrow \underline{1}} \max_{\zeta \in \omega} H(\zeta) \geq H_{\min}(\partial B) = \Gamma_{wa}, \quad (5.125)$$

By combining (5.124) and (5.125) we immediately obtain

$$\Phi(\underline{0}, \underline{1}) := \Gamma_{wa} \quad (5.126)$$

Note that to prove (5.126) we have applied the argument developed in ref. [56] with some small variations. In ref. [56], the set $\partial^+ \mathcal{B}_{wa}$ (external boundary of $\mathcal{B}_{wa}$, see (2.5)) was considered, while here we use the set $\partial \mathcal{B}_{wa}$ of exiting moves from $\mathcal{B}_{wa}$ (see (5.8)), so that in the present case $H_{\min}(\partial \mathcal{B}_{wa})$ substitutes $H(F(\partial^+ \mathcal{B}_{wa}))$.

The argument used to prove (5.126) also implies that $\mathcal{P}_{wa}$ is a gate. Indeed given any optimal path ω , it has to leave $\mathcal{B}_{wa}$ with a move in $(\partial \mathcal{B}_{wa})_{\min}$ otherwise, by proposition 5.11 we would have $\max_i H(\omega) > \Gamma_{wa}$. To conclude we use (5.110).

5.4 Theorems for the Gate

5.4.1 Reduction

In this section we first prove the following proposition.

Proposition 5.14. *There exists $\Gamma_0 < \Gamma_{wa}$ such that $\mathcal{X}_{\Gamma_0} \subseteq \{\underline{0}, \underline{1}\}$, i.e.:*

$$\begin{aligned} & \forall \eta \neq \underline{0}, \underline{1} \quad \exists \eta \in \mathcal{X} \text{ and a path } \omega : \eta \rightarrow \eta' \\ & \text{such that } H(\eta) < H(\eta'), \quad \max_{\zeta \in \omega} H(\zeta) < H(\eta) + \Gamma_0. \end{aligned} \quad (5.127)$$

In the second part of this section, as a corollary of this proposition, we will identify the stable and metastable states.

Proposition 5.15. *If the side L of the box Λ is large enough ($L > 2l_1^*$ is a possible choice), then $V_{\underline{0}} = (\underline{0}, \underline{1})$ and $\underline{1} = \mathcal{X}^s$, $\underline{0} = \mathcal{X}^m$.*

• Reduction Outside $\{\underline{0}, \underline{1}\}$

To prove proposition 5.14 we first characterize the set $\mathcal{X}_{U_1+U_2}$ of configurations which are not $(U_1 + U_2)$ -reducible, as follows.

We introduce some geometrical definitions. Let $\eta \in \mathcal{X}$ be given.

- (i) A site $x \in \Lambda$ is connected trough empty (full) sites to $\partial^- \Lambda$ if there exists $x_1, \dots, x_n$ a connected chain of nearest neighbor empty (full) sites namely, $x_1 \in nn(x), x_2 \in nn(x_1), \dots, x_n \in nn(x_{n-1}), x_n \in \partial^- \Lambda$ and $\eta(x_1) = \eta(x_2) = \dots = \eta(x_n) = 0$ ($\eta(x_1) = \eta(x_2) = \dots = \eta(x_n) = 1$).

- (ii) An external corner of a set $A \subset \Lambda$ is a site $x \notin A$ such that $\sum_{y \in nn(x): (x,y) \in \Lambda_{0,h}^*} \chi_A(y) = 1$ and $\sum_{y \in nn(x): (x,y) \in \Lambda_{0,v}^*} \chi_A(y) = 1$, where χ_A is the characteristic function of the set A .
- (iii) An internal corner of a set $A \subset \Lambda$ is a site $x \in A$ such that $\sum_{y \in nn(x): (x,y) \in \Lambda_{0,h}^*} \chi_A(y) = 1$ and $\sum_{y \in nn(x): (x,y) \in \Lambda_{0,v}^*} \chi_A(y) = 1$.
- (iv) Let η^{ext} be the set of sites $x \in \Lambda_0$ such that $\eta(x) = 1$ and x is connected through empty sites with $\partial^- \Lambda$.

Proposition 5.16. *Any configuration $\eta \in \mathcal{X}_{U_1+U_2}$ has no free particles and it has only rectangular clusters with minimal side larger than 1.*

Proof. If η has a free particle then η is obviously 0-reducible, i.e., $\eta \notin \mathcal{X}_{U_1+U_2}$. The reducing path ω satisfying (5.127) is immediately obtained by bringing the free particle outside Λ or attaching it to a cluster.

Thus for each $\eta \in \mathcal{X}_{U_1+U_2}$ we have $\eta = \eta_{cl}$. Let $C_1(\eta), \dots, C_n(\eta)$ be the clusters of η and let $\bar{C}_1(\eta), \dots, \bar{C}_n(\eta)$ be the minimal simply connected sets of $\mathcal{R}^2$ containing $\eta = \eta_{cl}$. Let $C_1(\eta), \dots, C_n(\eta)$, i.e., the clusters whose holes have been filled up. We next show the following:

- a. the sets $\bar{C}_i$ are rectangles with minimal side larger than one,
 - b. there are no holes inside the clusters: $C_i(\eta) = \bar{C}_i(\eta)$ for any i .
- a. By definition the Euclidean distance between two different clusters in $\mathcal{R}^2$ is at least one. This implies that if there is a set $\bar{C}_i(\eta)$, which is not a rectangle, then there is an external corner x of η connected through empty sites $x_1, \dots, x_n$ to $\partial^- \Lambda$. This implies that η can be Δ -reduced. Indeed the reducing path, i.e., the path $\omega : \eta \rightarrow \eta'$ with $H(\eta') < H(\eta)$ and such that $\max_{\zeta \in \omega} H(\zeta) \leq H(\eta) + \Delta$, is given by the sequence of configurations ω_i with the same clusters as η plus a free particle that moves along the sequence $x_n, \dots, x_1$, ($x_n \in \partial^- \Lambda$, x_1 , a nearestneighbor of the external corner x). In the final configuration ω_{n+1} the free particle is attached to the cluster in the site x . We have $H(\omega_i) \leq H(\eta) + \Delta$ for $i = 1, \dots, n$ and $H(\omega_{n+1}) \leq H(\eta) + \Delta - (U_1 + U_2) < H(\eta)$.

If a set $\bar{C}_i(\eta)$ is made by a unique row (or a unique column) then the configuration is obviously U_1 -reducible (U_2 -reducible) by removing a particle of the row (column) and bringing it out of Λ .

- b. If one of the clusters of η has a hole, i.e., if there exists $\bar{C}_i(\eta)$, which is not simply connected, then η can be $(U_1 + U_2)$ -reduced (see Fig. 5.13).

Indeed, if such a cluster $C_i(\eta)$ exists, there exists also a cluster $C_{i_0}(\eta)$, possibly equal to $C_i(\eta)$, with holes and with $C_{i_0}(\eta) \cap \eta^{ext} \neq \emptyset$.

Let y be an internal corner of a hole of $C_{i_0}(\eta)$, connected to an internal corner y_n of $C_{i_0}(\eta)$ through full sites $y_1, y_2, \dots, y_n$ and such that $y_n \in \eta^{ext}$. Such corners y and y_n exist since every set has at

least four internal corners and since $C_{i_0}(\eta) \cap \eta^{ext} \neq \emptyset$.

Let $\eta_1, \eta_2, \dots, \eta_n$ be the configurations obtained by moving the empty site from y to y_n through $y_1, \dots, y_{n-1}$.

For any $i = 1, \dots, n-1$, by using that y has at least 2 *n.n.* non-opposite occupied sites and that y_n has 2 *n.n.* non-opposite empty sites we have:

$$H(\eta_i) - H(\eta) \leq U_1 + U_2 \quad \text{and} \quad H(\eta_n) \leq H(\eta). \quad (5.128)$$

Moreover, by definition, y_n is an external corner of η_n , connected through empty sites to $\partial^- \Lambda$, so that η_n can be Δ -reduced as in point a. By joining the path $\eta_1, \eta_2, \dots, \eta_n$ with the path realizing the Δ -reduction of η_n we obtain the $U_1 + U_2$ -reduction of η . $\square$

Proof of proposition 5.14. Suppose that $\eta \in \mathcal{X}_{U_1+U_2}$ and $\eta \neq 0, 1$, from proposition 5.16 η has only rectangular clusters which are connected through empty sites to $\partial^- \Lambda$, i.e., $\eta^{ext} = \partial^- \eta$.

Suppose now that a rectangular cluster of η has a vertical subcritical side, i.e., $l_2 < l_2^*$, then it is possible to reduce with the path described in Fig. 5.2 that removes a column of length l_2 with energy barrier $\Delta H(\text{remove column}) = U_1 + U_2 + \epsilon(l_2 - 2) < 2\Delta - U_1$.

Otherwise if any rectangle in η has vertical supercritical sides, $l_2 \geq l_2^*$, it is possible to reduce η with the path described in Fig. 5.2 that adds a column with energy barrier $\Delta H(\text{add column}) = 2\Delta - U_1$.

The proof is complete by defining $\Gamma_0 := 2\Delta - U_1 < \Gamma_{wa}$.

• Stable and Metastable States

Proof of proposition 5.15. Since $\mathcal{X}_s \subseteq \mathcal{X}_V$ for any $V \geq 0$ and since, if the side L of the volume Λ is large enough, we have $H(\underline{0}) > H(\underline{1})$, using also that by proposition 5.14 we have $\mathcal{X}_{\Gamma_0} \subseteq \{\underline{0}, \underline{1}\}$, we can immediately conclude that $\mathcal{X}_s = \underline{1}$. If we are able to prove that

$$V_{\underline{0}} = \Phi(\underline{0}, \underline{1}) = \Gamma_{wa} > \Gamma_0 \quad (5.129)$$

we can immediately conclude that $\underline{0} \in \mathcal{X}^m$.

Let us now prove (5.129). By definition we have that $V_{\underline{0}} \leq \Phi(\underline{0}, \underline{1})$. We argue by contradiction: suppose that $V_{\underline{0}} < \Phi(\underline{0}, \underline{1})$. Then, by definition, there exists $\eta^{(1)}$ with $H(\eta^{(1)}) < H(\underline{0})$ and $\Phi(\underline{0}, \eta^{(1)}) = V_{\underline{0}} < \Phi(\underline{0}, \underline{1})$. This implies that $\eta^{(1)}$ can not be equal to $\underline{1}$, so since by $\mathcal{X}_{\Gamma_0} \subseteq \{\underline{0}, \underline{1}\}$, we know that $\eta^{(1)} \in \mathcal{X}_{\Gamma_0}$ we can iterate this argument by obtaining a sequence $H(\underline{0}) > H(\eta^{(1)}) > H(\eta^{(2)}) > \dots > H(\eta^{(n)})$ with $\Phi(\eta^{(i)}, \eta^{(i+1)}) \leq H(\eta^{(i)}) + \Gamma_0 < \Phi(\underline{0}, \underline{1})$ if $\eta^{(i)} \neq \underline{1}$. The number of these iterations must be finite since the sequence $\eta^{(i)}$ has a strictly decreasing energy and the state space is finite. Moreover, the sequence stops at $\eta^{(n)} \in \mathcal{X}_{\Gamma_0}$ and we have $\eta^{(n)} = \underline{1}$ since $\mathcal{X}_{\Gamma_0} \subseteq \{\underline{0}, \underline{1}\}$ and $H(\eta^{(0)}) > H(\eta^{(n)})$. We obtain

$$\Phi(\underline{0}, \underline{1}) = \Phi(\underline{0}, \eta^{(n)}) \leq \max\{\Phi(\underline{0}, \eta^{(1)}), \Phi(\eta^{(1)}, \eta^{(2)}), \dots, \Phi(\eta^{(n-1)}, \eta^{(n)})\} < \Phi(\underline{0}, \underline{1}) \quad (5.130)$$

which is absurd.

5.4.2 Proof of Theorem 5.3

To prove theorem 5.3 we need the notion of cycle that is one of the main tools used in the general theory of Freidlin Wentzell Markov chains. We shortly recall the definition in our case.

The following result represents the main property of cycles (see for instance [43] and [56] theorem 2.36 with large probability every state in a cycle is visited by the process before the exit).

Proposition 5.17. *Let C be a cycle. There exists $K > 0$ such that for any $\eta, \eta' \in C$ and for all sufficiently large β*

$$P_\eta(\tau_{\eta'} < \tau_{\partial+C}) \geq 1 - e^{-K\beta} \quad (5.131)$$

By using this result, to prove theorem (5.3) it is sufficient to show the following:

- (i) if η is a rectangular configuration contained in $R(l_2^* - 1, l_2^* - 1)$, then there exists a cycle $C_{\underline{0}}$ containing η and $\underline{0}$ and not containing $\underline{1}$;
- (ii) if η is a rectangular configuration containing $R(l_2^*, l_2^*)$, then there exists a cycle $C_{\underline{1}}$ containing η and $\underline{1}$ and not containing $\underline{0}$.

We start by showing (i). Let $C_{\underline{0}}$ be the maximal connected set containing $\underline{0}$ such that $\max_{\eta' \in C_{\underline{0}}} H(\eta') < \Gamma_{wa}$. By definition $C_{\underline{0}}$ is a cycle containing $\underline{0}$. It does not contain $\underline{1}$ since $\Phi(\underline{0}, \underline{1}) = \Gamma_{wa}$. We have only to prove that $C_{\underline{0}}$ contains η . This can be easily obtained by constructing a path $\omega^{\eta, \underline{0}}$ going from η to $\underline{0}$ keeping the energy less than Γ_{wa} . $\omega^{\eta, \underline{0}}$ is obtained by erasing site by site, each column of η and by showing that all the configurations of this path are in $C_{\underline{0}}$.

More precisely, let $\eta = \{(x, y) \in \mathbb{Z}^2; x \in (n, n + l_1], y \in (m, m + l_2]\} \in R(l_1, l_2)$ for some $n, m \in \mathbb{Z}$, and let $\{\bar{\omega}_i^{\eta, \underline{0}}\}_{i=0, \dots, l_1}$ be a path of rectangular configurations, starting from η and ending in $\underline{0}$, given by

$$\{\bar{\omega}_i^{\eta, \underline{0}}\} = \{(x, y) \in \mathbb{Z}^2; x \in (n, n + l_1 - i], y \in (m, m + l_2]\} \quad (5.132)$$

To complete the construction we can use now the same idea applied in the definition of the reference path ω^* : between every pair $\{\bar{\omega}_i^{\eta, \underline{0}}\}, \{\bar{\omega}_{i+1}^{\eta, \underline{0}}\}$ we can insert a sequence $\{\tilde{\omega}_{i,0}^{\eta, \underline{0}}\}, \dots, \{\tilde{\omega}_{i,l_2}^{\eta, \underline{0}}\}$ where $\{\tilde{\omega}_{i,0}^{\eta, \underline{0}}\} = \{\bar{\omega}_i^{\eta, \underline{0}}\}$ and for $j > 0$, $\{\tilde{\omega}_{i,j}^{\eta, \underline{0}}\}$ is obtained by $\{\bar{\omega}_i^{\eta, \underline{0}}\}$ by erasing j sites:

$$\{\tilde{\omega}_{i,j}^{\eta, \underline{0}}\} = \{\bar{\omega}_i^{\eta, \underline{0}}\} \setminus \{(x, y) \in \mathbb{Z}^2; x = n + l_1 - i, y \in (m + l_2 - j, m + l_2]\} \quad (5.133)$$

Again, as in the reference path ω^* , the last interpolation consists in inserting between every pair of consecutive configurations in $\tilde{\omega}^{\eta, \underline{0}}$ a sequence of configurations with a free particle in a suitable sequence of sites going from the site previously occupied by the erased particle to $\partial\Lambda$. Since for any $l_1 \leq l_1^* - 1$ and

$l_2 \leq l_2^* - 1$ we have $H(R(l_1, l_2)) < H(R(l_1^* - 1, l_2^*))$, for the path $\omega^{\eta, \underline{0}}$ obtained in this way we have:

$$\max_i H(\omega_i^{\eta, \underline{0}}) = \max_{l \in [1, l_1 - 1]} H(R(l, l_2)) + 2\Delta - U_1 < \Gamma_{wa} \quad (5.134)$$

The proof of (ii) is similar. Let $C_{\underline{1}}$ be the maximal connected set containing $\underline{1}$ such that $\max_{\eta' \in C_{\underline{1}}} H(\eta') < \Gamma_{wa}$. Again $C_{\underline{1}}$ is by definition a cycle containing $\underline{1}$ and not containing $\underline{0}$ since $\Phi(\underline{0}, \underline{1}) = \Gamma_{wa}$. To prove that $C_{\underline{1}}$ contains η we define now a path $\omega^{\eta, \underline{1}}$ going from η to $\underline{1}$ obtained by reaching first of all the standard shape and, from there, following the path ω^* . As before, it is easy to show that all the configurations of this path have an energy smaller than Γ_{wa} so that they are in $C_{\underline{0}}$.

Going into the details, let $\eta \in R(l_1, l_2)$; let us suppose that $[l_1 + l_2 - \bar{l}]_2 = [0]_2$, since the other case, $[l_1 + l_2 - \bar{l}]_2 = [1]_2$, can be treated in a similar way. If $l_1 - l_2 = \bar{l}$ then η is standard and $\omega^{\eta, \underline{1}}$ can be chosen as the part of the reference path ω^* going from η to $\underline{1}$. If $l_1 - l_2 < \bar{l}$ then first add columns to η , with the mechanism similar to the time reversal of the one used in the construction of $\omega^{\eta, \underline{0}}$, until we reach the standard rectangle in $R(l_2 + \bar{l}, l_2)$. The remaining part of the path follows ω^* from $R(l_2 + \bar{l}, l_2)$ to $\underline{1}$. If $l_1 - l_2 > \bar{l}$ then first move columns to rows following the mechanism given in steps a.3 and b.2, until we reach a standard rectangle. From there, follow the reference path ω^* . For the path $\omega^{\eta, \underline{1}}$ obtained in this way, by using that in our parameter regime $\Delta + U_1 - U_2 < 2\Delta - U_1$, and that $H(R(l_1, l_2)) < H(R(l_1^* - 1, l_2^*))$, for any $l'_1 \geq l_1^*$ and $l'_2 \geq l_2^*$, we obtain:

$$\max_i H(\omega_i^{\eta, \underline{1}}) \leq \max_{l'_1 \geq l_1^*, l'_2 \geq l_2^*} H(R(l'_1, l'_2)) + 2\Delta - U_1 < \Gamma_{wa} \quad (5.135)$$

so that $\omega_i^{\eta, \underline{1}} \in C_{\underline{1}}$ for any i and the proof of theorem 5.3 is complete.

Chapter 6

Metastability for lattice gas model under Kawasaki dynamics: Strong Anisotropy

In this thesis we analyze metastability and nucleation in the context of a local version of the Kawasaki dynamics for the two-dimensional anisotropic Ising lattice gas at very low temperature. Let $\Lambda \subset \mathbb{Z}^2$ be a sufficiently large finite box. Particles perform simple exclusion on Λ , but when they occupy neighboring sites they feel a binding energy $-U_1 < 0$ in the horizontal direction and $-U_2 < 0$ in the vertical direction; we assume $U_1 \geq U_2$, and condition of strong anisotropy: $0 < \epsilon \ll U_2$ and $U_1 > 2U_2 - 2\epsilon$. Along each bond touching the boundary of Λ from the outside, particles are created with rate $\rho = e^{-\Delta\beta}$ and are annihilated with rate 1, where β is the inverse temperature and $\Delta > 0$ is an activity parameter. Thus, the boundary of Λ plays the role of an infinite gas reservoir with density ρ .

We take $\Delta \in (U_1, U_1 + U_2)$ where the totally empty (full) configuration can be naturally associated to metastability (stability). We investigate how the transition from empty to full takes place under the dynamics. In particular, we identify the size and some characteristics of the shape of the critical droplet and the time of its creation in the limit as $\beta \rightarrow \infty$. We compare the different behavior in the weakly or strongly anisotropic case. In both case we find that Wulff shape is not relevant for the nucleation pattern.

6.1 Definition of the Model and Main Results

Let $\Lambda \subset \mathbb{Z}^2$ be a finite box centered at the origin that will be chosen large enough. Let $\partial^-\Lambda$ be the interior boundary of Λ and let $\Lambda_0 = \Lambda \setminus \partial^-\Lambda$ be the interior of Λ . With each $x \in \Lambda$ we associate an occupation variable $\eta(x)$, as-

suming values 0 or 1. A lattice configuration is denoted by $\eta \in \mathcal{X} = \{0, 1\}^\Lambda$. We often identify η with its support, i.e. the set of occupied sites in η .

Each configuration $\eta \in \mathcal{X}$ has an energy given by the following Hamiltonian in

$$H(\eta) = -U_1 \sum_{(x,y) \in \Lambda_{0,h}^*} \eta(x)\eta(y) - U_2 \sum_{(x,y) \in \Lambda_{0,v}^*} \eta(x)\eta(y) + \Delta \sum_{x \in \Lambda} \eta(x) \quad (6.1)$$

where $\Lambda_{0,h}^*$ (resp. $\Lambda_{0,v}^*$) is the set of the horizontal (vertical) un-oriented bonds joining *n.n.* points in Λ_0 . Thus the interaction is acting only inside Λ_0 ; the binding energy associated to a horizontal (vertical) bond is $-U_1 < 0$, $(-U_2 < 0)$. We can suppose without loss of generality that $U_1 \geq U_2$. Recall the Kawasaki dynamics as in chapter 4, section 4.3.2.

6.1.1 Horizontal and Vertical Rectangles

We denote by $\mathcal{R}(l_1, l_2)$ the set of configurations whose single contour is a rectangle $R(l_1, l_2)$, with $l_1, l_2 \in N$. For any $\eta, \eta' \in \mathcal{R}(l_1, l_2)$ we have immediately

$$H(\eta) = H(\eta') = H(R(l_1, l_2)) = U_1 l_2 + U_2 l_1 - \epsilon l_1 l_2 \quad (6.2)$$

where

$$\epsilon := U_1 + U_2 - \Delta \quad (6.3)$$

A configuration η is *s-minimal* if it minimizes the energy in v_s , i.e., if it belongs to $F(v_s)$.

Definition 6.1. A rectangle $R(l_1, l_2)$ is called *(L)-Horizontal rectangle* if $l_2 = L$. i.e., $R(l_1, L)$.

Definition 6.2. Similarly a rectangle $R(l_1, l_2)$ is called *(L)-Vertical rectangle*, if $l_1 = L$. i.e., $R(L, l_2)$.

In this thesis, We show *(L)-Horizontal* and *(L)-Vertical* rectangles, $\mathcal{R}^{[L]-h}$ and $\mathcal{R}^{[L]-v}$, respectively.

As it will be clear in section 6.2; we do not need to introduce *Horizontal and Vertical* rectangles (see Fig. 6.4). They act an important role in constructing the *reference path*.

Note that: in this chapter we use the definition of **Domino and quasi domino rectangles** with the condition $1 \leq l_2 \leq l_2^*$.

6.1.2 Main Results for transition time

Let

$$\underline{0} = \{\eta \in \mathcal{X} : \eta(x) = 0 \ \forall x \in \Lambda\} \quad (6.4)$$

be the configuration with Λ empty and

$$\underline{1} = \{\eta \in \mathcal{X} : \eta(x) = 1 \ \forall x \in \Lambda_0, \ \eta(x) = 0 \ \forall x \in \Lambda \setminus \Lambda_0\} \quad (6.5)$$

be the configuration with Λ_0 full and $\Lambda \setminus \Lambda_0$ empty.

We write

$$\begin{aligned} \Gamma_{sa} &:= \Phi(\underline{1}, \underline{0}) - H(\underline{0}) = H(\mathcal{P}_{sa}) - H(\underline{0}) \\ &= U_1 l_2^* + U_2(2l_2^* - 3) - (U_1 + U_2 - \Delta)l_2^*(2l_2^* - 3) + 2\Delta - U_1 \\ &= U_1(l_2^* - 1) + U_2(2l_2^* - 1) \\ &\quad - (U_1 + U_2 - \Delta)(l_2^* - 1)(2l_2^* - 1) + \Delta - U_2 + U_1 \end{aligned} \quad (6.6)$$

Recall the definition of $\tau_{\underline{1}}$ from chapter 3.

Strong Anisotropy Condition

As discussed heuristically in section 6.2, the behavior of the model strongly depends on the different values of the parameters. In this chapter we assume *strong anisotropy*:

$$0 < \epsilon \ll U_2 \text{ and } U_1 > 2U_2 - 2\epsilon \quad (6.7)$$

where $\ll$ means sufficiently smaller; for instance $\epsilon \leq U_2/100$ is enough. Note that this is not a significant restriction since the case of large values of the critical sizes l_1^* , l_2^* is the relevant case from a physical point of view. The isotropic case $U_1 = U_2$ has been already treated in refs. [32] and [36] and chapter 4.

The main results about the asymptotic of the tunneling time and the gate to stability are contained in the following:

Theorem 6.3. *Let U_1, U_2, Δ be such that $U_2/(U_1 + U_2 - \Delta)$ is not integer and (6.7) holds. Let Λ be a box with side $L + 2$. For L sufficiently large and for any $\delta > 0$,*

$$\lim_{\beta \rightarrow \infty} P_{\underline{0}}(e^{\beta(\Gamma_{sa} - \delta)} \leq \tau_{\underline{1}} \leq e^{\beta(\Gamma_{sa} + \delta)}) = 1 \quad (6.8)$$

$$\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \log E_{\underline{0}} \tau_{\underline{1}} = \Gamma_{sa}, \quad (6.9)$$

and moreover if we define $T_\beta := \inf\{n \geq 1 : P_{\underline{0}}(\tau_{\underline{1}} \leq n) \geq 1 - e^{-1}\}$ then,

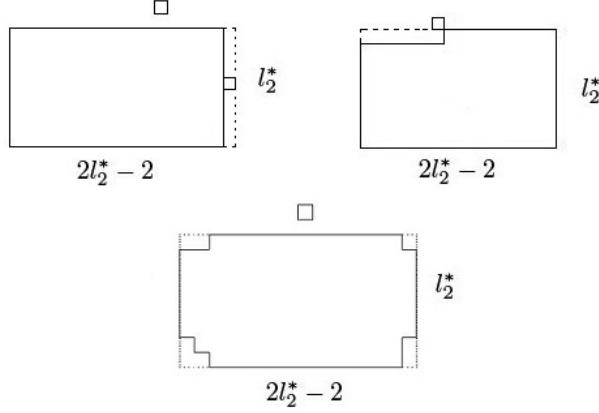
$$\lim_{\beta \rightarrow \infty} P_{\underline{0}}(\tau_{\underline{1}} > tT_\beta) = e^{-t} \quad (6.10)$$

and

$$\lim_{\beta \rightarrow \infty} \frac{E_{\underline{0}}(\tau_{\underline{1}})}{T_\beta} = 1 \quad (6.11)$$

Theorem 6.3, equation (6.8): For $\beta \rightarrow \infty$ the nucleation time from $\underline{0}$ to $\underline{1}$ behaves asymptotically, in probability, as $\Gamma_{sa}\beta + o(\beta)$.

Theorem 6.3 equations (6.8) and (6.10): The nucleation time from $\underline{0}$ to $\underline{1}$ has mean value asymptotically given, for large β , by $e^{\Gamma_{sa}\beta}$ and its distribution, after a suitable re scaling, is asymptotically exponential.

Figure 6.1: Configurations in $\mathcal{P}_{sa}$.

6.1.3 Main Results of the Gate

We write:

$$l_2^* = \lceil \frac{U_2}{U_1 + U_2 - \Delta} \rceil \quad (6.12)$$

$$s^* = 3l_2^* - 3 \quad (6.13)$$

with l_i^* , $i = 1, 2$ defined as in (5.25) (recall (5.13)). See Fig. 6.1 for an example of configuration in $\mathcal{P}_{sa}$. From (5.50), it follows that $H(\eta)$ is constant on $\mathcal{P}_{sa}$. and

$$\mathcal{P}_{sa} := \{\eta : n(\eta) = 1, v(\eta) = l_2^* - 1, \eta_{cl} \text{ is connected monotonic}$$

$$\text{and with circumscribed rectangles in } R(2l_2^* - 2, l_2^*)\} \quad (6.14)$$

Theorem 6.4. *Let U_1, U_2, Δ be such that $U_2/(U_1 + U_2 - \Delta)$ is not integer and (6.7) holds. Let Λ be a box with side $L + 2$. For L sufficiently large,*

$$\lim_{\beta \rightarrow \infty} P_{\underline{0}}(\theta_{\underline{0}, \underline{1}} < \theta_{\underline{0}, \mathcal{P}_{sa}, \underline{1}} < \tau_{\underline{1}}) = 1 \quad (6.15)$$

Theorem 6.4 says the the set $\mathcal{P}_{sa}$ is a gate for the nucleation: all paths from the metastable state $\underline{0}$ to the stable state $\underline{1}$ pass through this set with a probability tending to 1 as $\beta \rightarrow \infty$. Note that we do not establish in this theorem the minimality of the gate $\mathcal{P}_{sa}$ (see definition above), which would involve a much more detailed analysis.

Theorem 6.5. *Let U_1, U_2, Δ be such that $U_2/(U_1 + U_2 - \Delta)$ is not integer and (6.7) holds. Let Λ be a box with side $L + 2$ and let $\mathcal{R}^{\leq(l_1, l_2)}, \mathcal{R}^{\geq(l_1, l_2)}$ be the set of configurations whose single contour is a rectangle contained in (containing) a rectangle with sides l_1, l_2 . Then, for L sufficiently large,*

$$\begin{aligned} \text{if } \eta \in \mathcal{R}^{\leq(2l_2^*-1, l_2^*-1)} &\implies \lim_{\beta \rightarrow \infty} P_{\eta}(\tau_{\underline{0}} < \tau_{\underline{1}}) = 1 \\ \text{if } \eta \in \mathcal{R}^{\leq(2l_2^*-3, l_2^*)} &\implies \lim_{\beta \rightarrow \infty} P_{\eta}(\tau_{\underline{0}} < \tau_{\underline{1}}) = 1 \end{aligned} \quad (6.16)$$

$$\text{if } \eta \in \mathcal{R}^{\geq(2l_2^*-2, l_2^*)} \implies \lim_{\beta \rightarrow \infty} P_\eta(\tau_{\underline{1}} < \tau_{\underline{0}}) = 1 \quad (6.17)$$

Theorem 6.5, and equation (6.16) say that l_2^* is the critical sizes, i.e., sub-critical rectangles shrink to $\underline{0}$, while equation (6.17) says that super-critical rectangles grow to $\underline{1}$.

6.2 Heuristics

As we was in section 5.2.1 the static heuristic is not appropriate intuitively to justify the weak and strong anisotropic behavior. Therefore, here we begin with the following subsection.

6.2.1 Dynamic Heuristics

What follows is a heuristic discussion aimed to characterize the nucleation pattern. As we said in section 6.1 the locally conservative character of our dynamics makes difficult to determine, on rigorous grounds, the tube of typical trajectories realizing the transition from metastability to stability. However, we think that our heuristic arguments are quite convincing but, for a full proof, some more effort is needed. To help the reader we rewrite the first part of the section 5.2.2 which is needed to the comparison of the energy barriers in the strong anisotropic case given in formulas (6.19) and (6.21).

Key transitions

We start with a coarse graining description: we will restrict ourselves to determine the sequence of rectangles visited by typical trajectories. This is justified since, starting from any configuration, the process will relatively fast go to a rectangle and subsequently it will stay for a long period inside a cycle that plays the role of a generalized basin of attraction of this rectangle. The full tube should also specify the proper interpolation between contiguous rectangles. Our heuristic discussion will also include some information about these interpolations.

By the continuity properties of the dynamics it is reasonable to expect that only transitions between neighboring rectangles have to be taken into consideration. More precisely, starting from a configuration $\eta \in R(l_1, l_2)$, with $l_1, l_2 \geq 2$, the possible successive rectangles in the tube have to belong to one of the following classes: $R(l_1 + 1, l_2)$, $R(l_1, l_2 + 1)$, $R(l_1 - 1, l_2)$, $R(l_1, l_2 - 1)$, $R(l_1 - 1, l_2 + 1)$, and $R(l_1 + 1, l_2 - 1)$. So we shall consider the following transitions:

- From $R(l_1, l_2)$ to $R(l_1, l_2 + 1)$, corresponding to vertical growth, that will be denominated *add row* and symbolically denoted by the arrow $\uparrow$ pointing north direction.
- From $R(l_1, l_2)$ to $R(l_1 + 1, l_2)$, corresponding to horizontal growth, that will be denominated *add column* and denoted by the arrow $\rightarrow$ pointing east.

- From $R(l_1, l_2)$ to $R(l_1 + 1, l_2)$, corresponding to horizontal growth, that will be denominated *add column* and denoted by the arrow $\rightarrow$ pointing east.
- From $R(l_1, l_2)$ to $R(l_1, l_2 - 1)$, corresponding to vertical contraction, that will be denominated *remove row* and denoted by the arrow $\downarrow$ pointing south.
- From $R(l_1, l_2)$ to $R(l_1 - 1, l_2)$, corresponding to horizontal contraction, that will be denominated *remove column* and denoted by the arrow $\leftarrow$ pointing west.
- From $R(l_1, l_2)$ to $R(l_1 - 1, l_2 + 1)$, corresponding to a readjustment of the edges, making higher and narrower the rectangle by removing a column and simultaneously adding a row. It will be denominated *column to row* and denoted by the arrow $\nwarrow$ pointing northwest.
- From $R(l_1, l_2)$ to $R(l_1 + 1, l_2 - 1)$, corresponding to a readjustment opposite to the previous one. It will be denominated *row to column* and denoted by the arrow $\searrow$ pointing southeast.

The transition from $R(l_1, l_2)$ to $R(l_1 - 1, l_2 - 1)$ and $R(l_1 + 1, l_2 + 1)$ are not considered as elementary since, as it can be easily seen, a suitable combination of two of the above transitions takes place with larger probability.

At first sight the optimal interpolation paths realizing the above transitions between contiguous rectangles are the ones depicted in Figs. 6.2-4. Let us call $\Omega^{(1)}$ the set of paths as the one depicted in Fig. 6.2. They are the natural candidates to realize, in an optimal way, the transition $\uparrow$. For the transition $\rightarrow$ we have an analogous set of paths that we call $\Omega^{(1)}$.

Let us call B the time-reversal operator acting on finite paths; we have for $\omega = \omega_1, \dots, \omega_T$

$$B\omega = \omega', \text{ with } \omega'_i = \omega_{T+1-i}, \quad i = 1, \dots, T \quad (6.18)$$

For the transition $\downarrow$ we choose the set of paths $\Omega^{(3)}$ obtained by time reversal from the paths, analogous to the ones in $\Omega^{(1)}$, that realize the transition $R(l_1 - 1, l_2)$ to $R(l_1, l_2)$.

Similarly, for the transition $\leftarrow$ we use the set of paths $\Omega^{(4)}$ obtained by time-reversal from the paths, analogous to the ones in $\Omega^{(3)}$, that realize the transition $R(l_1, l_2 - 1)$ to $R(l_1, l_2)$. The set of paths that we consider as the optimal interpolation for the transition from $R(l_1, l_2)$ to $R(l_1 - 1, l_2 + 1)$ in the two cases $l_1 < l_2$, $l_1 \geq l_2$, are called $\Omega^{(5)}$ and $\bar{\Omega}^{(5)}$, respectively. A path in $\bar{\Omega}^{(5)}$ is represented in Fig. 3. where each arrow corresponds to a move and the quantities under the arrows represent the corresponding energy barriers ΔH . Dotted arrows indicate sequences of moves. The maximal energy along the path is reached in the configuration (2). A path in $\Omega^{(5)}$ is represented in Fig. 4 where to simplify we indicate under the dotted arrows the sum of the corresponding ΔH . Along this path the maximal energy is reached in configuration (5). In a similar way we define the optimal interpolation paths $\Omega^{(7)}$ and $\bar{\Omega}^{(7)}$ for the transition from $R(l_1, l_2)$ to $R(l_1 + 1, l_2 - 1)$. We call canonical the paths in the above sets.

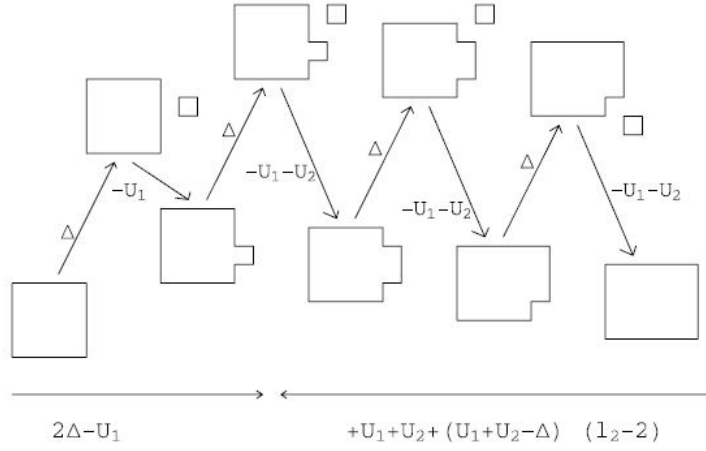
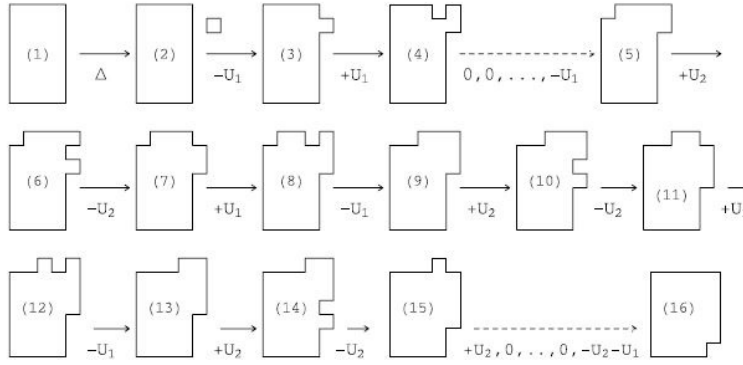


Figure 6.2: The procedure to grow a column

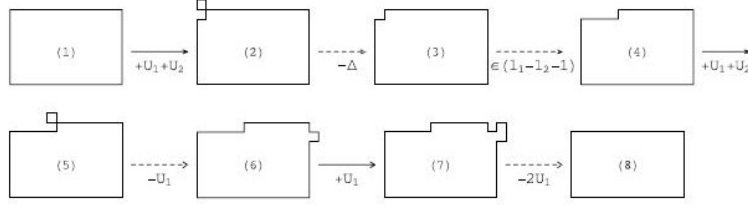
Figure 6.3: A path in $\Omega^{(5)}$.

Given (l_1, l_2) , to determine the most probable transition between $R(l_1, l_2)$ and one of the previous six contiguous rectangles, we will use the criterion of the smallest energy barrier, defined as the difference between the communication height and $H(R(l_1, l_2))$. We call *energy barrier from η to η'* along the path $= (\omega_1 = \eta, \dots, \omega_n = \eta')$ the difference between the maximal height reached along this path and $H(\eta)$. We compute the energy barriers along the canonical paths and we use them to estimate the true energy barriers. We denote by $\Delta H(\text{add row})$ the energy barrier along the paths in $\Omega^{(1)}$; similarly for the other transitions.

From Figs. 6.2-4 via easy computations, we get:

$$\Delta H(\text{add row}) = 2\Delta - U_2$$

$$\Delta H(\text{add column}) = 2\Delta - U_1$$

Figure 6.4: A path in $\bar{\Omega}^{(5)}$.

$$\begin{aligned}
\Delta H(\text{remove row}) &= \epsilon(l_1 - 2) + U_1 + U_2 \\
\Delta H(\text{remove column}) &= \epsilon(l_2 - 2) + U_1 + U_2 \\
\Delta H(\text{row to column}) &= \Delta \text{ if } l_1 < l_2 \\
\Delta H(\text{row to column}) &= \epsilon(l_1 - l_2) + U_1 + U_2 \text{ if } l_1 \geq l_2 \\
\Delta H(\text{column to row}) &= \Delta - U_2 + U_1 \text{ if } l_1 < l_2 \\
\Delta H(\text{column to row}) &= \Delta - U_2 + U_1 + \epsilon(l_2 - l_1 + 1) \text{ if } l_1 \geq l_2
\end{aligned} \tag{6.19}$$

These estimated energy barriers are, of course, larger than or equal to the true ones; the equality does not hold in general, since the above canonical paths sometimes happen to be non-optimal. For example, a deeper analysis leads to the conclusion that to add a row, instead of using a path in $\bar{\Omega}^{(1)}$, it is more convenient to compose $\Omega^{(2)}$ and $\Omega^{(5)}$, resp. $\bar{\Omega}^{(5)}$, when $l_1 < l_2$, resp. $l_1 \geq l_2$.

Let us now make a comparison in case of strong anisotropy

$$U_1 > 2U_2 - 2\epsilon, \tag{6.20}$$

corresponding to strong anisotropy where, since

$$\begin{aligned}
2\Delta - U_1 &< 2\Delta - U_2, \quad 2\Delta - U_1 < \Delta - U_2 + U_1 \text{ and} \\
U_1 + U_2 + \epsilon(l_2 - 2) &< U_1 + U_2 + \epsilon(l_1 - 2)
\end{aligned} \tag{6.21}$$

we deduce that we have only to compare $\Delta H(\text{remove column})$, $\Delta H(\text{add column})$, and $\Delta H(\text{row to column})$. We get

$$\Delta H(\text{remove column}) < \Delta H(\text{add column}) \iff l_2 < l_2^*, \tag{6.22}$$

$$\Delta H(\text{row to column}) < \Delta H(\text{add column}) \iff l_1 < l_2 + l_2^* - 2. \tag{6.23}$$

We have immediately that: in the set $A' = \{l_2 \leq l_2^* - 1, l_1 > 2l_2 - 2\}$ the minimal estimated energy barrier is $\Delta H(\text{remove column})$;

In the set $B' = \{l_1 < l_2 + l_2^* - 2, l_1 < 2l_2 - 2\}$ the minimal estimated energy barrier is $\Delta H(\text{row to column})$;

In the set $C' = \{l_2 \geq l_2^*, l_1 \geq l_2 + l_2^* - 2\} \cup \{l_1 \leq l_2\}$ the minimal estimated energy barrier is $\Delta H(\text{add column})$.

In the set $D' = \{l_2 \leq l_2^* - 1, l_1 = 2l_2 - 2\}$ we have degeneracy of the minimal estimated energy barrier: $\Delta H(\text{remove column}) = \Delta H(\text{row to column})$.

Note that $B' = \{l_2 \leq l_2^* - 1, l_1 < 2l_2 - 2\} \cup \{l_2 \geq l_2^*, l_1 < l_2 + l_2^* - 2\}$, so that again $A' \cup B' \cup C' \cup D' = \{l_1 > l_2\}$. We visualize these results in Fig. 6.1, using the same graphical representation introduced in the case weak anisotropy.

In the strongly anisotropic case, from Fig. 6.2, it is evident that in the plane (l_1, l_2) there is a connected attractive region T' consisting of three parts $T'_1 = \{(l_1, l_2) : l_2 < l_2^* \text{ and } 2l_2 - 3 \leq l_1 \leq 2l_2 - 1\} \cup R(2l_2^* - 3, l_2^*)$ containing domino shape rectangles, $T'_2 = \{(l_1, l_2) : l_2 = l_2^* \text{ and } l_2 + l_2^* - 2 \leq l_1 < L\}$, and $T'_3 = \{(l_1, l_2) : l_2^* \leq l_2 \text{ and } L - 1 \leq l_1 \leq L\}$.

The properties of T'_1 can be discussed in analogy with the weakly anisotropic case. For every configuration in T'_2 the minimal estimated energy barrier is $\Delta H(\text{add column})$, which implies that the rectangles in T'_2 will indefinitely grow in the horizontal direction until they become a complete horizontal strip with length L .

In T'_3 the minimal estimated energy barrier is $\Delta H(\text{add row})$, which implies that every horizontal strip with $l_1 = L$ will indefinitely grow in the vertical direction until it covers the whole box.

As in the previous case we can deduce from this discussion a conjecture on the tube of typical paths during the first excursion from $\underline{0}$ to $\underline{1}$.

As far as the strongly anisotropic case is concerned we do not have rigorous results; in particular we do not know any gate for the transition from $\underline{0}$ to $\underline{1}$ but we expect that the first super-critical rectangular configuration is contained in $R(2l_2^* - 2, l_2^*)$. We can construct, like before, a cycle path T'_{sub} describing the tube of typical paths going from the maximal sub-critical rectangles in $R(2l_2^* - 3, l_2^*) \cup R(2l_2^* - 1, l_2^* - 1)$ to $\underline{0}$ and a cycle path T'_{sup} going from the minimal super-critical rectangles in $R(2l_2^* - 2, l_2^*)$ to $\underline{1}$. Like in the weakly anisotropic case the tube of typical nucleating paths, describing the first excursion from $\underline{0}$ to $\underline{1}$, can be obtained by suitably joining the time-reversed of T'_{sub} with T'_{sup} .

Summarizing: the nucleation pattern in the strongly anisotropic case contains a sequence of increasing domino shaped rectangles up to $R(2l_2^* - 2, l_2^*)$; then a sequence of rectangles with $l_2 = l_2^*$ and l_1 going up to L (the size of the container); finally a sequences of horizontal strips whose width grows from l_2^* to L . We can say that the nucleation pattern, in the strongly anisotropic case, is T'_2 very similar to the one that we would have for non-conservative Glauber dynamics for any anisotropy.

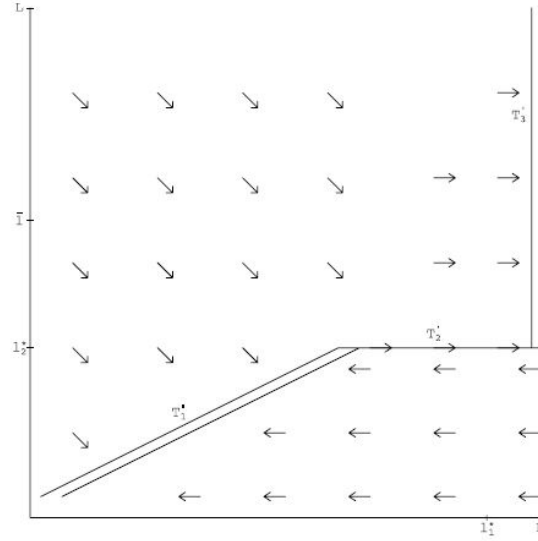


Figure 6.5: Strong anisotropy: minimal transitions and tube of typical trajectories.

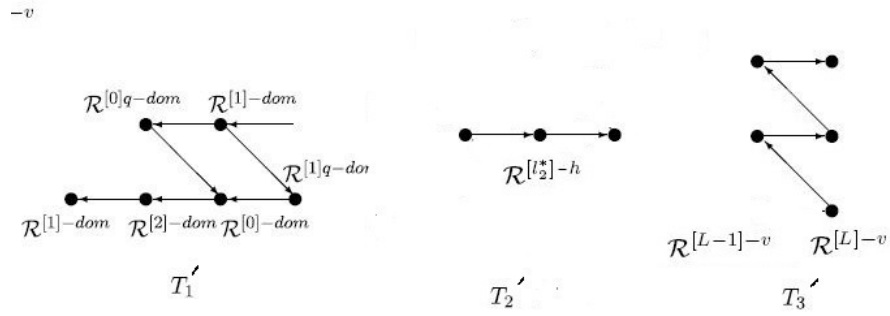


Figure 6.6: We introduce the minimal saddles with arrows between them: first picture T_1' for $s^* \leq 3l_2^* - 3$, second picture T_2' if $3l_2^* \leq s^* \leq L + 3l_2^*$, and third picture T_3' if $s^* \geq L + 3l_2^*$.

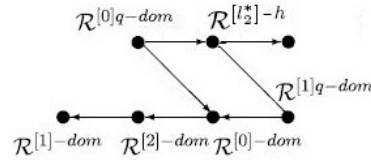


Figure 6.7: Minimal Saddles for $3l_2^* - 3 \leq s^* \leq 3l_2^* - 1$

6.3 Proofs of the theorems for the Transition time

In order to prove theorem 6.3, and 6.4 we will follow the strategy explained at the beginning of the section 2.11. For what concern the definition of the reference path is important to recall formula (2.83). Using the theorem 2.43, theorem 2.46, theorem 2.47, and theorem 2.49, we obtain theorems 6.3, and theorem 6.4 as an immediate consequence of the following:

- (a) $H(\mathcal{P}_{sa}) =: \Gamma = \Phi(\underline{0}, \underline{1})$,
- (b) there exists $\Gamma_0 < \Gamma_{sa}$ such that $\mathcal{X}_{\Gamma_0} \subseteq \{\underline{0}, \underline{1}\}$,
- (c) $\mathcal{P}_{sa}$ is a gate for the transition $\underline{0} \rightarrow \underline{1}$.

Point (a) means that we are able to compute explicitly the communication height between $\underline{0}$ and $\underline{1}$.

Point (b) means that each configuration $\eta \notin \{\underline{0}, \underline{1}\}$ is Γ_0 -reducible i.e., we can find a configuration with smaller energy, $\eta' \in \psi_\eta$, with $\Phi(\eta, \eta') \leq H(\eta) + \Gamma_0$. In other words, there are no too deep wells in the energy landscape, no deeper than the well with bottom $\underline{0}$. We will call *reduction* this step of the proof treated in section 6.4.1.

To prove (a) and (c) the general strategy is to find a suitable set of states $\mathcal{B}_{sa}$ containing $\underline{0}$ and not containing $\underline{1}$ so that $\partial\mathcal{B}_{sa}$ has to be crossed by every path going from $\underline{0}$ to $\underline{1}$ (see section 6.3.2). Moreover we find a reference path $\omega^* : \underline{0} \rightarrow \underline{1}$ (see section 6.3.1) such that the maximum of the energy in ω^* is reached when crossing $\partial\mathcal{B}_{sa}$ and this maximal energy in ω^* is equal to $H_{min}(\partial\mathcal{B}_{sa})$. As shown in section 6.3.3, these two ingredients are sufficient to determine the communication height $(\underline{0}, \underline{1})$. Moreover by characterizing geometrically the moves producing the crossing of $\partial\mathcal{B}_{sa}$, we will obtain the gate for the transition $\underline{0} \rightarrow \underline{1}$. In section we will prove point (b) and we will also easily show that (a) and (b) imply that $\bar{\Gamma} := V_{\underline{0}} = (\underline{0}, \underline{1}) = \Gamma_{sa}$ and $\underline{0} = \mathcal{X}^m$ and $\underline{1} = \mathcal{X}^s$, if the side L of the volume Λ is large enough. Theorems 6.3, and 6.4 are therefore immediate consequences of theorems 2.43, 2.46, 2.47, and 2.49.

In section 6.4.1, we prove a preliminary result on configurations of minimal energy at given s . The proof of theorem 6.5 is obtained in section 6.4.3.

6.3.1 Construction of the reference path

We construct now a particular reference path $\omega^* : \underline{0} \rightarrow \underline{1}$ that will be the proof of theorems 6.3, and 6.4. It will be given by a particular sequence of growing domino, l_2^* -horizontal and L -vertical rectangles, such that the maximum of the energy on ω^* , $\{arg \max_{\omega^*} H\}$, is reached on particular configurations called critical configurations given by a rectangle $R(2l_2^* - 3, l_2^*)$ with a protuberance on the shorter side and a free particle.

We will prove in section 6.3.3 that $\omega^* \in (\underline{0} \rightarrow \underline{1})_{opt}$ so that $\{arg \max_{\omega^*} H\} \subset$

$S(\underline{0}, \underline{1})$. We want to recall here that in this thesis we get only a partial solution to the problem of the determination of the tube of typical paths, i.e., the set of paths followed by the process with high probability during the transition from $\underline{0}$ to $\underline{1}$. It is easy to prove that a typical path is in the set $(\underline{0} \rightarrow \underline{1})_{opt}$. Note that this set is much larger than the tube of typical paths. However, we conjecture that the path ω^* , that we are going to construct, is not only optimal but also it suggests the structure of the tube of typical paths.

The idea of the construction of ω^* is the following: we first construct a skeleton path $\{\bar{\omega}_s\}_{s=2}^{2L}$ given by a sequence of rectangles with semi-perimeter s . For $s \leq 3l_2^* - 3$ these are domino rectangles (of type 0, 1, or 2) and for $3l_2^* - 2 \leq s \leq L + l_2^*$ these are (l_2^*) -horizontal rectangles (the rectangles satisfying $l_2 = l_2^*$) and for $L + l_2^* \leq s \leq 2L$ are L or $L - 1$ -vertical rectangles (the rectangles satisfying $l_1 = L$ or $l_1 = L - 1$). Obviously $\bar{\omega}_s$ is not a path in the sense that the transition from $\bar{\omega}_s$ to $\bar{\omega}_{s+1}$ can not be given in a single step of the dynamics, since $\bar{\omega}_s$ and $\bar{\omega}_{s+1}$ are rectangles. Thus to obtain a path we have to interpolate each transition of the skeleton path $\bar{\omega}$. This is done in two different steps. We first introduce between $\bar{\omega}_s$ and $\bar{\omega}_{s+1}$ a sequence of configurations $\tilde{\omega}_{s,1}, \dots, \tilde{\omega}_{s,i_s}$, is given by $\bar{\omega}_s$ plus a growing row or column; again these configurations are given by a single increasing droplet. This step is non-trivial since, as explained in more detail later on, there are cases in which to grow a row we first grow a column and then we move this column to a new row with a motion along the border of the droplet. Indeed it turns out that this is more convenient from an energetic point of view and this strategy is crucial near the boundary from $\mathcal{B}$ (see proof of theorems 6.3 and 6.4). The last interpolation, to obtain from the sequence of configurations $\tilde{\omega}_{s,i}$ a path ω^* , i.e., with $P(\omega_j^*, \omega_{j+1}^*) > 0$, consists in inserting between every couple of consecutive configurations in $\tilde{\omega}$ for which the cluster is increased by one particle, a sequence of configurations with a new particle initially created at the boundary of the box and then brought to the correct site with a sequence of consecutive moves of this free particle.

Skeleton: $\bar{\omega}$

Let us construct a sequence of rectangular configurations $\bar{\omega} = \{\bar{\omega}_s\}$ with $s = 0, \dots, 2L$, i.e.,

$$\bar{\omega}_1 = \underline{0}, \quad \bar{\omega}_2 = \{x_0\}, \dots, \quad \bar{\omega}_{2L} = F(\mathcal{X}) \in \underline{1} \quad (6.24)$$

Step a. For any $s \leq 3l_2^* - 3$, $\{\bar{\omega}_s\}$ is a growing sequence of domino rectangles, depending on the value of s . Indeed, if $[s]_3 = [0]_3$ in $\mathcal{Z}_3$, i.e., $s = 3l_2$ for some $l_2 \leq l_2^*$, we have $\bar{\omega}_s \in R(2l_2, l_2)$ is a 0-domino rectangle; if $[s]_3 = [1]_3$ in $\mathcal{Z}_3$, i.e., $s = 3l_2 - 2$ for some l_2 , we have $\bar{\omega}_s \in R(2l_2 - 2, l_2)$ is a 1-domino rectangle; if $[s]_3 = [2]_3$ in $\mathcal{Z}_3$, i.e., $s = 3l_2 - 1$ for some l_2 , we have $\bar{\omega}_s \in R(2l_2 - 1, l_2)$ is a 2-domino rectangle.

Step b. For $3l_2^* - 2 \leq s \leq L + l_2^*$, $\{\bar{\omega}_s\}$ is a growing sequence of (l_2^*) -horizontal rectangles. We add a vertical column as in Fig. 6.2 until we reach $\tilde{\omega}_{s,i_s} \in R(L - 1, l_2^*)$.

Step c. For $s \geq L + l_2^*$, $\{\bar{\omega}_s\} \in R(L, s - L)$. $(L - 1)$ and (L) -vertical rectangles.

First interpolation: $\tilde{\omega}$

For any choice for $\bar{\omega}_s$, we can construct the path $\tilde{\omega}_{s,i}$ such that $\tilde{\omega}_{s,0} = \bar{\omega}_s$ and between each pair $(\tilde{\omega}_s, \tilde{\omega}_{s+1})$, $\forall s$ we insert a sequence of configurations $\tilde{\omega}_{s,i}$ for $i = 0, 1, \dots, i_s$.

Step a.1 If $s \leq 3l_2^* - 3$ and $[s]_3 = [1]_3$ add a vertical column as in Fig. 6.2 passing from $\tilde{\omega}_{s,0} \in R(2l_2, l_2 + 1)$ to the 2-domino rectangle $\tilde{\omega}_{s,i_s} \in R(2l_2 + 1, l_2 + 1)$. More precisely $\tilde{\omega}_{s,1}$ is the configuration obtained creating a particle on the column (as in Fig. 6.2). We repeat this step for other $l_2 - 1$ particles that are created in the same column, so the configuration $\tilde{\omega}_{s,i_s} \in R(2l_2 + 1, l_2 + 1)$ is a 2-domino rectangle.

step a.2 If $s \leq 3l_2^* - 3$ and $[s]_3 = [2]_3$ add a vertical column as in Fig. 6.2 passing from $\tilde{\omega}_{s,0} \in R(2l_2 - 1, l_2)$ to $\tilde{\omega}_{s,i_s} \in R(2l_2, l_2)$ that is a 0-domino rectangle.

Step a.3 If $s \leq 3l_2^* - 3$ and $[s]_3 = [0]_3$ add a vertical column as in Fig. 6.2 passing from $\tilde{\omega}_{s,0} \in R(2l_2, l_2)$ to the quasi-domino rectangle $\tilde{\omega}_{s,l_2} \in R(2l_2 + 1, l_2)$ as described in the previous case a.1. Then use the path described in Fig. 6.4 (move a column to a row following the reverse path of Fig. 6.4) to define the path from $\tilde{\omega}_{s,l_2} \in R(2l_2 + 1, l_2)$ to $\tilde{\omega}_{s,i_s} \in R(2l_2, l_2 + 1)$ that is a 1-domino rectangle.

Step b.1 If $3l_2^* - 2 \leq s \leq L + l_2^*$ and $l_2 = l_2^*$ we have $\bar{\omega}_s \in R(2l_2^* - 1, l_2^*)$, add a vertical column as in Fig. 6.2 to obtain $\tilde{\omega}_{s,i_s} \in R(L - 1, l_2^*)$.

Step c.1 Use first the path given by the time-reversal of the one represented in Fig. 6.4 to define a first interpolation between $R(L, s - L) = \bar{\omega}_s$ and $R(L - 1, s - L + 1)$, and then use the path described in Fig. 6.2 to add a column to $R(L - 1, s - L + 1)$ in order to reach $R(L, s - L + 1) = \bar{\omega}_{s+1}$.

Second interpolation: ω^*

For any pair of configurations $(\tilde{\omega}_{s,i}, \tilde{\omega}_{s,i+1})$ such that $|\tilde{\omega}_{s,i}| < |\tilde{\omega}_{s,i+1}|$, by construction of the path $\tilde{\omega}_{s,i}$ the particles are created along the external boundary of the clusters. So there exists $x_1, \dots, x_{j_i}$ a connected chain of nearest neighbor empty sites of $\tilde{\omega}_{s,i}$ such that $x_1 \in \partial^- \Delta$ and x_{j_i} is the site where is located the additional particle in $\tilde{\omega}_{s,i+1}$.

Define the following:

$$\omega_{s,i,0}^* = \tilde{\omega}_{s,i}, \quad \omega_{s,i,j_i}^* = \tilde{\omega}_{s,i+1}, \quad \forall s = 0, \dots, 2(L + 2) \quad (6.25)$$

Insert between each pair $(\tilde{\omega}_{s,i}, \tilde{\omega}_{s,i+1})$, a sequence of configurations $\omega_{s,i,j}^*$, for $j = 1, \dots, j_i - 1$, where the free particle is moving from $x_1 \in \partial^- \Delta$ to the cluster until it reaches the position x_{j_i} .

Otherwise for any pair of configurations $(\tilde{\omega}_i, \tilde{\omega}_{i+1})$ such that $|\tilde{\omega}_{s,i}| = |\tilde{\omega}_{s,i+1}|$, we define $\omega_{s,i,0}^* = \tilde{\omega}_{s,i}$; $\omega_{s,i+1,0}^* = \tilde{\omega}_{s,i+1}$. This conclude the definition of the reference path.

We want now to describe in more details the reference path $\omega_{s,i,j}^*$ near the critical value $s^* = 3l_2^* - 3$.

Lemma 6.6. (i) *The energy function $H(R(2l_2^* + t, l_2^*))$ with $-3 < t < L - 2l_2^*$, is a decreasing function.*

(ii) *The energy function $H(R(2l_2^* + t, l_2^* - 1))$ with $-3 < t < L - 2l_2^*$, is an increasing function.*

(iii) *The energy function $H(R(s^*)) = H(R(3l_2^* - 3 - l_2, l_2))$ with $s^* = 3l_2^* - 3$ for $l_2 \geq l_2^* - 1$, is an increasing function.*

(iv) *The energy function $H(R(s^* - 1)) = H(R(3l_2^* - 4 - l_2, l_2))$ with $s^* - 1 = 3l_2^* - 4$ for $l_2 \geq l_2^* - 1$,*

(v) *The energy function $H(R(s^* - 2)) = H(R(3l_2^* - 5 - l_2, l_2))$ with $s^* - 2 = 3l_2^* - 5$ for $l_2 \geq l_2^* - 1$,*

(vi) *The energy function $H(R(s^* - 3)) = H(R(3l_2^* - 6 - l_2, l_2))$ with $s^* - 3 = 3l_2^* - 6$ for $l_2 \geq l_2^* - 1$,*

Proof. (i) Since $T_2' = \{(l_1, l_2) : l_2 = l_2^* \text{ and } l_2 + l_2^* - 2 \leq l_1 < L\}$ the set of l_2^* -horizontal rectangles. The energy function is:

$$\begin{aligned} H(R(2l_2^* + t, l_2^*)) &= U_1(2l_2^* + t) + U_2l_2^* - \epsilon l_2^*(2l_2^* + t) \\ &= (2U_1 + U_2)l_2^* - 2\epsilon l_2^{*2} + (U_2 - \epsilon l_2^*)t \end{aligned} \quad (6.26)$$

which is a line with negative slope $(U_2 - \epsilon l_2^*)$.

(ii) For $(l_2^* - 1)$ -horizontal rectangles with apply same the argument i.e.,

$$\begin{aligned} H(R(2l_2^* + t, l_2^* - 1)) &= U_1(2l_2^* + t) + U_2l_2^* - \epsilon l_2^*(2l_2^* + t) \\ &= U_1(l_2^* - 1) + U_2(2l_2^* + t) - \epsilon(l_2^* - 1)2(l_2^* + t) \\ &\quad tU_2 - \epsilon(2l_2^{*2} + (t - 2)l_2^* - t) \\ &= U_1l_2^* - U_1 + 2U_2l_2^* - \epsilon 2l_2^{*2} + 4\epsilon l_2^* \\ &\quad + tU_2 + t\epsilon - \epsilon(t - 2)l_2^* \\ &= -2\epsilon l_2^{*2} + (U_1 + 2U_2 + 4\epsilon)l_2^* - U_1 + t(U_2 + \epsilon - \epsilon l_2^*) \end{aligned}$$

Which is a line with a positive slope $(U_2 + \epsilon(1 - l_2^*))$.

(iii) The energy function is a parabola.

$$\begin{aligned} H(R(s^*)) &= H(R(3l_2^* - 3 - l_2, l_2)) = U_1l_2 + U_2(3l_2^* - 3 - l_2) - \epsilon l_2(3l_2^* - 3 - l_2) \\ &= \epsilon(l_2)^2 + (U_1 - U_2 + 3\epsilon)l_2 - 3U_2 + 3U_2l_2^* \end{aligned} \quad (6.27)$$

That reaches it minimum in $l_0 = \frac{U_2 - U_1 - 3\epsilon}{2\epsilon}$, since $l_2^* - 1 > l_0$. we conclude the result.

(iv)

$$\begin{aligned}
H(R(s^*+1)) &= H(R(3l_2^*-2-l_2, l_2)) = U_1 l_2 + U_2(3l_2^*-2-l_2) - \epsilon l_2(3l_2^*-2-l_2) \\
&= \epsilon(l_2)^2 + (U_1 - U_2 + 2\epsilon)l_2 - 2U_2 + 3U_2 l_2^*. \tag{6.28}
\end{aligned}$$

As a function on $\mathcal{R}$, $H(R(s^*))$ reaches its minimum in reaches it minimum in $l_0 = \frac{U_2 - U_1 - 2\epsilon}{2\epsilon}$; moreover its graph is a parabola w.r.t the axis $x = l_0$, since $l_2^* - 1 > l_0$ we conclude the result. We use the same argument to prove (iv) until (viii). $\square$

Recall the definition of Domino and quasi domino rectangles from chapter 5.

Lemma 6.7. *On T_1' the energy of domino and quasi domino configurations is an increasing function of n , for $s \leq 3l_2^* - 3$.*

More precisely the five functions:

(i)

$$\begin{aligned}
h^{(0-dom)}(n) &:= H(R(2n, n)) = (U_1 + 2U_2)n - 2\epsilon n^2, \\
n &= 2, \dots, l_2^* - 1, \tag{6.29}
\end{aligned}$$

(ii)

$$\begin{aligned}
h^{(1-dom)}(n) &:= H(R(2n-2, n)) = nU_1 + 2U_2(n-1) - 2\epsilon n(n-1) \\
n &= 2, \dots, l_2^* - 1, \tag{6.30}
\end{aligned}$$

(iii)

$$\begin{aligned}
h^{(2-dom)}(n) &:= H(R(2n-1, n)) = nU_1 + U_2(2n-1) - \epsilon n(2n-1), \\
n &= 2, \dots, l_2^* - 1, \tag{6.31}
\end{aligned}$$

(iv)

$$\begin{aligned}
h^{(0q-dom)}(n) &:= H(R(2n-3, n)) = nU_1 + U_2(2n-3) - \epsilon n(2n-3), \\
n &= 2, \dots, l_2^*, \tag{6.32}
\end{aligned}$$

(v)

$$\begin{aligned}
h^{(1q-dom)}(n) &:= H(R(2n+1, n)) = nU_1 + U_2(2n+1) - \epsilon n(2n+1), \\
n &= 0, \dots, l_2^* - 1, \tag{6.33}
\end{aligned}$$

are increasing functions of n .

Proof. Recall the definition of domino rectangles from chapter 5.

The function

$$h^{(0-dom)}(n) := H(R^{0-dom}(3n)) = (U_1 + 2U_2)n - 2\epsilon n^2, \quad n = 0, \dots, l_2^* - 1, \quad (6.34)$$

As a function on $\mathcal{R}$, $h^{(0-dom)}(n)$ has its maximum in $n_0 = \frac{U_1 + 2U_2}{4\epsilon}$. Moreover its graph is a parabola symmetric w.r.t the axis $x = n_0$.

Claim

$$l_2^* - 1 \leq \frac{U_1 + 2U_2}{4\epsilon}$$

Since $l_2^* = \lceil \frac{U_2}{\epsilon} \rceil$ we have:

$$l_2^* = \frac{U_2}{\epsilon} + 1 - \delta$$

for some positive δ Hence,

$$\frac{U_2}{\epsilon} + 1 - \delta - 1 \leq \frac{U_1 + 2U_2}{4\epsilon}$$

Since ϵ is positive we have:

$$2U_2 - \delta\epsilon \leq U_1$$

which is correct by strong anisotropy condition.

The claim has been proved; therefore, our energy function is ascending on $n = 0, \dots, l_2^* - 1$.

For 1-domino, 2-domino, 0q-domino, and 1q-domino rectangles we apply the same argument. $\square$

Remark 6.8. (i) In the reference path ω^* the l_2^* -rectangle regime starts before s^* :

$$s^* = 3l_2^* - 3 \quad (6.35)$$

(ii) The domino and quasi domino rectangle with semi-perimeter s^* have sides:

$$\begin{aligned} l_1(s^*) &= 2l_2^* - 3, \quad l_2(s^*) = l_2^*, \quad \text{if } 0q\text{-domino}, \\ l_1(s^*) &= 2l_2^* - 2, \quad l_2(s^*) = l_2^* - 1, \quad \text{if } 0\text{-domino}. \end{aligned} \quad (6.36)$$

(iii) The domino and quasi domino rectangles with semi-perimeter $s^* + 1$ have sides

$$\begin{aligned} l_1(s^* + 1) &= 2l_1^* - 2, \quad l_2(s^* + 1) = l_2^* \quad \text{if } 1\text{-domino}, \\ l_1(s^* + 1) &= 2l_1^* - 1, \quad l_2(s^* + 1) = l_2^* - 1, \quad \text{if } 1q\text{-domino}. \end{aligned} \quad (6.37)$$

(iv) The domino rectangle with semi-perimeter $s^* - 1$ has sides $l_1(s^* - 1) = 2l_2^* - 3$ and $l_2(s^* - 1) = l_2^* - 1$ if 1-domino.

Proposition 6.9. *If the hypothesis (S.A) holds, we have: On the reference path the rectangle which has the maximal energy is: $R(2l_2^* - 3, l_2^*)$. i. e.,*

$$\operatorname{argmax}_{R \in \{R^{dom} \cup R^{[l_2^*] - h} \cup R^{[L] - v}\}} H(R) = R(2l_2^* - 3, l_2^*) \quad (6.38)$$

Proof. To prove lets first assume $s \leq 3l_2^* - 3$.

- (a) By lemma 6.7 (i) the maximal energy for 0-domino rectangles happens on $R(2l_2^* - 2, l_2^* - 1)$ and $H(R(2l_2^* - 3, l_2^*)) > H(R(2l_2^* - 2, l_2^* - 1))$.
- (b) By lemma 6.7 (ii) the maximal energy for 1-domino rectangles happens on $R(2l_2^* - 3, l_2^* - 1)$ and $H(R(2l_2^* - 3, l_2^*)) > H(R(2l_2^* - 3, l_2^* - 1))$.
- (b) By lemma 6.7 (v) the maximal energy for 1q-domino rectangles happens on $R(2l_2^* - 1, l_2^* - 1)$ and $H(R(2l_2^* - 3, l_2^*)) > H(R(2l_2^* - 1, l_2^* - 1))$.
- (c) By lemma 6.6 (i) $H(R(2l_2^* - 3, l_2^*)) > H(R(2l_2^* - 2, l_2^*))$.

(a), (b) and (c) imply the result. □

Proposition 6.10. *If $U_1 > 2U_2 - 2\epsilon$, $\epsilon = U_1 + U_2 - \Delta$ is sufficiently small and L large enough, we have that*

$$\{\operatorname{arg max}_{\omega^*} H\} = \omega^* \cap \mathcal{P}_{sa}. \quad (6.39)$$

Proof. Let us consider the skeleton path $\{\bar{\omega}_s\}_{s=0, \dots, 2(L+2)}$, and let $\omega^*(\bar{\omega}_s, \bar{\omega}_{s+1})$ be the part of ω^* between $\bar{\omega}_s$ and $\bar{\omega}_{s+1}$, i.e., the interpolation of one step of the skeleton path. Defining

$$g(s) := \max_{\eta \in \omega^*(\bar{\omega}_s, \bar{\omega}_{s+1})} H(\eta) \quad (6.40)$$

We have:

$$\max_{\eta \in \omega^*} H(\eta) = \max_{s=0, \dots, 2(L+2)} g(s) \quad (6.41)$$

By the definition of ω^* we have that the function $g(s)$ takes the following values:

$$g(s) = \begin{cases} H(\bar{\omega}_s) + \Delta - U_2 + U_1 & \text{if } s \leq 3l_2^* - 2 \text{ and } l_2 \leq 2l_2^* - 1, \text{ or } l_2^* + L \leq s \leq 2L, \\ H(\bar{\omega}_s) + 2\Delta - U_1 & \text{if } 3l_2^* - 3 \leq s \leq l_2^* + L \text{ and } l_2 = l_2^*. \end{cases} \quad (6.42)$$

For $s \leq 3l_2^* - 2$ and $l_2 \leq 2l_2^* - 1$, We are on T'_1 and have domino and quasi domino rectangles, Since by strong anisotropy row to column $\Delta - U_2 + U_1$ Fig 6.4 is bigger than add a column $2\Delta - U_1$, Fig 6.2. We have $g(s) = H(\bar{\omega}_s) + \Delta - U_2 + U_1$.

And by lemma 6.7 (v) and 6.6 (ii), we can conclude:

$$\begin{aligned} \max_{s \leq 3l_2^* - 2 \text{ and } l_2 \leq 2l_2^* - 1} g(s) &= H(R(2l_2^* - 1, l_2^* - 1)) + \Delta - U_2 + U_1 \\ &= U_1(l_2^* - 1) + U_2(2l_2^* - 1) - (U_1 + U_2 - \Delta)(l_2^* - 1)(2l_2^* - 1) + \Delta - U_2 + U_1. \end{aligned} \quad (6.43)$$

For $3l_2^* - 3 \leq s \leq l_2^* + L$ and $l_2 = 2l_2^*$, We are on T_2' and have (l_2^*) -horizontal rectangles, and have add a column $2\Delta - U_1$, Fig 6.2. We have $g(s) = H(\bar{\omega}_s) + 2\Delta - U_1$.

And by lemma 6.7 (iv) and 6.6 (i), we can conclude:

$$\begin{aligned} & \max_{3l_2^* - 3 \leq s \leq l_2^* + L \text{ and } l_2 = 2l_2^*} g(s) = H(R(2l_2^* - 3, l_2^*)) + 2\Delta - U_1 \\ & = U_1 l_2^* + U_2(2l_2^* - 3) - (U_1 + U_2 - \Delta)l_2^*(2l_2^* - 3) + 2\Delta - U_1 \end{aligned} \quad (6.44)$$

Comparing (6.43) and (6.44), We have:

$$\begin{aligned} & H(R(2l_2^* - 3, l_2^*)) + 2\Delta - U_1 \\ & = U_1 l_2^* + U_2(2l_2^* - 3) - (U_1 + U_2 - \Delta)l_2^*(2l_2^* - 3) + 2\Delta - U_1 \\ & = H(R(2l_2^* - 1, l_2^* - 1)) + \Delta - U_2 + U_1 \\ & = U_1(l_2^* - 1) + U_2(2l_2^* - 1) - (U_1 + U_2 - \Delta)(l_2^* - 1)(2l_2^* - 1) + \Delta - U_2 + U_1. \end{aligned} \quad (6.45)$$

Which are the configurations on $\omega^* \cap \mathcal{P}_{sa}$. $\square$

6.3.2 The Exit from the Set $\mathcal{B}_{sa}$

Note that in the definition of $\mathcal{B}_{sa}$ we don't put any conditions on free particles; i.e., $n(\eta)$ can have any value.

Recall the definition of $s^* = 3l_2^* - 3$ and $s = l_1 + l_2$.

We define: $\mathcal{B}_{sa} = \mathcal{B}_1 \cup \mathcal{B}_2 \cup \mathcal{B}_3 \cup \mathcal{B}_4$ such that:

- $$\mathcal{B}_1 = \{\eta : s(\eta) \leq s^*\}, \quad (6.46)$$

- $$\begin{aligned} \mathcal{B}_2 := \{\eta : s^* + 2 \leq s(\eta) \leq l_2^* + L, \ v(\eta) \geq p_{max}(\eta) - 1, \ \eta_{cl} \text{ is connected} \\ \text{and with circumscribed rectangle in } R(l_1, l_2^*)\} \end{aligned} \quad (6.47)$$

- $$\begin{aligned} \mathcal{B}_3 = \{\eta : s^* + 1 \leq s(\eta) \leq L + l_2^* - 1, \ 1 \leq l_2 \leq l_2^* - 1, \ \eta_{cl} \text{ is with} \\ \text{circumscribed rectangles contained in } R(l_1, l_2)\} \end{aligned} \quad (6.48)$$

- $$\begin{aligned} \mathcal{B}_4 = \{\eta : s(\eta) = s^* + 1, \ v(\eta) \geq l_2^* - 1, \ \eta_{cl} \text{ is with circumscribed} \\ \text{rectangle in } R(2l_2^* - 2, l_2^*) \text{ or } R(2l_2^* - 3, l_2^* + 1)\} \end{aligned} \quad (6.49)$$

where s^* is defined before and $p_{min}(\eta) = p_1(\eta) \wedge p_2(\eta)$. The main result of this section is given by the following proposition. Note that $\mathcal{P}_{sa} \subseteq \mathcal{B}_4$.

Recall formula (5.8) for boundary, (5.9) for $H_{min}(\partial A)$, (5.10) for $(\partial A)_{min}$ and definition 2.1. Recall definition of $s(\eta)$ and $v(\eta)$ in (5.10).

Proposition 6.11. *Let Γ_{sa} as in (6.6) and $\mathcal{P}_{sa}$ as in (6.14), we have:*

$$H_{min}(\partial\mathcal{B}_{sa}) = \Gamma_{sa} \quad (6.50)$$

In order to prove this proposition and in particular, in order to analyze the exiting move from $\mathcal{B}_{sa}$, we prove a preliminary result on single moves.

Let $(\bar{\eta}, \eta)$ be a move, i.e., $P(\bar{\eta}, \eta) > 0$, we define

$$\Delta(s) := s(\eta) - s(\bar{\eta}). \quad (6.51)$$

In order to prove (6.50), we use one of these two strategies:

$$(1) \quad \begin{array}{l} \text{if } \bar{\eta} \in \partial^-\mathcal{B}_{sa} \cap \mathcal{P}_{sa}, \text{ then } H(\bar{\eta}) = \Gamma_{sa} \\ \text{and if } \eta \in \partial^+\mathcal{B}_{sa}, \text{ then } H(\eta) < \Gamma_{sa}. \end{array} \quad (6.52)$$

$$(2) \quad \begin{array}{l} \text{if } \bar{\eta} \in (\partial^-\mathcal{B}_{sa}) \setminus \mathcal{P}_{sa}, \text{ and } \eta \in (\partial^+\mathcal{B}_{sa}) \\ \text{then either } H(\bar{\eta}) > \Gamma_{sa} \text{ or } H(\eta) > \Gamma_{sa}. \end{array} \quad (6.53)$$

We have the following lemma:

Lemma 6.12. *Let $p_{min}(\eta) \geq 4$, we have*

- (i) $|\Delta(s)| \leq 5$
- (ii) if $|\Delta(s)| = 1$ then $v(\eta) \geq p_{min}(\eta) - 3$,
if $|\Delta(s)| = 2$ then $n(\bar{\eta}) \geq 1$ and $v(\eta) \geq 2p_{min}(\eta) - 5$,
if $|\Delta(s)| = 3$ then $n(\bar{\eta}) \geq 2$ and $v(\eta) \geq 3p_{min}(\eta) - 6$,
if $|\Delta(s)| = 4$ then $n(\bar{\eta}) \geq 3$ and $v(\eta) \geq 4p_{min}(\eta) - 7$,
if $|\Delta(s)| = 5$ then $n(\bar{\eta}) \geq 4$ and $v(\eta) \geq 5p_{min}(\eta) - 8$.
- (iii) if $|\Delta(s)| = 1$ and $v(\eta) < p_{min}(\eta) - 1$, then $n(\bar{\eta}) \geq 2$.

Proof. We say that a line r (column or row in $\mathcal{Z}^2$) becomes active in the move from $\bar{\eta}$ to η if it was not active in $\bar{\eta}$ (i.e., $r \cap \bar{\eta}_{cl} = \emptyset$) and it is active in η , $\eta_{cl} \cap r \neq \emptyset$. In a single move at most five lines can become active: these are the row and the column containing the new position of the moved particle, (we will call these lines r_1 and r_2 , where r_1 is the line of the move, and r_2 is the line orthogonal to it), and the three lines through the three nearest neighbor sites x_3, x_4 , and x_5 of the particle after the move, excluding the site that it occupied in $\bar{\eta}$ (lines r_3, r_4 , and r_5) (see Fig. 6.8).

Lines r_3, r_4 , and r_5 become active only if in the corresponding sites x_3, x_4 , and x_5 , there was a free particle in $\bar{\eta}$, and the line r_1 , corresponding to the move, becomes active only if the moving particle was free before the move, otherwise it was already present in $\bar{\eta}$. Each line of types r_3, r_4 , and r_5 becoming active, brings in the new configuration at least $p_{min}(\eta) - 1$, vacancies; indeed $|r_i \cap \eta_{cl}| = 1$ for $i = 3, 4, 5$ since $r_i \cap \bar{\eta}_{cl} = \emptyset$; the line r_1 brings at least $p_{min}(\eta) - 2$, vacancies, and the line r_2 brings at least $p_{min}(\eta) - 3$ vacancies. Points (i) and (ii) immediately follow from this. To prove (iii) suppose

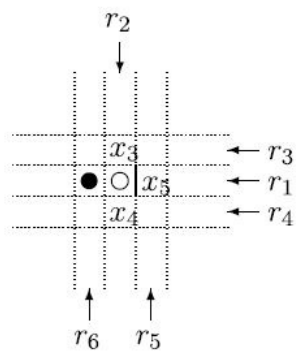


Figure 6.8:

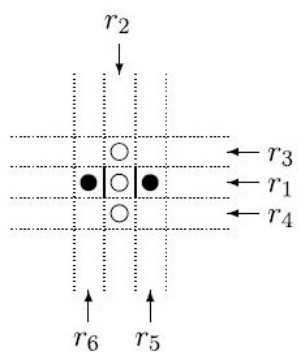


Figure 6.9:

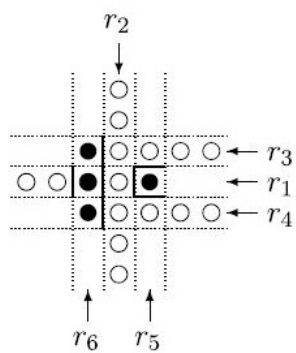


Figure 6.10:

first that $\Delta s = 1$ with $k \geq 2$ activated lines and k_1 deactivated lines (i.e., lines which were active in $\bar{\eta}$ and that are not active in η). Since $k \geq 2$ activated lines bring at least $2p_{\min}(\eta) - 5$ vacancies, and $p_{\min}(\eta) \geq 4$ in this case $v(\eta) \geq 2p_{\min}(\eta) - 5 \geq p_{\min}(\eta) - 1$. So the only possibility to have $\Delta s = 1$ and $v(\eta) < p_{\min}(\eta) - 1$ is when there is only one line activated by the move and no deactivated lines, and this activated line is r_1 or r_2 . If the activated line is r_1 and if it brings only $p_{\min}(\eta) - 2$ vacancies this means that in this line, in $\bar{\eta}$ there are two free particles, one of which is the moving particle. If the activated line is r_2 , it brings $p_{\min}(\eta) - 3$ vacancies only if it contains 2 free particles before the move in the sites x_3 and x_4 (see Fig. 6.8); it brings $p_{\min}(\eta) - 2$ vacancies if it contains a free particle in sites x_3 or x_4 before the move. If the moving particle is free in $\bar{\eta}$, we have $n(\bar{\eta}) \geq 2$, if the moving particle is not free in $\bar{\eta}$, then line r_6 (see Fig. 6.8) was active in $\bar{\eta}$ and it is continue to be active in η . Due to the fact that r_2 is the unique line that become active, the line orthogonal to r_2 through this free particle (i.e., lines r_3 or r_4 , say r_3 for concreteness) must be active in $\bar{\eta}$ and remains active in η . So we can conclude that there is an additional vacancy in η in the site $r_6 \cap r_3$, this implies that in this case $v(\eta) \geq p_{\min}(\eta) - 2 + 1$. Point (iii) is thus proved. $\square$

Remark 6.13. We note that if $n(\bar{\eta}) = 0$ the unique line that can become active is r_2 and in this case in $\bar{\eta}$ sites x_3 and x_4 are empty and $x_5 \in \bar{\eta}_{cl}$, where $x_5 \in r_1$ (see Figs. 6.8 and 6.9), so that $\bar{\eta}$ is not monotonic ($g'_1(\bar{\eta}) + g'_2(\bar{\eta}) \geq 1$) in this case.

Proof. of the proposition 6.11. Let $(\bar{\eta}, \eta) \in \partial\mathcal{B}_{sa}$ be the exiting move from $\mathcal{B}_{sa}$ and Δs be its corresponding variation of s . If $p_{\min}(\eta) \leq 3$, for $\epsilon \leq U_2$, from explicit computations it follows:

$$H(\eta) > \Gamma_{sa}. \quad (6.54)$$

Suppose from now on $p_{\min}(\eta) \geq 4$.

By using lemma 6.12, we can distinguish seven different cases corresponding to $\Delta s = -1, 0, 1, 2, 3, 4, 5$.

Case $\Delta s = -1$. In this case we have to consider these cases:

- (a) $\bar{\eta} \in \mathcal{B}_2$.
- (b) $\bar{\eta} \in \mathcal{B}_3$.

- In the case (a), it is impossible to leave $\mathcal{B}_{sa}$. Indeed, by remark 6.13 it is impossible to activate lines and $\Delta s = -1$ is obtained by a unique line becoming inactive. So, we have $\Delta v = v(\eta) - v(\bar{\eta}) \geq -(l_2^* - 1)$, because the minimal side of configuration in $\mathcal{B}_2$ is l_2^* . We obtain

$$v(\eta) \geq v(\bar{\eta}) - (l_2^* - 1) \geq 2l_2^* - 2 - (l_2^* - 1) = l_2^* - 1 \quad (6.55)$$

Hence, if $l_1 = 2l_2^* - 2$ we have $s = s^* + 1$ so $\eta \in \mathcal{B}_4$. If $2l_2^* - 1 \leq l_1 \leq L$, we have either $\eta \in \mathcal{B}_2$, if $v(\eta) \geq p_{\max}(\eta) - 1 = l_1 - 1$, either $\eta \in \partial^+\mathcal{B}_{sa}$ if $l_2^* \leq v(\eta) \leq l_1 - 2$. In the latter by lemma 6.6 (ii) for $2l_2^* \leq l_1 \leq L$ we have $H(\eta) \geq H(R(l_1, l_2^* - 1)) + \Delta - U_2 + U_1 > \Gamma_{sa}$.

- In case (b) since $\Delta s = -1$ and $\bar{\eta} \in \mathcal{B}_3$ then $\bar{\eta}_{cl}$ is contained in $R(l_1, l_2^* - 1)$ for $2l_2^* - 1 \leq l_1 \leq L$, so either $\eta \in \mathcal{B}_3$ or $\eta \in \mathcal{B}_1$, and is against $(\bar{\eta}, \eta) \in \partial\mathcal{B}_{sa}$.

Case $\Delta s = 0$. This is a case of the minimal exit from $\mathcal{B}_{sa}$. We have to consider these cases, indeed if $\Delta s = 0$, then $(\bar{\eta}, \eta) \in \partial\mathcal{B}_{sa}$ only if

(a) $\bar{\eta} \in \mathcal{B}_2$, and $\Delta v \leq -1$,

(b) $\bar{\eta} \in \mathcal{B}_3$,

(c) $\bar{\eta} \in \mathcal{B}_4$ and $\Delta v \leq -1$,

- In case (b) since $\Delta s = 0$ and $\bar{\eta} \in \mathcal{B}_3$ then $\bar{\eta}_{cl}$ is contained in $R(l_1, l_2^* - 1)$ for $2l_2^* - 1 \leq l_1 \leq L$, no line becomes active or deactive, therefore; $\eta \in \mathcal{B}_3$, and is against $(\bar{\eta}, \eta) \in \partial\mathcal{B}_{sa}$.
- Let us consider the cases (a) and (c). Since the number of vacancies can decrease only if either $p_1(\eta) - p_1(\bar{\eta}) = p_2(\bar{\eta}) - p_2(\eta) \neq 0$, or $p_1(\eta) - p_1(\bar{\eta}) = p_2(\bar{\eta}) - p_2(\eta) = 0$ but $|\eta_{cl}| - |\bar{\eta}_{cl}| > 0$, which implies that in both cases (a) and (c) we have
 - (i) either $n(\bar{\eta}) \geq 1$ or
 - (ii) $n(\bar{\eta}) = 0$ and, by remark 6.13, $g'_1(\bar{\eta}) + g'_2(\bar{\eta}) \geq 1$ and r_2 become active bringing at least $p_{min}(\eta) - 1$ vacancies in η .

Case (a-i) contains a minimal exit from $\mathcal{B}_{sa}$. If $\bar{\eta} \in \mathcal{B}_2$ and $n(\bar{\eta}) \geq 1$, by lemma 5.7 and lemma 6.6 (ii), we have:

$$H(\bar{\eta}) \geq H(R(2l_2^* - 1, l_2^* - 1)) + 2\Delta - U_2 > \Gamma_{sa} \quad (6.56)$$

since $2\Delta - U_2 > \Delta - U_2 + U_1$.

- Case (c-i), first suppose that $n(\bar{\eta}) = 1$, $\bar{\eta}_{cl} \in R(2l_2^* - 2, l_2^*)$ and $v(\bar{\eta}) = l_2^* - 1$, then $\bar{\eta} \in \mathcal{P}_{sa} \cap \partial^-\mathcal{B}_{sa}$ and using $\Delta v \leq -1$ we have $\eta \in \partial^+\mathcal{B}_{sa}$, and $H(\bar{\eta}) = \Gamma_{sa}$. Since $\eta \in \partial^+\mathcal{B}_{sa}$, we have $v(\eta) < l_2^* - 1$, and by lemma 5.7 we can conclude:

$$H(\eta) < H(R(2l_2^* - 2, l_2^*)) + \epsilon(l_2^* - 1) + \Delta = \Gamma_{sa}. \quad (6.57)$$

- if $\bar{\eta}_{cl} \in R(2l_2^* - 3, l_2^* + 1)$, and $n(\bar{\eta}) = 1$, if $\bar{\eta} \in \partial^-\mathcal{B}_{sa}$ and $\eta \in \partial^+\mathcal{B}_{sa}$, we have either,

$$H(\bar{\eta}) \geq H(R(2l_2^* - 3, l_2^* + 1)) + 2\Delta - U_1 > \Gamma_{sa} \quad (6.58)$$

since $H(R(2l_2^* - 3, l_2^* + 1)) > H(R(2l_2^* - 3, l_2^*))$.

- Otherwise, if $n(\bar{\eta}) > 1$ then $\bar{\eta} \notin \mathcal{P}_{sa}$. and by again by lemma 5.7 we have:

$$H(\bar{\eta}) \geq 2\Delta + H(R(2l_2^* - 2, l_2^*)) + \epsilon(l_2^* - 1) > \Gamma_{sa} \quad (6.59)$$

since $H(R(2l_2^* - 2, l_2^*)) < H(R(2l_2^* - 3, l_2^* + 1))$.

- In case (a-ii) and (c-ii), the number of vacancies increases at least by $p_{min}(\eta) - 1$ so $\eta \in \mathcal{B}_2$ and $\eta \in \mathcal{B}_4$, respectively, is against $(\bar{\eta}, \eta) \in \partial\mathcal{B}_{sa}$.

Case $\Delta s = 1$. We consider these cases:

- (a) $\bar{\eta} \in \mathcal{B}_2$,
- (b) $\bar{\eta} \in \mathcal{B}_3$,
- (c) $\bar{\eta} \in \mathcal{B}_4$,
- (d) $\bar{\eta} \in \mathcal{B}_1$,

Since $\Delta s = 1$ by using lemma 6.12 we consider these cases:

- (i) $v(\eta) \geq p_{min}(\eta) - 3$,
- (ii) if $v(\eta) < p_{min}(\eta) - 1$ then $n(\bar{\eta}) \geq 2$.
 - Cases (a-ii), and (c-ii) can be treated as in point $\Delta s = 0$ (see (6.56) and (6.59)).
 - Case (b) let $\bar{\eta} \in \mathcal{B}_3$ and $\Delta(s) = 1$, if the move is in the horizontal direction then $\eta_{cl} \in R(l_1, l_2^* - 1)$ so $\eta \in \mathcal{B}_3$ is against $(\bar{\eta}, \eta) \in \partial\mathcal{B}_{sa}$. If the move is in the vertical direction.

Case (b-i) if the move is in the vertical direction then line r_2 is horizontal becomes active and brings at least $2l_2^* - 2$ vacancies, so $\eta \in \mathcal{B}_2$ is against $(\bar{\eta}, \eta) \in \partial\mathcal{B}_{sa}$.

Case (b-ii) By lemma 6.6 (ii) and lemma 5.7, we have:

$$H(\bar{\eta}) \geq 2\Delta + H(R(2l_2^* - 1, l_2^* - 1)) > \Gamma_{sa} \quad (6.60)$$

- Case (d) let $\Delta s = 1$, suppose that $s(\bar{\eta}) = s^*$; if $\eta \notin \mathcal{B}_{sa}$, i.e., $\eta \notin \mathcal{B}_2 \cup \mathcal{B}_3 \cup \mathcal{B}_4$, then $\eta_{cl} \notin R(l_1, l_2^*)$. Again we have these cases
 - (1) If the move is in the vertical direction, then $3 \leq l_1 < 2l_2^* - 4$ and $l_2^* + 1 \leq l_2 < 2l_2^* - 4$.
 - (2) If the move in the horizontal direction then $3 \leq l_1 < 2l_2^* - 5$ and $l_2^* + 2 \leq l_2 < 2l_2^* - 3$.

In case (d-1-i) by lemma 6.6 (iii) and lemma 5.7 we have

$$\begin{aligned} H(\eta) &\geq H(R(2l_2^* - 4, l_2^* + 1)) + \Delta - U_2 = \\ &= H(R(2l_2^* - 3, l_2^*) + \Delta - U_2 + 4U_1 + U_2 - 3\Delta + \delta\epsilon \\ &= H(R(2l_2^* - 3, l_2^*) + 4U_1 - 2\Delta + \delta\epsilon > \Gamma_{sa} \end{aligned} \quad (6.61)$$

Since $4U_1 - 2\Delta + \delta\epsilon > 2\Delta - U_1$.

In case (d-2-i) by lemma 6.6 (iii) and lemma 5.7 we have

$$\begin{aligned} H(\eta) &\geq H(R(2l_2^* - 5, l_2^* + 2)) + \Delta - U_1 = \\ &= H(R(2l_2^* - 3, l_2^*) + \Delta - U_1 + 10U_1 + 4U_2 - 8\Delta + 5\delta\epsilon \\ &= H(R(2l_2^* - 3, l_2^*) + 9U_1 + 4U_2 - 7\Delta + 5\delta\epsilon > \Gamma_{sa} \end{aligned} \quad (6.62)$$

Since $9U_1 + 4U_2 - 2\Delta + 5\delta\epsilon > 2\Delta - U_1$.

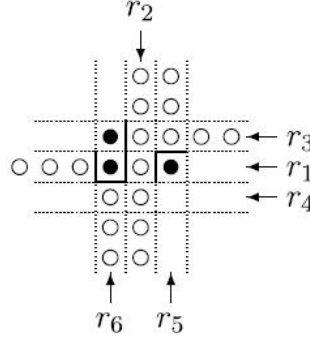


Figure 6.11:

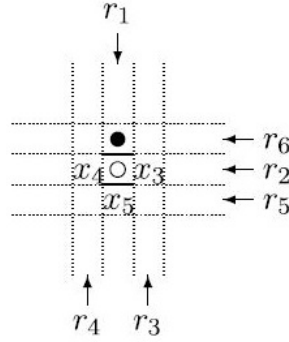


Figure 6.12:

In case (d-ii), since $n(\bar{\eta}) \geq 2$ by lemma 6.6 (iii) and lemma 5.7 we can conclude:

$$H(\bar{\eta}) \geq H(R(2l_2^* - 4, l_2^* + 1)) + 2\Delta > \Gamma_{sa} \quad (6.63)$$

See (6.61).

Case $\Delta s = 2$. We consider these cases:

- (a) $\bar{\eta} \in \mathcal{B}_2$,
 - (b) $\bar{\eta} \in \mathcal{B}_3$,
 - (c) $\bar{\eta} \in \mathcal{B}_4$,
 - (d) $\bar{\eta} \in \mathcal{B}_1$,
- Cases (a) and (c), since $n(\eta) \geq 1$ can be treated as before (see (6.56) and (6.59)).
 - For case (b) and (d), $\Delta s = 2$ means two lines r_1 and r_2 become active, so we have one move in the vertical and one in the horizontal direction.

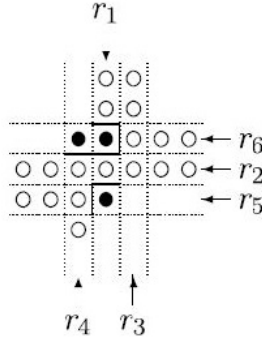


Figure 6.13:

In case (b) and (d), since $\Delta s = 2$ by lemma 6.12 we have $n(\bar{\eta}) \geq 1$ and $v(\eta) \geq 2p_{min} - 5$. If $n(\bar{\eta}) \geq 2$ we conclude like case $\Delta s = 1$, (b-ii) and (d-ii), (see (6.60) and (6.63)), respectively.

So we are left with the case: $n(\bar{\eta}) = 1$.

If the unique free particle is the moving particle we can not have $\Delta s = 2$. Indeed r_3 , r_4 , and r_5 can not be activated and, in order to have $\Delta s = 2$, r_1 and r_2 have to become active. This implies that the sites x_3 , x_4 , and x_5 must be empty, but then $\Delta s = 0$.

If $g'_1(\bar{\eta}) + g'_2(\bar{\eta}) \geq 1$ we have

$$\begin{aligned} H(\eta) &\geq H(R(2l_2^*, l_2^*)) + 5\Delta - 5U_1 - 3U_2 + U_2 \\ &= H(R(2l_2^* - 1, l_2^* - 1)) + 7\Delta - 6U_2 - 6U_2 > \Gamma_{sa} \end{aligned} \quad (6.64)$$

So we have to consider only the case $n(\bar{\eta}) = 1$, $g'_1(\bar{\eta}) = g'_2(\bar{\eta}) = 0$.

We distinguish two cases:

- (a) the free particle is in site x_i , with i equal 3 or 4 the lines that become active are r_2 and r_i . Due to $g'_1(\bar{\eta}) = g'_2(\bar{\eta}) = 0$ the site x_5 is empty, and the site $\{x_3, x_4\} \setminus \{x_i\}$ is empty.
- (b) the free particle is in site x_5 the lines that become active are r_2 and r_5 and the sites x_3 and x_4 are empty

In both cases if the moving particle has in $\bar{\eta}$ at least one vertical and one horizontal bond connecting it to other particles, then $\Delta H \geq U_2$ and so $H(\eta) \geq H(\bar{\eta}) + U_2 \geq H(R(2l_2^* - 1, l_2^* - 1)) + \Delta + U_2 > \Gamma_{sa}$.

If the moving particle has in $\bar{\eta}$ either two bonds orthogonal to the move, or only one vertical or only one horizontal bond connecting it to other particles, then it is impossible to leave $\mathcal{B}_{sa}$. Indeed in this case there exists a line r ($r = r_1$ or $r = r_6$) such that its intersection with $\bar{\eta}$ is only the

moving particle. If $r = r_6$ then this line become inactive after the move against $\Delta s = 2$. If $r = r_1$ then the number of vacancies in η are at least the vacancies induced by the two activating lines and r_1 . This means that in case (a) r_i and r_2 becomes active

$$|r_1 \cap \eta_{cl}| = 1, \quad |r_2 \cap \eta_{cl}| = 2, \quad |r_i \cap \eta_{cl}| = 1, \quad (6.65)$$

so that

$$v(\eta) \geq p_1 - 1 + p_2 - 2 + p_{min}(\eta) - 1 = s(\eta) + p_{min}(\eta) - 4 = s^* + p_{min}(\eta) - 2. \quad (6.66)$$

In case (b), lines r_5 and r_2 become active and

$$|r_1 \cap \eta_{cl}| = 2, \quad |r_2 \cap \eta_{cl}| = 1, \quad |r_5 \cap \eta_{cl}| = 1, \quad (6.67)$$

and so $\eta \in \mathcal{B}_{sa}$ against $(\bar{\eta}, \eta) \in \partial \mathcal{B}_{sa}$.

- In case (d-i), since $n(\bar{\eta}) \geq 1$ we can conclude like case $\Delta s = 1$, (d-i).

Case $\Delta s = 3$. Again we consider these cases:

- (a) $\bar{\eta} \in \mathcal{B}_2$,
- (b) $\bar{\eta} \in \mathcal{B}_3$,
- (c) $\bar{\eta} \in \mathcal{B}_4$,
- (d) $\bar{\eta} \in \mathcal{B}_1$,

- Cases (a) and (c), can be treated as before (see (6.56) and (6.59)).

For cases (b) and (d), by lemma 6.12, three lines r_1 , r_2 and r_i , ($i = 3, 4, 5$) become active, so we have one line in horizontal and two lines in vertical direction or vice-versa.

- Case (b)
 - If we have one move in the vertical and two moves in the horizontal direction, since by lemma 6.12, $\Delta s = 3$ implies that $n(\bar{\eta}) \geq 2$, we can conclude like case $\Delta s = 1$, (b-ii), (see 6.60).
 - If we have two moves in the vertical and one move in the horizontal direction, since by lemma 6.12 $\Delta s = 3$, we have:

$$H(\bar{\eta}) \geq 2\Delta + H(R(2l_2^* - 1, l_2^* - 1)) > \Gamma_{sa} \quad (6.68)$$

- Case (d), if $(\bar{\eta}, \eta) \in \partial \mathcal{B}_{sa}$ only if $s(\bar{\eta}) \geq s^* - 1$, and $\eta_{cl} \notin R(l_1, l_2^*)$; hence, $l_2 \geq l_2^* - 1$, by lemma 6.12 we know that $n(\bar{\eta}) \geq 2$. Therefore, by lemma 6.6 (iv) and again lemma 5.7 we have:

$$H(\bar{\eta}) \geq 2\Delta + H(R(s^* - 1)) > \Gamma_{sa}. \quad (6.69)$$

Since, $H(R(2l_2^* - 3, l_2^* - 1)) = H(R(2l_2^* - 3, l_2^*)) + U_1 - 2U_2 + \epsilon - 2\delta\epsilon$ there the equation (6.69) becomes

$$\begin{aligned} H(\bar{\eta}) &\geq 2\Delta + H(R(2l_2^* - 3, l_2^* - 1)) \\ &= 2\Delta + H(R(2l_2^* - 3, l_2^*)) + U_1 - 2U_2 + \epsilon - 2\delta\epsilon \\ &> H(R(2l_2^* - 3, l_2^*)) + 2\Delta - U_1 = \Gamma_{sa}. \end{aligned} \quad (6.70)$$

Case $\Delta s = 4$. In this case by lemma 6.12, four lines r_1, r_2, r_i , and r_j ($i, j = 3, 4, 5$) become active, so we have two lines in horizontal and two lines in vertical direction. If $(\bar{\eta}, \eta) \in \partial\mathcal{B}_{sa}$ only if $s(\bar{\eta}) \geq s^* - 2$, and by lemma 6.12, we know that $n(\bar{\eta}) \geq 3$. Therefore, by lemma 5.7 and lemma 6.6 (v) we have $H(\bar{\eta}) \geq 3\Delta + H(R(s^* - 2)) > \Gamma_{sa}$ as before.

Case $\Delta s = 5$. In this case by lemma 6.12, all lines r_1, r_2, r_3, r_4 , and r_5 become active, so we have two lines in horizontal and three lines in vertical direction or vice-versa. If $(\bar{\eta}, \eta) \in \partial\mathcal{B}_{sa}$ only if $s(\bar{\eta}) \geq s^* - 3$, and by lemma 6.12, we know that $n(\bar{\eta}) \geq 4$. Therefore, by lemma 5.7 and lemma 6.6 (vi), we have $H(\bar{\eta}) \geq 4\Delta + H(R(s^* - 3)) > \Gamma_{sa}$ as before. $\square$

6.3.3 Communication Height and Gate

By definition of communication height $\Phi(\underline{0}, \underline{1})$, by proposition 6.10 we have immediately:

$$\Phi(\underline{0}, \underline{1}) := \max_i H(\omega_i^*) = H(\mathcal{P}_{sa}) = \Gamma_{sa}, \quad (6.71)$$

where $\mathcal{P}_{sa}$ and Γ_{sa} are defined in (6.6) and (6.14), respectively. On the other side, since every path going from $\underline{0}$ to $\underline{1}$ has to leave $\mathcal{B}_{sa}$, we have by proposition 6.11 that

$$\Phi(\underline{0}, \underline{1}) := \min_{\omega: \underline{0} \rightarrow \underline{1}} \max_{\zeta \in \omega} H(\zeta) \geq H_{min}(\partial\mathcal{B}_{sa}) = \Gamma_{sa}, \quad (6.72)$$

By combining (6.71) and (6.72) we immediately obtain

$$\Phi(\underline{0}, \underline{1}) := \Gamma_{sa} \quad (6.73)$$

Note that to prove (6.73) we have applied the argument developed in ref. [43] with some small variations. In ref. [43], the set $\partial^+\mathcal{B}_{sa}$ (external boundary of $\mathcal{B}_{sa}$, see (2.5)) was considered, while here we use the set $\partial\mathcal{B}_{sa}$ of exiting moves from $\mathcal{B}_{sa}$ (see (5.8)), so that in the present case $H_{min}(\partial\mathcal{B}_{sa})$ substitutes $H(F(\partial^+\mathcal{B}_{sa}))$.

The argument used to prove (6.73) also implies that $\mathcal{P}_{sa}$ is a gate. Indeed given any optimal path ω , it has to leave $\mathcal{B}$ with a move in $(\partial\mathcal{B})_{min}$ otherwise, by proposition 6.11 we would have $\max_i H(\omega) > \Gamma_{sa}$. To conclude we use (6.53).

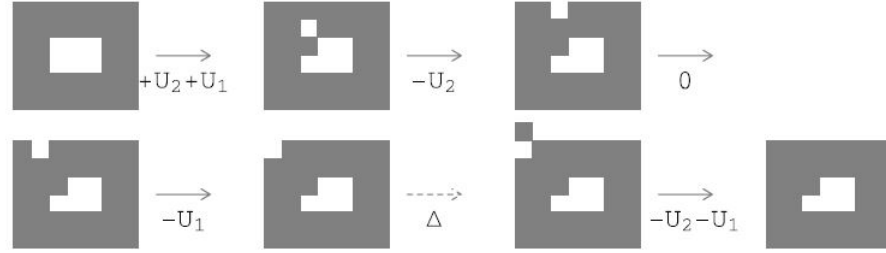
6.4 Theorems for the Gate

6.4.1 Reduction

In this section we first prove the following proposition.

Proposition 6.14. *There exists $\Gamma_0 < \Gamma_{sa}$ such that $\mathcal{X}_{\Gamma_0} \subseteq \{\underline{0}, \underline{1}\}$, i.e.:*

$$\begin{aligned} &\forall \eta \neq \underline{0}, \underline{1} \quad \exists \eta \in \mathcal{X} \text{ and a path } \omega : \eta \rightarrow \eta' \\ &\text{such that } H(\eta) < H(\eta'), \quad \max_{\zeta \in \omega} H(\zeta) < H(\eta) + \Gamma_0. \end{aligned} \quad (6.74)$$

Figure 6.14: $(U_1 + U_2)$ -reduction of a rectangle with a hole

In the second part of this section, as a corollary of this proposition, we will identify the stable and metastable states.

Proposition 6.15. *If the side L of the box Λ is large enough ($L > 2l_1^*$ is a possible choice), then $V_0 = (0, 1)$ and $1 = \mathcal{X}^s$, $0 = \mathcal{X}^m$.*

• **Reduction Outside $\{0, 1\}$**

To prove proposition 6.14 we first characterize the set $\mathcal{X}_{U_1+U_2}$ of configurations which are not $(U_1 + U_2)$ -reducible, as follows.

We introduce some geometrical definitions. Let $\eta \in \mathcal{X}$ be given.

- (i) A site $x \in \Lambda$ is connected trough empty (full) sites to $\partial^- \Lambda$ if there exists $x_1, \dots, x_n$ a connected chain of nearest neighbor empty (full) sites namely, $x_1 \in nn(x), x_2 \in nn(x_1), \dots, x_n \in nn(x_{n-1}), x_n \in \partial^- \Lambda$ and $\eta(x_1) = \eta(x_2) = \dots = \eta(x_n) = 0$ ($\eta(x_1) = \eta(x_2) = \dots = \eta(x_n) = 1$).
- (ii) An external corner of a set $A \subset \Lambda$ is a site $x \notin A$ such that $\sum_{y \in nn(x): (x,y) \in \Lambda_{0,h}^*} \chi_A(y) = 1$ and $\sum_{y \in nn(x): (x,y) \in \Lambda_{0,v}^*} \chi_A(y) = 1$, where χ_A is the characteristic function of the set A .
- (iii) An internal corner of a set $A \subset \Lambda$ is a site $x \in A$ such that $\sum_{y \in nn(x): (x,y) \in \Lambda_{0,h}^*} \chi_A(y) = 1$ and $\sum_{y \in nn(x): (x,y) \in \Lambda_{0,v}^*} \chi_A(y) = 1$.
- (iv) Let η^{ext} be the set of sites $x \in \Lambda_0$ such that $\eta(x) = 1$ and x is connected trough empty sites with $\partial^- \Lambda$.

Proposition 6.16. *Any configuration $\eta \in \mathcal{X}_{U_1+U_2}$ has no free particles and it has only rectangular clusters with minimal side larger than 1.*

Proof. Done in chapter 5. □

Proof of proposition 6.14. Suppose that $\eta \in \mathcal{X}_{U_1+U_2}$ and $\eta \neq 0, 1$, from proposition 6.16 η has only rectangular clusters which are connected through empty sites to $\partial^- \Lambda$, i.e., $\eta^{ext} = \partial^- \eta$.

Suppose now that a rectangular cluster of η has a vertical subcritical side, i.e., $l_2 < l_2^*$, then it is possible to reduce η with the path described in Fig. 6.2 that

removes a column of length l_2 with energy barrier $\Delta H(\text{remove column}) = U_1 + U_2 + \epsilon(l_2 - 2) < 2\Delta - U_1$.

Otherwise the rectangle in η have vertical supercritical sides, $l_2 \geq l_2^*$, We have two different cases

- (i) if $l_1 = L - 1$, it is possible to reduce η with the path described in Fig. 6.2 that is (add a column) with energy barrier $\Delta H(\text{add a column}) = 2\Delta - U_1$.
- (ii) if $l_1 = L$, it is not possible to reduce η with the path described in Fig. 6.2 that adds a column. Therefore, it is only possible to reduce η with the path described in Fig. 6.4 that is (column to row) with energy barrier $\Delta H(\text{column to row}) = \Delta - U_2 + U_1$.

The proof is complete by defining $\Gamma_0 := \Delta - U_2 + U_1 < \Gamma$.

6.4.2 Stable and Metastable States

Proof of proposition 6.15. Since $\mathcal{X}^s \subseteq \mathcal{X}_V$ for any $V \geq 0$ and since, if the side L of the volume Λ is large enough, we have $H(\underline{0}) > H(\underline{1})$, using also that by proposition 6.15 we have $\mathcal{X}_{\Gamma_0} \subseteq \{\underline{0}, \underline{1}\}$, we can immediately conclude that $\mathcal{X}_s = \underline{1}$. If we are able to prove that

$$V_{\underline{0}} = \Phi(\underline{0}, \underline{1}) = \Gamma_{sa} > \Gamma_0 \quad (6.75)$$

we can immediately conclude that $\underline{0} \in \mathcal{X}^m$.

Let us now prove (6.75). By definition we have that $V_{\underline{0}} \leq \Phi(\underline{0}, \underline{1})$. We argue by contradiction: suppose that $V_{\underline{0}} < \Phi(\underline{0}, \underline{1})$. Then, by definition, there exists $\eta^{(1)}$ with $H(\eta^{(1)}) < H(\underline{0})$ and $\Phi(\underline{0}, \eta^{(1)}) = V_{\underline{0}} < \Phi(\underline{0}, \underline{1})$. This implies that $\eta^{(1)}$ can not be equal to $\underline{1}$, so since by $\mathcal{X}_{\Gamma_0} \subseteq \{\underline{0}, \underline{1}\}$, we know that $\eta^{(1)} \notin \mathcal{X}_{\Gamma_0}$ we can iterate this argument by obtaining a sequence $H(\underline{0}) > H(\eta^{(1)}) > H(\eta^{(2)}) > \dots > H(\eta^{(n)})$ with $\Phi(\eta^{(i)}, \eta^{(i+1)}) \leq H(\eta^{(i)}) + \Gamma_0 < \Phi(\underline{0}, \underline{1})$ if $\eta^{(i)} \neq \underline{1}$. The number of these iterations must be finite since the sequence $\eta^{(i)}$ has a strictly decreasing energy and the state space is finite. Moreover, the sequence stops at $\eta^{(n)} \in \mathcal{X}_{\Gamma_0}$ and we have $\eta^{(n)} = \underline{1}$ since $\mathcal{X}_{\Gamma_0} \subseteq \{\underline{0}, \underline{1}\}$ and $H(\eta^{(0)}) > H(\eta^{(n)})$. We obtain

$$\begin{aligned} \Phi(\underline{0}, \underline{1}) &= \Phi(\underline{0}, \eta^{(n)}) \leq \max\{\Phi(\underline{0}, \eta^{(1)}), \Phi(\eta^{(1)}, \eta^{(2)}), \dots, \Phi(\eta^{(n-1)}, \eta^{(n)})\} \\ &< \Phi(\underline{0}, \underline{1}) \end{aligned} \quad (6.76)$$

which is absurd.

6.4.3 Proof of Theorem 6.5

To prove theorem 6.5 we need the notion of cycle that is one of the main tools used in the general theory of Freidlin Wentzell Markov chains.

The following result represents the main property of cycles (see for instance

[43] and [56] theorem 2.36): with large probability every state in a cycle is visited by the process before the exit.

Recall the definition of cycle from chapter 2.

Proposition 6.17. *Let C be a cycle. There exists $K > 0$ such that for any $\eta, \eta' \in C$ and for all sufficiently large β*

$$P_\eta(\tau_{\eta'} < \tau_{\partial+C}) \geq 1 - e^{-K\beta} \quad (6.77)$$

By using this result, to prove theorem 6.5 it is sufficient to show the following:

- (i) if η is a rectangular configuration contained in $R(2l_2^* - 1, l_2^* - 1)$, or $R(2l_2^* - 3, l_2^*)$ then there exists a cycle $C_{\underline{0}}$ containing η and $\underline{0}$ and not containing $\underline{1}$;
- (ii) if η is a rectangular configuration containing $R(2l_2^* - 2, l_2^*)$, then there exists a cycle $C_{\underline{1}}$ containing η and $\underline{1}$ and not containing $\underline{0}$.

We start by showing (i). Let $C_{\underline{0}}$ be the maximal connected set containing $\underline{0}$ such that $\max_{\eta' \in C_{\underline{0}}} H(\eta') < \Gamma_{sa}$. By definition $C_{\underline{0}}$ is a cycle containing $\underline{0}$. It does not contain $\underline{1}$ since $\Phi(\underline{0}, \underline{1}) = \Gamma_{sa}$. We have only to prove that $C_{\underline{0}}$ contains η . This can be easily obtained by constructing a path $\omega^{\eta, \underline{0}}$ going from η to $\underline{0}$ keeping the energy less than Γ_{sa} . $\omega^{\eta, \underline{0}}$ is obtained by erasing site by site, each column of η and by showing that all the configurations of this path are in $C_{\underline{0}}$. More precisely, let $\eta = \{(x, y) \in \mathcal{Z}^2; x \in (n, n + l_1], y \in (m, m + l_2)\} \in R(l_1, l_2)$ for some $n, m \in \mathcal{Z}$, and let $\{\bar{\omega}_i^{\eta, \underline{0}}\}_{i=0, \dots, l_1}$ be a path of rectangular configurations, starting from η and ending in $\underline{0}$, given by

$$\{\bar{\omega}_i^{\eta, \underline{0}}\} = \{(x, y) \in \mathcal{Z}^2; x \in (n, n + l_1 - i], y \in (m, m + l_2)\} \quad (6.78)$$

To complete the construction we can use now the same idea applied in the definition of the reference path ω^* : between every pair $\{\bar{\omega}_i^{\eta, \underline{0}}\}, \{\bar{\omega}_{i+1}^{\eta, \underline{0}}\}$ we can insert a sequence $\{\tilde{\omega}_{i,0}^{\eta, \underline{0}}\}, \dots, \{\tilde{\omega}_{i,l_2}^{\eta, \underline{0}}\}$ where $\{\tilde{\omega}_{i,0}^{\eta, \underline{0}}\} = \{\bar{\omega}_i^{\eta, \underline{0}}\}$ and for $j > 0$, $\{\tilde{\omega}_{i,j}^{\eta, \underline{0}}\}$ is obtained by $\{\bar{\omega}_i^{\eta, \underline{0}}\}$ by erasing j sites:

$$\{\tilde{\omega}_{i,j}^{\eta, \underline{0}}\} = \{\bar{\omega}_i^{\eta, \underline{0}}\} \setminus \{(x, y) \in \mathcal{Z}^2; x = n + l_1 - i, y \in (m + l_2 - j, m + l_2)\} \quad (6.79)$$

Again, as in the reference path ω^* , the last interpolation consists in inserting between every pair of consecutive configurations in $\tilde{\omega}^{\eta, \underline{0}}$ a sequence of configurations with a free particle in a suitable sequence of sites going from the site previously occupied by the erased particle to $\partial\Lambda$. Since for any $l_1 \leq 2l_2^* - 1$ and $l_2 \leq l_2^* - 1$ we have $H(R(l_1, l_2)) < H(R(2l_2^* - 3, l_2^*))$, for the path $\omega^{\eta, \underline{0}}$ obtained in this way we have:

$$\max_i H(\omega^{\eta, \underline{0}}) = \max_{l \in [1, 2l_2 - 1]} H(R(l, l_2)) + 2\Delta - U_1 < \Gamma_{sa} \quad (6.80)$$

The proof of (ii) is similar. Let $C_{\underline{1}}$ be the maximal connected set containing $\underline{1}$ such that $\max_{\eta' \in C_{\underline{1}}} H(\eta') < \Gamma_{sa}$. Again $C_{\underline{1}}$ is by definition a cycle containing $\underline{1}$ and not containing $\underline{0}$ since $\Phi(\underline{0}, \underline{1}) = \Gamma_{sa}$. To prove that $C_{\underline{1}}$ contains η we define now a path $\omega^{\eta, \underline{1}}$ going from η to $\underline{1}$ obtained by reaching first of all the l_2^* -horizontal rectangles and, from there, following the path ω^* . As before, it

is easy to show that all the configurations of this path have an energy smaller than Γ_{sa} so that they are in $C_{\underline{0}}$.

Going into the details, let $\eta \in R(l_1, l_2)$; let us suppose that $l_2 \geq l_2^*$. If $l_1 - l_2 = l_2^* - 2$ then η is standard and $\omega^{\eta, \underline{1}}$ can be chosen as the part of the reference path ω^* going from η to $\underline{1}$. The remaining part of the path follows ω^* from $R(2l_2^* - 2, l_2^*)$ to $\underline{1}$. If $l_1 - l_2 > l_2^*$ then first move columns to rows following the mechanism given in steps a.3 and b.2, until we reach a standard rectangle. From there, follow the reference path ω^* . For the path $\omega^{\eta, \underline{1}}$ obtained in this way, by using that in our parameter regime $2\Delta - U_1 < \Delta + U_1 - U_2$, and that $H(R(l_1, l_2)) < H(R(2l_2^* - 1, l_2^* - 1))$, for any $l'_1 \geq 2l_2^* - 1$ and $l'_2 \geq l_2^*$, we obtain:

$$\max_i H(\omega_i^{\eta, \underline{1}}) \leq \max_{l'_1 \geq l_1^*, l'_2 \geq l_2^*} H(R(l'_1, l'_2)) + \Delta - U_2 + U_1 < \Gamma_{sa} \quad (6.81)$$

so that $\omega_i^{\eta, \underline{1}} \in C_{\underline{1}}$ for any i and the proof of theorem 6.5 is complete.

Bibliography

- [1] D. Aldous, M. Brown, Inequalities for rare events in time reversible Markov chains I,” in Stochastic Inequalities, Lecture Notes of the Institute of Mathematical Statistics,. Vol 22., 1-16, (1992).
- [2] L. Alonso and R. Cerf, The three-dimensional polyominoes of minimal area, Electron. J. Combin. 3 (1996) Research Paper 27.
- [3] J. Beltran, C. Landim, Tunneling and metastability of continuous time Markov chains”, J. Stat. Phys. 140 no. 6, 1065-1114, (2010).
- [4] G. Ben Arous and R. Cerf, Metastability of the three-dimensional Ising model on a torus at very low temperature, Electron. J. Probab. 1 (1996) Research Paper 10.
- [5] O. Benois, C. Landim, C. Hitting Times of Rare Events in Markov Chains, J. Stat. Phys. vol 153, 967–990, (2013).
- [6] A. Bianchi, A. Gaudilliere, Metastable states, quasi-stationary and soft measures, mixing time asymptotics via variational principles, arXiv., 1103–143, (2011).
- [7] S. Bigelis, E. N. M. Cirillo, J.L. Lebowitz, E.R. Speer, Commun. Critical droplets in metastable probabilistic cellular automata, Phys. 59, 3935 (1999).
- [8] A. Bovier, F. den Hollander, F.R. Nardi, Sharp asymptotic for Kawasaki dynamics on a finite box with open boundary, Probab. Theory Relat. Fields 135, 265–310, (2006).
- [9] A. Bovier, F. den Hollander, C. Spitoni, Homogeneous nucleation for Glauber and Kawasaki dynamics in large volumes at low temperature, An Probab. Theory Relat. Fields 135, 38, (2010).
- [10] A. Bovier, M. Eckhoff, V. Gayrard and M. Klein, Metastability in stochastic dynamics of disordered mean-field models, Prob. Theory Related Fields. Phys. 119, 99–161, (2001).
- [11] A. Bovier, M. Eckhoff, V. Gayrard and M. Klein, Metastability in reversible diffusion processes. I. Sharp asymptotics for capacities and exit times. J. Eur. Math. Soc. 119, 399–242, (2004).

- [12] A. Bovier, M. Eckhoff, V. Gayrard and M. Klein, Metastability and low lying spectra in reversible Markov chains, *Commun. Math. Phys.* 228, 219–255, (2002).
- [13] A. Bovier and F. Manzo, Metastability in Glauber dynamics in the low-temperature limit: beyond exponential asymptotics, *J. Stat. Phys.* 107, 757–779, (2002).
- [14] M. Cassandro, A. Galves, E. Olivieri, M.E. Vares, Metastable behavior of stochastic dynamics A pathwise approach, *Phys. Stats.* 35, 603–634, (1984).
- [15] O. Catoni, R. Cerf, The exit path of a Markov chain with rare transitions, *Probab. Theory Relat. ESAIM*, 1, 95–144, (1997).
- [16] O. Catoni, Simulated annealing algorithms and Markov chains with rare transitions”, *Seminaire de Probabilites*, XXXIII 1709, 69–119, (1999).
- [17] O. Catoni, A. Trounev, Parallel annealing by multiple trials: a mathematical study. *Simulated annealing* 129–143, Wiley-Intersci. Ser. Discrete Math., (1992).
- [18] R. Cerf, F. Manzo, Nucleation and growth for the Ising model in d dimensions at very low temperatures, *Ann. of Prob.* 41, 3697–3785, (2013).
- [19] E. N. M. Cirillo, J. L. Lebowitz, Metastability in the two-dimensional Ising model with free boundary conditions, *Stat. Phys.* 90, 211–226, (1998).
- [20] E. N. M. Cirillo, F. R. Nardi, Metastability for a stochastic dynamics with a parallel heat bath updating rule, *Journ. Stat. Phys.* 110, 183–217, (2003).
- [21] E. N. M. Cirillo, F. R. Nardi, Relaxation height in energy landscapes: an application to multiple metastable states, *Stat. Phys.*, 150, 1080–1114, (2013).
- [22] E. N. M. Cirillo, F. R. Nardi, C. Spitoni, Metastability for reversible probabilistic cellular automata with self-interaction, *Journ. Stat. Phys.* 132, 431–471, (2008).
- [23] E. N. M. Cirillo, F. R. Nardi, C. Spitoni, Competitive nucleation in reversible Probabilistic Cellular Automata, *Physical Review E* 78. 040601(R), (2008).
- [24] E. N. M. Cirillo, F. R. Nardi, C. Spitoni, Competitive nucleation in metastable systems, *Communications to SIMAI Congress 3*, ISSN 1827-2015 (2009).
- [25] E. N. M. Cirillo, F. R. Nardi, A.D. Polosa, Magnetic order in the Ising model with a parallel dynamics”, *Journ. Phys. Rev. E* 64, 057103, (2001).
- [26] E. N. M. Cirillo, E. Olivieri, Metastability and nucleation for the Blume-Capel model: different mechanisms of transition, *Stat. Phys.* 83, 473–554, (1996).

- [27] P. Dehghanpour, R. Schonmann, Metropolis dynamics relaxation via nucleation and growth, *Commun. Math. Phys.* 188, 89-119 (1997).
- [28] F. den Hollander, F. R. Nardi, E. Olivieri and E. Scoppola, Droplet growth for three-dimensional Kawasaki dynamics, *Probab. Theory Relat. Fields* 125, 153–194, (2003).
- [29] F. den Hollander, F. R. Nardi, A. Troiani, Kawasaki dynamics with two types of particles : critical droplets., *Stat. Phys.* 149(6), 1013–1057, (2012).
- [30] F. den Hollander, F. R. Nardi, A. Troiani, Kawasaki dynamics with two types of particles: stable/metastable configurations and communication heights, *Journ. Stat. Phys.* 145(6), 1423-1457 (2011).
- [31] F. den Hollander, F. R. Nardi, A. Troiani, Metastability for low temperature Kawasaki dynamics with two types of particles, *Elect. Prob.* 17, 1–26, (2012).
- [32] F. den Hollander, E. Olivieri, E. Scoppola, Metastability and nucleation for conservative dynamics, *Math. Phys.* 41, 1424–1498, (2000).
- [33] M. I. Freidlin, A. D. Wentzell, Random perturbations of dynamical systems”, *Grundlehren der Mathematischen Wissenschaften*, J. Springer-Verlag,. New York. (1984).
- [34] R. Fernandez, F. Manzo, F. R. Nardi, J. Sohler, Asymptotically exponential hitting times and metastability, a pathwise approach without reversibility; (2015).
- [35] R. Fernandez, F. Manzo, F. R. Nardi, E. Scoppola, Conditioned quasi stationary restricted measure and escape from metastable states ; (2016).
- [36] A. Gaudilliere, E. Olivieri, E. Scoppola, Nucleation pattern at low temperature for local kawasaki dynamics in two-dimensions, *Markov Processes Relat. Fields*, 11, 553–628, (2005).
- [37] A. Gaudilliere, F. R. Nardi, An upper bound for front propagation velocities inside moving populations, *Commun. Math. Stats.* 24, 256–278, (2010).
- [38] A. Gaudilliere, F. den Hollander, E. Olivieri, and E. Scoppola, approximation for a two dimensional rarefied gas under Kawasaki dynamics, *Commun. Math. Stats.* 119 (2009) 737–774.
- [39] R. Kotecky, E. Olivieri, Shapes of growing droplets - a model of escape from the metastable phase, *Stat. Phys.* 75, 409–506, (1994).
- [40] R. Kotecky, E. Olivieri, Droplet dynamics for asymmetric Ising model, *Stat. Phys.* 70, 1121–1148, (1991).
- [41] R. Kotecky, E. Olivieri, Shape of growing droplets-A model of escape from a metastable phase, *Stat. Phys.* 75, 409–507, (1994).

- [42] H. Larralde, F. Leyvraz, Metastability for Markov Processes with Detailed Balance, *Phys. Rev.* 94, 160201 (2005).
- [43] F. Manzo, F. R. Nardi, E. Olivieri, and E. Scoppola, On the essential features of metastability: tunnelling time and critical configurations, *J. Stats. Phys.* 115, (2004).
- [44] F. Manzo E. Olivieri, Relaxation patterns for competing metastable states a nucleation and growth model”, *Markov Process. Relat. Fields* 4, 549-570, (1998).
- [45] F. Manzo, E. Olivieri, Dynamical Blume-Capel model: competing metastable states at infinite volume”, *sJourn. Stat. Phys.* 115, 591-641, (2001).
- [46] F. R. Nardi, S. C. Borst, A. Zocca,, Tunneling behavior of Ising and Potts models in the low temperature regime, (2017).
- [47] F. R. Nardi, E. Olivieri, Low temperature stochastic dynamics for an Ising model with alternating field”, *Markov Processes fields* 2, 117-166, (1996).
- [48] F. R. Nardi, E. Olivieri, and E.Scoppola, Anisotropy Effects in Nucleation for Conservative Dynamics, *Commun. Math. Phys.* 137, 539–595, (2005).
- [49] F. R. Nardi, E. Olivieri, E. Scoppola, Anisotropy effects in nucleation for conservative dynamics, *Journ. Stat. Phys.* 119, 539-595 (2005).
- [50] F. R. Nardi, C. Spitoni, Sharp Asymptotics for Stochastic Dynamics with Parallel Updating Rule with self-interaction, *Journal of Statistical Physics* 146, 701-718, (2012).
- [51] F. R. Nardi, A. Zocca,, Tunneling behavior of Ising and Potts models in the low temperature regime, (2017).
- [52] E. J. Neves and R.H. Schonmann, Critical droplets and metastability for a Glauber dynamics at very low temperature, *Commun. Math. Phys.* 137, 209–230, (1991).
- [53] E. J. Neves, R.H. Schonmann, Behavior of droplets for a class of Glauber dynamics at very low temperature, *Prob. Theory Related Fields* 91(3-4), 331-354, (1992).
- [54] E. Olivieri, E. Scoppola, Markov chains with exponentially small transition probabilities: First exit problem from general domain II. The general case, *Journ. Stat. Phys.* 84, 987-1041 (1996).
- [55] E. Olivieri, E. Scoppola, Markov chains with exponentially small transition probabilities: First exit problem from general domain I. The reversible case”, *Journ. Stat. Phys.* 79, 613-647, (1995).
- [56] E. Olivieri and M. E. Vares,, Large Deviations and Metastability, *Commun.* (Cambridge University Press, 2005).
- [57] O. Penrose, J. L. Lebowitz, Rigorous treatment of metastable states in the van der Waals Maxwell theory, *Stat. Phys.* 3, 211 (1971).

- [58] R. H. Schonmann, S. Shlosman, Wulff droplets and metastable relaxation of Kinetic Ising models, *Commun. Math. Phys.* 194, 389–462, (1998).
- [59] R.H. Schonmann, Slow droplets driven relaxation of stochastic Ising models in the vicinity of phase coexistence region, *Commun. Math. Phys.* 161, 1-49 (1994).
- [60] E. Scoppola, Metastability for Markov chains: a general procedure based on renormalization group ideas, *Probability and phase transition* (Cambridge, 1993), NATO Adv. Sci. Inst. Ser. C Math. Phys. Sci., vol. 420, pp. 303-322, (1994).
- [61] A. Trounev, Cycle decomposition and simulated annealing, *SIAM J. control and optimization* 34, 966–985, (1996).
- [62] A. Trounev, Partially parallel simulated annealing: low and high temperature approach of the invariant measure, *Applied stochastic analysis* (New Brunswick, NJ, 1991), 262– 278, *Lecture Notes in Control and Inform. Sci.* 177, Springer, Berlin, (1992).