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An introduction to metastability through random walks

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Abstract. This paper gives a didactic introduction to the problem of metastability by taking elementary examples from the theory of random walks. Some mathematical tools of the theory are presented briefly with precise references. The main ideas used in recent results about the conservative case, are discussed in the last section, through simplified models of random walks.

1 Introduction

The aim of the paper is to give a brief introduction to the main ideas of metastability, providing some mathematical tools necessary to construct a general theory. We will start from physics, from a ferromagnet, but we will use it just as an example to understand the problem and to single out the interesting questions. Due to limited space we will not mention the application of the theory to other fields.

Metastability is a dynamical phenomenon taking place in the vicinity of a first-order phase transition. It is a difficult topic, because of the many different aspects of the problem. Different mathematical methods are involved in the construction of a theory of metastability, like the Freidlin and Wentzell results on small random perturbations of dynamical systems or analytical methods to control the convergence to equilibrium of a random process by means of the spectral properties of its generator. Also, geometrical problems like isoperimetric inequalities are involved to describe the cooperative effect of a large deviation. The different mathematical tools necessary to a complete analysis of the problem are presented in the paper in brief by simple examples and with precise references for the interested reader.

Some recent results, concerning the more difficult conservative case, are discussed in the last section and the main ideas are presented there in a simplified way.

The paper is not a complete review on metastability but, rather, a guide for beginners. In particular we will not discuss many interesting regimes of metastability like the infinite volume results proved by Dehghampour and Schonmann for the Glauber dynamics in two dimensions (see [10,11,41,42]), or the results by Schonmann and Shlosman for the Ising model in the regime of temperature $T < T_c$ small but fixed, $h \to 0$ (see [40,43]).

A review of different regimes of the Glauber dynamics can be found in [39], Chapter 7.

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1.1 The physical problem and the model

We present a model in which metastability can be studied, starting from its physical origin. Consider a **ferromagnet** at low temperature T, say, sufficiently below the Curie temperature, and measure its magnetization m for different values of the external magnetic field h. The result of such an experiment is recalled in Figure 1.

The phenomenon of *spontaneous magnetization* takes place so that

$$\lim_{h\to 0^+} m(h) > 0, \qquad \lim_{h\to 0^-} m(h) < 0.$$

Suppose we now change the value of the external magnetic field, starting from a small negative value, going to zero and then to small positive values. Under suitable experimental conditions, we can construct in this way a state, called *metastable*, with magnetization opposite to h, in apparent equilibrium, until an external perturbation or a spontaneous, large-enough fluctuation will *nucleate* the stable phase with magnetization parallel to h, starting an irreversible process leading to global equilibrium. A similar behavior is observed in the opposite direction, from positive to negative h. Metastable states correspond to the dashed line in the picture. At high temperature this phenomenon disappears. A more detailed description of this physical phenomenon can be found, for instance, in [1].

A simple model to describe some aspect of ferromagnetism is the **Ising model**. Consider a finite volume $\Lambda \subset \mathbb{Z}^d$. With each site $x \in \Lambda$ is associated a spin variable $\sigma(x) \in \{-1, +1\}$. The interaction between spin variables is given by the following Hamiltonian:

$$H(\sigma) = -\frac{J}{2} \sum_{(x,y)\in\Lambda^*} \sigma(x)\sigma(y) - \frac{h}{2} \sum_{x\in\Lambda} \sigma(x), \tag{1.1}$$

where the first sum is over the set Λ^* of all the pairs (x, y) of nearest-neighbor sites, $J > 0$ is the pair interaction, $h > 0$ is the external magnetic field, and we

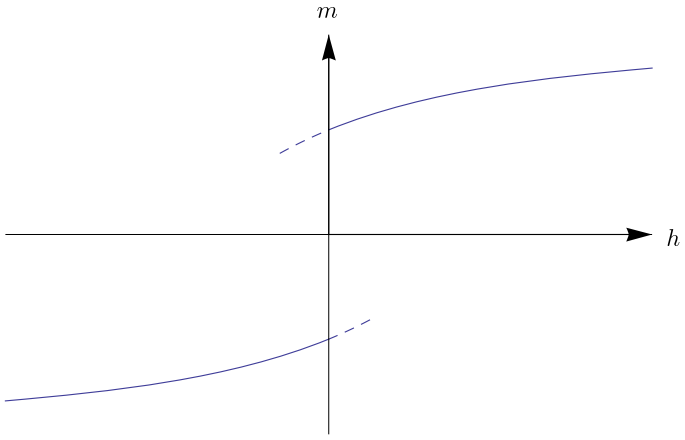

Figure 1 *Spontaneous magnetization and metastable states (dashed line).*

assume periodic boundary conditions on Λ. Denote by $\mathcal{X} = \{+1, -1\}^\Lambda$ the space of all possible spin configurations σ. These spin variables represent a crude description of atom spins.

Following the general ideas of equilibrium statistical mechanics, to describe a macroscopic physical system, instead of analyzing the microscopic variables describing the system, we look at families of probability measures on the state space, called *statistical ensembles*. Each statistical ensemble depends on some parameters. In particular, for the ferromagnet we are considering, we introduce a measure depending on the volume Λ, on the external magnetic field h and on the temperature: the *grand-canonical Gibbs measure*

$$\mu(\sigma) = \frac{e^{-\beta H(\sigma)}}{Z} \qquad (\sigma \in \mathcal{X}), \text{ where } Z = \sum_{\sigma \in \mathcal{X}} e^{-\beta H(\sigma)}, \tag{1.2}$$

and $\beta > 0$ is the inverse temperature. To describe macroscopic physical quantities, we have to consider the *thermodynamic limit* $\Lambda \to \mathbb{Z}^d$.

A short introduction to equilibrium statistical mechanics can be found in [39], Section 3.3, where Gibbs measures in the thermodynamic limit are rigorously defined. In that chapter the reader can also find a first description of phase transitions and in particular a rigorous proof of the existence of a phase transition at low temperature for the Ising model when $d \geq 2$. See also [16] for a more detailed analysis.

The Ising model turns out to be sufficiently simple to be rigorously studied and on the other hand not trivial so that interesting physical aspects, like phase transitions, can be described in its framework. More information on the Ising model can be found in classical Statistical Mechanics books like [24].

We now want to describe the **evolution of a metastable state**, and in particular its decay to the stable equilibrium through the nucleation of the stable phase. Different strategies can be adopted to this purpose, since a general theory of nonequilibrium statistical mechanics is still lacking. A metastable state can be described as a Gibbs measure conditioned to a suitable subset $\mathcal{R}$ of the state space corresponding to the metastable phase. This approach was originally developed by Lebowitz and Penrose [29]. More details can also be found in [39], Section 4. In these notes we will rather adopt the *pathwise approach* introduced in [7] by Cassandro et al.

We define a dynamics on the state space $\mathcal{X}$ by means of a **Markov chain** (MC) on $\mathcal{X}$ with *invariant measure* given by the equilibrium Gibbs measure (1.2), corresponding to the stable phase. Let $(\sigma_t)_{t \in \mathbb{N}_0}$ be the discrete-time MC with transition probabilities given by the *Glauber–Metropolis algorithm*: the transitions from a configuration σ are allowed only towards the configurations σ^x, $x \in \Lambda$, where

$$\sigma^x(y) = \begin{cases} \sigma(y), & \text{if } x \neq y, \\ -\sigma(y), & \text{if } x = y. \end{cases} \tag{1.3}$$

Each transition $\sigma \to \sigma^x$ occurs at rate given by the *Metropolis rate*: $e^{-\beta[H(\sigma^x)-H(\sigma)]_+}$, where $[a]_+ := a \vee 0$. This means that the transition probability

of the chain is given by

$$P(\sigma,\sigma') = \begin{cases} \dfrac{1}{|\Lambda|} e^{-\beta[H(\sigma^x)-H(\sigma)]_+}, & \text{if } \sigma' = \sigma^x \text{ for some } x, \\ 1 - \displaystyle\sum_{x\in\Lambda} \frac{1}{|\Lambda|} e^{-\beta[H(\sigma^x)-H(\sigma)]_+}, & \text{if } \sigma' = \sigma, \\ 0, & \text{otherwise.} \end{cases} \tag{1.4}$$

This dynamic is *nonconservative* in the sense that the total magnetization is not a conserved quantity. It is easy to check that the *reversibility* condition

$$\mu(\sigma)P(\sigma,\sigma') = \mu(\sigma')P(\sigma',\sigma) \tag{1.5}$$

is satisfied with μ the Gibbs measure defined in (1.2) so that μ is the invariant measure of the chain. Moreover the chain is irreducible and aperiodic, which implies that the t-step transition probability P^t converges to the invariant measure as $t \to \infty$:

$$\lim_{t\to\infty} P^t(\sigma_0,\sigma) = \mu(\sigma) \tag{1.6}$$

for any starting configuration $\sigma_0 \in \mathcal{X}$ and any $\sigma \in \mathcal{X}$.

Metastability takes place when the MC is such that this convergence to equilibrium is realized through a *large deviation* mechanism. This implies that there exists an initial measure which is almost invariant for large times. In this way the decay of the metastable state turns out to be described by the convergence to equilibrium of the Markov chain starting from an initial measure corresponding to the metastable state.

In Section 2 we will clarify what we mean by "metastability through large deviations" with a very simple example.

1.2 More references on Markov chains

Markov chains are an important subject in probability theory and are a crucial tool in metastability. A beautiful, easy and self-contained introduction to the theory of Markov chains can be found in [23] in which applications are also considered. In particular the Markov chain Monte Carlo method (MCMC) for sampling is illustrated with several examples. This method is actually strictly related to mestastability, since a rigorous analysis of the convergence to equilibrium, that is, of the method's efficiency, requires the discussion of possible metastable states. For the MCMC method see also the review by Jerrum and Sinclair [25].

We also mention here the connection between Markov chains and electric networks. A very interesting approach to the study of Markov chains and their convergence to the stationary measure is based on *potential theory*. Indeed, several probabilistic quantities, like the mean value of the first hitting time to a given set, can be studied in terms of electrostatic quantities like capacities and equilibrium potential. See the very informative paper by Doyle and Snell [14], and the useful

review on this subject given by Gaudillière in [18] for the lecture notes of the XIIth Brazilian School of Probability (Ouro Preto, 2008).

These ideas turn out to give rise to an alternative approach to metastability ([3–5]) with respect to that of large deviations, providing sharp estimates on the *mean decay time* of metastable states with a control not only in the logarithmic asymptotic sense. This means that following the approach based on large deviations, quite rough estimates can be obtained, since prefactors of exponentially small quantities are not taken into account. The potential theoretical approach, on the other hand, takes into account also these prefactors providing in this way sharper estimates.

We will follow in these notes the large deviations ideas because more information can be obtained in this way on the decay of the metastable state.

2 Metastability in finite state space

When $|\mathcal{X}|$ does not depend on β, for large β, the stable states coincide with the configurations with minimal energy, on which the invariant measure is concentrated. In a similar way the metastable states are configurations corresponding to local minima.

2.1 A toy model: 1D-RW

Consider a random walk $\{X_t\}_{t\in\mathbb{N}}$ on $\mathcal{X} = \{0, 1, \ldots, n\}$ reversible w.r.t. the following measure:

$$\mu(x) = \frac{e^{-\beta H(x)}}{Z}, \qquad Z = \sum_{x=0}^{n} e^{-\beta H(x)}$$

where the Hamiltonian $H(x)$ is given by the double well shown in Figure 2.

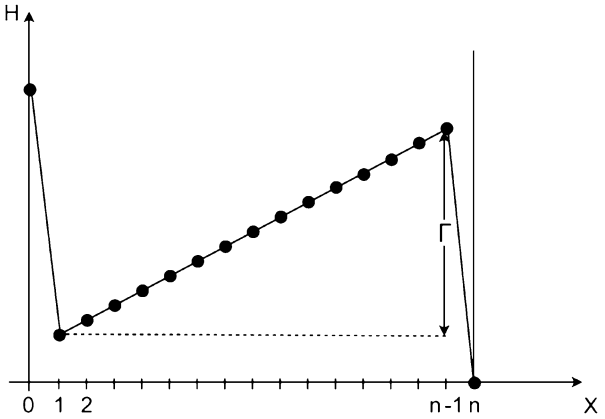

Figure 2 *Double well for the 1D-RW.*

This means that, for each $x, y \in \mathcal{X}$, the transition probabilities of the chain are given by the Metropolis rule

$$P(x,y) = \begin{cases} \frac{1}{2} e^{-\beta[H(y)-H(x)]_+}, & \text{if } |x-y| = 1, \\ 0, & \text{if } |x-y| > 1, \\ 1 - \frac{1}{2} \sum_{y:|x-y|=1} e^{-\beta[H(y)-H(x)]_+}, & \text{if } x = y, \end{cases} \tag{2.1}$$

where we can consider $H(-1) = H(n+1) = \infty$, in order to have the random walk in the interval $[0, n]$, and we consider the regime of large β at fixed n. We can look at this random walk as a simple case of a birth and death chain.

The measure μ, which is the invariant measure of the chain, is concentrated on the state of minimal energy, that is, the state n. Due to the convergence result recalled in Equation (1.6), the chain X_t in a sufficiently long time will reach this stable state n, with probability converging to one as $\beta \to \infty$. All the other states have a measure which is exponentially smaller in β. Among these, when $\beta \to \infty$, the state 1 has the largest measure, it is a local minimum. Actually the chain can be viewed as a small stochastic perturbation of a random walk $X_t^{(0)}$, that we call 0-*temperature dynamics*, with absorbing states 1 and n obtained by Equation (2.1) in the limit $\beta \to \infty$. This means that the transition probabilities of this 0-temperature dynamics are given by

$$\begin{aligned} P^{(0)}(x,x) = P^{(0)}(x,x-1) = \tfrac{1}{2}, \\ P^{(0)}(x,x+1) = 0 \qquad \text{for } x = 2, \dots, n-2, \end{aligned} \tag{2.2}$$

$$P^{(0)}(0,0) = P^{(0)}(0,1) = \tfrac{1}{2}, \tag{2.3}$$

$$P^{(0)}(n-1,n) = P^{(0)}(n-1,n-2) = \tfrac{1}{2}, \qquad P^{(0)}(n-1,n-1) = 0, \tag{2.4}$$

so that the state $n-1$ represents the saddle configuration:

$$P^{(0)}(1,1) = P^{(0)}(n,n) = 1, \tag{2.5}$$

so that 1 and n are absorbing states. The random walk $X_t^{(0)}$, when moving, that is, not considering the steps $i \to i$, is subject to a drift towards the left from $n-1$ to 1 and a drift towards the right from 0 to 1 and from $n-1$ to n.

This dynamics, with large probability, reaches its absorbing states, 1 or n, in a time n^α for $\alpha \geq 2$. Indeed the probability that the absorbtion time is larger than t is smaller than

$$\sum_{i-0}^{n-1} \binom{t}{i} 2^{-t} \leq e^{-c(t-n\ln t)}$$

for a suitable constant c.

For large β the process X_t is close to this 0-temperature dynamics $X_t^{(0)}$ and again its evolution reaches the set $\{1, n\}$ with large probability in a short time. Starting from this set the process X_t typically remains in the same state for a time exponentially large in β, at least of order $e^{\delta\beta}$ where $\delta := H(2) - H(1)$.

Consider now the evolution of the chain X_t starting at the state 1. After many unsuccessful attempts to leave this state, coming back after small fluctuations, there will be a large fluctuation corresponding to a motion against the drift, producing a fast transition to n.

We summarize the behavior of the above-described chain with the following proposition that we prove in this very simple case in order to present in the simplest context some ideas and techniques that are used in more general situations. The general version of these results is developed in the Freidlin Wenzell theory, as discussed in Section 3.

We denote by τ_A the first hitting time to the set $A \subset \mathcal{X}$, and shortly τ_x when $A = \{x\}$, and by $\mathbb{P}_x$ the probability conditioned to the starting point x and by $\mathbb{E}_x$ the corresponding mean.

Proposition 2.1. *For every positive* ε:

(1) *Uniformly in* $x \in \mathcal{X}$

$$\mathbb{P}_x\big(\tau_{\{1,n\}} > e^{\varepsilon\beta}\big) = SES,$$

where SES means super exponentially small in β. *Moreover for any* $x < n-1$

$$\lim_{\beta\to\infty} \mathbb{P}_x(\tau_1 < \tau_n) = 1.$$

(2) *If* $\Gamma = H(n-1) - H(1)$ *uniformly in* $x < n-1$ *we have*

$$\lim_{\beta\to\infty} \mathbb{P}_x\big(e^{\beta(\Gamma-\varepsilon)} < \tau_n < e^{\beta(\Gamma+\varepsilon)}\big) = 1.$$

(3) *For any* $x < n-1$

$$\lim_{\beta\to\infty} \frac{1}{\beta} \ln \mathbb{E}_x(\tau_n) = \Gamma.$$

(4) *If* $\tau_{\{0,n-1\}}$ *is the first exit time from the interval* $[1, n-2]$, *for any* x *in this interval we have*

$$\mathbb{P}_x\big(X_{\tau_{\{0,n-1\}}} = 0\big) \le e^{-\beta[H(0)-H(n-1)-\varepsilon]}.$$

2.2 Proof of Proposition 2.1

(1) Starting from every $x \in \mathcal{X}$, we define the *decreasing path* starting at x, as the sequence of states in $\mathcal{X}$, $\{\phi_t^d(x)\}_{t=0,1,\dots,n}$, satisfying
- $\phi_t^d(x) = x$ for all t, for $x = 1$ or n;
- $\phi_t^d(x) = (x-t) \vee 1$, for $x = 2, 3, \dots, n-1$;

- $\phi_t^d(0) = (x+t) \wedge 1$.

Note that the decreasing paths are the paths of the 0-temperature dynamics when cutting out the steps $i \to i$, with the exclusion of the transition $n-1 \to n$, having probability $\frac{1}{2}$ for the process $X^{(0)}$. Indeed for the saddle point $n-1$ it is possible to define the decreasing path to the left (as done in the previous definition) or to the right, to the absorbing state n.

The event $D_n := \{X_t = \phi_t^d(X_0), \text{ for } t = 0, 1, \dots, n\}$, that is, the process follows the decreasing path, implies the arrival to the set $\{1, n\}$ and, for β large it has a probability at least of order 2^{-n} so that the event $\tau_{\{1,n\}} > e^{\varepsilon\beta}$ implies that in each of the $\frac{e^{\varepsilon\beta}}{n}$ subintervals of length n of the interval of length $e^{\varepsilon\beta}$ the event D_n is not realized. We can conclude

$$\mathbb{P}_x\big(\tau_{\{1,n\}} > e^{\varepsilon\beta}\big) \le (1-2^{-n})^{e^{\varepsilon\beta}/n} = SES.$$

Note that we are considering the regime n fixed and β large. The second claim of this point immediately follows by looking at the motion at 0-temperature and noting that every step "against the flow," that is, following the increasing direction of H, has a probability smaller or equal to $e^{-\delta\beta}$, so that the probability that the process X_t follows a path which is not a trajectory of $X_t^{(0)}$ in a time interval exponentially shorter than $e^{\delta\beta}$, is exponentially small in β.

(2) To prove that

$$\mathbb{P}_x\big(\tau_n > e^{\beta(\Gamma+\varepsilon)}\big) = SES$$

we can proceed as in the previous point. We define the event "go to the right": $R_n := \{X_t = (X_0 + t) \wedge n, t = 0, 1, \dots, n\}$. R_n implies $\{\tau_n \le n\}$ and indeed its probability can be estimated from below uniformly in the starting point x by $e^{-\beta(\Gamma+\varepsilon/2)}$, for β sufficiently large, so that we can conclude as before: for each $t \ge e^{\beta(\Gamma+\varepsilon)}$

$$\mathbb{P}_x(\tau_n > t) \le \big(1 - e^{-\beta(\Gamma+\varepsilon/2)}\big)^{t/(2n)} \le e^{-te^{-\beta(\Gamma+\varepsilon/2)}/(2n)} = SES. \tag{2.6}$$

The opposite bound can be proved by using reversibility. By point (1) it is sufficient to consider the case $x = 1$ since

$$\mathbb{P}_x\big(\tau_n < e^{\beta(\Gamma-\varepsilon)}\big) \le \mathbb{P}_x\big(\tau_1 < \tau_n < e^{\beta(\Gamma-\varepsilon)}\big) + \mathbb{P}_x(\tau_1 \ge \tau_n)$$

and $\mathbb{P}_x(\tau_1 < \tau_n < e^{\beta(\Gamma-\varepsilon)}) \le \mathbb{P}_1(\tau_n < e^{\beta(\Gamma-\varepsilon)})$.

We have

$$\mathbb{P}_1\big(\tau_n < e^{\beta(\Gamma-\varepsilon)}\big) \le \mathbb{P}_1\big(\tau_{n-1} \le e^{\beta(\Gamma-\varepsilon)}\big) = \sum_{t=1}^{e^{\beta(\Gamma-\varepsilon)}} \sum_{\substack{\omega=\{\omega_0=1,\omega_1,\dots,\omega_t=n-1\} \\ \omega_i \ne n-1, i=1,\dots,t-1}} P(\omega)$$

where by time reversal

$$\begin{aligned} P(\omega) &:= P(\omega_0,\omega_1)P(\omega_1,\omega_2)\cdots P(\omega_{t-1},\omega_t) \\ &= \frac{\mu(n-1)}{\mu(1)} P(\omega_t,\omega_{t-1})\cdots P(\omega_2,\omega_1)P(\omega_1,\omega_0) =: \frac{\mu(n-1)}{\mu(1)} P(\overleftarrow{\omega}), \end{aligned}$$

so that

$$\mathbb{P}_1\big(\tau_{n-1} \le e^{\beta(\Gamma-\varepsilon)}\big) = \frac{\mu(n-1)}{\mu(1)} \sum_{t=1}^{e^{\beta(\Gamma-\varepsilon)}} \sum_{\substack{\omega=\{\omega_0=1,\omega_1,\dots,\omega_t=n-1\} \\ \omega_i\neq n-1, i=1,\dots,t-1}} P(\overleftarrow{\omega}).$$

Since the last sum is the probability that starting at $n-1$ the process reaches 1 at t without visiting the sites $n-1$ and n in between, and so it's smaller than one, we can conclude

$$\mathbb{P}_1\big(\tau_{n-1} \le e^{\beta(\Gamma-\varepsilon)}\big) \le e^{\beta(\Gamma-\varepsilon)} \frac{\mu(n-1)}{\mu(1)} = e^{-\beta\varepsilon}.$$

(3) For any $\varepsilon > 0$

$$\begin{aligned}\mathbb{E}_x\tau_n &= \sum_{t=0}^{\infty} t\mathbb{P}_x(\tau_n = t) \ge \sum_{t=e^{\beta(\Gamma-\varepsilon)}}^{e^{\beta(\Gamma+\varepsilon)}} t\mathbb{P}_x(\tau_n = t) \\ &\ge e^{\beta(\Gamma-\varepsilon)}\mathbb{P}_x\big(e^{\beta(\Gamma-\varepsilon)} < \tau_n < e^{\beta(\Gamma+\varepsilon)}\big).\end{aligned}$$

On the other hand, for a discrete stopping time we have

$$\mathbb{E}_x\tau_n = \sum_{t=0}^{\infty} \mathbb{P}_x(\tau_n > t) \le e^{\beta(\Gamma+\varepsilon)} + \sum_{t>e^{\beta(\Gamma+\varepsilon)}} \mathbb{P}_x(\tau_n > t)$$

and by (2.6) and by using that ε is arbitrarily small we obtain

$$\lim_{\beta\to\infty} \frac{1}{\beta} \ln \mathbb{E}_x(\tau_n) = \Gamma.$$

(4) The proof of the last point is straightforward

$$\begin{aligned}&\mathbb{P}_x(X_{\tau_{\{0,n-1\}}} = 0) \\ &\quad= \sum_{t=1}^{\infty} \mathbb{P}_x\big(\{X_{\tau_{\{0,n-1\}}} = 0\} \cap \big\{\tau_{\{0,n-1\}} = t\big\}\big) \\ &\quad= P(1,0) \sum_{t'=0}^{\infty} \mathbb{P}_x\big(\{X_{t'} = 1\} \cap \big\{\tau_{\{0,n-1\}} > t'\big\}\big) \le P(1,0)\mathbb{E}_x\tau_{\{0,n-1\}} \\ &\quad\le P(1,0)\mathbb{E}_x\tau_{n-1} \le P(1,0)\mathbb{E}_x\tau_n \le e^{-\beta[H(0)-H(n-1)-\varepsilon]}.\end{aligned}$$

2.3 Preliminary remarks on metastability

The main features of the toy model of Section 2.1, those describing its metastable behavior, can be summarized as follows:

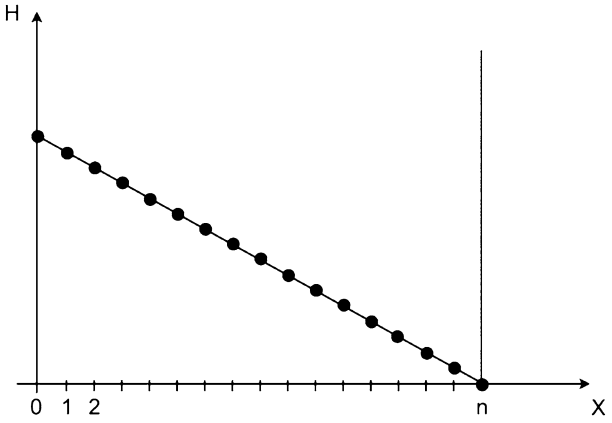

Figure 3 *A 1D-RW without metastable behavior.*

- There are two minima of the Hamiltonian H: a local minimum 1 that can be called a *metastable state* and a global minimum n representing the *stable state* where the invariant measure is concentrated. This is a very important feature of metastability. For instance the situation is completely different if we consider the random walk on $\mathcal{X} = \{0, \dots, n\}$ reversible w.r.t. the Hamiltonian shown in Figure 3.

  The time τ_n is almost deterministic in this case and it is of order n, *there is not a metastable behavior.*
- The dynamics X_t can be seen as a small random perturbation of the 0-temperature dynamics $X_t^{(0)}$, and it reaches the states $1, n$ with large probability, in a time shorter than the time necessary to go from 1 to n.
- Starting at the metastable state 1 the system performs small fluctuations around it, staying in its vicinity an exponentially long time, every time coming back to 1, remaining in the interval $[1, 2, \dots, n-2]$.
- After this time exponentially large in β a large deviation takes place with motion against the drift, leading the process X_t out of $[1, 2, \dots, n-2]$, exiting at $n-1$, which is the point of the boundary with lowest energy. From the saddle $n-1$ the stable state n is reached following the drift.
- The asymptotics of the first hitting time to the stable state starting from the metastable one has been studied in probability and in L^1. This convergence can also be studied in distribution, as explained for instance at the end of the notes [18] in a more general context (see also [30]).

2.4 A result on 2D Glauber dynamics

Consider now the two-dimensional Glauber dynamics, defined in Section 1.1, in the **metastable, finite-volume (MFV) regime**:

$$\Lambda \text{ is large but finite (independent of } \beta), \qquad h \in (0, 2J), \qquad \beta \to \infty. \quad (2.7)$$

To justify this denomination we give two arguments showing that there is a critical size l_c such that clusters smaller than l_c have the tendency to shrink while clusters larger than l_c have the tendency to grow. A first rough preliminary discussion of the energy landscape is the following: let

$$\begin{aligned} \boxplus &= \text{the configuration with } \sigma(x) = +1 \text{ for all } x \in \Lambda, \\ \boxminus &= \text{the configuration with } \sigma(x) = -1 \text{ for all } x \in \Lambda. \end{aligned} \tag{2.8}$$

In the MFV regime (2.7) the Gibbs measure will be concentrated around $\boxplus$, which is the unique ground state of H. Clearly, $\boxminus$ is only a local minimum of H that we call *metastable state*. Indeed, for $l \in \mathbb{N}$, let

$$E(l) = H(\sigma_{l\times l}) - H(\boxminus), \tag{2.9}$$

where $\sigma_{l\times l}$ is the configuration in which the $(+1)$-spins form an $l \times l$ square in a sea of (-1)-spins. It follows from (1.1) that $E(l) = 4Jl - hl^2$, which is maximal for $l = \frac{2J}{h}$; see Figure 4.

This means that, even though an arbitrarily small, nonvanishing magnetic field determines the phase, its effect is relevant only on sufficiently large space scales, namely $l \geq l_c$ with

$$l_c = \left\lceil \frac{2J}{h} \right\rceil. \tag{2.10}$$

Only on such scales the volume energy dominates the surface energy and a larger square of $(+1)$-spins is energetically more favorable than a smaller square. Note that the MFV regime implies $l_c \geq 1$.

We want to consider now the energy landscape in more details not only on square configurations. Denoting by $\sigma_{l\times l'}$, a *quasi-square* configuration in which

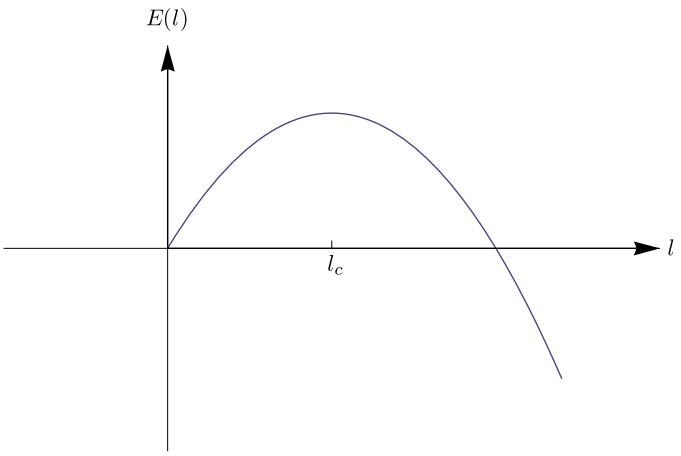

Figure 4 *The energy of a square droplet as a function of its side.*

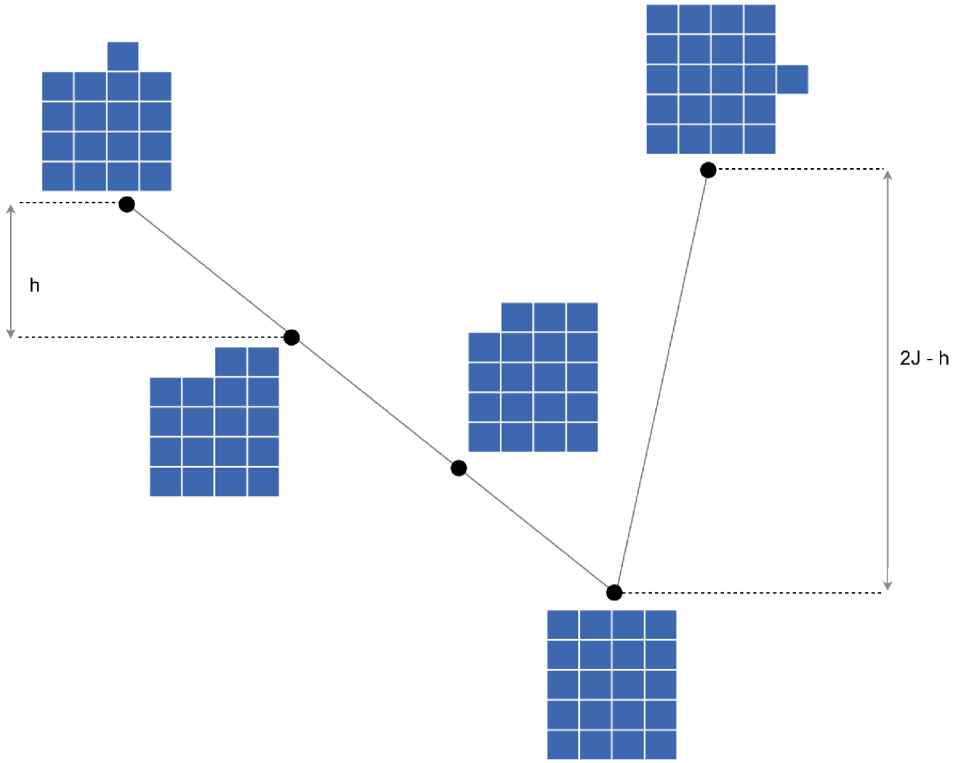

Figure 5 *Energy well for the Glauber dynamics around a quasi-square.*

the $(+1)$-spins form a $l \times l'$ rectangle in a sea of (-1)-spins, where $|l - l'| \leq 1$, we look at the energy barriers between $\sigma_{l\times l}$ and $\sigma_{l\times(l-1)}$ and between $\sigma_{l\times l}$ and $\sigma_{l\times(l+1)}$ in order to compare the probabilities of shrinking or growing. Around each quasi-square the energy landscape is like a well, as shown in Figure 5.

The energy barrier between $\sigma_{l\times l}$ and $\sigma_{l\times(l-1)}$ is given by $h(l-1)$, while the energy barrier between $\sigma_{l\times l}$ and $\sigma_{l\times(l+1)}$ is given by $2J - h$. If l is such that $h(l-1) > 2J - h$, that is, $l > l_c$ with l_c given by (2.10), then the cluster tends to grow, while if $l < l_c$ then the energy barrier on the left in the picture is lower than that on the right so that the cluster tends to shrink.

The above heuristic arguments have been developed in a rigorous way by Neves and Schonmann [34,35] (see also Schonmann [40–42]). Let

$$\tau_A = \min\{t \in \mathbb{N}_0 : \sigma_t \in A\} \tag{2.11}$$

be the *first hitting time* of the set $A \subset \mathcal{X}$, as before we use τ_η in the case $A = \{\eta\}$, and let

$$\tau_{\eta,\eta'} = \max\{t < \tau_{\eta'} : \eta_t = \eta\}$$

be the *time of the last visit to* η *before visiting* η'.

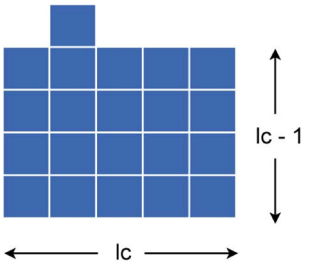

Figure 6 *The critical droplet.*

The main result for metastability in MFV regime reads:

Theorem 2.1 ([34,35]). *Suppose that Λ is sufficiently large. Suppose that $h \in (0, 2J)$, with $\frac{2J}{h}$ not integer, and put $l_c = \lceil \frac{2J}{h} \rceil$.*

(a) *Let $\mathcal{R}$ be the set of configurations where the $(+1)$-spins form a rectangle in a sea of (-1)-spins. For $\sigma \in \mathcal{R}$, let $l_1(\sigma) \times l_2(\sigma)$ be the rectangle of $(+1)$-spins in σ, and let $l(\sigma) = \min\{l_1(\sigma), l_2(\sigma)\}$. Then for any $\sigma \in \mathcal{R}$*

$$l(\sigma) < l_c: \qquad \lim_{\beta\to\infty} \mathbb{P}_\sigma(\tau_{\boxminus} < \tau_{\boxplus}) = 1, \tag{2.12}$$

$$l(\sigma) \geq l_c: \qquad \lim_{\beta\to\infty} \mathbb{P}_\sigma(\tau_{\boxplus} < \tau_{\boxminus}) = 1. \tag{2.13}$$

(b) *Let $\mathcal{C}r$ be the set of configurations where the $(+1)$-spins form a rectangle $l_c \times (l_c - 1)$ or $(l_c - 1) \times l_c$ with a protuberance attached anywhere to one of the sides of length l_c. Let $\bar{\tau}_{\mathcal{C}r} = \min\{t > \tau_{\boxminus,\boxplus} : \sigma_t \in \mathcal{C}r\}$. Then*

$$\lim_{\beta\to\infty} \mathbb{P}_{\boxminus}(\bar{\tau}_{\mathcal{C}r} < \tau_{\boxplus}) = 1. \tag{2.14}$$

(c) *Let $\Gamma(J, h) = 4Jl_c - h(l_c^2 - l_c + 1)$. Then*

$$\lim_{\beta\to\infty} \frac{1}{\beta} \log \mathbb{E}_{\boxminus}(\tau_{\boxplus}) = \Gamma(J, h). \tag{2.15}$$

Moreover, $\tau_{\boxplus}/\mathbb{E}_{\boxminus}(\tau_{\boxplus})$ converges in distribution to an exponential random variable with mean one.

Note that $\Gamma(J, h)$ is the energy of the critical droplet $\mathcal{C}r$ shown in Figure 6.

2.5 Different aspects of the problem and different approaches to metastability

Metastability in this case of Glauber dynamics is a much richer phenomenon than the one-dimensional random walk treated in Section 2.1 (1D-RW). We have here a more complicated energy landscape and a new ingredient becomes relevant now:

there is a *critical size* of the droplet representing the saddle configuration emerging from the competition in the energy between volume and perimeter of the cluster. Indeed, to have an idea of the energy landscape, consider also in this case the 0-temperature dynamics, where only moves not increasing the energy are accepted. It is immediate to see that there is a lot of local minima of H; every configuration in which the plus spins form rectangular clusters at distance larger than two from each other is a local minimum. As discussed above, looking at configurations with a unique cluster close to a square, we expect that the energy landscape is again a sort of double well, with a local minimal configurations $\boxminus$ and the absolute minimum $\boxplus$, but with many additional local minima, as shown in Figure 5, and with a saddle given by the critical configuration $\mathcal{C}r$ described in the Theorem 2.1. Again the process can be seen as a small random perturbation of a dynamical system, the 0-temperature dynamics, so that the motion against the drift is still a crucial ingredient for the nucleation of the critical droplet. As mentioned above, the results given in the case of the double well in Proposition 2.1, can be generalized to any energy landscape within the Freidlin Wentzell theory so that they constitute a general part of the theory. This is discussed in details in Freidlin and Wentzell [15], Catoni and Cerf [6], Olivieri and Scoppola [36–38] and [44], under rather general hypotheses on the Markov chain. However, this is only a first ingredient of metastability.

The more geometrical aspect involved in the discussion of the energy landscape, which is crucial when considering interacting particle systems, is an important model-dependent part of the problem in the study of metastability in concrete situations. This can be difficult even in the case of finite volume we are considering at the moment. We mention results in more than two dimensions [2], the anisotropic case [27], Ising model with nearest and next nearest neighbor interaction [28], Ising with alternating field [31,33], Blume–Capel model [9] and probabilistic cellular automata [8]. There are cases in which it is a difficult task to have a complete analysis of the full state space. In these cases the application of the general results of the Freidlin Wentzell theory is too difficult, since the complete control of the energy landscape is missing. This difficulty actually forces a reconsideration of the problem also from a general point of view, then it becomes interesting to know what is the minimal knowledge on the structure of the state space necessary to have the different results on metastability. We refer to [30] for this discussion.

The geometrical model-dependent analysis of the state space is also crucial to discuss the *tube of typical paths* followed in the transition from the metastable to the stable state. Actually, a very interesting physical question is how nucleation takes place. The study of the tube of typical paths is strictly related to the point of view of the pathwise approach where, indeed, the main point is to single out typical trajectories and to look at the statistics along such paths. So the tube of typical paths suggests the relevant part of the energy landscape which is important to analyze in order to control metastability in the pathwise approach.

We refer for this to [6,36,38,40] and [2].

As a final remark we note that this question on the tube of typical paths clearly shows that metastability is not only a problem of convergence to equilibrium in the sense of the control on nucleation time and the analytical methods to control convergence to equilibrium are not able to solve this aspect of the problem.

2.6 Back to one-dimensional random walks

We will not give here the proof of Theorem 2.1 given in [35], but we will discuss the main ideas necessary to this proof, again with our toy model introduced in Section 2.1. In this way we separate the geometrical aspects of the problem from the probabilistic ones.

The *geometrical problem* involved in the discussion of the Glauber dynamics can be summarized as follows:

> given an integer $i \in \{0, 1, \dots, |\Lambda|\}$, look for the minimal energy obtained among the configurations with i plus spins:

$$\mathcal{E}(i) := \min_{\sigma : \sum_x [\sigma(x)]_+ = i} H(\sigma).$$

This can be viewed as an isoperimetrical problem, if we note that the energy (1.1) of a spin configuration can be written as

$$H(\sigma) = Jp(\sigma) - ha(\sigma) + \text{const}, \tag{2.16}$$

where $p(\sigma)$ and $a(\sigma)$ are respectively the perimeter and the area of the union of unit squares associated to the sites where σ is $+1$. This region, corresponding to the configuration σ, is called *polyomino* in [2], where this geometrical problem is completely solved also in three dimensions. In two dimensions the plyominos minimizing the perimeter at a given area, can be found as the regions closest to squares, like in the Figure 5.

We can then consider the random walk defined in Section 2.1 with $n = |\Lambda|$ and with Hamiltonian $\mathcal{E}(i)$. This energy landscape is similar to the double well of the toy model 1D-RW, with minima in 0 and $|\Lambda|$, but now *decorated* by many additional local minima, as given in Figure 5.

The goal of the following three sections is to provide the basic tools necessary to explain:

(1) how to generalize the results of Proposition 2.1 to this more complicated energy landscape;
(2) why this one-dimensional random walk is a good representation of the original Glauber dynamics.

3 Freidlin and Wentzell results

The main ideas used to study metastability come out from the Freidlin and Wentzell (F–W) theory of diffusion processes describing small random perturbations of dynamical systems.

The crucial point of the F–W theory is to perform large deviation estimates for such a process in terms of simpler processes defined on much smaller state spaces. More precisely, it is possible to study a diffusion process, say in $\mathbb{R}^d$, in the regime of small diffusion, in terms of a Markov chain on a smaller state space $\gamma \subset \mathbb{R}^d$, which can be reduced further to a Markov chain on a finite state space L. In particular, results on the invariant measure and on the first exit from a given region can be obtained for the diffusion process in terms of similar results for a much easier finite Markov chain.

These key results of the F–W theory are given in the lemmas stated in Section 3.3, crucial to extend the analysis given in the case of 1-d random walk to general situations. They are obtained by using the not widely known tool of W-graphs recalled in what follows. We want to stress that the F–W theory is developed under general hypotheses and in particular reversibility is not required.

This reduction procedure is used later on in the so-called renormalization procedure and will be crucial in the discussion of metastability for the conservative case where the state space is exponentially large in β.

Another result of the F–W theory, based on W-graphs and concerning the spectrum of the generator of the process, is recalled in Section 5.3.

For the reader's convenience we decided to adopt in this section and in Section 6 the notation of [15] even though this is not in agreement with the notation in the rest of the paper. In particular, the large deviation parameter is $\frac{1}{\varepsilon^2}$ here, instead of β. This choice is useful to make references to [15] for details and proofs. We warn the reader about this.

3.1 From a diffusion process to a Markov chain

Consider a dynamical system in $\mathbb{R}^d$

$$\dot{x}_t^0 = b(x_t^0). \tag{3.1}$$

A small random perturbation of this system can be written in its simplest form as

$$\dot{x}_t^\varepsilon = b(x_t^\varepsilon) + \varepsilon \dot{w}_t, \tag{3.2}$$

where w_t is the Wiener process and ε a small parameter, under suitable hypotheses on b (see again [47] for definitions and general results).

Suppose that all the long time limit sets (the ω-limit sets) of the unperturbed dynamical system (3.1), say the equilibrium points and the limit cycles, are contained in a set $K = K_1 \cup \cdots \cup K_l$ given by a finite number of compacta K_i.

To make the ideas more concrete, let us consider the example of a diffusion process on $\mathbb{R}$ with $b(x) = -\frac{dU}{dx}(x)$ with $U(x)$ a symmetric double well $U(x) = (x^2-1)^2$. (See [26] for a more general one-dimensional example.) There are three equilibria in this case, $K = \{-1, 0, +1\}$. All the solutions x_t^0 of (3.1) starting in $x > 0$ ($x < 0$) will converge to the equilibrium $+1$ (-1), for $t \to \infty$. The saddle point 0 is an unstable equilibrium.

For small ε the diffusion process defined by (3.2) follows with large probability the flow defined by (3.1). So with large probability, in a time independent of ε, the diffusion process reaches the set K and remains around it under the effect of small fluctuations. Looking at the process on sufficiently large time intervals, under the effect of a large deviation, it is possible to see the diffusion process jumping from an equilibrium K_i to another, going *against the flow*, for short time intervals, using the F–W terminology. In our example this means that also transitions from -1 to 0 or from $+1$ to 0 are performed, under the effect of a large fluctuation.

Here the large deviation theory is more complicated than the easy case of the one-dimensional random walk discussed in Section 2.1. For general references on large deviation theory, see [12] and [39].

In this case the large deviation functional describing the concentration of random paths around the deterministic ones, is given by

$$I_T(\phi) = \int_0^T |\dot{\phi}(s) - b(\phi(s))|^2 \, ds.$$

Therefore I_T is zero along paths of the unperturbed system (3.1). This means that the probability that a trajectory x_t^ε in the interval $0 \le t \le T$ is close to a function $\phi(t)$, where $\phi(0) = x$ is the starting point of x_t^ε, is approximately equal to

$$\exp\left\{-\frac{1}{2\varepsilon^2} I_T(\phi)\right\}.$$

Define

$$V(x, y) = \inf_{T>0} \inf_{\phi:\phi_0=x,\phi_T=y} I_T(\phi),$$

and the equivalence relation: $x \sim y$ if $V(x, y) = V(y, x) = 0$.

Suppose the compacta $K_1 \cup \cdots \cup K_l$ are such that for any $i \in L := \{1, \ldots, l\}$

$$x \sim y \qquad \forall x, y \in K_i, \qquad x \not\sim y \qquad \text{if } x \in K_i, y \notin K_i.$$

We define

$$V_{ij} = V(x, y) \qquad \forall x \in K_i, y \in K_j.$$

To describe the behavior of the process in a simpler way, for each compactum K_i we can construct a pair of neighborhoods with smooth boundaries γ_i and Γ_i.

Let $\gamma = \bigcup_{i \in L} \gamma_i$ and $\Gamma = \bigcup_{i \in L} \Gamma_i$ and define

$$\tau_0 = 0, \qquad \sigma_n = \inf\{t \ge \tau_{n-1} : x_t^\varepsilon \in \Gamma\}, \qquad \tau_n = \inf\{t \ge \sigma_n : x_t^\varepsilon \in \gamma\}$$

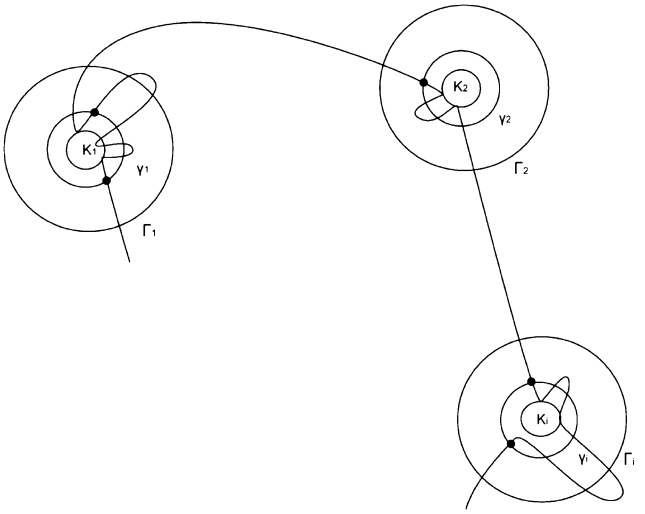

Figure 7 *Construction of the Markov chain (dots along the path correspond to the states of the MC).*

and the *Markov chain on* γ given by $z_n = x^{\varepsilon}_{\tau_n}$ (see Fig. 7).

In our example we can choose, for instance, intervals of length 0.1 and 0.2 around the points $-1, 0, 1$, respectively, for γ_i and Γ_i, with $i \in \{-1, 0, 1\} = L$.

We have that for each $h > 0$ there is an $r > 0$ such that for any choice of the two neighborhoods inside the r-neighborhoods of K_i, and for ε sufficiently small, for $x \in \gamma$:

$$e^{-V_{ij}-h/(2\varepsilon^2)} < P(x, \gamma_j) < e^{-V_{ij}+h/(2\varepsilon^2)}. \tag{3.3}$$

Briefly we will write $P(x, \gamma_j) \asymp e^{-V_{ij}/(2\varepsilon^2)}$. More broadly we use this symbol to denote estimates in the logarithmic asymptotic sense. We write $A \asymp e^{B/(2\varepsilon^2)}$ if for any $h > 0$ and any ε sufficiently small we have

$$e^{B-h/(2\varepsilon^2)} < A < e^{B+h/(2\varepsilon^2)}. \tag{3.4}$$

3.2 *W*-graphs

For this kind of Markov chain, F–W theory provides estimates on the invariant measure, on the mean number of steps until the first entrance in a given set $\bigcup_{i\in W} \gamma_i$ and on the typical first entrance in this set by using the following graphs of arrows.

Let $L = \{1, \ldots, l\}$ and $W \subset L$, a graph of arrows $m \to n$ with $m \in L\backslash W$ and $n \in L$ is called a *W-graph* if:

(1) every point $m \in L\backslash W$ is the initial point of exactly one arrow,
(2) there are no closed cycles in the graph.

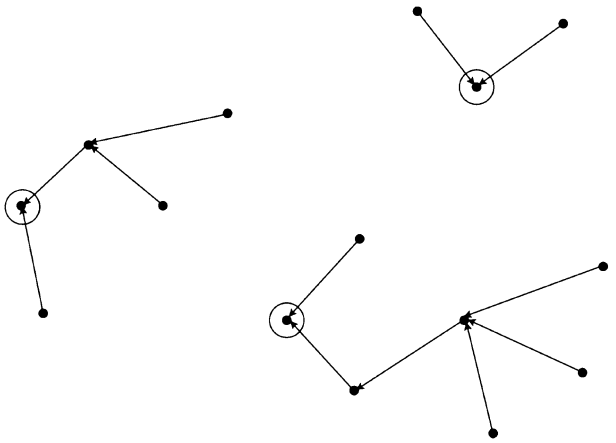

Figure 8 *A W-graph (dots represent states in L, dots within a circle states in W).*

Condition (2) can be replaced with

(2′) for every point $m \in L \setminus W$ there exists a sequence of arrows leading from it to some point in W.

This means that a W-graph can be seen as a forest with arrows directed to the roots of the trees which are points in W. Figure 8 is an example of W-graph. We will denote by $G(W)$ the set of W-graphs, and if $p_{ij}, i, j \in L$ are numbers given by $p_{ij} = e^{-V_{ij}/2\varepsilon^2}$, given a graph $g \in G(W)$ let $\pi(g) = \prod_{(m\to n)\in g} p_{mn}$.

3.3 Lemmas on Markov chains

The first exit problem and the invariant measure of the diffusion process can be studied (see [15], Chapter 6) by using the following general results on Markov chains on a state space $\gamma = \bigcup_{i\in L} \gamma_i$ such that

$$a^{-1} p_{ij} \le P(x, \gamma_j) \le a p_{ij}, \qquad x \in \gamma_i, i \ne j,$$

for some $a > 1$.

Note that this hypothesis is verified for the Markov chain defined in Section 3.1 (see [3.3]), with $a = e^{h/(2\varepsilon^2)}$.

Suppose that for every $i \in L$ and $x \in \gamma$, there exists s such that $P^s(x, \gamma_i) > 0$, that is, every γ_i can be reached from any state x, sooner or later.

Lemma 3.1. *The invariant measure ν satisfies*

$$a^{2-2l}\Big(\sum_{i\in L} Q_i\Big)^{-1} Q_i \le \nu(\gamma_i) \le a^{2l-2}\Big(\sum_{i\in L} Q_i\Big)^{-1} Q_i,$$

where

$$Q_i = \sum_{g \in G(\{i\})} \pi(g).$$

For $i \in L \backslash W$, $j \in W$ we denote by $G_{ij}(W)$ the set of W-graphs in which the sequence of arrows leading from i into W ends at the point j. We also denote by $q_W(x, \gamma_j)$ the probability that at the first entrance time of $\bigcup_{k \in W} \gamma_k$ the chain starting from x hits γ_j.

Lemma 3.2. *If the number of points in $L \backslash W$ is r then*

$$a^{-4r} \frac{\sum_{g \in G_{ij}(W)} \pi(g)}{\sum_{g \in G(W)} \pi(g)} \leq q_W(x, \gamma_j) \leq a^{4r} \frac{\sum_{g \in G_{ij}(W)} \pi(g)}{\sum_{g \in G(W)} \pi(g)}$$

with $x \in \gamma_i$, $i \in L \backslash W$, $j \in W$.

Let $m_W(x)$ be the mean number of steps until the first entrance on the set $\bigcup_{i \in W} \gamma_i$ starting from x.

Lemma 3.3. *If the number of points in $L \backslash W$ is r then for $x \in \gamma_i$, $i \in L \backslash W$:*

$$\begin{aligned} & a^{-4r} \frac{\sum_{g \in G(W \cup \{i\})} \pi(g) + \sum_{j \in L \backslash W, j \neq i} \sum_{g \in G_{ij}(W \cup \{i\})} \pi(g)}{\sum_{g \in G(W)} \pi(g)} \\ & \quad \leq m_W(x) \\ & \quad \leq a^{4r} \frac{\sum_{g \in G(W \cup \{i\})} \pi(g) + \sum_{j \in L \backslash W, j \neq i} \sum_{g \in G_{ij}(W \cup \{i\})} \pi(g)}{\sum_{g \in G(W)} \pi(g)}. \end{aligned}$$

3.4 Remarks on F–W results

- We do not give here the proofs of these lemmas, which can be found in Chapter 6 of [15]; we strongly recommend these to the interested reader. Indeed, after only looking at these proofs it becomes clear that a W-graph is an important tool producing simple and very elegant proofs.
- As discussed above, metastability in finite volume can be described in terms of the first arrival of the process to the stable state of minimal energy. This means that the results on the typical exit from a given region given by Lemmas 3.2 and 3.3, represent the main tool for the discussion of metastability in this regime. In particular, not only the asymptotic of the first hitting time to the stable state can be obtained but, as discussed below, information on the tube of typical paths followed in the transition from the metastable state to the stable one can also be derived in terms of typical exits from a suitable sequence of sets. Note that the results recalled in this section are very general and, in particular, reversibility is not required. In the reversible case, similar results can be obtained without the help of W-graphs, as discussed in the following section (see also [36]).

- Note that with the construction of the Markov chain we have a first reduction of the state space from $\mathbb{R}^d$ to γ. Moreover, it is possible to study the chain on γ through a finite Markov chain on L. Indeed, consider the MC on L with

$$p_{ij} = \frac{1}{\nu(\gamma_i)} \int_{\gamma_i} \nu(dx) P(x, \gamma_j).$$

Recall that for each i, j there exists s such that $P^s(x, \gamma_i) > 0$, with $x \in \gamma_j$, so $\nu(\gamma_i) > 0$ for all i. This finite Markov chain clearly satisfies the hypotheses of the lemmas with $a = 1$, so that the invariant measure and the exit from a given region for the diffusion process can be actually studied in terms of the same quantities evaluated for this finite chain.

Coming back to our example, we can then describe our diffusion process by means of a Markov chain on the state space $\{-1, 0, +1\}$ with transition probabilities: $p_{ij} = e^{-V_{i,j}/(2\varepsilon^2)}$ where, by symmetry, $V_{0,1} = V_{0,-1} = 0$, since there exists a solution of the unperturbed system x_t^0 going from δ to $1 - \delta$ for any positive, arbitrarily small δ, and so a path ϕ going from 0 to 1 arbitrarily close to x_t^0. For transitions in the opposite direction we have $V_{-1,0} = V_{1,0} = 4U(0) = 4$ since in the gradient case $b(x) = -U'(x)$ it is easy to estimate the large deviation functional:

$$\begin{aligned} V_{1,0} &= \inf_{T>0} \inf_{\phi:\phi_0=1,\phi_T=0} \int_0^T |\dot{\phi}(s) + U'(\phi(s))|^2 \, ds \\ &= \inf_{T>0} \inf_{\phi:\phi_0=1,\phi_T=0} \int_0^T \big(|\dot{\phi}(s) - U'(\phi(s))|^2 + 4\dot{\phi}(s)U'(\phi(s))\big) \, ds \qquad (3.5) \\ &\geq 4\big(U(0) - U(1)\big) = 4. \end{aligned}$$

On the other hand $V_{1,0} \leq I_T(\psi)$, where ψ is a path going from 1 to 0, arbitrarily close to a solution of the equation $\dot{\phi} = -b(\phi) = U'(\phi)$ going from $1 - \delta$ to δ, for arbitrarily small δ. We have

$$I_T(\psi) = \int_0^T |2b(\psi(s))|^2 = 4 \int_0^T \dot{\psi}(s) U'(\psi(s)) \, ds = 4.$$

- W-graphs are a very interesting and powerful tool of the theory. We have to note that even if they provide very general results with elegant proofs, however their application, when $|L| = l$ is large it involves difficult combinatorial problems since the set of W-graphs considered in the sums have a large cardinality. In other words, W-graphs are not a simple tool for explicit calculations for finite chains with large state space.

4 The reversible case

In the reversible case, that is, when the transition probabilities of the MC satisfy (1.5) and can be defined by means of an energy landscape H, the first exit problem

can be solved without W-graphs, by using the function H. Since both the toy model 1D-RW and the Glauber dynamics are reversible MC, we briefly discuss in this section the theory in this reversible case. We first introduce the main tool of the theory in this case: the *cycles*.

4.1 Cycles

We need first of all some definition and notation.

Let $\sigma, \sigma' \in \mathcal{X}$, we denote by $\varphi : \sigma \rightsquigarrow \sigma'$ a *path*, that is, a finite sequence σ_0, $\sigma_1, \dots, \sigma_n$ of configurations such that, for any $i < n$, $P(\sigma_i, \sigma_{i+1}) > 0$, starting at σ and ending at σ'.

We will denote by $\overleftarrow{\varphi}$ the *time reversal of* φ, defined by

$$\overleftarrow{\varphi} := (\sigma_n, \dots, \sigma_1, \sigma_0).$$

A subset $\mathcal{V}$ of $\mathcal{X}$ is said to be *connected* if for any σ and σ' in $\mathcal{V}$ there exists a path $\varphi : \sigma \rightsquigarrow \sigma'$ which never leaves $\mathcal{V}$.

For any subset $\mathcal{V}$ of $\mathcal{X}$ we will denote by $\partial\mathcal{V}$ its *border*:

$$\partial\mathcal{V} := \{\sigma' \in \mathcal{X} \setminus \mathcal{V} : \exists \sigma \in \mathcal{V}, P(\sigma, \sigma') > 0\}.$$

We say that the connected set of configurations $\mathcal{C} \subset \mathcal{X}$ is a **cycle** if it satisfies one at least of the two following conditions:

(i) $\mathcal{C}$ is a singleton;
(ii) $\inf H(\partial\mathcal{C}) > \sup H(\mathcal{C})$ [with the convention: $\inf H(A) = \inf_{\sigma \in A} H(\sigma)$, the same for sup, and $H(\varnothing) = +\infty$].

A cycle which satisfies the first condition only is called *trivial cycle*. A cycle which satisfies the second condition is called a *nontrivial cycle*.

The *height* $h(\mathcal{C})$ and the *depth* $d(\mathcal{C})$ of a cycle $\mathcal{C}$ are defined by

$$h(\mathcal{C}) := \begin{cases} \min H(\partial\mathcal{C}), & \text{if } \mathcal{C} \text{ is a nontrivial cycle,} \\ H(\mathcal{C}), & \text{if } \mathcal{C} \text{ is a trivial cycle,} \end{cases}$$

and

$$d(\mathcal{C}) := h(\mathcal{C}) - \min H(\mathcal{C}).$$

To have an idea we consider the example of one-dimensional random walk with Hamiltonian given in Figure 9, where $C_1 = \{1, 2, 3\}$, $C_2 = \{1, 2, 3, 4, 5, 6\}$ and $C_3 = \{12, 13, 14, 15, 16, 17\}$.

Cycles were introduced by Freidlin Wentzell to study the system on different time scales. Actually, their method provides a control of the time typically spent by the system in each cycle, and we know that, again in a typical way, the process visits a whole cycle before leaving it. Furthermore, we can identify the configuration through which the system leaves a given cycle.

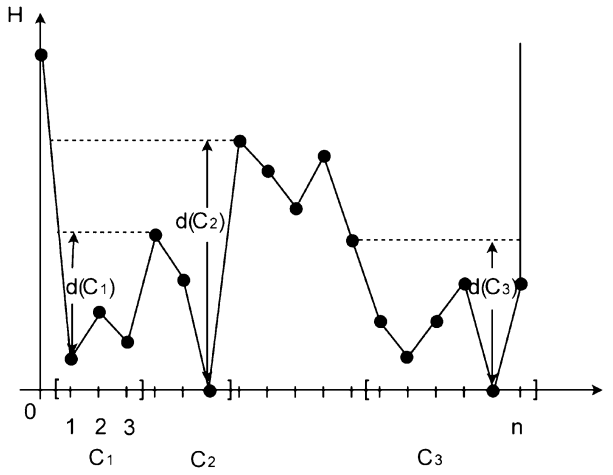

Figure 9 *Cycles.*

4.2 Cycle theorem

The main result on cycles can be summarized as follows. (We refer to [39] for more details and for the proof; see also [6] for analogous results.)

Theorem 4.1. *Let $\mathcal{C} \subset \mathcal{X}$ be a nontrivial cycle. For any $\delta > 0$, there exists $\alpha > 0$ such that*:

(i) *for any η in $\mathcal{C}$*

$$\limsup_{\beta\to+\infty} \frac{1}{\beta} \ln \mathbb{P}_\eta\big(\tau_{\partial\mathcal{C}} \notin \big[e^{(d(\mathcal{C})-\delta)\beta}, e^{(d(\mathcal{C})+\delta)\beta}\big]\big) \le -\alpha,$$

(ii) *for any η and η' in $\mathcal{C}$*

$$\limsup_{\beta\to+\infty} \frac{1}{\beta} \ln \mathbb{P}_\eta(\tau_{\eta'} > \tau_{\partial\mathcal{C}}) \le -\alpha.$$

Furthermore, for any $\eta \in \mathcal{C}$ and any $\eta'' \in \partial\mathcal{C}$,

$$\liminf_{\beta\to+\infty} \frac{1}{\beta} \ln \mathbb{P}_\eta(\eta_{\tau_{\partial\mathcal{C}}} = \eta'') \ge -[H(\eta'') - h(\mathcal{C})]_+,$$

and for any $\eta \in \mathcal{C}$

$$\lim_{\beta\to\infty} \frac{1}{\beta} \log \mathbb{E}_\eta(\tau_{\partial\mathcal{C}}) = d(\mathcal{C}).$$

Moreover, $\tau_{\partial\mathcal{C}}/\mathbb{E}_\eta(\tau_{\partial\mathcal{C}})$ converges in distribution to an exponential random variable with mean one.

4.3 Strategy

Cycles turn out to be a crucial tool to study metastability and, actually, Theorem 2.1 can be proved by using these results on cycles with the following general strategy:

1. Define the stable state as the configurations in which H reaches its absolute minimum. To simplify the exposition we assume that this ground state is given by a unique configuration denoted by σ_s.

   Given a pair of configuration $\sigma, \sigma' \in \mathcal{X}$ we define their *communication height*:

   $$\Phi(\sigma, \sigma') = \min_{\varphi:\sigma\rightsquigarrow\sigma'} \max_{\zeta\in\varphi} H(\zeta). \tag{4.1}$$

   Among the local minima of H, find the configuration such that its communication height with σ_s is largest. Suppose again that this is a unique configuration that we call the metastable state σ_m.
2. Define the *metastable cycle* $\mathcal{C}_{\sigma_m}^{\Phi(\sigma_m,\sigma_s)}$ as the nontrivial cycle made of all the configurations reached from σ_m by some path staying stricly below the communication height $\Phi(\sigma_m, \sigma_s)$ and study the first exit time from it. By definition the metastable cycle does not contain the stable state and is the deepest cycle with this property, so that the decay of the metastable state is equivalent to the exit from the metastable cycle.

The results on the decay of the metastable state, τ_{σ_s} (c) in Theorem 2.1 can then be derived by Theorem 4.1. By point (ii) also point (a) of Theorem 2.1 can be obtained. To control the critical configuration, point (b), and more generally to get the tube of typical paths, we summarize as follows the remaining strategy:

3. Denote now by $\mathcal{S}(\sigma, \sigma')$ the *set of minimal saddles* from σ to σ' in $\mathcal{X}$:

   $$\mathcal{S}(\sigma, \sigma') = \{\zeta : \exists \varphi : \sigma \rightsquigarrow \sigma', \zeta \in \varphi, H(\zeta) = \max H(\varphi) = \Phi(\sigma, \sigma')\}, \tag{4.2}$$

   and consider the *set of optimal paths* between σ and σ':

   $$(\eta \rightsquigarrow \eta')_{\mathrm{opt}} = \{\varphi : \sigma \rightsquigarrow \sigma' : \max H(\varphi) = \Phi(\sigma, \sigma')\}. \tag{4.3}$$

   Find the *gates* from σ_m to σ_s, that is, the subset $\mathcal{G}$ of the set of minimal saddles $\mathcal{S}(\sigma_m, \sigma_s)$ such that for any $\varphi \in (\sigma_m \rightsquigarrow \sigma_s)_{\mathrm{opt}}$ we have $\varphi \cap \mathcal{G} \neq \varnothing$;
4. If we define a *cycle path* as a sequence $\Phi = (\Phi_0, \Phi_1, \ldots, \Phi_n)$ of cycles such that

   $$\forall i \in \{1, \ldots, n\} \qquad \Phi_i \cap \partial\Phi_{i-1} \neq \varnothing$$

   and a *downhill cycle path* as a cycle path $\Phi = (\Phi_0, \Phi_1, \ldots, \Phi_n)$ such that

   $$\forall i \in \{1, \ldots, n\} \qquad h(\Phi_i) \leq h(\Phi_{i-1}),$$

   then we have to look for the downhill cycle paths from the gates to the metastable state and from the gate to the stable state.

5. By using reversibility we describe the typical exit with the typical descent:

$$\forall \Omega \in \Omega^*(\sigma, \sigma') := \{\varphi = (\sigma_0 = \sigma, \sigma_1, \ldots, \sigma_n = \sigma') : \\ \sigma_i \neq \sigma, \sigma' \ \forall i = 1, \ldots, n-1\},$$

$$\mathbb{P}_\sigma\big(\{\sigma_t\}_{t\in[\tau_{\sigma,\sigma'},\tau_{\sigma'}]} \in \Omega\big) = P_{\sigma'}\big(\{\sigma_t\}_{t\in[\tau_{\sigma',\sigma},\tau_{\sigma'}]} \in \overleftarrow{\Omega}\big)$$

with $\overleftarrow{\Omega} = \{\overleftarrow{\varphi}, \varphi \in \Omega\}$.

Remarks.

- The previous strategy is general, however, to implement each step a general control of the configuration space $\mathcal{X}$ is necessary, and this is the model-dependent part of the problem. The min–max problem in the first step of the strategy can be studied in the case of Glauber dynamics by solving an isoperimetrical problem. Indeed, to go from $\boxminus$ to $\boxplus$ with single spin–flip dynamics, all the magnetizations between $-|\Lambda|$ and $+|\Lambda|$ must be crossed; moreover, for a given magnetization, the configurations with minimal energy turn out to have a unique plus cluster whose shape is as close as possible to a square. With this idea, the min–max problem can be solved easily; see [2].
- As described in this strategy, metastable decay in finite volume implies the exit from the metastable cycle. We can call this exit the *event of first nucleation*. In this case of finite state space, when σ_m is a unique metastable state, the metastable cycle is the deepest one, so that the first nucleation actually corresponds to the main part of the *event of decay to the stable state*. Indeed, to go from the metastable state to the stable one, the longer portion of time is spent in the effort to leave the metastable cycle, by nucleating the critical droplet. Once a saddle configuration is reached, in the gate, the rest of the story can be discussed again by a sequence of problems of first exit from a sequence of suitable domains, the cycles constituting the cycle path. However, since these cycles have a smaller depth, the time necessary to follow the cycle path from the gate to the stable state is exponentially shorter in β. This is exactly what we saw in the 1D-RW example where the metastable cycle was given by the interval $[1, n-2]$ and $n-1$ was the gate configuration.

  This strict relation between metastable decay and first exit from the metastable cycle actually can produce the identification of the two problems. We prefer to distinguish between first nucleation, that is, exit from the metastable cycle, and decay to the stable state. In the case of conservative dynamics in exponentially large volumes, these two problems are very different and between first nucleation and arrival to the stable state, many additional physical problems are involved, during the supercritical growth.

5 Recurrence and renormalization

The main idea of the F–W theory to study a diffusion process or a Markov chain in terms of a simpler Markov chain can be applied iteratively by constructing a sequence of simpler and simpler Markov chains describing the original process on an increasing sequence of time scales. This theory has been introduced in [44] (see also [45]) and turned out to be a useful tool in many different applications (see, e.g., [30]). In particular, it provides answers to the two questions at the end of Section 2.6.

As in the F–W theory, we present the idea of renormalization under very general hypotheses; the reversible case is discussed, as a particular case, in Section 5.2.

Consider a discrete time Markov chain X_t on a finite state space $\mathcal{X}$ with transition probabilities satisfying for each $x \neq y$ $P(x,y) \asymp \exp\{-\beta\Delta(x,y)\}$, with $\Delta(x,y)$ assuming a finite number of values $\Delta_0 = 0 < \Delta_1 < \cdots < \Delta_n < \infty$. We define $\Delta(x,y) = \infty$ if $P(x,y) = 0$. Using the same strategy introduced by F–W we can define the functional $I_T(\phi) = \sum_{i=0}^{T-1} \Delta(\phi_i, \phi_{i+1})$, where we define $\Delta(x,x) = 0$. Note that we are considering now paths ϕ given by sequences of states $\phi_i \in \mathcal{X}$ such that $P(\phi_i, \phi_{i+1}) > 0$. Clearly, here the exponential weigh (the large deviation functional) of each path ϕ of length T is given by $I_T(\phi)$.

We introduce the equivalence relation $x \sim y$ iff $V(x,y) = V(y,x) = 0$, where as before $V(x,y) = \inf_{T\in\mathbb{N}} \inf_{\phi:\phi_0=x,\phi_T=y} I_T(\phi)$. We say that $x \in \mathcal{X}$ is a *minimum* iff for any $y \not\sim x$ we have $V(x,y) > 0$. Note that we are not assuming reversibility, even though the name "minimum" becomes evident in the context of reversible chains. Denote by $\mathcal{M} \subset \mathcal{X}$ the set of configurations which are minima. We have the following *recurrence property on* $\mathcal{M}$ (see Proposition 2.2 of [44]):

Proposition 5.1. *Let $\delta = 2\delta_0|\mathcal{X}|$, for any β sufficiently large and for any $t > e^{\delta\beta}$*

$$\sup_{x\in\mathcal{X}} \mathbb{P}_x(\tau_{\mathcal{M}} > t) \le \exp\left\{-\exp\left\{\frac{\delta\beta}{2}\right\}\right\} = SES,$$

where $\tau_{\mathcal{M}}$ is the first hitting time to $\mathcal{M}$.

5.1 Rescaled and renormalized chain

Let θ be the shift operator for the Markov chain X_t, that is, $\theta(\{x_0, x_1, \ldots, x_n, \ldots\}) = \{x_1, x_2, \ldots, x_{n+1}, \ldots\}$, and θ_p be its pth power. We define

$$V_1 = \inf_{x\in\mathcal{M}, y\in\mathcal{X}, x\not\sim y} V(x,y), \qquad t_1 = e^{V_1\beta}$$

and define recursively a sequence of stopping times:

$$\sigma = \inf\{t > 0 : X_t \not\sim X_0\}, \qquad \tau = \inf\{t \ge \sigma : X_t \in \mathcal{M}\},$$

$$\zeta_1 = \begin{cases} t_1, & \text{if } \sigma > t_1, \\ \tau, & \text{if } \sigma \le t_1, \end{cases}$$

and for all $n > 1$

$$\zeta_n = \zeta_{n-1} + \zeta_1 \circ \theta_{\zeta_{n-1}}.$$

It is easy to prove that ζ_n are stopping times and that $\bar{X}_n = X_{\zeta_n}$ is an homogeneous Markov chain on $\mathcal{M}$ with transition probabilities satisfying the following: $\forall x, y \in \mathcal{M}, x \not\asymp y$ $\bar{P}(x, y) \asymp t_1 \exp\{-\bar{\Delta}(x, y)\beta\}$ with

$$\bar{\Delta}(x, y) = \inf_{\substack{t, \phi; \phi_0 = x, \phi_t = y \\ \phi_s \notin \mathcal{M}_{x,y} \forall s \in (0,t)}} I_{[0,t]}(\phi),$$

where $\mathcal{M}_{x,y}$ is the set of minima with the exception of the states x and y and all the states which are equivalent to x and y.

Let $\mathcal{M} = \{m_1, \dots, m_r\}$ be the partition of $\mathcal{M}$ in maximal equivalence classes; on the state space $\mathcal{X}^{(1)} = \{1, \dots, r\}$ we can define a Markov chain $X^{(1)}$ similar to X_t but on a smaller state space with transition probabilities

$$P^{(1)}(i, j) = \frac{1}{\bar{\nu}(m_i)} \sum_{x \in m_i} \bar{\nu}(x) \sum_{y \in m_j} \bar{P}(x, y)$$

and corresponding to X_t on scale t_1 in the following sense: for $B^{(1)} \subset W^{(1)} \subset \mathcal{X}^{(1)}$ by denoting with $B \subset W$ the corresponding sets in $\mathcal{M}$ we have (see Theorem 2.1 in [44]):

Theorem 5.1. *For any β sufficiently large, $x \in m_i$, $i \in \mathcal{X}^{(1)} \setminus W^{(1)}$, $j \in W^{(1)}$*

$$\exp\{-4r\delta\beta\} q^{(1)}_{W^{(1)}}(i, j) \le q_W(x, m_j) \le \exp\{4r\delta\beta\} q^{(1)}_{W^{(1)}}(i, j),$$

$$e^{-\delta'\beta} t_1 E_i \tau^{(1)}_{W^{(1)}} \le E_x \tau_W \le e^{\delta'\beta} t_1 E_i \tau^{(1)}_{W^{(1)}},$$

$$t_1 e^{-\delta''\beta} \nu^{(1)}\big(B^{(1)}\big) \le \nu(B) \le t_1 e^{\delta''\beta} \nu^{(1)}\big(B^{(1)}\big),$$

where $\delta, \delta', \delta'' \to 0$ as $\beta \to \infty$.

By *iteration* we obtain a sequence of Markov chains $X^{(i)}$ on smaller and smaller state spaces $\mathcal{X}^{(i)}$ corresponding to the initial chain X_t on a sequence of larger and larger time scales $T_i = t_1 t_2 \cdots t_i$.

By the cycle theory we can associate with each state $x \in \mathcal{X}^{(i)}$ a cycle in the original state space $\mathcal{X}$ corresponding to the states visited by the chain X_t before the chain $X^{(i)}$ leave the state x. In particular, it is easy to associate with each path of the chain X_t a corresponding path of the renormalized chain $X^{(n)}$ by looking at the realization of the stopping times ζ_i on the path. On the other hand, it is possible to associate with each transition of the renormalized chain $X^{(n)}$ a tube of paths of the original chain X_t (see [37]).

This remark suggests another strategy to study metastability in finite volume based on renormalization. Indeed, we can:

1. apply the renormalization procedure up to a state space containing only the metastable and the stable states;
2. reconstruct the tube of paths corresponding to the trivial trajectory *metastable* $\to$ *stable* for this renormalized chain.

A global control of the state space is necessary for reduction, but the control of local details is not necessary to have L^1 estimates on tunneling time.

5.2 The reversible and nondegenerate case

Suppose that the transition probabilities of the chain satisfy $P(x, y) \asymp e^{-\beta \Delta(x,y)}$, with

$$\Delta(x, y) = H(x, y) - H(x)$$

and

$$H(x, y) = H(y, x) \geq H(x) \vee H(y). \tag{5.1}$$

In the Metropolis case $H(x, y) = H(x) \vee H(y)$. Moreover we assume a nondegeneracy condition

$$H(x) \neq H(y) \qquad \forall x \neq y.$$

This hypothesis is called *approximately reversible nondegenerate condition* in [39] (see Section 6.9).

In this case the renormalization procedure can be simplified by using the energy landscape and the fact that there are no equivalent states. At each step of the iteration the chain is reversible and nondegenerate and the iteration scheme can be view directly on the functions $H(x)$ and $H(x, y)$:

$$H^{(k)}(x) = H(x), \qquad H^{(k+1)}(x, y) = H(x) + \inf_{t, \phi^{(k)}: x \to y} I^{(k)}_{[0,t]}(\phi^{(k)}) - V_{k+1}.$$

This means that with the renormalization procedure the local minima are ordered in terms of their increasing *stability level*, that is, the height of the barrier separating them from lower energy states.

In Figure 10 we consider the 1D-RW example; see [45] for more details.

5.3 Time scales of renormalization and the spectrum of the generator

Freidlin and Wentzell proved the following result. Let $\mathcal{L} = \mathbf{P} - \mathbf{1}$ be the generator associated to a finite Markov chain X_t with transition matrix $(\mathbf{P})_{i,j} \asymp e^{-V_{ij}/\varepsilon^2}$ where $\mathbf{1}$ is the identity matrix and the relation $\asymp$ is defined in (3.4). Denote by $\lambda_1 = 0, \lambda_2, \ldots$ the eigenvalues of the matrix $-\mathcal{L}$ arranged in order of increasing real part (real eigenvalues in the reversible case) and define

$$\mathcal{V}_k = \min_{W; |W| = k} \min_{g \in G(W)} \sum_{(i \to j) \in g} V_{ij}. \tag{5.2}$$

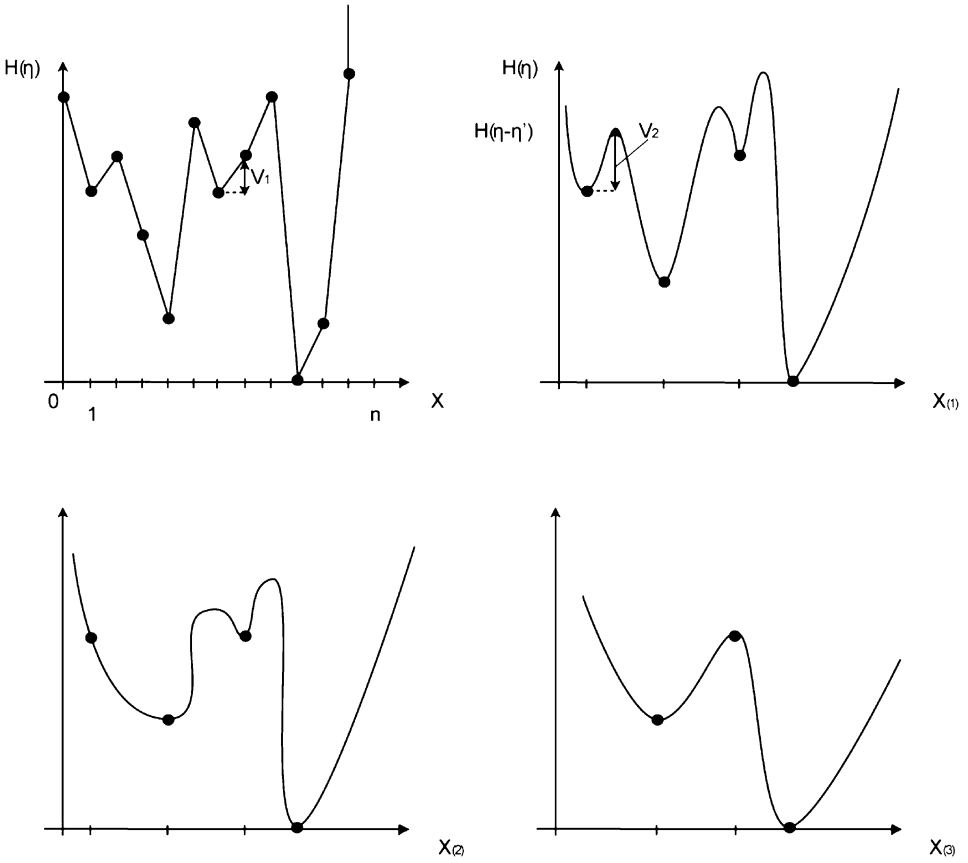

Figure 10 *The renormalization procedure.*

Lemma 5.1.

$$\lim_{\varepsilon\to 0} -\frac{1}{2\varepsilon^2}\log(\mathcal{R}e\lambda_k) = \mathcal{V}_{k-1} - \mathcal{V}_k.$$

See [15], Chapter 7 for the proof. By using this lemma we have

Theorem 5.2.

$$\lim_{\beta\to\infty} -\frac{1}{\beta}\log(\mathcal{R}e\lambda_k) = \lim_{\beta\to\infty} -\frac{1}{\beta}\log T_{N_k} = V_1 + V_2 + \cdots + V_{n_k},$$

where $N_k = \min\{n : |\mathcal{X}^{(n)}| < k\}$.

The main point in the proof of this theorem (see [46]) is that the renormalization strategy can be applied to the F–W theory of W-graphs in particular to find the graphs $g \in G(W)$ maximizing $\pi(g)$, call it $\bar{g}(W)$, which are crucial in the large

deviation regime studied by F–W. More precisely given $W \subset \mathcal{X}^{(k)}$ there is a correspondence between $\bar{g}^{(k)}(W)$ and $\bar{g}^{(k-1)}(W)$. This correspondence turns out to be a powerful tool in the W-graph theory because $\bar{g}^{(k)}(W)$ are easily found for sufficiently large k.

6 The conservative case

In this final section we consider a lattice-gas model in order to describe metastability for a supersaturated gas. This is a more difficult situation and we will discuss the new problems arising in this conservative case again by means of examples of random walks.

6.1 The model

With each site x in a box $\Lambda \subset \mathbb{Z}^2$, we associate a variables $\eta(x) \in \{0, 1\}$, [$\eta(x) = 0$ means the site x is empty, and $\eta(x) = 1$ means the site x contains a particle]. The interaction between particles is given by the analog of the Ising Hamiltonian

$$H(\eta) = -U \sum_{(x,y)\in\Lambda^*} \eta(x)\eta(y), \qquad \eta \in \mathcal{X} = \{0, 1\}^\Lambda \tag{6.1}$$

with 0 boundary conditions, where $-U < 0$ is the binding energy and, as before, the sum is over all the pairs of nearest-neighbor sites in Λ. Consider now a fixed particle density in Λ: $\frac{n}{|\Lambda|} =: \rho = e^{-\Delta\beta}$, with $n = \sum_{x\in\Lambda} \eta(x)$, where $\Delta > 0$. On the set $\mathcal{N}_n$ of configurations with n particles, we define the *canonical Gibbs measure*

$$\nu_n(\eta) = \frac{e^{-\beta H(\eta)} \mathbf{1}_{\mathcal{N}_n}(\eta)}{Z_n} \qquad (\eta \in \mathcal{X}), \qquad Z_n = \sum_{\eta\in\mathcal{N}_n} e^{-\beta H(\eta)}. \tag{6.2}$$

In order to have at least a particle we need now to consider *exponentially large volumes*, moreover, metastability in this case is given by the **Kawasaki metastable regime**:

$$\Lambda = \Lambda_\beta \qquad \text{with } |\Lambda_\beta| = e^{\Theta\beta}, \qquad \Delta \in (U, 2U),$$
$$\beta \to \infty, \qquad n = e^{-\Delta\beta}|\Lambda_\beta| \to \infty.$$

In order to explain why $\rho = e^{-\Delta\beta}$ with $\Delta \in (U, 2U)$ is the interesting regime of density, we consider the grand-canonical Gibbs measure associated to the model

$$\mu_\lambda(\eta) = \frac{e^{-\beta H_\lambda(\eta)}}{Z_\lambda},$$

where $H_\lambda(\eta) = H(\eta) - \lambda n$, $\lambda \in \mathbb{R}$ is an activity parameter. It turns out that the canonical and the grand-canonical ensembles are equivalent in the thermodynamic limit if ρ and λ are related by the equation $\rho = e^{\lambda\beta}$. We define $\Delta = -\lambda$.

Writing now the grand-canonical Hamiltonian in terms of spin variables, by using the relation $\eta(x) = \frac{1+\sigma(x)}{2}$, for which $\eta(x) = 1(0)$ corresponds to $\sigma(x) = 1(-1)$, we obtain

$$\begin{aligned} H_\lambda(\sigma) &= -U \sum_{(x,y)\in\Lambda} \frac{1+\sigma(x)}{2}\frac{1+\sigma(y)}{2} - \lambda \sum_{x\in\Lambda} \frac{1+\sigma(x)}{2} \\ &= \frac{U}{4} \sum_{(x,y)\in\Lambda} \sigma(x)\sigma(y) - \frac{2U-\Delta}{2} \sum_{x\in\Lambda} \sigma(x) + \text{const.} \end{aligned} \tag{6.3}$$

This Hamiltonian is equal to that in (1.1) with $J = \frac{U}{2}$ and $h = 2U - \Delta$ so that the metastable regime can be derived for these variables as $\Delta \in (U, 2U)$ corresponding to $h \in (0, 2J)$.

$\Delta \in (0, U)$ represents the *unstable gas*, $\Delta = U$ the *spinodal point*, $\Delta \in (U, 2U)$ the *metastable gas*, $\Delta = 2U$ the *condensation point*, and $\Delta \in (2U, \infty)$ the *stable gas*.

If we consider now a finite box $\Lambda_0 \subset \Lambda_\beta$ independent of β, we will call *local grand-canonical energy* the Hamiltonian (6.3) restricted to it:

$$H_{lgc}(\eta) = -U \sum_{(x,y)\in\Lambda_0^*} \eta(x)\eta(y) + \Delta \sum_{x\in\Lambda_0} \eta(x). \tag{6.4}$$

For this Hamiltonian metastability can be discussed as before in the spin variables, so we expect a critical length $l_c = \lceil \frac{U}{2U-\Delta} \rceil$.

Kawasaki dynamics: the dynamics are defined by a continuous time Markov chain $(\eta_t)_{t\geq 0}$ with state space $\mathcal{N}_n = \{\eta \in \{0,1\}^{\Lambda_\beta} : \sum_{x\in\Lambda_\beta} \eta(x) = n\}$. With each bond $b \in \Lambda_\beta^*$ we associate a Poissonian random clock. When the clock at $b = (x, y)$ rings, we look at the present configuration (say η), define the configuration $\eta^{(x,y)}$ obtained by exchanging $\eta(x) \to \eta(y)$, and jump from η to $\eta^{(x,y)}$ with a Metropolis rate given by

$$c((x, y), \eta) = e^{-\beta[H(\eta^{(x,y)}) - H(\eta)]_+}. \tag{6.5}$$

It is easily verified that the reversibility condition holds w.r.t. the canonical measure ν_n.

6.2 The problem

The main difference between the conservative and nonconservative case is that in the nonconservative case particles are "created ex nihilo" so that the gas is like a constant reservoir acting everywhere; it produces an effect on the cluster behavior but the cluster change doesn't affect the gas behavior. In the conservative case particles must "arrive" at a given point to construct a cluster, coming from somewhere in the gas. Gas and clusters are interacting in a stronger sense: there are effects not only of the gas on the cluster but also of the cluster on the gas. What is difficult

is to combine the behavior of gas and clusters in the conservative case and to describe them *jointly*. In the analysis of metastability, we can say that the difficulty in controlling many different aspects of the problem at the same time reaches its top in the conservative case, and a complete discussion of metastability is a long-term objective. As a first, simpler problem we can describe the first nucleation of a critical droplet when the volume $|\Lambda_\beta|$ is sufficiently small to have a unique nucleation. By calling $\mathcal{R}$ the set of subcritical configurations, corresponding to the metastable phase

$$\mathcal{R} := \{\eta \in \{0;1\}^{\Lambda_\beta} : \text{all clusters have volume} \le l_c(l_c-1)+2\},$$

we suppose to start from $\mu_{\mathcal{R}}$ the grand-canonical Gibbs measure conditioned to $\mathcal{R}$, with $Z_{\mathcal{R}}$ the corresponding partition function,

$$\mu_{\mathcal{R}}(\eta) := \frac{1}{Z_{\mathcal{R}}} \exp\left\{-\left(H(\eta) + \Delta \sum_{x\in\Lambda_\beta} \eta(x)\right)\beta\right\} \mathbf{1}_{\mathcal{R}}(\eta) \qquad \text{for } \eta \in \{0;1\}^{\Lambda_\beta}.$$

Indeed, we expect that in this first stage of the dynamics, clusters do not deplete the gas, so that the gas density is constant and equal to $e^{-\Delta\beta}$.

This problem was studied introducing some simplified models, again to discuss separately the different aspects of the interaction gas–cluster. In [13] the authors study a model with interaction only in a finite box in order to discuss the cluster nucleation while in [19] is discussed the behavior of the gas particle. The complete result on the first nucleation for the Kawasaki dynamics in exponentially large volumes uses all these preliminary results and is in preparation, [21].

6.3 The 1D-RW corresponding to the local dynamics

We believe that the best way to introduce the reader to the analysis of the conservative case, which is not easy involving different models, is again through random walks. As before, we want to discuss the Kawasaki dynamics as a one-dimensional random walk with states given by the volume of a growing cluster, at least up to the nucleation of a supercritical cluster, that is, up to the first exit from $\mathcal{R}$. The Kawasaki analog of the random walk introduced in Section 2.6 for the finite volume Glauber dynamics is the following: for $i = 0, 1, \dots, l_c(l_c-1)+2$

$$\begin{aligned} P(i,i+1) &= \tfrac{1}{2}e^{-\Delta\beta}, \qquad P(i,i-1) = \tfrac{1}{2}e^{-f(i)\beta}, \\ P(i,i) &= 1 - P(i,i+1) - P(i,i-1), \end{aligned} \tag{6.6}$$

with

$$f(i) = \begin{cases} \infty, & \text{if } i = 0, \\ 0, & \text{if } i = 1, \\ U, & \text{if } i = 2,3 \text{ or } i = l_1 \times l_2 + 1, i > 4, \\ 2U, & \text{otherwise,} \end{cases} \tag{6.7}$$

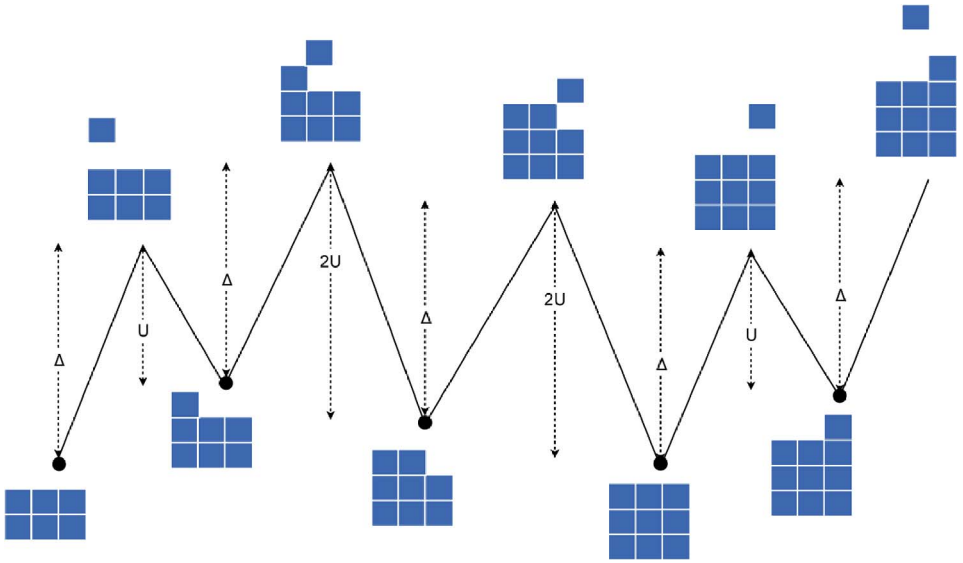

Figure 11 *Energy landscape for the Kawasaki dynamics.*

here l_1 and l_2 are two integers such that $l_2 \geq l_1 > 1$ and $l_2 - l_1 \leq 1$. As in the Glauber case, if we consider the geometrical isoperimetrical problem, that is, the minimization of the grand-canonical local energy at fixed area of the cluster i: $\mathcal{E}(i) = \min_{\eta:|\eta|=i} H_{lgc}(\eta)$, again we have that the minimizing configurations can be be found as those clusters closest to squares, like in Figure 11.

The function $f(i)$ turns out to be the energy barrier to overcome to go from the area i to $i-1$. This means that this chain is reversible w.r.t. the Hamiltonian given by $\mathcal{E}(i)$, if we consider the pair energy $H(i, i+1) \equiv H(i+1, i) := \mathcal{E}(i) + \Delta$ [see(5.1)]. Indeed, we have $P(i, i+1) = e^{-(H(i,i+1)-\mathcal{E}(i))}$ and $P(i, i-1) = e^{-(H(i-1,i)-\mathcal{E}(i))}$ and $H(i-1, i) - \mathcal{E}(i) = \mathcal{E}(i-1) + \Delta - \mathcal{E}(i) = f(i)$.

This chain is a good description of the *completely local model* introduced in [13] (see also [23,34]), given by the Kawasaki dynamics in a finite box Λ_0 with creation and annihilation of particle at the boundary with rates ρ and 1 respectively. This is a simple model to study the behavior of the cluster, it captures and releases particles, describing the *effect of the gas on the cluster*. The process of creation and annihilation of particles at the boundary is like a constant reservoir outside the box, there is no conservation, and there are *no effects of the cluster on the gas* in this model.

6.4 A two-dimensional model for the gas: 2D-gas

If we now adopt the point of view of the gas in the reservoir outside the finite box mentioned above, we can consider a gas of identical and indistinguishable particles moving in an exponentially large two-dimensional box, with density $e^{-\Delta\beta}$.

All the gas particles move in this model like independent simple random walks everywhere except at site 0, which represents a kind of trap. When a gas particle arrives at 0, it is captured and can be released with a rate depending on the number of particles which are at 0 at that moment. This dynamic can be realized by associating with each particle a Poissonian clock. When a clock rings, the corresponding particle moves from its position x to one of the four neighboring sites $y : |x - y| = 1$, with equal probability which is equal to $\frac{1}{4}$ if $x \neq 0$ (independently from the position of the other particles), and $\frac{1}{8}e^{-f(i)\beta}$ if $x = 0$, where i is the number of particles at 0 at this time and $f(i)$ is the function defined in (6.7), and remaining at 0 with probability $1 - \frac{1}{2}e^{f(i)\beta}$. In other words, we are assuming that the site 0 behaves like a cluster capturing and releasing particles as described in the previous model of Section 6.3.

The gas dynamics defined in this way are clearly very close to a system of IRW and a coupling can be easily defined between the two systems. Gas particles perform in this model *Quasi Random Walks* (QRW), that is, RW with possible pauses in 0 and the interaction among them is only related to these pauses.

A general theory for QRW is developed in [19], by using the important result on the control of collisions for a finite system of IRW given in [17]. In particular, it is proved that particle trajectories are nonsuperdiffusive and have a diffusive, spread-out property.

6.5 The local interaction model

The two previous models, 1D-RW and 2D-gas, can be combined together to describe the behavior of a cluster (with 1D-RW) in a gas (with 2D-gas), with the following coupling. Start from the state i for the 1D-RW and with the same number i of particles in the origin for the 2D-gas. Define the dynamics of the 2D-gas exactly as in the previous section. The evolution of the 1D-RW is now defined by considering i independent Poissonian clocks, coinciding with the clocks of the particles in the trap in the 2D-gas model. When such a clock rings the transition $i \to i - 1$ is done by using the same random variables used for the exit from the trap in the 2D-gas. The transition $i \to i + 1$ is realized only when a new particle arrives at 0 in the 2D-gas. This implies that, with this coupling, the number of particles at the origin for the 2D-gas model coincides, at every time, with the state of the 1D-RW. Of course, the probability $P(i, i + 1)$ for the 1D-RW depends in this case on the original configuration of the gas particles not in 0 of the 2D-gas model. If the gas particles not at 0 are at a distance of order $e^{\beta\Delta/2}$ from the origin, in the initial configuration, then we expect that the transition $i \to i + 1$ takes place in a time of order $e^{\beta\Delta}$, as in the case of the model of Section 6.3.

By using the ideas of recurrence developed in Section 3, we can prove that the gas configurations in which there are no particles outside the origin within a radius $e^{\beta\Delta/2}$ are *recurrent* for the gas so that these become the typical configurations on

a time scale $e^{\beta\Delta}$. This implies that on this time scale this combined model behaves like the 1D-RW Section 6.3, as far as its cluster behavior is concerned.

With this combined model we obtain the main idea at the origin of the *local interaction model* introduced in [13] where the dynamics η_t is Kawasaki in the finite box and a process of independent random walks (IRW) outside. In this case the control of the gas–cluster interaction is not too difficult: particles arrive in the box with an IRW law, they are caught and released by the cluster as in the completely local model, described in Section 6.3, they can return to the gas outside. Gas and cluster are studied jointly in this case.

6.6 A system of RWs for the Kawasaki dynamics in an exponentially large volume

Looking now at the original problem of the Kawasaki dynamics in exponentially large volume, some questions arise:

- There is no longer a fixed interaction box, there are many clusters and they can be everywhere in Λ_β;
- What is actually the gas? Does the gas behave independently in different regions? Is there propagation of the effects of a cluster on the gas?

In this case we obtain in [21] a result on the first nucleation in the regime of homogeneous nucleation, that is, when the volume $|\Lambda_\beta|$ is sufficiently small to have a unique nucleation. We can prove the following.

Result. If $|\Lambda_\beta| = e^{\Theta\beta}$, with $\Theta < \Gamma - (2\Delta - U)$ then:

(i) For all $\delta > 0$,

$$\limsup_{\beta\to+\infty} \frac{1}{\beta} \ln P_{\mu_{\mathcal{R}}}\left(\tau_{\mathcal{R}^c} \notin \left[\frac{e^{\Gamma\beta}}{|\Lambda_\beta|}e^{-\delta\beta}; \frac{e^{\Gamma\beta}}{|\Lambda_\beta|}e^{+\delta\beta}\right]\right) < 0;$$

(ii) With probability exponentially close to 1 the system will nucleate a wandering cluster visiting in dimensions the full increasing sequence of the quasi-squares, and that, after the exit from $\mathcal{R}$, will grow in the same way up to a square $l(\beta) \times l(\beta)$ for any unbounded and nondecreasing function $l(\beta)$ such that

$$l(\beta) \ln l(\beta) = o(\ln \beta).$$

This square $l(\beta) \times l(\beta)$ will be reached from the exit of $\mathcal{R}$ in a time exponentially smaller than that used to reach $\mathcal{R}^c$. In addition there will be some fluctuations in the dimensions of the growing cluster between two successive q.s. of different dimensions, both in the subcritical and supercritical evolution: denoting by l and L the shortest and longest side length of its circumscribed rectangle, fluctuations of order

$$0 \le L - l \le 2\sqrt{l_c}$$

will be typical (will occur with probability exponentially close to 1) and fluctuations of order

$$0 \le L - l \le 2\sqrt{L} + 1$$

will be nonnegligible (will occur with nonexponentially small probability).

We are looking at the *escape from metastability* by looking at the first exit from $\mathcal{R}$ starting from a measure concentrated on subcritical configurations. This occurs by nucleation of a supercritical cluster in any place of the box Λ_β and that is why we are talking of homogeneous nucleation. This is reflected by the spatial entropic factor $\frac{1}{|\Lambda_\beta|}$ in the asymptotics of the exit time.

We can look at the supercritical growth only up to a small size $l(\beta)$; indeed, the growth of macroscopical cluster implies gas depletion and this is a difficult open problem.

As before we will not give the proof of this result, but we go back again to our random walk model in order to give some ideas. Indeed it is possible to prove the theorem by studying the first nucleation in a box of volume $e^{(2\Delta - U - \gamma)\beta}$ for a suitable small γ. By a priori estimates of large deviations for $\mu_{\mathcal{R}}$, we can prove that the number of clusters in such a box is not exponentially large in β, say, smaller than m, with probability super exponentially close to one.

On the other hand we have to note that the results on QRW obtained in [19] are sufficiently robust and a large (though not exponentially large) number of traps, say m, can be considered obtaining results essentially independent of their location.

This suggests that the Kawasaki dynamics can be studied in terms of a family of m copies of the 1d-RW, $\{\xi_k\}_{k=1,\dots,m}$, describing the size of the clusters, with m not exponentially large in β, and a 2D-gas of indistinguishable particles performing QRW. With each 1D-RW ξ_k not in 0 a trap is associated in the 2D-gas of QRW. In this way, the geometrical problems arising in the Kawasaki dynamics are completely overtaken.

This family of 1D-RW can be studied along the same lines described above. This is discussed in [20], by using again the idea of reduction of the F–W theory.

The proof that the Kawasaki dynamics can be reduced to this family of 1D-RWs is given in [21] and is far from trivial. Indeed, for the Kawasaki dynamics, clusters evolve, in general, not independently one from the other. Consider, for instance, the possible coalescence of two different clusters. Of course it is difficult to control these dependent evolutions. However, by using again the idea of recurrence, we can over pass this problem since with large probability, the Kawasaki process visits the set $\mathcal{V}$ of configurations without any cluster in a time exponentially smaller than $\frac{e^{\Gamma\beta}}{|\Lambda_\beta|}$. Starting from this set $\mathcal{V}$ it is possible to construct an event of nucleation along trajectories with a unique growing cluster.

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