

Abnormal droplet formation in a metastable model in infinite volume

F. Manzo, e-mail: manzo.fra@gmail.com

ABSTRACT. We study a simple nucleation-and-growth model with a very rich behavior. Unlike other models, here the microscopic details of the critical cycle can influence the pattern and time of decay from a metastable state. Depending on the speed of growth, the system goes through four different regimes: 1) both the “shape of the critical droplet” and the typical relaxation time are the same as in finite volume; 2) the “shape of the critical droplet” and its “formation rate” are the same as in finite volume but the “relaxation time” is shorter; 3) the “shape of the critical droplet” is the same as in finite volume while the nucleation rate and the “relaxation time” are smaller; 4) the “shape of the critical droplet” is different from what we have in finite volume and its formation rate is smaller than the formation rate of the finite-volume droplet.

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1. Introduction.

Metastability is a typical phenomenon for thermodynamic systems out of equilibrium in the vicinity of phase coexistence regions. Suppose you have a thermodynamic system in a state A and you change abruptly one of the thermodynamic parameters to a value that corresponds to a new phase B . Many systems, instead of undergoing immediately the phase transition, remain for a very long time in an apparent equilibrium A' , often “close” to the old phase.

A natural interpretation of metastability is that the metastable state corresponds to a local minimum in the free energy, a reminiscence of the stable phase beyond the transition. The system is somehow trapped in this local minimum and has to overcome a barrier or go through a bottleneck to reach the equilibrium.

Unfortunately, make this picture a rigorous argument or at least a clear heuristics is quite complicated. First of all, it is clear that the role of the dynamics is crucial: if the dynamics allows to go directly (i.e. without any barrier) from A' to the new stable

state B , we do not have any metastable behavior, if on the contrary the dynamics is non-ergodic, we never see the relaxation.

The barrier in the naïf picture above is due both to a bottleneck of the dynamics and to an energy barrier to overcome. In other words, we need to find the relationship between the microscopic point of view of the dynamics and the macroscopic point of view of the free energy. In general, this correspondence is not clear.

While a physical theory of metastability is still lacking, in the last fifteen years metastability was successfully studied in the framework of lattice spin models with stochastic dynamics. For these systems we have rigorous results and, in some specific regimes, a full understanding of the problem. Provided we are able to describe the energy landscape in a suitable way, the methods developed allow to understand completely this phenomenon in two cases: the finite volume, low temperature limit and the mean field, many particle limit.

In these regimes, we are able to transform the heuristic picture in a rigorous argument and answer the questions in full generality. The key idea is to regard the problem as the exit of a Markov process from a general domain, under the condition (to be verified in the given model) that starting in the trap it is very unlikely that the system exits the trap before reaching the "metastable state". Each time the system reaches this state, it loses memory of its past, and since it typically needs many attempts to exit, the exit time has an exponential behavior. In the reversible case, the trap can be seen as a deep well in the free-energy landscape, and the relaxation time is characterized by the depth of this well, a free-energy barrier that the system must cross in order to reach the equilibrium.

The finite-volume case and the mean field case, share a key feature: the entropic contribution to the measure is trivial to compute. Indeed, in the finite volume case this contribution is always negligible when the temperature goes to zero, while in the mean field case, the projection of the dynamics onto the space of macroscopic variables is a close markovian dynamics, so that the problem can be stated directly in macroscopic terms.

Behind these cases, the relaxation to the stable state was described only in a few Ising-like ferromagnetic models, by means of model-specific extensions of the finite volume ideas and techniques. In particular, two key properties needed to link finite volume and infinite volume results are the low range and attractivity (ferromagnetism) of the microscopic energy. A typical feature of Ising-like ferromagnetic models is that the relaxation from the metastable phase is triggered by the formation of a suitable "nucleus": a well described droplet that grows until eventually coalesce with other droplets or fill the entire volume. The easiest of these regimes is the infinite-volume, low temperature limit, analyzed in [DS2], [CM] for the Ising model in two or higher dimensions, respectively, and in [MO2] for the two-dimensional Blume-Capel model. The other remarkable case is the coexistence limit (infinite volume, vanishing magnetic field) for the two-dimensional Ising model studied in [ShSch].

In these cases, the shape of the nucleus can be understood as the minimizer of the free-energy at a critical value of the magnetization. In other words, in all the models analyzed, few macroscopic characteristics of the free-energy landscape are needed to describe the relaxation to the equilibrium.

Still, a fundamental question remains open: is it possible, in general, to give a thermodynamic description of the phenomenon, including the metastable state, the two time-scales, and the relaxation path? In other terms, is it possible to understand the mechanism that traps the system and to describe the relaxation in terms the macroscopic variables? Despite the encouraging examples cited above, we give here a negative answer.

The paper is written for non experts, and can be used as an introduction to metastability methods in statistical mechanics. The model we study is simple enough to be analyzed directly, without any previous knowledge of the general theorems. The setting is the easiest of the regimes where the entropic contribution is non-negligible: the low temperature limit in infinite volume.

The model is largely inspired to the kinetic Ising model (KI in the following), studied in the infinite volume, low temperature regime in [DS2] in dimension 2 and in [CM] for higher dimensions. In these papers, the results rely on the finite volume analysis, in particular [DS2] on the description of the energy landscape obtained in [NS].

In the KI model in a finite volume Λ , the configuration space is $\{-1, 1\}^\Lambda$ (very high-dimensional). The a single flip Metropolis dynamics turns out to produce plenty of local wells. In the finite volume regime, general results ensure that these details do not need to be taken into account to determine the relaxation time or the shape of the critical nucleus: the only relevant quantity to compute is the height of the energy barrier to the stable state. In infinite volume, this is not the case: the details can play a role and modify the scenario changing the nucleation rate and the nucleus itself. This is what will happen in the model studied here, while in both the models studied in the literature in this regime, the KI model and the Blume-Capel model studied in [MO2], the energy landscape is "smooth enough" to preserve the shape of the critical droplet and its formation rate.

Notice that since the dynamics allows only single spin flips, the system must take all the values of the magnetization in order to go from the configuration with all minuses $\underline{-1}$ (the metastable configuration) to the configuration with all pluses $\underline{+1}$ (stable).

Let Γ be the energy gap between the saddle point and $\underline{-1}$ and τ_+ the hitting time to $\underline{+1}$. In finite volume, for β large enough,

$$\mathbb{E}(\tau_+) = ce^{\beta\Gamma}(1 + o), \quad (1.1)$$

$$\mathbb{P}(\tau_+ > \mathbb{E}(\tau_+)t) = e^{t(1+o)}(1 + o), \quad (1.2)$$

where c is a constant computed in [BM] and o is exponentially small with β . Moreover, during the last excursion from $\underline{-1}$ to $\underline{+1}$, the process visits a critical nucleus with probability exponentially close to 1 (see e.g. [MNOS]).

When the volume is infinitely large, a nucleus is formed immediately somewhere. We look at a local observable, say near the origin, and compute the time when it changes from the value it assumes in the $\underline{-1}$ configuration to the value it assumes in the $\underline{+1}$ configuration. Since the speed of growth in the KI model is limited, it is clear that the droplet that invades the origin does not come from too far away. A good heuristic assumption to compute the invasion time for the KI model in dimension d consists in assuming that the critical nuclei originate independently of each other with rate $e^{-\beta\Gamma_d}$ and grow with speed $e^{-\beta\nu}$. Let us consider the “space-time cone” with vertex in (o, t) and slope $e^{-\beta\nu}$. By definition, if a critical droplet is generated into the cone, it reaches the origin within t . The value t_c of the typical time required by the droplet to reach the origin is given by

$$t_c (e^{-\beta\nu} t_c)^d e^{-\beta\Gamma_d} \sim 1, \quad (1.3)$$

which gives

$$t_c \sim e^{\beta \frac{\Gamma_d + d\nu}{d+1}}. \quad (1.4)$$

In [CM] is shown that in the KI model the growth speed is determined by a $(d-1)$ -dimensional metastability problem in infinite volume and it is the multiplicative inverse of the invasion time in dimension $(d-1)$. With an inductive argument,

$$t_c \sim e^{\beta \frac{\sum_{k=0}^d \Gamma_k}{d+1}}. \quad (1.5)$$

The value in the r.h.s. of (1.4) has to be compared with the typical nucleation time at finite volume, that is $e^{\beta\Gamma}$.

The ansatz that the formation time of a critical droplet is exponential with rate $e^{-\beta\Gamma_d}$ for times of order t_c is verified a posteriori, but it is clear that it is a much stronger assumption than (1.2).

2. Notation and results.

We denote by $[x]_+ := \max\{x, 0\}$ the *positive part* of the real number x .

The model. We consider a one-dimensional spin system on the lattice \mathbb{Z} where the spin variable $\sigma(i)$ can take values in $\Omega := \{-1, 0, 1, 2, 3\}$. The values 1 and 2 of the spin variable should be thought of as “inner degrees of freedom” (sub-critical droplets) of the system, while $-1, 0$, and 3 as observable states.

The *single site Hamiltonian* is

$$\begin{aligned}
 H(-1) &= \frac{40}{36} \\
 H(0) &= 0 \\
 H(1) &= \frac{33}{36} \\
 H(2) &= \frac{3}{36} \\
 H(3) &= 1
 \end{aligned} \tag{2.1}$$

and is shown in Fig. 1.

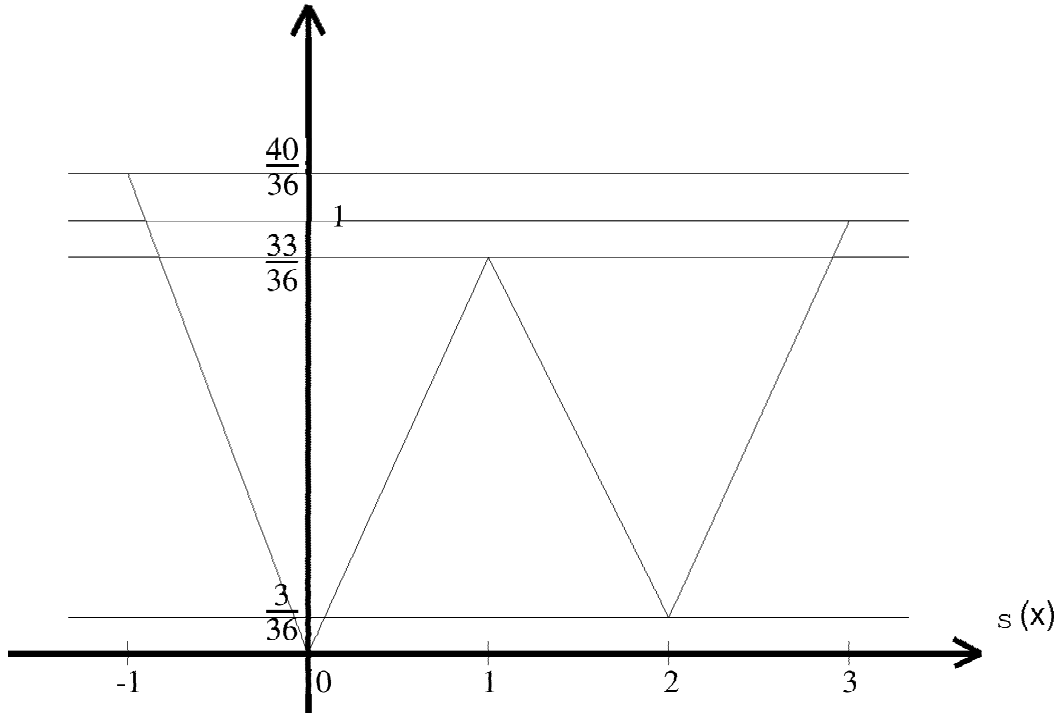


FIGURE 1. Single-site Hamiltonian.

The *single site dynamics* is given by the following transition rates:

For $a \notin \{-1, 3\}$,

$$c_\beta(b, a) := \begin{cases} e^{-\beta[H(b)-H(a)]_+} & \text{if } a = b \pm 1 \\ 0 & \text{otherwise.} \end{cases} \tag{2.2}$$

If $a = -1$ or $a = 3$, then $c_\beta(a, b) \equiv 0$ and no transition is allowed. This dynamics is Metropolis reversible in $\{0, 1, 2\}$ with absorbing states in -1 and in 3 . Therefore, we will be allowed to use the results in [OS] and [MO2] about reversible Markov chains up to the hitting time to $\{-1, 3\}$.

The parameter β has the meaning of the *inverse temperature*.

We denote by σ_t^* the *single-site process* on Ω distributed according with the above defined dynamics and by

$$\tau_Q^* := \min \left\{ t; \sigma_t^* \in Q \right\}, \quad (2.3)$$

$$\tau^* := \tau_{-1,3}^*. \quad (2.4)$$

The *infinite volume dynamics* is defined as follows: at time $t = 0$ the initial configuration is $\underline{0}$ (all zeroes). Afterwards, the sites evolve according to their single-site dynamics (namely, with the same law of σ^*) until they have one nearest neighbor with spin -1 or 3 . Then, they assume the value of the spin of their nearest neighbor with spin -1 or 3 with rate

$$e^{-\beta\nu}. \quad (2.5)$$

If a site has both nearest neighbors with spin in $\{-1, 3\}$, it will assume one of the two values with uniform probability and rate $e^{-\beta\nu}$. ν is the only parameter in our model and $e^{-\beta\nu}$ has the meaning of growth speed of super-critical configurations.

This model can be considered as the counterpart of the nucleation-and-growth model introduced in [DS1]. While in that case Dehghanpour and Schonmann focused their attention on the supercritical growth, here we are interested on how the speed of growth influence the nucleation pattern.

Given a volume $\Phi \subset \mathbb{Z}$ and a configuration ρ (boundary condition), we define the *restriction* $\sigma_{\Phi,t}^\rho$ of the process to Φ by freezing the spins outside Φ to $\rho(i)$.

We focus our attention on the following hitting time

$$\tau := \min \left\{ t; \sigma_t(0) \in \{-1, 3\} \right\}. \quad (2.6)$$

For $\Phi \subset \mathbb{Z}$, we consider the auxiliary hitting time:

$$\hat{\tau}^\rho(\Phi) := \min \left\{ t; \exists i \in \Phi \ \sigma_{\Phi,t}^\rho(i) \in \{-1, 3\} \right\}. \quad (2.7)$$

We omit the volume from notation if $\Phi = \mathbb{Z}$ and the boundary condition if $\rho = \underline{0}$.

Obviously, if $\Phi' \subseteq \Phi''$ and for all i , $\rho'(i) \leq \rho''(i)$, then

$$\hat{\tau}^{\rho'}(\Phi') \leq \hat{\tau}^{\rho''}(\Phi'') \quad (2.8)$$

We call the first appearance of a -1 or a 3 in a given volume *nucleation*, the site where we see this -1 or 3 *critical droplet* and the value of this spin *shape of the critical droplet*. If $\nu < 1/3$, we say that the -1 -droplets are of the *right kind* whereas the 3 -droplet are of the *wrong kind*; if $\nu > 1/3$, it is vice versa.

Let us introduce some useful notation before stating our main result.

Given a set $B \subset \Omega$, we define $F(B)$ as the set of the minima of the Hamiltonian H in B . We denote by ∂B its *outer boundary* and the energy of the points in this set by $H(F(B))$.

A *cycle* $A \subset \Omega$ is a connected set such that $H(F(\partial A)) > \max_{a \in A} H(a)$ (in our case, $\{0\}$, $\{2\}$, and $\{0, 1, 2\}$ are cycles). Given a cycle A , we define its *depth* as $\Gamma(A) := H(F(\partial A)) - H(F(A))$ and its *largest inner resistance* $\Theta(A)$ as the maximal depth of a sub-cycle $A' \subset A$ that does not contain the whole $F(A)$:

$$\Theta(A) := \max_{F(A) \not\subset A' \subset A} \Gamma(A') \quad (2.9)$$

if such a sub-cycle does not exist, we set $\Theta(A) := 0$. We will use results about the exit from cycles from [OS] and [MO2].

Let us introduce some useful functions of ν :

$$k^a(\nu) := \frac{20}{36} + \frac{\nu}{2} \quad (2.10)$$

$$k^b(\nu) := \frac{22}{36} + \frac{\nu}{3} \quad (2.11)$$

$$k^c(\nu) := \frac{1}{2} + \frac{\nu}{2} \quad (2.12)$$

$$k^d(\nu) := 1 \quad (2.13)$$

The time of the first appearance of a stable phase in the origin is characterized by the following exponent:

$$k(\nu) := \min \left\{ k^a, k^d, \max \left\{ k^b, k^c \right\} \right\} \quad (2.14)$$

In Fig. 2, k is plotted v.s. ν .

$\partial_\nu k(\nu)$ has three discontinuity points for the values $\nu = 1/3$, $2/3$, and 1. These points correspond to “dynamical phase transitions”, namely to changes in the nucleation patterns. We remark once more that the single-point energy landscape does not depend on ν and thus these transitions have no finite-volume counterpart.

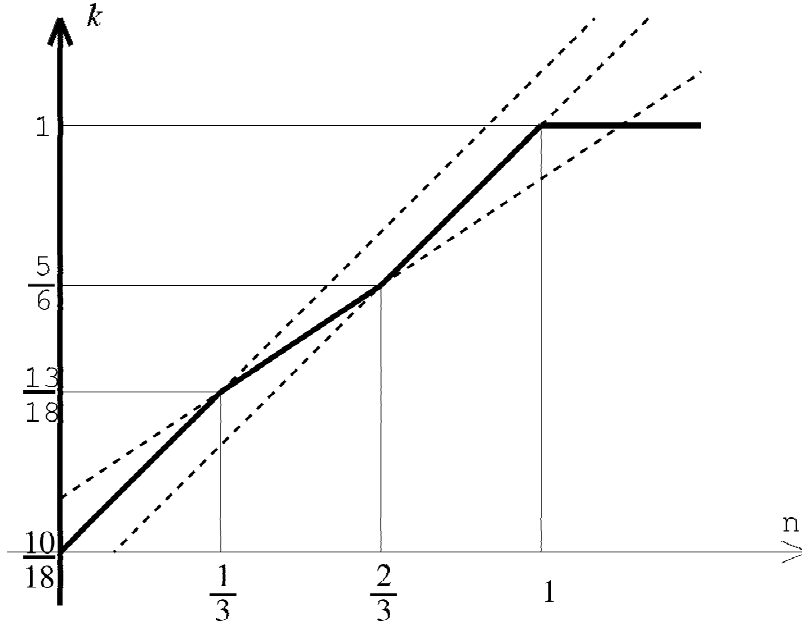
Notice that $k(\nu)$ is strictly monotonic for $\nu \leq 1$. We denote the inverse function of $k(\nu)$ by

$$\nu(\kappa) : [\frac{5}{9}, 1] \rightarrow [0, 1]. \quad (2.15)$$

A particular role will be played by the slab

$$\Lambda := \left\{ - \lfloor e^{\beta(k(\nu)-\nu)} \rfloor, \dots, \lfloor e^{\beta(k(\nu)-\nu)} \rfloor \right\} \quad (2.16)$$

that corresponds to the heuristic notion of base of the “critical space-time cone” described in the introduction (see (1.3)).

FIGURE 2. k v.s. ν .

Our main result is contained in the following Theorem:

Theorem 2.1. $\forall \nu > 0, \forall \varepsilon > 0$ in the limit $\beta \uparrow \infty$,

$$\mathbb{P}_{\underline{0}}(\tau > e^{\beta(k(\nu)-\varepsilon)}) \rightarrow 1 \quad (2.17)$$

$$\mathbb{P}_{\underline{0}}(\tau < e^{\beta(k(\nu)+\varepsilon)}) \rightarrow 1. \quad (2.18)$$

Moreover,

$$\mathbb{P}(\sigma_{\tau}(0) = -1) \rightarrow 1 \text{ if } \nu < \frac{1}{3} \quad (2.19)$$

$$\mathbb{P}(\sigma_{\tau}(0) = 3) \rightarrow 1 \text{ if } \nu > \frac{1}{3} \quad (2.20)$$

The Theorem above shows that both the exit time and the exit state may depend on the inner structure of the critical cycle. This dependence shows up only at very high speed of growth and it is hidden in the Ising and Blume-Capel model studied in [DS1], [DS2], [MO1], and [MO2] where the speed of growth is not independent of the energy of the critical droplet. Depending on the parameter, we detect in our model four different nucleation behaviors:

- i) for $\nu > 1$ (where $k(\nu) = k^d(\nu)$), the system behaves like in finite volume, and both the exit time and state are “the same” as in finite volume;

- ii) for $2/3 < \nu < 1$ (where $k(\nu) = k^c(\nu)$), the system is in the Dehghanpour and Schonmann regime: the typical exit time is $\exp\left(\beta\left(\frac{1+\nu}{2}\right)\right)$ and the exit state is the same as in finite volume; both this case and case i were described in [DS1] (see the introduction for the heuristic discussion of case ii).
- iii) for $1/3 < \nu < 2/3$ (where $k(\nu) = k^b(\nu)$), the inner structure of the cycle $\{0, 1, 2\}$ in Fig. 1 becomes relevant. Indeed, since it is very unlikely that the process once reached 2 goes back to 0, both the exit from $\{0\}$ and the exit from $\{2\}$ are rare event to take into consideration. The exit rate is therefore lower than the one we get from the heuristics in [DS1] while the exit state is the same as in previous cases;
- iv) for $\nu < 1/3$ (where $k(\nu) = k^a(\nu)$), like in case iii, the exit trough 3 entails two rare events and its probability is so low that it is more likely to exit from -1 ; the exit rate is consistently affected. In this case the system reaches the “state” where value of the spin is a.s. -1 despite of the fact that the Gibbs measure gives a.s. the value 3 and the fact that the energy barrier between 0 and -1 is higher than that between 0 and 3.¹

3. Basic tools.

In this Section, we review the basic results about finite-volume metastability in the context of [OS] and [MO2]. The setting is that of Markov chains with exponentially small transition rates (e.g. Metropolis dynamics in the $\beta \rightarrow \infty$ limit) with finite state-space.

The extension to the continuous-time case is immediate (via large-deviation estimates) as far as exponential times are concerned.

We will use these results to bound the probability of exit through a given state at a given time from above and from below.

The following Lemma gives the desired upper bound:

Lemma 3.1 (Lemma 3.1 in [OS]). *For all a, b such that $H(b) > H(a)$, for all $\kappa > 0$ and $\varepsilon > 0$*

$$\mathbb{P}_a(\tau_b^* \leq e^{\beta\kappa}) \leq e^{-\beta(H(b)-H(a)-\varepsilon)} \tag{3.1}$$

If $\kappa < \Gamma(A)$, we immediately get the bound

$$\mathbb{P}_a(\tau_{\partial A}^* = \tau_b^*, \tau_b^* \leq e^{\beta\kappa}) \leq e^{-\beta(H(b)-H(a)-\varepsilon)}. \tag{3.2}$$

In particular, when $\kappa < \Gamma(A)$, the exit probability goes to zero. The counterpart of this fact is the content of the following Lemma from [OS]:

¹In a reversible situation, the system would go to the intermediate state and then reach the Gibbs state at a later time.

Lemma 3.2 (Proposition 3.7 in [OS] i and iii). *For all $a \in A$, for all $\varepsilon > 0$*

$$\mathbb{P}_a \left(\tau_{\partial A}^* < e^{\beta(I(A)+\varepsilon)} \right) \geq 1 - e^{-\beta c} \quad (3.3)$$

for some positive constant c and sufficiently large β .

Moreover, for all $a \in A$, $b \in \partial A$, for all $\varepsilon > 0$,

$$\mathbb{P}_a \left(\tau_{\partial A}^* = \tau_b^* \right) \geq e^{-\beta(H(b)-H(F(\partial A))-\varepsilon)} \quad (3.4)$$

While the two previous Lemmata give sharp bounds on the exit time at finite volume, their results are not sufficient to deal with the infinite-volume case.

The following Lemma from [MO2] shows that if the exit time is not too small, the inner details of the cycle do not influence the exit state. In this case, the bound on the exit probability is “exponentially equivalent” to the bound (3.2).

Lemma 3.3. (Lemma 4.3 in [MO2].) *Given a non-trivial cycle A and a positive number κ such that*

$$\Theta(A) < \kappa \leq \Gamma(A),$$

we have $\forall a \in A, \forall b \in \partial A, \forall \varepsilon > 0$ and β sufficiently large

$$\mathbb{P}_a \left(\tau_{\partial A}^* < e^{\beta \kappa}, \tau_{\partial A}^* = \tau_b^* \right) \geq e^{-\beta(H(b)-H(F(A))-\kappa+\varepsilon)}. \quad (3.5)$$

4. Proof of Theorem 2.1.

We now focus on the model described in §2. In the following key Lemma we estimate the exit probability at a given time T , showing that the most likely exit state depends on T .

Lemma 4.1. *For all $0 < \kappa < 1, \forall \varepsilon > 0$ and sufficiently large β ,*

$$e^{-\beta(\kappa-\nu(\kappa)+\varepsilon)} \leq \mathbb{P}_0 \left(\tau^* \leq e^{\beta \kappa} \right) \leq e^{-\beta(\kappa-\nu(\kappa)-\varepsilon)}. \quad (4.1)$$

Moreover,

$$\mathbb{P}_0 \left(\tau^* = \tau_3^* \mid \tau^* \leq e^{\beta \kappa} \right) \quad (4.2)$$

tends to 0 if $\kappa < 26/36$ (i.e. $\nu(\kappa) < 1/3$) and to 1 if $\kappa > 26/36$.

PROOF. We split the proof into three parts:²

²In the general case, the analogue of this proof would be to pass to a “renormalized Markov chain” (see [S]) where the state space is partitioned into the subsets of states that are “equivalent” at time T (meaning that starting from any state in a subset all the other states in the same subset are visited within T with large probability). The probability of a transition is “exponentially equivalent” to the probability of the best path in this renormalized Markov chain (the product of the transition probabilities in the path).

a) $\kappa < 26/36$ (i.e. $\nu(\kappa) < 1/3$).

By applying Lemma 3.3 on the cycle $\{0\}$:

$$\mathbb{P}_0 \left(\left\{ \tau^* = \tau_{-1}^* \right\} \cap \left\{ \tau^* \leq e^{\beta\kappa} \right\} \right) \geq e^{-\beta(40/36 - \kappa + \varepsilon)} \quad (4.3)$$

while, from 3.2

$$\mathbb{P}_0 \left(\left\{ \tau^* = \tau_{-1}^* \right\} \cap \left\{ \tau^* \leq e^{\beta\kappa} \right\} \right) \leq e^{-\beta(40/36 - \kappa)} \quad (4.4)$$

On the other hand, the exit passing through 3 entails a transition from 0 to 1 and a transition from 2 to 3; therefore, by using Lemma 3.1 and the Markov property, we get

$$\mathbb{P}_0 \left(\left\{ \tau^* = \tau_3^* \right\} \cap \left\{ \tau^* \leq e^{\beta\kappa} \right\} \right) \leq e^{-2\beta(33/36 - \kappa)} \quad (4.5)$$

Since $40/36 - \kappa = \kappa - \nu(\kappa) < 66/36 - 2\kappa$, by (4.3), (4.4) and (4.5), we get (4.1) in case a). By (4.3) and (4.5) we get (4.2):

$$\mathbb{P}_0 \left(\left\{ \tau^* = \tau_3^* \right\} \mid \left\{ \tau^* \leq e^{\beta\kappa} \right\} \right) \leq \frac{\mathbb{P}_0 \left(\left\{ \tau^* = \tau_3^* \right\} \cap \left\{ \tau^* \leq e^{\beta\kappa} \right\} \right)}{\mathbb{P}_0 \left(\left\{ \tau^* = \tau_1^* \right\} \cap \left\{ \tau^* \leq e^{\beta\kappa} \right\} \right)} \rightarrow 0 \quad (4.6)$$

b) if $26/36 \leq \kappa < 30/36$ (i.e. $1/3 \leq \nu(\kappa) < 2/3$) then we still have the bounds in (4.4) and (4.5) but now $\kappa - \nu(\kappa) = 66/36 - 2\kappa$ and the leading term is (4.5). To get a lower bound on the probability to exit through 3, we observe that

$$\begin{aligned} & \mathbb{P}_0 \left(\left\{ \tau^* = \tau_3^* \right\} \cap \left\{ \tau^* \leq e^{\beta\kappa} \right\} \right) \geq \\ & \mathbb{P}_0 \left(\tau_1^* \leq \frac{1}{2}e^{\beta\kappa} \right) \mathbb{P}_1 \left(\tau_2^* \leq 1 \right) \mathbb{P}_2 \left(\tau_3^* \leq \frac{1}{2}e^{\beta\kappa} - 1 \right) \geq \\ & e^{-2\beta(33/36 - \kappa + \varepsilon)}, \end{aligned} \quad (4.7)$$

where, to get the last inequality, we used Lemma 3.3 on the cycles $\{0\}$ and $\{2\}$. By (4.3), (4.4) and (4.7), we get (4.1) in case b). By (4.4) and (4.7) we get (4.2):

$$\mathbb{P}_0 \left(\left\{ \tau^* = \tau_1^* \right\} \mid \left\{ \tau^* \leq e^{\beta\kappa} \right\} \right) \leq \frac{\mathbb{P}_0 \left(\left\{ \tau^* = \tau_{-1}^* \right\} \cap \left\{ \tau^* \leq e^{\beta\kappa} \right\} \right)}{\mathbb{P}_0 \left(\left\{ \tau^* = \tau_3^* \right\} \cap \left\{ \tau^* \leq e^{\beta\kappa} \right\} \right)} \rightarrow 0 \quad (4.8)$$

c) $30/36 < \kappa < 1$ (i.e. $2/3 < \nu(\kappa)$). In this case, we can deal directly with the cycle $\{0, 1, 2\}$. By (3.2) and Lemma 3.3, respectively, we get the following bounds on the probability to exit through 3:

$$\mathbb{P}_0 \left(\left\{ \tau^* = \tau_3^* \right\} \cap \left\{ \tau^* \leq e^{\beta\kappa} \right\} \right) \leq e^{-\beta(1 - \kappa)} \quad (4.9)$$

and

$$\mathbb{P}_0 \left(\left\{ \tau^* = \tau_3^* \right\} \cap \left\{ \tau^* \leq e^{\beta\kappa} \right\} \right) \geq e^{-\beta(1-\kappa+\varepsilon)}. \quad (4.10)$$

By (4.3), (4.4) and (4.10), we get (4.1) in case c). By the same procedure leading to (4.8) we get (4.2). \square

THE LOWER BOUND ON τ (PROOF OF (2.17)).

We use Lemma 4.1 when $\kappa = k(\nu) - \varepsilon$ (notice that if $\nu > 1$ this choice gives $\kappa - \nu(\kappa) = \varepsilon$).

Since the spins are independent from each other until time $\hat{\tau}(\Lambda)$,

$$\mathbb{P}_0 (\hat{\tau}(\Lambda) < t) = 1 - (1 - \mathbb{P}_0 (\tau^* < t))^\Lambda \quad (4.11)$$

by using the definition of Λ (see (2.16)), we get from (4.11)

$$\begin{aligned} \mathbb{P}_0 (\hat{\tau}(\Lambda) < e^{\beta(k(\nu)-\varepsilon)}) &\leq \\ \lfloor e^{\beta(k(\nu)-\nu)} \rfloor e^{-\beta(\lfloor k(\nu)-\nu \rfloor_+)} e^{-\beta\varepsilon'} &\rightarrow 0; \end{aligned} \quad (4.12)$$

namely, it is very unlikely that the nucleation occurs into Λ within time $e^{\beta(k(\nu)+\varepsilon)}$.

Next, we prove that L is too large to be crossed within the allotted time:

$$\mathbb{P}_\Omega (\tau < e^{\beta(k(\nu)-\varepsilon)} \mid \hat{\tau}(\Lambda) > e^{\beta(k(\nu)-\varepsilon)}) \leq 2 \mathbb{P} \left(\sum_{n=0}^{\lfloor e^{\beta(k(\nu)-\nu)} \rfloor} \zeta(n) < e^{\beta(k(\nu)-\varepsilon)} \right), \quad (4.13)$$

where the $\zeta(n)$'s are i.i.d. exponential variables with rate $e^{-\beta\nu}$. Let Z be a Poisson variable with mean $e^{\beta(k(\nu)-\nu-\varepsilon)}$ r.h.s. of (4.13) is equal to

$$2\mathbb{P} (Z \geq \lfloor e^{\beta(k(\nu)-\nu)} \rfloor) \leq \frac{e^{\beta(k(\nu)-\nu-\varepsilon)}}{\lfloor e^{\beta(k(\nu)-\nu)} \rfloor} \rightarrow 0, \quad (4.14)$$

where in the last inequality we used Chebychev inequality.

This concludes the proof of the lower bound (2.17). \square

UPPER BOUND ON τ (PROOF OF (2.18)). Let us start by considering the case $\nu < 1$ (so that $k(\nu) + \varepsilon$ can be taken smaller than 1). By using Lemma 4.1 and (4.11), we see that Λ is so large that (with large probability) nucleation in it occurs within $e^{\beta(k(\nu)+\varepsilon)}$.

Now we show that Λ is small enough to be crossed in the allotted time: by the same procedure of (4.13), we get

$$\mathbb{P}_\Omega (\tau > e^{\beta(k(\nu)+\varepsilon)} \mid \hat{\tau}(\Lambda) > e^{\beta(k(\nu)+\varepsilon)}) \leq \mathbb{P}_\Omega \left(\sum_{n=0}^{\lfloor e^{\beta(k(\nu)-\nu)} \rfloor} \zeta(n) > e^{\beta(k(\nu)+\varepsilon)} \right), \quad (4.15)$$

where the $\zeta(n)$'s are i.i.d. exponential variables with mean $e^{\beta\nu}$. By using Chebychev inequality, we bound r.h.s. of (4.15) by

$$\frac{\lfloor e^{\beta(k(\nu)-\nu)} \rfloor e^{\beta\nu}}{e^{\beta(k(\nu)+\varepsilon)}} \rightarrow 0 \tag{4.16}$$

In the case $\nu \geq 1$, Lemma 3.2 applied on the cycle $\{0, 1, 2\}$ gives

$$\mathbb{P}_0(\tau^* = \tau_3^*, \tau^* < e^{\beta(1+\varepsilon)}) \geq 1 - e^{-\beta c}. \tag{4.17}$$

Since with large probability nucleation occurs in the origin within the allotted time $e^{\beta(1+\varepsilon)}$ and since, by (2.8), nucleation in other sites can only help, we conclude the proof. \square

THE SHAPE OF THE DROPLET (PROOF OF (2.19) AND (2.20)). By the same procedure leading to (4.12), we immediately show that with overwhelming probability all the droplets of the “wrong” kind formed within $e^{\beta(k(\nu)+\varepsilon)}$ are very far away from the origin (more than $\lfloor e^{\beta(k(\nu)-\nu)} \rfloor e^{\beta\delta}$ for some $\delta > 0$). Since the presence of droplets of the “right” kind does not increase the speed of growth of the the droplets of the “wrong kind” (indeed, they prevent the growth), we can proceed as for (4.14) and conclude the proof. \square

References

[BBG1] G. Ben Arous, A. Bovier, V. Gayrard “Glauber dynamics for the random energy model I: metastable motion on the extreme states” in preparation (2001).
 [BBG2] G. Ben Arous, A. Bovier, V. Gayrard “Glauber dynamics for the random energy model II: Aging below the critical temperature” in preparation (2001).
 [BEGK1] A. Bovier, M. Eckhoff, V. Gayrard, M. Klein “Metastability in stochastic dynamics of disordered mean-field models” *Probab. Theory Related Fields* **119** (2001), 99–161.
 [BEGK2] A. Bovier, M. Eckhoff, V. Gayrard, M. Klein “Metastability and low-lying spectra in reversible Markov chains” WIAS-preprint 601 (2000).
 [BM] A. Bovier, F. Manzo “Metastability in Glauber Dynamics in the Low-Temperature limit: Beyond Exponential Asymptotics” WIAS-preprint 663 (2001).
 [C] O. Catoni “Sharp large deviations estimates for simulated annealing algorithms” *Ann. Inst. Henri Poincaré, Probab. Stat.* **27**, No.3, 291-383 (1991).
 [CC] O. Catoni, R. Cerf “The exit path of a Markov chain with rare transitions.” *ESAIM, Probab. Stat.* **1** (1997), 95-144 (1996).
 [CGOV] M. Cassandro, A. Galves, E. Olivieri, M.E. Vares “Metastable behavior of stochastic dynamics: a pathwise approach” *J. Statist. Phys.* **35** (1984), 603–634.
 [CO] E.N.M. Cirillo, E. Olivieri “Metastability and nucleation for the Blume-Capel model. Different mechanisms of transition” *J. Stat. Phys.* **83**, No.3-4, 473-554 (1996).
 [DS1] P. Dehghanpour, R. Schonmann: “A Nucleation-and-growth model”. *Probab. Theory Relat. Fields.* **107**, 123-135 (1997)
 [DS2] P. Dehghanpour, R. Schonmann: “Metropolis dynamics relaxation via nucleation and growth”. *Commun. Math. Phys.* **188**, 89-119 (1997)
 [FW] M. Freidlin, A. Wentzell: “Random perturbations of Dynamical Systems”, Springer, (1984)

- [HOS] F. den Hollander, E. Olivieri, E. Scoppola “Metastability and nucleation for conservative dynamics” *Markov Process. Relat. Fields* **7**, No.1, 51-53 (2001)
- [KO] R. Kotecký, E. Olivieri “Droplet dynamics for asymmetric Ising model” *J. Stat. Phys.* **70**, No.5-6, 1121-1148 (1993).
- [KS] H. Kesten, R.H. Schonmann “On some growth models with a small parameter.” *Probab. Theory Relat. Fields* **101**, No.4, 435-468 (1995)
- [LP] Lebowitz, J.L.; Penrose, O. “Rigorous treatment of metastable states in the van der Waals-Maxwell theory” *J. Stat. Phys.* **3**, 211-236 (1971)
- [MO1] F.Manzo, E.Olivieri “Relaxation patterns for competing metastable states: a nucleation and growth model”. *Markov Proc. Rel. Field* **4**, 549-570 (1998)
- [MO2] F.Manzo, E.Olivieri “Dynamical Blume-Capel Model: Competing Metastable States at Infinite Volume” *Journal of Statistical Physics* 104(5/6): 1029-1090, September 2001
- [NS] E.J. Neves, R.H. Schonmann, “Critical droplets and metastability for a Glauber dynamics at very low temperatures” *Comm. Math. Phys.* **137** (1991), no. 2, 209–230.
- [NO] F. R. Nardi, E. Olivieri “Low temperature stochastic dynamics for an Ising model with alternating field” *Markov Process. Relat. Fields* **2**, No.1, 117-166 (1996)
- [OS] E. Olivieri, E. Scoppola “Markov chains with exponentially small transition probabilities: First exit problem from a general domain -I. The reversible case”. *JSP* **79**, 613 (1995)
- [T] A. Trouvé “Convergence optimale pour les algorithmes de recrutis généralisés” *C. R. Acad. Sci., Paris, Sr. I* **315**, No.11, 1197-1202 (1992).
- [S] E. Scoppola “Renormalization group for Markov chains: a general procedure” based on renormalization group ideas, *Jour. Stat. Phys.* **73** nos. 1/2 (1993), 83–121
- [SS] R.H. Schonmann, S.B. Shlosman “Wulff droplets and the metastable relaxation of kinetic Ising models” *Comm. Math. Phys.* **194** (1998), 389–462.