Metastability under stochastic dynamics *

F. den Hollander
EURANDOM, P.O. Box 513,
5600 MB Eindhoven, The Netherlands.

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Abstract

This paper is a tutorial introduction to some of the mathematics behind metastable behavior of interacting particle systems. The main focus is on the formation of so-called critical droplets, in particular, on their geometry and the time of their appearance. Special attention is given to Ising spins subject to a Glauber spin-flip dynamics and lattice particles subject to a Kawasaki hopping dynamics. The latter is one of the hardest models that can be treated to date and therefore is representative for the current state of development of this research area.

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1 Introduction

We begin with a phenomenological description of metastability. Concrete models will be described later.

Consider a thermodynamic system in equilibrium at a point P in phase space (= the space of thermodynamic parameters, such as temperature, pressure, density or external field). The point P is assumed to lie on one side of a curve at which the system undergoes a *first-order* phase transition (= a transition requiring energy). Suppose that the parameters are rapidly – essentially instantaneously – changed to a point P' on the *opposite* side of the curve, lying *close* to the curve (see Fig. 1.1). Then, instead of rapidly undergoing the phase transition, the system persists for a long time in the old equilibrium at P, now called *metastable state*, until it tunnels to the new equilibrium at P' under the influence of random fluctuations, either internal or external. Since the system has to overcome the energy barrier when making the transition, it takes time for the random fluctuations to achieve the crossover.

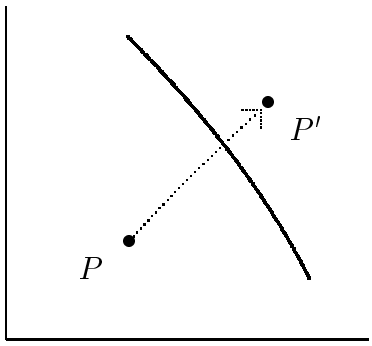

Fig. 1.1: A metastable transition.

The phase transition occurs only after the system creates a sufficiently large droplet of the new phase inside the old phase, called *critical droplet*, which triggers the crossover. The metastable state is characterized by *many unsuccessful attempts* to create a critical droplet.

The above phenomenon occurs in the following examples:

(1) A wrongly magnetized ferromagnet.
(2) A supersaturated gas.
(3) A supercooled liquid.

For (1), we imagine a system of spins (= microscopic magnets) that can point either up or down and that have a tendency to align among themselves (= for each pair of neighboring spins the interaction energy is negative when they are parallel and positive when they are anti-parallel) and to align with a magnetic field (= for each spin the interaction energy is negative when it is parallel to the magnetic field and positive

when it is anti-parallel). If we apply a strong negative magnetic field (P), then most spins will point downwards. If we rapidly change the magnetic field to a *small but positive* value (P'), then the spins will prefer to point upwards. Under the influence of a *Glauber dynamics* (= a Metropolis spin-flip dynamics), the spins will gradually flip upwards, but at low temperature this takes a long time. Indeed, initially a single spin will flip upwards, and in doing so it will loose energy because it aligns with the magnetic field, but it will gain energy because it no longer aligns with its neighboring spins. If the net result is positive, then the spin will tend to flip back. After some time, a random fluctuation will make a group of neighboring spins flip upwards. Again, all these spins loose energy because they align with the magnetic field, but some energy is gained because they no longer align with the spins along the boundary of the group. The net energy *per spin*, however, is lower than for the single flipped spin, because within the group the flipped spins align with each other. Perhaps the net energy is increasing with the number of spins, in which case the group has a *subcritical* size and the spins will tend to flip back again. Eventually, the group of flipped spins is so large that the net energy is decreasing with the number of spins (because the energy loss is proportional to the volume of the group while the energy gain is proportional to the surface). In that case the group has a *supercritical* size and is stable against random fluctuations. Now the spins along the boundary will tend to flip upwards, until eventually a majority of the spins in the system are pointing upwards and the system is positively magnetized.

In (2), we imagine a system of gas molecules that are subject to cohesive forces (= for each neighboring pair of molecules the interaction energy is negative). If we start with a low density system (P), then most molecules will be isolated. If we rapidly increase the density to a value *slightly above saturation* (P'), then the molecules will prefer to form a clump. Under the influence of a *Kawasaki dynamics* (= a Metropolis hopping dynamics), the molecules will gradually clump together, but at low temperature this takes a long time. Indeed, initially two molecules will meet, but since their interaction energy is only slightly negative they typically separate before a third molecule attaches itself. After some time, three molecules meet, but they may not stick together long enough before the fourth molecule arrives, in which case the group has a *subcritical* size. Eventually, the group of molecules is so large and its interaction energy so negative that it stays together until the next molecule arrives. In that case the group has a *supercritical* size and is stable against random fluctuations. Now other molecules will tend to attach themselves, until eventually the gas condenses.

In (3), we imagine a glass filled with water that is rapidly cooled from a temperature above its freezing point (P) to a temperature *slightly below* (P'). Ice may not appear immediately. But when we shake the glass or hit it with a stick, then the ice forms instantly. This is due to the formation of a critical droplet of ice that acts as a nucleus for the freezing of the system.

There are many other phenomena in nature where metastability plays a key role. For instance, dielectric breakdown (opposite charges are added to two plates with a thin isolation between them until current passes through), fracture growth (increasing pressure is applied to a rock until it cracks), protein folding (a long polymer rearranges itself when adopting different low energy configurations). In the present paper we will

restrict ourselves to examples (1) and (2). The main questions we will be interested in are:

What does the critical droplet look like?
How long does it take to complete the phase transition?
What is the system doing before it achieves the crossover?

2 Microscopic models

In this paper we focus on two particular microscopic models for (1) and (2), thereby entering the world of *non-equilibrium statistical mechanics*. The challenge is to explain the sudden crossover from the metastable state to the stable state, both qualitatively and quantitatively.

In all metastable situations a picture like the following sits in the background:

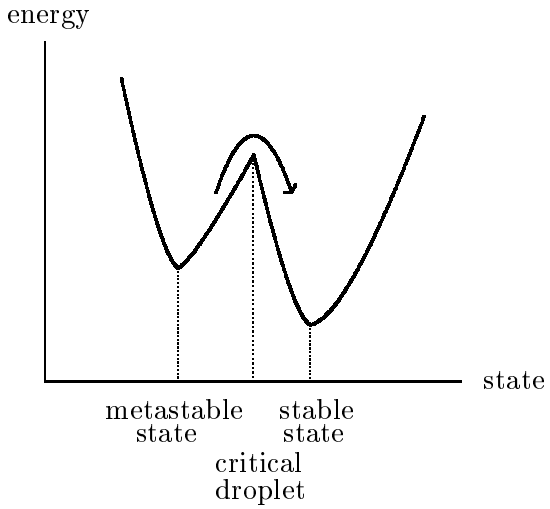

Fig. 2.1: The paradigm picture of the energy landscape.

The system starts in the metastable state, which is a local minimum at the bottom of a deep energy valley, and moves to the stable state, which is a global minimum at the bottom of another deep energy valley (see Fig. 2.1). Under the influence of fluctuations, induced by a *stochastic dynamics*, the system moves around in the first valley, until it manages to go over the hill that separates the two valleys and move into the second valley. At low temperature the crossover, once it occurs, is typically fast compared to the time spent in the first valley. How does the system start in the metastable state? This state may have been a global minimum before the rapid change of thermodynamic parameters and moved up in energy as a result of this change, so as to become a local minimum.

The picture in Fig. 2.1 is naive: typically the state space is neither ordered nor is the energy landscape a double well. In microscopic models typically the state space is high-

dimensional and the energy landscape is complex (small wells inside large wells, possibly plateaux, dead-ends, etc.) In addition, the top of the hill separating the two valleys may have a complex structure too. The three questions mentioned earlier translate into:

> What do the states on the top of the hill look like?
> How long does it take to move between the two valleys?
> How does the system move to the top?

The literature on metastability in physics and in chemistry is vast. What has happened mathematically? After the groundbreaking works of Eyring, Kramers and Wigner in the 1930's and 1940's (see van Kampen [27]), Lebowitz and Penrose [30] in 1971 were the first to derive a rigorous theory of metastability in the context of Van der Waals theory. Early subsequent results include Capocaccia, Cassandro and Olivieri [11] (Ising model) and Cassandro and Olivieri [13] (fluid models). Around the mid 1980's several papers addressing a number of different microscopic models appeared. Since the early 1990's the area is in full swing. Our bibliography contains a (fairly comprehensive) list of mathematical papers that deal with metastability for interacting particle systems, with the emphasis on droplet formation. In 2004, a monograph by Olivieri and Vares [45] will appear that describes the history and the recent development of metastability. For earlier overviews of specific parts, see Penrose and Lebowitz [47], Schonmann [52], [53], Scoppola [56], Vares [58], Olivieri and Scoppola [44], Bovier [4].

Currently there are two main approaches to metastability:

(I) The *pathwise* approach, which was initiated in 1984 by Cassandro, Galves, Olivieri and Vares [12]. Here, the analysis of metastability is based on large deviations for the path of the dynamics, in the spirit of Freidlin and Wentzell [21]. Typically this gives rather detailed information on the evolution of the system, but is hard to carry through in detail.

(II) The *potential theoretic* approach, which was initiated in 2002 by Bovier, Eckhoff, Gayrard and Klein [6]. Here, the analysis of metastability is based on a computation of capacities, in the spirit of Doyle and Snell [20]. Typically this gives less information on the evolution of the system, but leads to sharp results on the metastable transition time.

In Sections 3 and 4 we will address the above three questions for model (1) and (2), respectively, focussing on two dimensions and systems of *finite volume* at *low temperature*. For both models these results draw on approaches (I) and (II). In Section 5 we describe extensions to three dimensions. In Section 6 we compare the two models and discuss their main differences. In Section 7 we mention related work and list some open problems.

Metastability is closely linked with the *spectral properties* of the generator of the stochastic dynamics. This link, which has been pioneered by Davies, Holley, Kusuoka, Martinelli, Miclo, Stroock, Zegarlinski and others, is not discussed in the present paper. For a review we refer to Bovier, Eckhoff, Gayrard and Klein [7], [8].

3 Model (1) in two dimensions

3.1 Definitions

Let $\Lambda \subset \mathbb{Z}^2$ be a large finite box, with periodic boundary conditions. With each site $x \in \Lambda$ we associate an Ising-spin variable $\sigma(x) \in \{-1, +1\}$, indicating whether the spin at x is down or up. A spin configuration $\sigma = \{\sigma(x)\colon\ x \in \Lambda\}$ is an element of the configuration space $\mathcal{X} = \{-1, +1\}^{\Lambda}$ (see Fig. 3.1). With each configuration $\sigma \in \mathcal{X}$ we associate an energy given by the Hamiltonian

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

where Λ^* denotes the set of nearest-neighbor bonds in Λ, $J > 0$ is the *ferromagnetic pair potential* acting between neighboring spins and $h > 0$ is the *magnetic field* acting on single spins.

−	−	+	−	−
+	−	−	−	+
+	−	−	+	−
−	+	+	+	−
+	−	−	+	−

Ising spins
Glauber dynamics
non-conservative
periodic boundary

Fig. 3.1: A configuration in model (1).

We choose a stochastic dynamics on $\mathcal{X}$ given by the standard Metropolis algorithm:

$$\sigma \to \sigma' \qquad \text{at rate} \qquad e^{-\beta\{[H(\sigma')-H(\sigma)]\vee 0\}}$$

for all σ' obtainable from σ via:

– *spin flips* at single sites in Λ.

This is called *Glauber dynamics on a torus* at inverse temperature $\beta > 0$.

The Gibbs measure associated with H is

$$\mu_\beta(\sigma) = \frac{1}{Z_\beta}\, e^{-\beta H(\sigma)}, \quad \sigma \in \mathcal{X},$$

and is the *reversible equilibrium* of the Glauber dynamics.

The regime that will be considered is

$$h \in (0, 2J), \quad \beta \to \infty,$$

which is a low temperature limit. The restriction on h corresponds to the *metastable regime*. Indeed, let $\boxminus, \boxplus \in \mathcal{X}$ denote the configurations where all spins in Λ are -1,

respectively, $+1$. Then the energy of an $\ell \times \ell$ droplet of $(+1)$-spins in a sea of (-1)-spins, $\sigma_{\ell \times \ell}$, relative to the energy of $\boxminus$ equals

$$E(\ell) = H(\sigma_{\ell \times \ell}) - H(\boxminus) = J[4\ell] - h[\ell^2],$$

which achieves its maximal value at $\ell = 2J/h \in (1, \infty)$ (see Fig. 3.2). To avoid ties we assume that $2J/h$ is non-integer, in which case

$$\ell_c = \left\lceil \frac{2J}{h} \right\rceil$$

is the *critical droplet size*, i.e., droplets of size $\geq \ell_c$ prefer to grow, droplets of size $< \ell_c$ prefer to shrink.

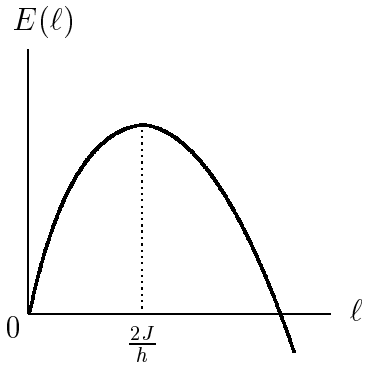

Fig. 3.2: Energy of an $\ell \times \ell$ droplet of $(+1)$-spins in a sea of (-1)-spins.

3.2 Main theorems

The results in this section are taken from Neves and Schonmann [40], [41], Schonmann [48], [49] and Neves [39]. For proofs we refer to these papers.

For $\sigma \in \mathcal{X}$, let $\mathbb{P}_\sigma$ be the law of the Glauber dynamics $(\sigma_t)_{t \geq 0}$ starting from $\sigma_0 = \sigma$. For $\mathcal{A} \subset \mathcal{X}$, let

$$\tau_{\mathcal{A}} = \{t \geq 0 \colon \sigma_t \in \mathcal{A}, \sigma_t \neq \sigma_0\}$$

denote the first hitting time of $\mathcal{A}$ (the restriction $\sigma_t \neq \sigma_0$ is put in because the dynamics runs in continuous time).

Let

$$\Gamma = \min_{\omega \colon \boxminus \to \boxplus} \max_{\sigma \in \omega} [H(\sigma) - H(\boxminus)]$$

be the *communication height* between $\boxminus$ and $\boxplus$, where the minimum runs over all *admissible* paths ω connecting $\boxminus$ and $\boxplus$ (where admissible means that the path only follows transitions that are allowed by the dynamics) and the maximum runs over all configurations σ encountered along ω. Let

$$\mathcal{S} = \left\{\zeta \in \mathcal{X} \colon \exists \omega \colon \boxminus \to \boxplus, \omega \ni \zeta \colon \max_{\sigma \in \omega} H(\sigma) = H(\zeta) = \Gamma\right\}$$

be the *communication level set* between $\boxminus$ and $\boxplus$ (also called the communication saddle). Note that $\boxplus$ is the global minumum of H, whereas $\boxminus$ is a local minimum.

Theorem 3.2.1 *(i)*

$$\lim_{\beta\to\infty} \mathbb{P}_{\boxminus}\left(e^{(\Gamma-\delta)\beta} < \tau_{\boxplus} < e^{(\Gamma+\delta)\beta}\right) = 1 \qquad \forall\, \delta > 0.$$

(ii)

$$\lim_{\beta\to\infty} \mathbb{P}_{\boxminus}(\tau_{\mathcal{S}} < \tau_{\boxplus} \mid \tau_{\boxplus} < \tau_{\boxminus}) = 1.$$

Theorem 3.2.1(i) shows that $\Gamma = H(\mathcal{S})$ is the *exponent* of the transition time. Theorem 3.2.1(ii) states that $\mathcal{S}$ is a *gate* for the transition, i.e., on its way from $\boxminus$ to $\boxplus$ the dynamics must pass through $\mathcal{S}$. Both statements are sharp in the limit as $\beta \to \infty$, and are general in the sense that they do not require any detailed knowledge of the model.

In order to compute Γ and to identify the geometry of the *relevant* configurations in $\mathcal{S}$, we define:

Definition 3.2.2 *(i) Let $\mathcal{C}^* = \bar{\mathcal{C}}^* \cup \widetilde{\mathcal{C}}^*$ with (see Fig. 3.3):*

- *$\bar{\mathcal{C}}^*$ the set of configurations where the $(+1)$-spins form an $(\ell_c - 1) \times \ell_c$ quasi-square anywhere in Λ with a single protuberance attached anywhere on a side of length ℓ_c.*
- *$\widetilde{\mathcal{C}}^*$ the set of configurations where the $(+1)$-spins form an $(\ell_c - 1) \times \ell_c$ quasi-square anywhere in Λ with a single protuberance attached anywhere on a side of length $\ell_c - 1$.*

In both sets the quasi-square may occur in either of two orientations.
(ii) Let $\Gamma^* = H(\mathcal{C}^*) - H(\boxminus) = J[4\ell_c] - h[\ell_c(\ell_c - 1) + 1]$.

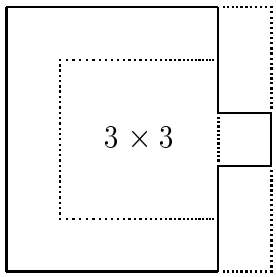

Fig. 3.3: A configuration in $\bar{\mathcal{C}}^*$ for $\ell_c = 5$. The $(+1)$-spins lie inside the solid contour, the (-1)-spins outside.

Theorem 3.2.3 *(i) $\mathcal{S} \supseteq \mathcal{C}^*$.*
(ii) $\Gamma = \Gamma^*$.
(iii)

$$\lim_{\beta\to\infty} \mathbb{P}_{\boxminus}(\tau_{\bar{\mathcal{C}}^*} < \tau_{\boxplus} \mid \tau_{\boxplus} < \tau_{\boxminus}) = 1.$$

Theorem 3.2.3(i) states that $\mathcal{C}^*$ is a subset of $\mathcal{S}$. Theorem 3.2.3(ii) identifies Γ in terms of the model parameters. Theorem 3.2.3(iii) shows that $\bar{\mathcal{C}}^*$ is a gate for the transition, while $\widetilde{\mathcal{C}}^*$ consists of *dead-ends*. We will see in Section 3.3 that $\bar{\mathcal{C}}^*$ is in fact a *minimal gate* for the transition. Thus, $\bar{\mathcal{C}}^*$ plays the role of the set of *critical droplets*. Think of Γ^* as the formation energy of the critical droplets.

Why are the configurations in $\bar{\mathcal{C}}^*$ critical? This is explained as follows:

- The cost of *adding* a bar of length ℓ to a droplet is $2J - h$: this is the energy necessary to add a single protuberance, after which the rest of the bar is added "downhill".
- The cost of *removing* a bar of length ℓ from a droplet is $(\ell - 1)h$: this is the energy necessary to remove the bar except for a single protuberance, after which the latter is removed "downhill".
- The two costs match when $\ell = 2J/h$ (recall Fig. 3.2). The configurations in $\bar{\mathcal{C}}^*$ are obtained by first creating a 1×1 square, then successively adding on bars of length $1, \ldots, \ell_c - 1$ following a growing sequence of quasi-squares,

$$1 \times 1 \quad 1 \times 2 \quad 2 \times 2 \quad 2 \times 3 \quad \ldots \quad (\ell_c - 1) \times (\ell_c - 1) \quad (\ell_c - 1) \times \ell_c,$$

  and finally adding on a single protuberance, thereby reaching the top of the hill.

Note that in $\widetilde{\mathcal{C}}^*$ the single protuberance is attached to the "wrong side": filling the bar along this side does not lead to a droplet that is supercritical, because one of the sides of the droplet still has length $< \ell_c$.

The proof of Theorem 3.2.3(i) uses standard discrete isoperimetric inequalities.

3.3 Refinements

The next theorem is an improvement of Theorem 3.2.3(i,iii).

Theorem 3.3.1 *(i)* $\mathcal{S} \supsetneq \mathcal{C}^*$.
(ii)

$$\lim_{\beta \to \infty} \mathbb{P}_{\boxminus}(\eta_{\tau_{\bar{\mathcal{C}}^*}} = \eta \mid \tau_{\bar{\mathcal{C}}^*} < \tau_{\boxplus}) = \frac{1}{|\bar{\mathcal{C}}^*|} \qquad \forall\, \eta \in \bar{\mathcal{C}}^*.$$

Theorem 3.3.1(i) shows that $\mathcal{S}$ is larger than $\mathcal{C}^*$. An example of a configuration in $\mathcal{S} \setminus \mathcal{C}^*$ is obtained by picking any configuration in $\mathcal{C}^*$, flipping down any spin next to the protuberance (at gain h) and afterwards flipping up any spin at a corner of the quasi-square (at cost h). Theorem 3.3.1(ii) says that the *entrance distribution of* $\bar{\mathcal{C}}^*$ *is uniform*. This fact is immediate from symmetry arguments.

The result is taken from Bovier and Manzo [10]. For the proof we refer to that paper.

Theorem 3.3.2 *(i)*

$$\mathbb{E}_{\boxminus}(\tau_{\boxplus}) = Ke^{\beta\Gamma^*}[1+o(1)] \qquad \textit{as } \beta \to \infty$$

with

$$K = K(\Lambda, \ell_c) = \frac{3}{4(2\ell_c - 1)} \frac{1}{|\Lambda|}.$$

(ii)

$$\mathbb{P}_{\boxminus}\left(\tau_{\boxplus} > t\mathbb{E}_{\boxminus}(\tau_{\boxplus})\right) = [1+o(1)]\, e^{-t[1+o(1)]} \qquad \textit{uniformly in } t \geq 0 \textit{ as } \beta \to \infty.$$

Theorem 3.3.2(i) is a sharp asymptotics for the average magnetization time. Theorem 3.3.2(ii) shows that the transition time is exponentially distributed, which is typical for "success occurs after many unsuccessful attempts", each unsuccessful attempt to create a critical droplet ending with a return to $\boxminus$ where the system starts from scratch.

The interpretation of the constant K is as follows. First, the average time it takes to enter $\bar{\mathcal{C}}^*$ is

$$\frac{1}{|\bar{\mathcal{C}}^*|}\, e^{\beta\Gamma^*}\, [1+o(1)] \qquad \text{as } \beta \to \infty.$$

Second, let $\pi(\ell_c)$ be the average probability (w.r.t. the uniform entrance distribution of $\bar{\mathcal{C}}^*$) that the critical droplet is exited in the direction of $\boxplus$ rather than $\boxminus$. Then the average number of attempts it takes to go over the hill in $\bar{\mathcal{C}}^*$ after reaching the top of the hill is

$$\frac{1}{\pi(\ell_c)}\, [1+o(1)] \qquad \text{as } \beta \to \infty.$$

The product of the last two displays is the average transition time, so that

$$K = \frac{1}{|\mathcal{C}^*|\, \pi(\ell_c)}.$$

Third, we have

$$|\bar{\mathcal{C}}^*| = |\Lambda|\, N(\ell_c) \quad \text{ with } \quad N(\ell_c) = 4\ell_c.$$

Indeed, the $(\ell_c - 1) \times \ell_c$ quasi-square can be centered anywhere in Λ (which is a torus) and can occur in two possible orientations, while the protuberance can be attached in $2\ell_c$ possible positions. Fourth, if the protuberance sits at one of the two extreme ends of the side of length ℓ_c it is attached to, then the probability is $\frac{1}{2}$ that its *one* neighboring spin on the same side flips upwards before the protuberance flips downwards. On the other hand, if the protuberance sits elsewhere, then the probability is $\frac{2}{3}$ that one of its *two* neighboring spins on the same side flips upwards before the protuberance flips downwards. Hence,

$$\pi(\ell_c) = \frac{1}{\ell_c} \left\{ 2\, \frac{1}{2} + (\ell_c - 2)\, \frac{2}{3} \right\} = \frac{1}{3\ell_c}\, (2\ell_c - 1).$$

The last three displays explain the formula for K.

On its way from $\boxminus$ to $\boxplus$ the dynamics may hit $\bar{\mathcal{C}}^*$ in only one configuration, implying that no strict subset of $\bar{\mathcal{C}}^*$ is a gate. Thus, $\bar{\mathcal{C}}^*$ is a minimal gate, as was claimed below Theorem 3.2.3.

The proof of Theorem 3.3.2(i) makes use of potential theory and sharp estimates for Dirichlet forms associated with the Glauber dynamics. The main idea is that K is determined by only a *tiny* part of the configuration space, namely, *the configurations in and directly communicating with* $\bar{\mathcal{C}}^*$. Establishing fast recurrence to either $\boxminus$ or $\boxplus$ from an arbitrary configuration is an important ingredient in the analysis. So is reversibility.

4 Model (2) in two dimensions

4.1 Definitions

Let $\Lambda \subset \mathbb{Z}^2$ be a large finite box. With each site $x \in \Lambda$ we associate an occupation variable $\eta(x) \in \{0,1\}$, indicating the absence or presence of a particle at x. A lattice gas configuration $\eta = \{\eta(x)\colon\ x \in \Lambda\}$ is an element of the configuration space $\mathcal{X} = \{0,1\}^\Lambda$ (see Fig. 4.1). With each configuration $\eta \in \mathcal{X}$ we associate an energy given by the Hamiltonian

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

where $\Lambda^{-,*}$ denotes the set of nearest-neighbor bonds in $\Lambda^- = \Lambda \setminus \partial\Lambda$ ($\partial\Lambda$ denotes the boundary of Λ), $-U < 0$ is the *binding energy* between neighboring particles and $\Delta > 0$ is the *activation energy* of single particles. Note that particles in $\partial\Lambda$ experience no interaction.

0	0	1	0	0
0	0	0	1	0
0	1	1	0	0
0	1	1	0	0
0	0	0	0	0

Lattice gas
Kawasaki dynamics
conservative
open boundary

Fig. 4.1: A configuration in model (2).

We choose a stochastic dynamics on $\mathcal{X}$ given by the standard Metropolis algorithm:

$$\eta \to \eta' \qquad \text{at rate} \qquad e^{-\beta\{[H(\eta')-H(\eta)]\vee 0\}}$$

for all η' obtainable from η via:

- an *exchange* of occupation numbers between neighboring sites in Λ,
- a *raising* or *lowering* of occupation numbers at single sites in $\partial\Lambda$,

which correspond to hopping of particles in Λ, respectively, to creation or annihilation of particles in $\partial\Lambda$, mimicking the presence of a gas reservoir in $\mathbb{Z}^2 \setminus \Lambda$. This is called *Kawasaki dynamics with an open boundary* at inverse temperature $\beta > 0$.

The Gibbs measure associated with H is

$$\mu_\beta(\eta) = \frac{1}{Z_\beta}\, e^{-\beta H(\eta)}, \quad \eta \in \mathcal{X},$$

and is the *reversible equilibrium* of the Kawasaki dynamics, describing the lattice gas in equilibrium with the gas reservoir, which has density $e^{-\Delta\beta}$, the rate at which particles are created at the boundary. The regime that will be considered is

$$\Delta \in (U, 2U), \quad \beta \to \infty,$$

which is a low temperature and low density limit. The restriction on Δ corresponds to the *metastable regime*. Indeed, the energy of an $\ell \times \ell$ droplet of particles, $\eta_{\ell\times\ell}$, equals

$$E(\ell) = H(\eta_{\ell\times\ell}) = -U[2\ell(\ell-1)] + \Delta\ell^2,$$

which achieves its maximal value at $\ell = U/(2U-\Delta) \in (1, \infty)$ (see Fig. 4.2). To avoid ties we assume that $U/(2U-\Delta)$ is non-integer, in which case

$$\ell_c = \left\lceil \frac{U}{2U-\Delta} \right\rceil$$

is the *critical droplet size*.

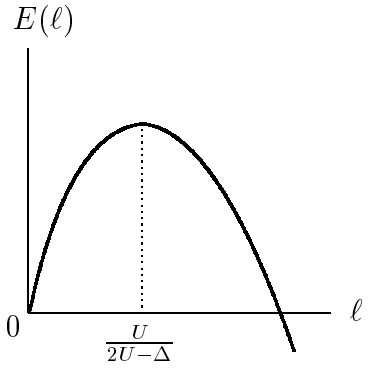

Fig. 4.2: Energy of an $\ell \times \ell$ droplet of particles.

4.2 Main theorems

The results in this section are taken from den Hollander, Olivieri and Scoppola [24], [25], [26]. For proofs we refer to these papers.

For $\eta \in \mathcal{X}$, let $\mathbb{P}_\eta$ be the law of the Kawasaki dynamics $(\eta_t)_{t\geq 0}$ starting from $\eta_0 = \eta$. For $\mathcal{A} \subset \mathcal{X}$, let

$$\tau_{\mathcal{A}} = \{t \geq 0 \colon\ \eta_t \in \mathcal{A},\ \eta_t \neq \eta_0\}$$

denote the first hitting time of $\mathcal{A}$.

Let $\square, \blacksquare \in \mathcal{X}$ denote the configurations where Λ is empty, respectively, full. We assume that Λ is so large that $H(\blacksquare) < H(\square) = 0$, in which case $\blacksquare$ is the global minimum. Let

$$\Gamma = \min_{\omega:\, \square \to \blacksquare} \max_{\eta \in \omega} H(\eta)$$

be the *communication height* between $\square$ and $\blacksquare$, where the minimum runs over all *admissible* paths ω connecting $\square$ and $\blacksquare$ and the maximum runs over all configurations η encountered along ω. Let

$$\mathcal{S} = \left\{ \zeta \in \mathcal{X} \colon\ \exists \omega \colon\ \square \to \blacksquare,\, \omega \ni \zeta \colon\ \max_{\eta \in \omega} H(\eta) = H(\zeta) = \Gamma \right\}$$

be the *communication level set* between $\square$ and $\blacksquare$. The analogue of Theorem 3.2.1 reads:

Theorem 4.2.1 *(i)*

$$\lim_{\beta \to \infty} \mathbb{P}_{\square} \left(e^{(\Gamma - \delta)\beta} < \tau_{\blacksquare} < e^{(\Gamma + \delta)\beta} \right) = 1 \qquad \forall\, \delta > 0.$$

(ii)

$$\lim_{\beta \to \infty} \mathbb{P}_{\square}(\tau_{\mathcal{S}} < \tau_{\blacksquare} \mid \tau_{\blacksquare} < \tau_{\square}) = 1.$$

The interpretation of Theorem 4.2.1 is similar to that of Theorem 3.2.1.

In order to compute Γ and to identify the geometry of the *relevant* configurations in $\mathcal{S}$, we need some more definitions. The following is the analogue of Definition 3.2.2 but is more complex.

Definition 4.2.2 *(i) Let $\mathcal{Q} = \bar{\mathcal{Q}} \cup \widetilde{\mathcal{Q}}$ with (Fig. 4.3):*

- *$\bar{\mathcal{Q}}$ the set of configurations where the particles are in Λ^- and form an $(\ell_c - 1) \times \ell_c$ quasi-square with a single protuberance attached on a side of length ℓ_c.*
- *$\widetilde{\mathcal{Q}}$ the set of configurations where the particles are in Λ^- and form an $(\ell_c - 1) \times \ell_c$ quasi-square with a single protuberance attached on a side of length $\ell_c - 1$.*

In both sets the droplet may be located anywhere in Λ^- and may occur in either of the two orientations.
(ii) Let $\mathcal{D} \supset \mathcal{Q}$ be the set of configurations that can be reached from some configuration in $\mathcal{Q}$ via a U-path, i.e.,

$$\omega \colon\ \eta \to \eta', \qquad \eta \in \mathcal{Q},\, \eta' \in \mathcal{D},$$

such that

$$\begin{aligned} &\max_{\xi \in \omega} H(\xi) \le H(\eta) + U, \\ &|\xi| = |\eta| = |\eta'| \text{ for all } \xi \in \omega, \\ &H(\eta) = H(\eta') \end{aligned}$$

(with $|\xi|$ the number of particles in ξ).
(iii) Let

$$\mathcal{C}^* = \mathcal{D} + \text{ free particle anywhere in } \Lambda.$$

(iv) Let

$$\begin{aligned} \Gamma^* &= H(\mathcal{C}^*) = H(\mathcal{D}) + \Delta = H(\mathcal{Q}) + \Delta \\ &= -U[(\ell_c - 1)^2 + \ell_c(\ell_c - 2) + 1] + \Delta[\ell_c(\ell_c - 1) + 2]. \end{aligned}$$

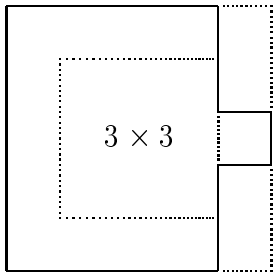

Fig. 4.3: A configuration in $\bar{\mathcal{Q}}$ for $\ell_c = 5$.
The particles lie inside the solid contour.

The analogue of Theorem 3.2.3 reads:

Theorem 4.2.3 *(i)* $\mathcal{S} \supseteq \mathcal{C}^*$.
(ii) $\Gamma = \Gamma^*$.
(iii)

$$\lim_{\beta\to\infty} \mathbb{P}_{\square}(\tau_{\mathcal{C}^*} < \tau_{\blacksquare} \mid \tau_{\blacksquare} < \tau_{\square}) = 1.$$

Theorem 4.2.3(i) states that $\mathcal{C}^*$ is a subset of $\mathcal{S}$. Theorem 4.2.3(ii) identifies Γ in terms of the model parameters. Theorem 4.2.3(iii) shows that $\mathcal{C}^*$ is a gate for the transition. The latter is different from Theorem 3.2.3(iii), where the smaller set $\bar{\mathcal{C}}^*$ appears as a gate. In Section 4.3 we will explain why. There we will see that $\mathcal{C}^*$ is in fact a *minimal gate* for the transition. Thus, $\mathcal{C}^*$ plays the role of the set of *critical droplets*. Think of Γ^* again as the formation energy of the critical droplets.

Why are the configurations in $\mathcal{C}^*$ critical? This is explained as follows:

- The cost of *adding* a bar of length ℓ to a droplet is $2\Delta - U$: this is the energy necessary to create a first particle (at cost Δ), move it to the droplet (at cost 0), attach it to the droplet (at gain U), create a second particle (at cost Δ), and move it to the droplet (at cost 0). The bar can then be completed "downhill", because the gain is $2U > \Delta$ when the second particle attaches itself next to the first one.

- The cost of *removing* a bar of length ℓ from a droplet is $(\ell - 2)(2U - \Delta) + 2U$: this is the energy necessary to, one by one, detach $\ell - 2$ particles (at cost $2U$), move them to the boundary of the box (at cost 0), and annihilate them (at gain Δ), and after that detach one more particle (at cost $2U$), and moving it to the boundary of the box (at cost 0). The rest is again "downhill".

– The two costs match when $\ell = U/(2U - \Delta)$ (recall Fig. 4.2). The configurations in $\mathcal{Q}$ are obtained by first creating a 1×1 square, then successively adding on bars of length $1, \ldots, \ell_c - 1$ following a growing sequence of quasi-squares,

$$1 \times 1 \quad 1 \times 2 \quad 2 \times 2 \quad 2 \times 3 \quad \ldots \quad (\ell_c - 1) \times (\ell_c - 1) \quad (\ell_c - 1) \times \ell_c,$$

and finally adding on a single protuberance, thereby reaching the top of the hill, similarly as for Glauber.

– The configurations in $\mathcal{D}$ are those configurations the dynamics can reach *after* hitting $\mathcal{Q}$ *before* the arrival of the next particle. Indeed, a U-path is completed in a time of order $e^{U\beta}$, while it takes a time of order $e^{\Delta\beta} \gg e^{U\beta}$ to create a new particle. This particle moves the configuration into $\mathcal{C}^*$ and completes the formation of the critical droplet.

Think of $\mathcal{Q}$ as the set of *canonical protocritical droplets* and $\mathcal{D}$ as the set of *protocritical droplets*.

The definition of $\mathcal{D}$ in Definition 4.2.2(ii) is in terms of a certain "environment" of $\mathcal{Q}$ (defined in terms of U-paths). In Section 4.3 we will give a *full geometric description* of the configurations in $\mathcal{D}$. This geometry will in turn allow us to get a better grip on the transition time.

4.3 Refinements

The results in this section are taken from Bovier, den Hollander and Nardi [9]. For proofs we refer to that paper.

Theorem 4.3.1 $\mathcal{D} = \bar{\mathcal{D}} \cup \widetilde{\mathcal{D}}$ *with (see Fig. 4.4):*

– $\bar{\mathcal{D}}$ *the set of configurations where the particles are in* Λ^- *and form an* $(\ell_c - 2) \times (\ell_c - 2)$ *square with four bars attached to the fours sides of lengths* $\bar{k}_i$ *satisfying*

$$1 \leq \bar{k}_i \leq \ell_c - 1, \qquad \sum_i \bar{k}_i = 3\ell_c - 3.$$

– $\widetilde{\mathcal{D}}$ *the set of configurations where the particles are in* Λ^- *and form an* $(\ell_c - 3) \times (\ell_c - 1)$ *square with four bars attached to the four sides of lengths* $\widetilde{k}_i$ *satisfying*

$$1 \leq \widetilde{k}_i \leq \ell_c - 1, \qquad \sum_i \widetilde{k}_i = 3\ell_c - 2.$$

In both sets the droplet may be located anywhere in Λ^- *and may occur in any possible orientation.*

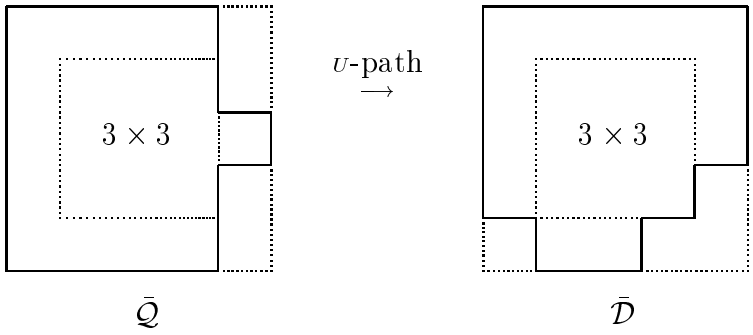

Fig. 4.4: Motion along the border for $\ell_c = 5$.

Note that $\bar{\mathcal{Q}}$ consists of precisely those configurations in $\bar{\mathcal{D}}$ where one bar has length 1 and the other bars have maximal length. Similarly for $\widetilde{\mathcal{Q}}$ and $\widetilde{\mathcal{D}}$. The case $\ell_c = 2$ is degenerate: in that case $\mathcal{Q} = \mathcal{D}$ is the set of configurations where 3 particles form an arbitrary cluster.

The configurations in $\mathcal{D}$ arise from those in $\mathcal{Q}$ via *motion of particles along the border of the droplet*, as follows. The protuberance in the first picture of Fig. 4.4 slides along the right side of the droplet (at cost 0), until it reaches the upper right corner. After that the right-most particle in the horizontal bar on top of the droplet slides on top of the protuberance (at cost U). The remaining particles in this bar re-attach themselves one by one (at cost 0), until the last particle re-attaches itself (at gain U). At this point the energy is back to where it started. Now there sits a vertical bar of length two on the right side of the droplet. Move the lower particle in this bar down (at cost U), and move the upper particle down so that it re-attaches itself (at gain U). At this point the energy is again back to where it started. After that the same mechanism can be repeated, etc. The motion along the border of the droplet is a feature that is special to Kawasaki dynamics.

As a result of the full geometry in Theorem 4.3.1, we can get sharper information on the transition path and the transition time, as stated in the three theorems below.

First we improve Theorem 4.2.3(i,iii) by stating the analogue of Theorem 3.3.1:

Theorem 4.3.2 *(i)* $\mathcal{S} \supsetneq \mathcal{C}^*$.
(ii)

$$\lim_{\beta\to\infty} \mathbb{P}_{\square}(\tau_{\mathcal{Q}} < \tau_{\mathcal{C}^*} < \tau_{\blacksquare} \mid \tau_{\blacksquare} < \tau_{\square}) = 1.$$

(iii)

$$\lim_{\beta\to\infty} \mathbb{P}_{\square}(\eta_{\tau_{\mathcal{C}^*}-} = \eta \mid \tau_{\mathcal{C}^*} < \tau_{\square}) = \frac{1}{|\mathcal{D}|} \qquad \forall\, \eta \in \mathcal{D}$$

with $\tau_{\mathcal{C}^*}-$ *the time just prior to* $\tau_{\mathcal{C}^*}$.

Theorem 4.3.2(i) shows that $\mathcal{S}$ is larger than $\mathcal{C}^*$. An example of a configuration in $\mathcal{S}\setminus\mathcal{C}^*$ is obtained by picking any configuration in $\mathcal{Q}^*$ ($= \mathcal{Q} +$ free particle anywhere in Λ), moving the free particle to any site at distance 2 from the single protuberance (at cost

0), detaching this protuberance from the protocritical droplet and attaching it to the free particle in a single jump (at cost 0), so that we end up with an $(\ell_c - 1) \times \ell_c$ quasi-square and a dimer. Other examples arise by picking any configuration in $(\mathcal{D} \setminus \mathcal{Q})^*$ $(= (\mathcal{D} \setminus \mathcal{Q}) +$ free particle anywhere in $\Lambda)$, moving the free particle to any bar on the side of the protocritical droplet (at cost 0), attaching the free particle on top of the bar (at gain U), and starting a motion of particles along the border of the droplet (at cost U).

Theorem 4.3.2(ii) states that the dynamics must first pass through $\mathcal{Q}$, then possibly through $\mathcal{D} \setminus \mathcal{Q}$, and finally through $\mathcal{C}^*$ (which is different from Theorem 3.2.3(iii)). Theorem 4.3.2(iii) says that the *entrance distribution of* $\mathcal{C}^*$ *is uniform*, i.e., all configurations in $\mathcal{D}$, seen just prior to the arrival of the free particle that moves the configuration into $\mathcal{C}^*$, occur with equal probability (which is the analogue of Theorem 3.3.1(ii)).

The analogues of Theorem 3.3.2 read:

Theorem 4.3.3 *(i) There exists a constant* $K = K(\Lambda, \ell_c)$ *such that*

$$\mathbb{E}_{\square}(\tau_{\blacksquare}) = K e^{\Gamma^* \beta}[1 + o(1)] \qquad \text{as } \beta \to \infty.$$

(ii)

$$\mathbb{P}_{\square}\left(\tau_{\blacksquare} > t\mathbb{E}_{\square}(\tau_{\blacksquare})\right) = [1 + o(1)]\, e^{-t[1+o(1)]} \qquad \text{uniformly in } t \geq 0 \text{ as } \beta \to \infty.$$

Theorem 4.3.4 *As* $\Lambda \to \mathbb{Z}^2$,

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

with

$$N(\ell_c) = \frac{1}{3}(\ell_c - 1)\ell_c^2(\ell_c + 1)$$

the cardinality of $\mathcal{D} = \mathcal{D}(\Lambda, \ell_c)$ *modulo shifts.*

The constant K in Theorem 4.3.3(i) is determined by the *geometry of the configurations in* $\mathcal{C}^*$ *and its boundary*, as was the case in Theorem 3.3.2(i). However, it turns out that this boundary is *rather complex*, due to the motion of particles along the border of the protocritical droplet that is triggered when the free particle is about to attach itself. Therefore, unlike Theorem 3.3.2(i), no explicit formula for K is available. Nevertheless, Theorem 4.3.4 shows that the asymptotics of K for large Λ is simple. The interpretation of this asymptotics is as follows (compare with the explanation given below Theorem 3.3.2). First, the average time it takes to enter $\mathcal{C}^*$ is

$$\frac{1}{|\mathcal{D}|\,|\partial\Lambda|}\, e^{\Gamma^* \beta}\,[1 + o(1)] \qquad \text{as } \beta \to \infty.$$

Second, let $\pi(\Lambda, \ell_c)$ be the average probability (w.r.t. the uniform entrance distribution of $\mathcal{C}^*$) that the critical droplet is exited in the direction of $\blacksquare$ rather than $\square$. Then the

average number of attempts it takes to go over the hill in $\mathcal{C}^*$ after reaching the top of the hill is

$$\frac{1}{\pi(\Lambda, \ell_c)} [1 + o(1)] \qquad \text{as } \beta \to \infty.$$

The product of the last two displays is the average transition time, so that

$$K = \frac{1}{|\mathcal{D}|\,|\partial\Lambda|\,\pi(\Lambda, \ell_c)}.$$

Third, we have

$$|\mathcal{D}| \sim N(\ell_c)\,|\Lambda| \qquad \text{as } \Lambda \to \mathbb{Z}^2.$$

Fourth, we have

$$|\partial\Lambda|\,\pi(\Lambda, \ell_c) \sim \frac{4\pi}{\log|\Lambda|} \qquad \text{as } \Lambda \to \mathbb{Z}^2.$$

Indeed, the latter is the probability that a particle detaching itself from the protocritical droplet reaches $\partial\Lambda$ before re-attaching itself. This probability is independent of the shape and the location of the protocritical droplet, as long as it is far from $\partial\Lambda$, due to the recurrence of simple random walk in two dimensions. By reversibility, the reverse motion has the same probability. The last three displays explain the asymptotics for K.

On its way from $\square$ to $\blacksquare$ the dynamics may hit $\mathcal{D}$ in only one configuration, implying that for no strict subset of $\mathcal{D}$ when we add the free particle we get a gate for the transition. Thus, $\mathcal{C}^*$ is a minimal gate for the transition, as was claimed below Theorem 4.2.3. Note that, contrary to what we saw for Glauber, $\bar{\mathcal{C}}^*$ alone is not a minimal gate, because it communicates with $\widetilde{\mathcal{C}}^*$ via the motion of particles along the border of the droplet.

5 Extension to three dimensions

5.1 Glauber

In Ben Arous and Cerf [2] and Bovier and Manzo [10], the results in Section 3 are extended to three dimensions. Although the geometry is more complex, it can be handled with the help of the discrete isoperimetric inequalities proven in Alonso and Cerf [1]. These inequalities lead to a *focalization of optimal paths*: all paths realizing the minimax defining $\mathcal{S}$ must cross sets of configurations with a certain specific fixed number of (+1)-spins in certain specific configurations.

The metastable regime is

$$h \in (0, 3J), \qquad \beta \to \infty.$$

Two critical droplet sizes play a role,

$$\ell_c = \left\lceil \frac{2J}{h} \right\rceil, \qquad m_c = \left\lceil \frac{4J}{h} \right\rceil,$$

and we assume that $4J/h$ is non-integer in order to avoid ties.

The analogue of Definition 3.2.2 reads:

Definition 5.1.1 *(i) Let $\mathcal{C}^* = \bar{\mathcal{C}}^* \cup \widetilde{\mathcal{C}}^*$ with:*

- *$\bar{\mathcal{C}}^*$ the set of configurations where the $(+1)$-spins form an $(m_c - 1) \times (m_c - 2 + a_c) \times m_c$ quasi-cube anywhere in Λ with, attached anywhere to one of its largest faces, an $(\ell_c - 1) \times \ell_c$ quasi-square with, attached anywhere to one of its largest sides, a single protuberance.*
- *$\widetilde{\mathcal{C}}^*$ the same but with either the quasi-cube or the protuberance attached elsewhere.*

Here,

$$a_c = \left\lceil 2 \left(1 + \frac{h}{4J} \epsilon_c \right) (1 - \epsilon_c) \right\rceil \in \{1, 2\} \quad \text{with} \quad \epsilon_c = m_c - \frac{4J}{h} \in (0, 1)$$

counts the number of sides of length m_c of the quasi-cube. In both sets the quasi-square and the quasi-cube may occur in any of the possible orientations.
(ii) Let

$$\Gamma^* = H(\mathcal{C}^*) - H(\boxminus),$$

for which an explicit formula can be written down.

Thus, the configurations in $\mathcal{C}^*$ consist of a *two-dimensional* critical droplet attached to a face of a *three-dimensional* quasi-cube that is maximally subcritical.

With these definitions, Theorems 3.2.1, 3.2.3 and 3.3.2 carry over. The only difference is that the constant K takes on a different form, as shown by Bovier and Manzo [10]:

$$K = K(\Lambda, \ell_c, m_c, a_c) = \frac{a_c}{16} \frac{1}{(2\ell_c - 1)(m_c - \ell_c)^{2-a_c}(m_c - \ell_c + 1)^{a_c}} \frac{1}{|\Lambda|}.$$

The interpretation of the constant K is similar as in two dimensions. The key observation is that

$$|\bar{\mathcal{C}}^*| = |\Lambda| \, N(\ell_c, m_c, a_c) \quad \text{with} \quad N(\ell_c, m_c, a_c) = \frac{24}{a_c} \ell_c (m_c - \ell_c)^{2-a_c} (m_c - \ell_c + 1)^{a_c}.$$

Indeed, there are $4\ell_c$ shapes and orientations for the two-dimensional critical droplet. For $a_c = 1$ the number of $(m_c - 1) \times m_c$ faces is 4, and the number of ways to place the two-dimensional critical droplet on such a face equals $(m_c - \ell_c)(m_c - \ell_c + 1)$. For $a_c = 2$ the number of $m_c \times m_c$ faces is 2, and the number of ways to place the two-dimensional critical droplet on such a face equals $(m_c - \ell_c + 1)^2$. The number of orientations of the quasi-cube is 3 in both cases, which explains the form of $N(\ell_c, m_c, a_c)$. We have

$$K = \frac{1}{|\Lambda| \, N(\ell_c, m_c, a_c) \, \pi(\ell_c)}$$

with $\pi(\ell_c)$ the same quantity as appearing at the end of Section 3.3, which explains the form of K.

5.2 Kawasaki

In den Hollander, Nardi, Olivieri and Scoppola [22] and Bovier, den Hollander and Nardi [9], the results in Section 4 are *partially* extended to three dimensions. Again, the discrete isoperimetric inequalities proven in Alonso and Cerf [1] play a key role, but the geometry is too complex to be handled in full detail.

The metastable regime is

$$\Delta \in (U, 3U), \qquad \beta \to \infty.$$

Two critical droplet sizes play a role,

$$\ell_c = \Big\lceil \frac{U}{3U-\Delta} \Big\rceil, \qquad m_c = \Big\lceil \frac{2U}{3U-\Delta} \Big\rceil,$$

and we assume that $2U/(3U-\Delta)$ is non-integer in order to avoid ties.

The analogue of Definition 4.2.2 reads as follows:

Definition 5.2.1 *(i) Let $\mathcal{Q} = \bar{\mathcal{Q}} \cup \widetilde{\mathcal{Q}}$ with (see Fig. 5.1):*

- *$\bar{\mathcal{Q}}$ the set of configurations where the particles are in Λ^- and form an $(m_c-1)\times(m_c+2-a_c)\times m_c$ quasi-cube with, attached to one of its largest faces, an $(\ell_c-1)\times\ell_c$ quasi-square with, attached to one of its largests sides, a single protuberance.*
- *$\widetilde{\mathcal{Q}}$ the same but with either the quasi-cube or the protuberance attached elsewhere.*

In both sets the droplet may be located anywhere in Λ^- and may occur in any possible orientation. Moreover, $a_c \in \{0,1\}$ is the same as for Glauber with the replacements $2J \to U$ and $h \to 3U-\Delta$.
(ii) Let $\mathcal{D} \supset \mathcal{Q}$ be the set of configurations that can be reached from some configuration in $\mathcal{Q}$ via a U-path if $\Delta \in (U, 2U)$, respectively, a $2U$-path if $\Delta \in (2U, 3U)$.
(iii) Let

$$\mathcal{C}^* = \mathcal{D} + \textit{free particle anywhere in } \Lambda.$$

(iv) Let

$$\Gamma^* = H(\mathcal{C}^*) = H(\mathcal{D}) + \Delta = H(\mathcal{Q}) + \Delta,$$

for which an explicit formula can be written down.

In a picture, the set $\mathcal{Q}^*$ ($= \mathcal{Q}$ + free particle anywhere in Λ) looks like (compare with Fig. 4.3):

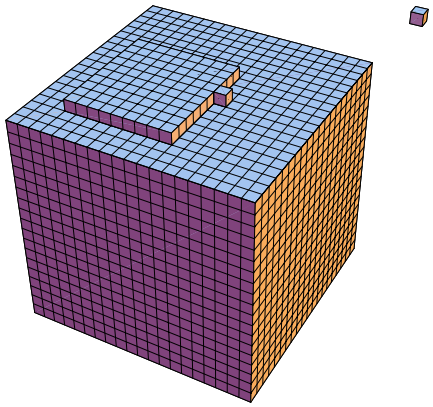

FIG. 5.1. A configuration in $\mathcal{Q}^*$ for $\ell_c = 10$, $m_c = 20$ and $a_c = 2$.

With these definitions, Theorems 4.2.3, 4.3.2 and 4.3.3 carry over. However, we have no complete geometric description of $\mathcal{D}$, due to the *complexity of the motion of particles along the border of the droplet* (see den Hollander, Nardi, Olivieri and Scoppola [22] for pictures). Consequently, we have no full analogues of Theorems 4.3.1 and 4.3.4, in particular, we have no formula for $N(\ell_c, m_c, a_c)$, the cardinality of $\mathcal{D}$ modulo shifts, nor for $\pi(\Lambda, \ell_c, m_c, a_c)$, the average probability that the critical droplet is exited in the direction of ■ rather than □. Partial results in Bovier, den Hollander and Nardi [9] include the statement that

$$K = \frac{1}{|\mathcal{D}|\,|\partial\Lambda|\,\pi(\Lambda, \ell_c, m_c, a_c)}$$

with

$$|\mathcal{D}| \sim N(\ell_c, m_c, a_c)\,|\Lambda| \qquad \text{as } \Lambda \to \mathbb{Z}^3,$$

as well as bounds on the inscribing and circumscribing cubes of the configurations in $\mathcal{D}$, leading to the asymptotics

$$|\partial\Lambda|\,\pi(\Lambda, \ell_c, m_c, a_c) \to \rho(\ell_c, m_c, a_c) \qquad \text{as } \Lambda \to \mathbb{Z}^3,$$

with upper and lower bounds on the limit. This limit is finite due to the transience of simple random walk in three dimensions, and satisfies

$$\rho(\ell_c, m_c, a_c) \sim \kappa m_c \qquad \text{as } m_c \to \infty$$

for some constant κ, corresponding to $\Delta \uparrow 2U$, the limit of weak supersaturation.

6 Comparison of Glauber and Kawasaki

As is evident from Sections 3, 4 and 5, there are many similarities and differences between Glauber and Kawasaki. We discuss the main differences:

– Glauber is a *non-conservative* dynamics (spins are not conserved on Λ), Kawasaki is a *conservative* dynamics (particles are conserved on the interior of Λ). Consequently, Glauber is local, whereas Kawasaki is both local and global: the droplet exchanges particles with $\partial\Lambda$ many times over long time intervals.

– Glauber does not allow for motion along the border of the droplet (spins flip, not hop), whereas Kawasaki does. Consequently, the droplet cannot shift about for Glauber, whereas it can for Kawasaki (see den Hollander, Nardi, Olivieri and Scoppola [22] for pictures).

– For Glauber the set $\mathcal{C}^*$ is simple: it falls apart into two disjoint subsets, $\bar{\mathcal{C}}^*$ and $\widetilde{\mathcal{C}}^*$, each consisting of a quasi-cube, a quasi-square and a single protuberance, the former playing the role of the set of critical droplets and the latter the role of a set of dead-ends. Moreover, all configurations in $\mathcal{C}^*$ are *isolated*, i.e., there are no direct transitions between them. For Kawasaki the situation is more difficult: $\mathcal{C}^*$ again falls apart into two disjoint subsets, $\bar{\mathcal{C}}^*$ and $\widetilde{\mathcal{C}}^*$, but these sets are more complex and communicate with each other due to the motion of particles along the border of the droplet. This is why only when put together do they form the set of critical droplets. Moreover, $\mathcal{C}^*$ consists of *plateaux* (corresponding to a free particle moving inside the box) and *wells* embedded in these plateaux (corresponding to the free particle attaching itself "improperly" to the protocritical droplet, i.e., on top of one of the bars of the protocritical droplet rather than next to one of the bars). As a consequence of all of this, the geometry of $\mathcal{C}^*$ and its immediate vicinity and the sharp asymptotics for the average metastable transition time are complete for Glauber, but are only partially complete for Kawasaki, particularly in three dimensions.

– The papers cited in Sections 3 and 5.1 contain a wealth of more detailed results for Glauber. For instance, it is known how subcritical droplets shrink and supercritical droplets grow, how long this shrinking and growing takes at the various stages of the metastable transition, what the entrance and the exit distribution are on the set of critical droplets, etc. In words, rather precise knowledge is available on the *tube of trajectories* for the metastable transition. For Kawasaki most of this knowledge is still missing. The references cited in Sections 4 and 5.2 contain only very partial information, the motion of particles along the border of the droplet again being the major complicating factor.

7 Related work and some open problems

The reader can find related work in:

- Martinelli, Olivieri and Scoppola [34] use metastability for Glauber to prove exponential mixing properties for the Ising model at low temperature.

- Dehghanpour and Schonmann [18], [19] investigate Glauber for $\Lambda = \mathbb{Z}^2$ and $\Lambda = \mathbb{Z}^3$ at low temperature. Droplets may appear anywhere, grow, move around, bump

into other droplets, until they invade the window of observation. (See also Manzo and Olivieri [32], [33].)

- Shlosman and Schonmann [54] consider Glauber for $\Lambda = \mathbb{Z}^2$ in the limit as $h \downarrow 0$ for $\beta > \beta_c$, i.e., the limit of a large critical droplet above the critical inverse temperature. They prove that the magnetization time near the origin behaves like

$$\exp\left\{\frac{\beta\lambda(\beta)}{h}[1+o(1)]\right\}, \qquad \text{as } h \downarrow 0,$$

  with $\lambda(\beta)$ calculable in terms of the "equilibrium Wulff shape" of the scaled critical droplet. See also Schonmann [50], [51], [52], [53].

- Various other types of models and dynamics have been looked at: Martinelli, Olivieri and Scoppola [35], [36] (Swendsen-Wang), Kotecký and Olivieri [28], [29] (anisotropic Ising and next-nearest-neighbor Ising), Peixoto [46] (Ising with stirring), Cirillo and Olivieri [17], Mathieu and Picco [37] (Curie-Weiss), Manzo and Olivieri [33] (Blume-Capel), Nardi and Olivieri [38] (Ising with alternating field), Cirillo [15], Cirillo and Nardi [16] (cellular automata).

- For results in a general Markov chain context, see Scoppola [55], [56], [57], Catoni and Cerf [14], Olivieri and Scoppola [42], [43], Bovier, Eckhoff, Gayrard and Klein [6].

- An analysis of metastability for disordered mean-field models is given in Bovier, Eckhoff, Gayrard and Klein [5], and for diffusion processes in Bovier, Eckhoff, Gayrard and Klein [7], [8].

- A general analysis of gate structure and its implications for metastable transition times can be found in Manzo, Nardi, Olivieri and Scoppola [31].

- In real experiments, theromodynamic parameters may not change rapidly enough to bring the system into a sharp metastable state. In that case hysteresis effects start to play a role. See e.g. Berglund and Gentz [3].

Here are some open problems for Kawasaki:

- Give a complete geometric description of the set of critical droplets $\mathcal{C}^*$ in three dimensions, i.e., find the analogue of Theorem 4.3.1 for two dimensions. This problem requires an extension of parts of Alonso and Cerf [1].

- Extend the results for the average nucleation time from finite Λ to exponentially large Λ, both in two and in three dimensions, i.e., find the analogues of Theorems 4.2.1(i), 4.3.3(i) and 4.3.4 when Λ grows exponentially fast with β. This problem is addressed in den Hollander, Nardi, Olivieri and Scoppola [23].

- What happens for $\Lambda = \mathbb{Z}^2$, $\beta > \beta_c$ and $\Delta \uparrow 2U$? Is there a result similar as for Glauber, with a scaled critical droplet taking on the equilibrium Wulff shape?

- What happens when there are two types of particles, with binding energies U_{11}, U_{22}, U_{12} and activation energies Δ_1, Δ_2? Identify the metastable regime and the set of critical droplets, both in two and in three dimensions.

We close with the remark that *ageing* in disordered media is a phenomenon deeply related to metastability: instead of tunneling from a metastable to a stable state, the system moves through a whole succession of metastable states. For simplified models quite some progress has been made in the past few years. See Bovier [4] for an overview and references.

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