Metastability under stochastic dynamics

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F. den Hollander

Mathematical Institute
Leiden University
P.O. Box 9512
2300 RA Leiden
The Netherlands

EURANDOM
P.O. Box 513
5600 MB Eindhoven
The Netherlands

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INTRODUCTION

In these lecture notes we describe the metastable behavior of Ising spins subject to Glauber dynamics and of lattice gas particles subject to Kawasaki dynamics, both in two dimensions. Attention focusses on the identification of the geometry of the critical droplet for the crossover from the metastable state to the stable state, and on the estimation of the crossover time. We consider three metastable regimes: (1) finite systems at low temperature; (2) large systems at low temperature; (3) large systems at positive temperature. These three regimes are progressively more challenging, and for the latter two regimes work is still in progress.

The present lectures are a continuation of the lectures given by Anton Bovier, in which a general theory of metastability is outlined for Markov processes. Our focus on Glauber dynamics and Kawasaki dynamics serves as an illustration of this general theory.

Acknowledgment: Part of the results described in these lectures is joint work with Anton Bovier, Alex Gaudilliere, Reda Messikh, Francesca Nardi, Enzo Olivieri and Elisabetta Scoppola.

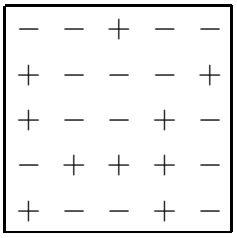
1 Lecture 1: Crude analysis for finite systems at low temperature

1.1 Glauber and Kawasaki

Let $\Lambda \subset \mathbb{Z}^2$ be a finite box. We consider two types of configurations:

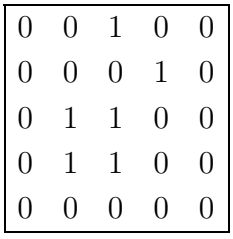
(I) *Ising spins*: $\eta = \{\eta(x)\colon\ x \in \Lambda\} \in \mathcal{X} = \{-1, +1\}^\Lambda$;
-1 = down-spin, $+1$ = up-spin (see Fig. 1).

(II) *Lattice gas*: $\eta = \{\eta(x)\colon\ x \in \Lambda\} \in \mathcal{X} = \{0, 1\}^\Lambda$;
0 = vacant, 1 = occupied (see Fig. 2).



Ising spins
periodic boundary

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



Lattice gas
open boundary

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

On the configuration space $\mathcal{X}$, we consider the Hamiltonians:

$$\begin{aligned} &\text{(I)}: \quad H(\sigma) = -\tfrac{J}{2} \sum_{\substack{x,y\in\Lambda \\ x\sim y}} \eta(x)\eta(y) - \tfrac{h}{2} \sum_{x\in\Lambda} \eta(x), \\ &\text{(II)} \quad H(\sigma) = -U \sum_{\substack{x,y\in\Lambda \\ x\sim y}} \eta(x)\eta(y) + \Delta \sum_{x\in\Lambda} \eta(x), \end{aligned} \tag{1.1}$$

where $x \sim y$ means that x and y are neighboring sites, in (I) we pick *periodic* boundary conditions and in (II) *open* boundary conditions (see (1.5–1.6) below). The parameters are: $J > 0$ the *ferromagnetic pair potential* and $h \in \mathbb{R}$ the *magnetic field*, respectively, $U > 0$ the *binding energy* and $\Delta > 0$ the *activation energy*.

Definition 1.1 *The Metropolis dynamics at inverse temperature $\beta \in (0,\infty)$ is the continuous-time Markov process $(\sigma(t))_{t\geq 0}$ on $\mathcal{X}$ with transition rates*

$$c(\eta,\eta') = \exp\{-\beta[H(\eta')-H(\eta)]_+\}, \qquad \eta,\eta' \in \mathcal{X}, \tag{1.2}$$

and allowed transitions

$$\begin{aligned} &\text{(I)}: \quad \eta' = \eta^x, \quad x \in \Lambda, \\ &\text{(II)}: \quad \eta' = \eta^{x,y}, \quad x,y \in \Lambda,\ x \sim y, \end{aligned} \tag{1.3}$$

where

$$\eta^x(y) = \begin{cases} \eta(y), & y \neq x, \\ -\eta(x), & y = x, \end{cases} \qquad \eta^{x,y}(z) = \begin{cases} \eta(z), & z \neq x,y, \\ \eta(x), & z = y, \\ \eta(y), & z = x. \end{cases} \tag{1.4}$$

In words, for Ising spins the dynamics consists of spin-flips at single sites, called *Glauber dynamics*, while for the lattice gas it consists of exchange of occupation numbers between neighboring sites, called *Kawasaki dynamics*.

In the second dynamics, we also allow particles to *enter* and *exit* Λ. To that end, we also allow transitions

$$\text{(II)}: \quad \eta' = \eta^{*,x}, \quad x \in \partial\Lambda, \tag{1.5}$$

where

$$\eta^{*,x}(y) = \begin{cases} \eta(y), & y \neq x, \\ 1-\eta(x), & y = x. \end{cases} \tag{1.6}$$

View this as mimicking the presence of an *infinite gas reservoir* in $\mathbb{Z}^2\backslash\Lambda$ that inserts particles at the sites of $\partial\Lambda$ at rate $e^{-\beta\Delta}$ and removes particles from the sites of $\partial\Lambda$ at rate 1.

A key observation is the following. The Metropolis dynamics has the *Gibbs measure*

$$\mu(\eta) = \frac{1}{Z_\beta}\, e^{-\beta H(\eta)}, \qquad \eta \in \mathcal{X}, \tag{1.7}$$

as its *reversible equilibrium*, i.e.,

$$\mu(\eta)c(\eta,\eta') = \mu(\eta')c(\eta',\eta), \qquad \forall\, \eta,\eta' \in \mathcal{X}. \tag{1.8}$$

Note that the two Hamiltonians in (1.1) can be transformed into each other via the transformation $\eta(x) \leftrightarrow \frac{1}{2}[1+\eta(x)]$, $h \leftrightarrow 2U-\Delta$, $J \leftrightarrow \frac{1}{2}U$ (modulo constant terms and boundary terms). However, the allowed transitions of the two dynamics are different: the first dynamics is *non-conservative*, the second dynamics is *conservative*.

1.2 Metastable regimes

We will study the two dynamics in the *low temperature* limit $\beta \to \infty$, in their so-called *metastable regimes*:

$$\begin{aligned} &\text{(I)}: \quad 0 < h < 2J, \quad \sigma(0) = \boxminus, \\ &\text{(II)}: \quad U < \Delta < 2U, \quad \sigma(0) = \square. \end{aligned} \tag{1.9}$$

Here, $\boxminus \equiv -1$ is the configuration with all spins down and $\square \equiv 0$ is the configuration with all sites vacant. We will be interested in how the dynamics tunnels to $\boxplus \equiv +1$, respectively, $\blacksquare \equiv 1$.

The parameter restrictions $h < 2J$ and $\Delta > U$ guarantee that $\boxminus$ and $\square$ are *local minima* of the Hamiltonian, which correspond to *metastable states*. Indeed, a spin-flip in $\boxminus$ costs an energy $2J - h > 0$, because it aligns the spin with the magnetic field but does not align it with its four neighbors. Similarly, creating a particle and attaching it to another particle that is already present costs an energy $\Delta - U > 0$. The parameter restrictions $h > 0$ and $\Delta < 2U$ guarantee that $\boxplus$ and $\blacksquare$ are *global minima* of the Hamiltonian, which correspond to *stable states* (in model (II) this requires Λ to be large enough, so that boundary effects are negligible). Thus, we have the following qualitative picture:

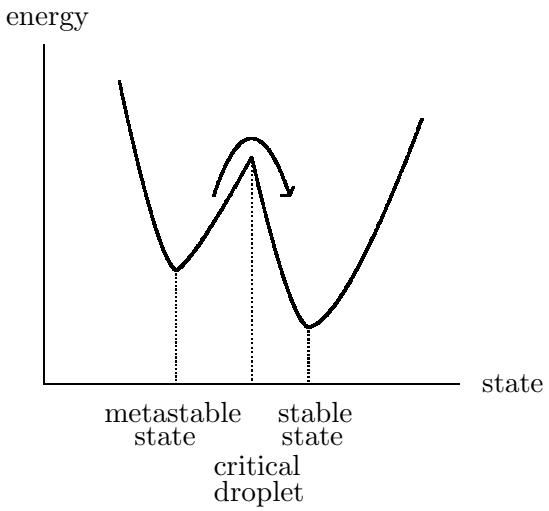


Fig. 3: The paradigm picture of the energy landscape.

We will address the following two questions:

(A) What are the *critical droplets* for the transitions $\boxminus \to \boxplus$ and $\square \to \blacksquare$?

(B) How large are the *crossover times* $\tau_{\boxplus}, \tau_{\blacksquare}$ starting from $\boxminus, \square$?

In the remainder of Lecture 1 we will provide a *crude answer* to these questions. In Lecture 2 we will describe some *refinements*.

1.3 Communication height and level set

Write $\omega\colon\ \eta \to \eta'$ to denote a path of allowed transitions from η to η'.

Definition 1.2 *The communication height between* $\boxminus$ *and* $\boxplus$ *is defined as*

$$\Gamma = \min_{\omega\colon\ \boxminus \to \boxplus} \max_{\xi \in \omega} [H(\xi) - H(\boxminus)]. \tag{1.10}$$

The corresponding communication level set is

$$\mathcal{S} = \Big\{\zeta \in \mathcal{X}\colon\ \exists\,\omega\colon\ \boxminus \to \boxplus \text{ with } \omega \ni \zeta \text{ such that } \max_{\xi\in\omega}[H(\xi) - H(\boxminus)] = H(\zeta) - H(\boxminus) = \Gamma\Big\}. \tag{1.11}$$

Similar definitions apply for $\square, \blacksquare$.

In words, Γ is the minimal amount the energy has to increase in a path that crosses over (note that $H(\boxminus) < 0$ and $H(\square) = 0$), while $\mathcal{S}$ is the set of saddle point configurations (recall Fig. 3).

Our *intuitive guess* for the answer to question (A) is that the critical droplet consists of all elements of $\mathcal{S}$, and for the answer to question (B) that

$$\tau_{\boxplus},\, \tau_{\blacksquare} \approx e^{\beta\Gamma} \quad \text{as } \beta \to \infty, \tag{1.12}$$

where the precise meaning of $\approx$ remains to be clarified. We will see that (1.12) is correct, but that the critical droplet actually is a smaller set than $\mathcal{S}$.

1.4 Geometry of prototype critical droplets

We begin by giving a geometric description of *prototype* critical droplets, thereby providing a crude answer to question (A). In Lecture 2 we will see that a description of *all* critical droplets is more involved for model (II).

Let us consider the energy of an $\ell \times \ell$ droplet, i.e.,

$$\begin{aligned} &\text{(I)}: \quad E(\ell) = H(\eta_{\ell\times\ell}) - H(\boxminus),\\ &\text{(II)}: \quad E(\ell) = H(\eta_{\ell\times\ell}), \end{aligned} \tag{1.13}$$

(recall that $H(\square) = 0$). An easy comptation given

$$\begin{aligned} &\text{(I)}: \quad E(\ell) = J[4\ell] - h\ell^2,\\ &\text{(II)}: \quad E(\ell) = -U[2\ell(\ell-1)] + \Delta\ell^2. \end{aligned} \tag{1.14}$$

In both cases, $\ell \mapsto E(\ell)$ is a downward parabola that assumes a maximum at

$$\ell_{max} = \frac{2J}{h}, \qquad \ell_{max} = \frac{U}{2U-\Delta}. \tag{1.15}$$

Hence, if both these ratios are non-integer, then the critical droplets are somewhere between a square of size $\ell_c - 1$ and a square of size ℓ_c, where

$$\ell_c = \left\lceil \frac{2J}{h} \right\rceil, \qquad \ell_c = \left\lceil \frac{U}{2U-\Delta} \right\rceil, \tag{1.16}$$

are the *critical droplet lengths*.

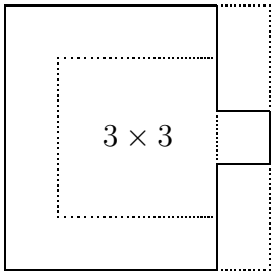


Fig. 4: A prototype critical droplet for $\ell_c = 5$ in model (I): the $+1$'s lie inside the solid contour, the -1's outside.

Theorem 1.3 (Neves and Schonmann [14]; den Hollander, Olivieri and Scoppola [12])
The set $\mathcal{S}$ contains the following prototype critical droplets:
(I) *An $\ell_c \times (\ell_c - 1)$ quasi-square of $(+1)$-spins in a sea of (-1)-spins, with a protuberance on one side of length ℓ_c.*
(II) *An $\ell_c \times (\ell_c - 1)$ quasi-square of particles, with a protuberance on one side of length ℓ_c, plus a free particle.*
(In both cases, the quasi-square can be centered anywhere in Λ and can occur in both orientations.)

Proof. (I) On its way from $\boxminus$ to $\boxplus$, the dynamics must pass through a configuration that has $\ell_c(\ell_c - 1)$ up-spins. Among the configurations with precisely this number of up-spins, those having an $\ell_c \times (\ell_c - 1)$ quasi-square of up-spins (of any orientation) have the smallest energy (due to a straightforward isoperimetric inequality; see e.g. Alonso and Cerf [1]). Continuing on its way from $\boxminus$ to $\boxplus$, the dynamics must flip one more spin upwards. The configurations with smallest energy are those where this spin is attached to one of the side of the quasi-square, forming a protuberance. Now, if this protuberance sits on one of the sides of length ℓ_c, then the dynamics can proceed downwards in energy to form an $\ell_c \times \ell_c$ square, and this square is "over the hill", i.e., there is a path from the quasi-square to $\boxplus$ that stays strictly below Γ (in other words, the quasi-square lies in the Γ-valley around $\boxplus$). On the other hand, if the protuberance sits on one of the sides of length $\ell_c - 1$, then the dynamics can proceed downwards in energy to form an $(\ell_c - 1) \times (\ell_c + 1)$ rectangle, but this rectangle is "not over the hill", i.e., there is no path from the rectangle to $\boxplus$ that stays strictly below Γ (in other words, the rectangle lies in the Γ-valley around $\boxminus$, not around $\boxplus$).
(II) For $\square, \blacksquare$ a similar argument applies, with the sole difference that after the protuberance has been formed the dynamics must create a new particle at the boundary and move it to the droplet. ♡

The protuberance indicates the initiation of the growth of a row or column that completes the square (see Fig. 4). In model (II), adding a row or colum of length ℓ costs $2\Delta - U$, while removing a row or colum of length ℓ costs $(2U - \Delta)(\ell - 2) + 2U$ (see Fig. 5). Hence, if the row or colum has length $\geq \ell_c$, then the dynamics more easily adds it than removes it, while the reverse is true when the row or colum has length $< \ell_c$. This provides another explanation of why ℓ_c is the critical droplet length.

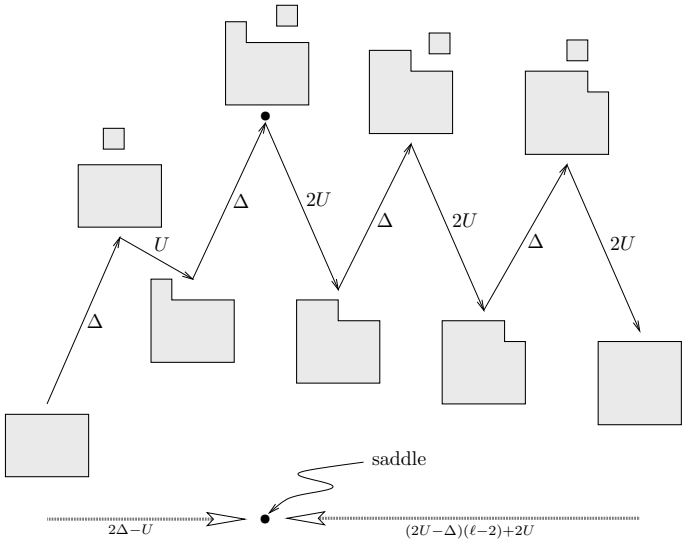


FIG. 5. Adding or removing a row or column of length ℓ.

Having identified a prototype element of $\mathcal{S}$, we are in a position to compute Γ, which is the energy of the configurations in $\mathcal{S}$. Indeed, we find

$$\begin{aligned} &\text{(I)}: \quad \Gamma = J[4\ell_c] - h[\ell_c(\ell_c-1)+1], \\ &\text{(II)}: \quad \Gamma = -U[(\ell_c-1)^2 + \ell_c(\ell_c-1)+1] + \Delta[\ell_c(\ell_c-1)+2]. \end{aligned} \tag{1.17}$$

1.5 Gate property and estimate of crossover time

Having computed Γ, we next give an estimate of the crossover time, thereby providing a crude answer to question (B).

Theorem 1.4 (Neves and Schonmann [14]; den Hollander, Olivieri and Scoppola [12])
For every $\delta > 0$,

$$\lim_{\beta\to\infty} \mathbb{P}_{\boxminus}\left(e^{\beta(\Gamma-\delta)} < \tau_{\boxplus} < e^{\beta(\Gamma+\delta)}\right) = 1. \tag{1.18}$$

A similar estimate applies for $\square, \blacksquare$.

Proof. One key ingredient in the proof is the *reversibility* of the dynamics expressed by (1.8). Fix $T > 0$ and a trajectory $\eta_{[0,T]}$ from $\eta(0) = \eta$ to $\eta(T) = \eta'$. Then

$$\mathbb{P}\big(\sigma_{[0,T]} \in d\eta_{[0,T]}\big) = \mathbb{P}\big(\sigma_{[0,T]} \in d\mathcal{R}\eta_{[0,T]}\big)\,\frac{\mu(\eta')}{\mu(\eta)}, \tag{1.19}$$

where $\mathcal{R}$ is the operator that reverses time, i.e., $R\eta_{[0,T]}(t) = \eta_{[0,T]}(T-t)$, $0 \le t \le T$.

Another key ingredient in the proof is the following. We have already seen that $\boxminus, \square$ are local minima and $\boxplus, \blacksquare$ are global minima of the Hamiltonian. In order for the crossover time to be determined entirely by the saddle point configurations in $\mathcal{S}$, we must ensure that there are no configurations in $\mathcal{X}$ that lie on the bottom of a well that is deeper than Γ. Indeed, if the dynamics were to go there, then it would get stuck for

a time much longer than the time we are targeting. The following lemma shows that in our two models such deep traps do not occur. The proof is somewhat technical and we refer the reader to the references cited.

Lemma 1.5 (Bovier and Manzo [7], den Hollander, Nardi, Olivieri and Scoppola [11])
For all $\eta \in \mathcal{X}\backslash\{\boxminus, \boxplus\}$,

$$\Gamma(\eta, \{\boxminus, \boxplus\}) < \Gamma, \tag{1.20}$$

where

$$\Gamma(\eta, \mathcal{A}) = \min_{\omega\colon\, \eta\to\mathcal{A}} \max_{\xi\in\omega} [H(\xi) - H(\eta)] \tag{1.21}$$

is the communication height between η *and the set* $\mathcal{A} \subset \mathcal{X}$. *A similar inequality holds for the pair* $\{\square, \blacksquare\}$.

We are now ready to prove (1.18).

Upper bound: We show that

$$\lim_{\beta\to\infty} \mathbb{P}_{\boxminus}\left(\tau_{\boxplus} < e^{\beta(\Gamma+\delta)}\right) = 1. \tag{1.22}$$

For $V > 0$, let

$$\mathcal{X}_V = \{\eta \in \mathcal{X}\colon\, \Gamma(\eta, I(\eta)) > V\}, \qquad I(\eta) = \{\zeta \in \mathcal{X}\colon\, H(\zeta) < H(\eta)\}. \tag{1.23}$$

In words, $\mathcal{X}_V$ is the set of all those configurations whose communication height to the set of configurations with lower energy exceeds V. It is straightforward to prove that for all $V, \delta > 0$,

$$\lim_{\beta\to\infty} \frac{1}{\beta} \log \max_{\eta\in\mathcal{X}\backslash\mathcal{X}_V} \mathbb{P}_\eta\left(\tau_{\mathcal{X}_V} > e^{\beta(V+\delta)}\right) = -\infty. \tag{1.24}$$

Therefore, to get (1.22), it suffices to pick $V = \Gamma$ and show that $\mathcal{X}_\Gamma = \{\boxplus\}$. To achieve the latter, we use Lemma 1.5, which implies that there exists a $V_0 < \Gamma$ such that $\mathcal{X}_{V_0} \subset \{\boxminus, \boxplus\}$. Since $\mathcal{X}_\Gamma \subset \mathcal{X}_{V_0}$ and since there is a path $\omega\colon \boxminus \to \boxplus$ with maximal height Γ, it follows that $\boxminus \notin \mathcal{X}_\Gamma$.

Lower bound: We show that

$$\lim_{\beta\to\infty} \mathbb{P}_{\boxminus}\left(\tau_{\boxplus} > e^{\beta(\Gamma-\delta)}\right) = 1. \tag{1.25}$$

Abbreviate $T = e^{\beta(\Gamma-\delta)}$ and

$$\mathcal{A}_{\boxminus} = \left\{\eta \in \mathcal{X}\colon\, \exists\,\omega\colon\, \eta \to \boxminus\colon\, \max_{\xi\in\omega} [H(\xi) - H(\boxminus)] < \Gamma\right\}. \tag{1.26}$$

Since $\boxplus \notin \mathcal{A}_{\boxminus}$, every path $\omega\colon \boxminus \to \boxplus$ has to cross $\partial\mathcal{A}_{\boxminus}$, the exterior boundary of $\mathcal{A}_{\boxminus}$. Therefore we have

$$\mathbb{P}_{\boxminus}\left(\tau_{\boxplus} \le T\right) \le \mathbb{P}_{\boxminus}\left(\tau_{\partial\mathcal{A}_{\boxminus}} \le T\right) = \sum_{\xi\in\partial\mathcal{A}_{\boxminus}} \int_0^T \mathbb{P}_{\boxminus}\left(\tau_{\partial\mathcal{A}_{\boxminus}} \in dt,\, \sigma(t) = \xi\right). \tag{1.27}$$

By (1.7) and the reversibility property in (1.19), we have

$$\begin{aligned}&\mathbb{P}_{\boxminus}\left(\tau_{\partial\mathcal{A}_{\boxminus}} \in dt,\, \sigma(t) = \xi\right)\\ &\quad = \frac{\mu(\xi)}{\mu(\boxminus)}\,\mathbb{P}_{\xi}\left(\sigma(s) \in \mathcal{A}_{\boxminus}\,\forall\, 0 \le s < t,\, \sigma(t) = \boxminus \mid \tau_{\partial\mathcal{A}_{\boxminus}} > t\right) dt.\end{aligned} \tag{1.28}$$

Combining (1.26–1.28), we get

$$\mathbb{P}_{\boxminus}\left(\tau_{\boxplus} \le T\right) \le |\partial\mathcal{A}_{\boxminus}|\, T\, e^{-\beta\Gamma} = |\partial\mathcal{A}_{\boxminus}|\, e^{-\beta\delta}, \tag{1.29}$$

which implies (1.25). ♡

The following theorem shows that the dynamics must pass through the communication level set $\mathcal{S}$.

Theorem 1.6 (Neves and Schonmann [14]; den Hollander, Olivieri and Scoppola [12])
$\lim_{\beta\to\infty} \mathbb{P}_{\boxminus}(\tau_{\mathcal{S}} < \tau_{\boxplus} \mid \tau_{\boxplus} < \tau_{\boxminus}) = 1$.

Proof. Any path from $\boxminus$ to $\boxplus$ that does not pass through $\mathcal{S}$ must hit a configuration η with $H(\eta) > \Gamma$. Therefore there exists a set $\mathcal{A} \subset \mathcal{X}$, with $\min_{\eta\in\mathcal{A}}[H(\eta) - H(\boxminus)] \ge \Gamma + \delta$ for some $\delta > 0$, such that

$$\mathbb{P}_{\boxminus}\left(\tau_{\boxplus} < \tau_{\mathcal{S}},\, \tau_{\boxplus} < \tau_{\boxminus}\right) \le \mathbb{P}_{\boxminus}\left(\tau_{\mathcal{A}} < \tau_{\boxminus}\right). \tag{1.30}$$

Estimate, with the help of (1.7) and the reversibility property in (1.19),

$$\begin{aligned}\mathbb{P}_{\boxminus}(\tau_{\mathcal{A}} < \tau_{\boxminus}) &\le \sum_{\eta\in\mathcal{A}} \mathbb{P}_{\boxminus}(\tau_{\eta} < \tau_{\boxminus}) = \sum_{\eta\in\mathcal{A}} \frac{\mu(\eta)}{\mu(\boxminus)}\,\mathbb{P}_{\eta}(\tau_{\boxminus} < \tau_{\eta})\\ &\le \sum_{\eta\in\mathcal{A}} e^{-\beta[H(\eta)-H(\boxminus)]} \le |\mathcal{X}|\, e^{-\beta(\Gamma+\delta)}.\end{aligned} \tag{1.31}$$

In a similar fashion, estimate

$$\begin{aligned}\mathbb{P}_{\boxminus}(\tau_{\boxplus} < \tau_{\boxminus}) &\ge \max_{\eta\in\mathcal{S}} \mathbb{P}_{\boxminus}\left(\tau_{\eta} < \tau_{\boxminus},\, \tau_{\eta} < \tau_{\boxplus}\right)\,\mathbb{P}_{\eta}\left(\tau_{\boxplus} < \tau_{\boxminus}\right)\\ &= \max_{\eta\in\mathcal{S}} \frac{\mu(\eta)}{\mu(\boxminus)}\,\mathbb{P}_{\eta}\left(\tau_{\boxminus} < \tau_{\eta},\, \tau_{\boxminus} < \tau_{\boxplus}\right)\,\mathbb{P}_{\eta}\left(\tau_{\boxplus} < \tau_{\boxminus}\right)\\ &\ge e^{-\beta\Gamma}\, C_1 C_2,\end{aligned} \tag{1.32}$$

where in the last line $C_1, C_2 > 0$ because $\mathcal{X}$ is finite and both trajectories from $\eta \in \mathcal{S}$ are going "downhill". Combine (1.30–1.32) to get

$$\mathbb{P}_{\boxminus}(\tau_{\boxplus} < \tau_{\mathcal{S}} \mid \tau_{\boxplus} < \tau_{\boxminus}) \le \frac{1}{C_1 C_2}\,|\mathcal{X}|\, e^{-\beta\delta}, \tag{1.33}$$

which proves the claim. ♡

Theorem 1.6 shows that $\mathcal{S}$ is a *gate* for the crossover. In Lecture 2 we will see that the full set of critical droplets for the crossover, i.e., the "minimal gate" for the crossover, is smaller than $\mathcal{S}$, i.e., $\mathcal{S}$ contains configurations that are *dead ends* for the crossover.

1.6 Extension to three dimensions

It is possible to extend the above analysis to $\mathbb{Z}^3$. For details, we refer to den Hollander, Nardi, Olivieri and Scoppola [11]. The geometry of droplets is considerably more delicate on $\mathbb{Z}^3$ than on $\mathbb{Z}^2$. Fortunately, most of the arguments can be carried over with the help of the powerful isoperimetric inequalites that are derived in Alonso and Cerf [1]. Thus, it is possible to compute Γ, and to obtain a rough idea of what the critical droplets look like. A prototype critical droplet is given in Fig. 6. This has *two* critical lengths:

$$\ell_c = \left\lceil \frac{U}{3U - \Delta} \right\rceil, \qquad m_c = \left\lceil \frac{2U}{3U - \Delta} \right\rceil. \tag{1.34}$$

Here, m_c is the size of the three-dimensional critical droplet, while ℓ_c is the size of the two-dimensional critical droplet that is attached to one of its faces and signals the threshold for completing the face that will push the three-dimensional critical droplet over the hill.

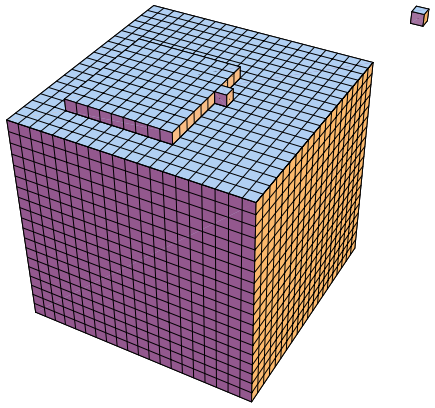


FIG. 6. A prototype critical droplet on $\mathbb{Z}^3$ for $\ell_c = 10$ and $m_c = 20$.

2 Lecture 2: Refined analysis for finite systems at low temperature

The results described in Lecture 1 constitute a crude analysis of metastability at low temperature. In Lecture 2 we give a more refined analysis, in which questions (A) and (B) receive more detailed answers. In particular, we identify the full set of critical droplets and obtain a sharp estimate of the crossover time.

2.1 Glauber

For model (I) we have the following.

Theorem 2.1 (Ben Arous and Cerf [2]; Bovier and Manzo [7])
Let $\mathcal{C}$ denote the set of configurations defined in Theorem 1.3(I)*. Then:*

$$\begin{aligned} &\lim_{\beta\to\infty} \mathbb{P}_{\boxminus}\left(\tau_{\mathcal{C}} < \tau_{\boxplus} \mid \tau_{\boxplus} < \tau_{\boxminus}\right) = 1, \\ &\lim_{\beta\to\infty} \mathbb{P}_{\boxminus}\left(\eta(\tau_{\mathcal{C}}) = \eta \mid \tau_{\mathcal{C}} < \tau_{\boxminus}\right) = |\mathcal{C}|^{-1} \quad \forall\, \eta \in \mathcal{C}. \end{aligned} \tag{2.1}$$

Theorem 2.2 (Bovier and Manzo [7])
(a) $\mathbb{E}_{\boxminus}(\tau_{\boxplus}) = Ke^{\beta\Gamma}[1 + o(1)]$ *as* $\beta \to \infty$*, with*

$$K = K(\Lambda, \ell_c) = \frac{3}{4(2\ell_c - 1)} \frac{1}{|\Lambda|}. \tag{2.2}$$

(b) $\lim_{\beta\to\infty} \mathbb{P}_{\boxminus}(\tau_{\boxplus} > t\, \mathbb{E}_{\boxminus}(\tau_{\boxplus})) = 1$ *uniformly in* $t \geq 0$.

Theorem 2.1 says that the set of prototype critical droplets is in fact the full set of critical droplets, i.e., is a "minimal gate" for the crossover, and that the dynamics enters this set uniformly (after which it may either cross or go back). Theorem 2.2 identifies the average crossover time up to a multiplicative factor that tends to 1, and shows that the crossover time is exponentially distributed.

The proof of these two theorems is beyond the scope of this lecture (later we indicate some of the techniques). Here is the *intuitive* idea. The uniform entrance distribution comes from the fact that for the critical droplet to grow a row or a column it must start with a protuberance. This protuberance must appear on one of the sides of length ℓ_c, otherwise it does not lead to the $\ell_c \times \ell_c$ square that is "over the hill". All locations of the protuberance are equally likely.

The exponential law comes from the fact that the crossover only occurs after many unsuccessful attempts to create a critical droplet and "go over the hill". To understand the fine asymptotics of the average crossover time, we argue as follows. The average time needed to enter $\mathcal{C}$ is

$$\frac{1}{|\mathcal{C}|} e^{\beta\Gamma}\,[1 + o(1)]. \tag{2.3}$$

Let $\pi(\ell_c)$ denote the average probability with respect to the uniform entrance distribution that the critical droplet is exited in the direction of $\boxplus$ rather than $\boxminus$. Then the average number of attempts to go over the hill in $\mathcal{C}$ after reaching the top is

$$\frac{1}{\pi(\ell_c)}\,[1+o(1)]. \tag{2.4}$$

The product of (2.3) and (2.4) is the average crossover time, and so

$$K = \frac{1}{|\mathcal{C}|\pi(\ell_c)}. \tag{2.5}$$

Now,

$$|\mathcal{C}| = |\Lambda|\,4\ell_c, \tag{2.6}$$

because the droplet can be centered anywhere in Λ, has 2 possible orientations, and the protuberance can sit in $2\ell_c$ places. Moreover,

$$\pi(\ell_c) = \frac{1}{\ell_c}\left(2\,\frac{1}{2} + (\ell_c - 2)\,\frac{2}{3}\right). \tag{2.7}$$

Indeed, if the protuberance sits at one of the two extreme ends of a side of length ℓ_c, 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, when the protuberance sits elsewhere, then it has *two* neighboring spins on the same side and so the probability for one of them to flip upwards before the protuberance flips downwards is $\frac{2}{3}$. Combining (2.5–2.7), we get (2.2).

2.2 Kawasaki

The situation is considerably more complex for model (II).

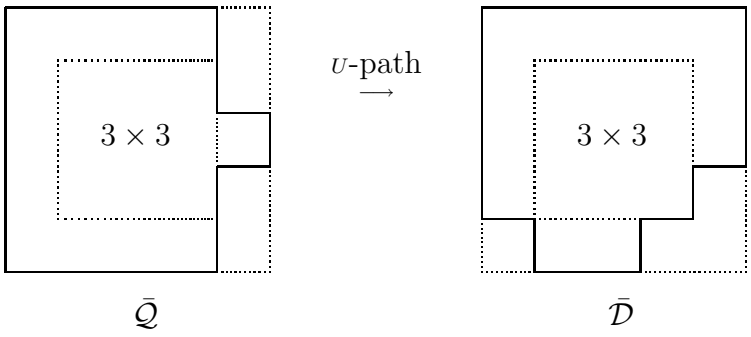


Fig. 7: Critical droplets without free particle for $\ell_c = 5$ in model (II): the 1's lie inside the solid contour, the 0's outside.

Theorem 2.3 (Bovier, den Hollander and Nardi [6])
Let

- $\bar{\mathcal{D}}$ *be the set of configurations where the particles form an* $(\ell_c-2)\times(\ell_c-2)$ *square with four bars attached to the four sides with total length* $3\ell_c-3$.
- $\tilde{\mathcal{D}}$ *be the set of configurations where the particles form an* $(\ell_c-3)\times(\ell_c-1)$ *rectangle with four bars attached to the four sides with total length* $3\ell_c-2$.

Let $\mathcal{D}=\bar{\mathcal{D}}\cup\tilde{\mathcal{D}}$, *and let* $\mathcal{C}$ *be the configurations in* $\mathcal{D}$ *plus a free particle. Then:*

$$\begin{aligned}&\lim_{\beta\to\infty}\mathbb{P}_{\square}\left(\tau_{\mathcal{C}}<\tau_{\blacksquare}\mid\tau_{\blacksquare}<\tau_{\square}\right)=1,\\&\lim_{\beta\to\infty}\mathbb{P}_{\square}\left(\eta(\tau_{\mathcal{C}}-)=\eta\mid\tau_{\mathcal{C}}<\tau_{\square}\right)=|\mathcal{D}|^{-1}\quad\forall\,\eta\in\mathcal{D}.\end{aligned}\tag{2.8}$$

Theorem 2.4 (Bovier, den Hollander and Nardi [6])
(a) $\mathbb{E}_{\square}(\tau_{\blacksquare})=Ke^{\beta\Gamma}[1+o(1)]$ *as* $\beta\to\infty$, *with*

$$K=K(\Lambda,\ell_c)\sim\frac{3}{4\pi\ell_c^2(\ell_c^2-1)}\,\frac{\log|\Lambda|}{|\Lambda|}\qquad\text{as }\Lambda\to\mathbb{Z}^2.\tag{2.9}$$

(b) $\lim_{\beta\to\infty}\mathbb{P}_{\square}(\tau_{\blacksquare}>t\,\mathbb{E}_{\square}(\tau_{\blacksquare}))=1$ *uniformly in* $t\geq 0$.

The intuitive idea behind Theorem 2.3 is as follows. Once the dynamics has created a configuration in the set defined in Theorem 1.3(II), it must wait for the next particle to arrive from the boundary, which takes a time of order $e^{\beta\Delta}$. Because $\Delta>U$, this time is much larger than $e^{\beta U}$, the time for the dynamics to make moves that cost U. Therefore the droplet will explore all shapes that can be reached from its prototype shape via a U-path, i.e., a path between two configurations with the same energy that never goes more than U above this energy. For instance, the protuberance may detach itself from the side of length ℓ_c and reattach itself to the side of length ℓ_c-1. But it is also possible for particles to *slide along the boundary of the droplet*, in a train-like motion around corners (see Fig. 8), so as to modify the four bars in the annulus of the droplet. Each of these configurations is equally likely to be visited the moment the next particle arrives from the boundary, which is why we get a uniform entrance distribution.

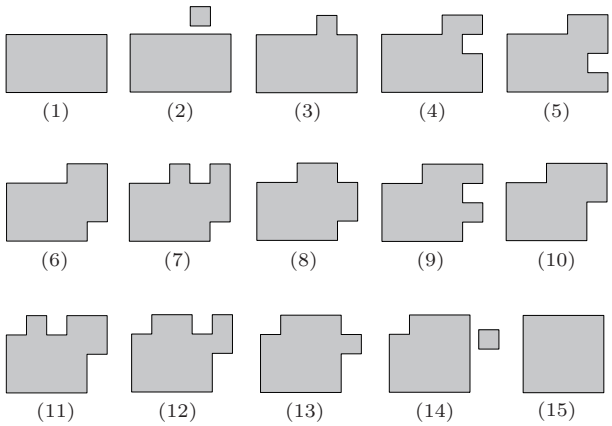


FIG. 8. Motion along the border of the droplet.

The prefactor in Theorem 2.4 can be explained as follows. The average time needed to enter $\mathcal{C}$ is

$$\frac{1}{|\mathcal{D}|\,|\partial\Lambda|}\,[1+o(1)] \quad \text{as } \beta\to\infty. \tag{2.10}$$

Let $\pi(\Lambda,\ell_c)$ denote the average probability with respect to the uniform entrance distribution that the critical droplet is exited in the direction of ■ rather than □. Then the average number of attempts to go over the hill in $\mathcal{C}$ after reaching the top is

$$\frac{1}{\pi(\Lambda,\ell_c)}\,[1+o(1)] \quad \text{as } \beta\to\infty. \tag{2.11}$$

The product of (2.3) and (2.4) is the average crossover time, and so

$$K=\frac{1}{|\mathcal{D}|\,|\partial\Lambda|\pi(\Lambda,\ell_c)}. \tag{2.12}$$

Now,

$$|\mathcal{D}|\sim|\Lambda|\,\frac{1}{3}\ell_c^2(\ell_c^2-1) \quad \text{as } \Lambda\to\mathbb{Z}^2, \tag{2.13}$$

where the first factor comes from centering the droplet anywhere in Λ not touching $\partial\Lambda$, while the second factor comes from a combinatorial calculation counting the number of locations of the four bars. Moreover,

$$|\partial\Lambda|\pi(\ell_c)\sim\frac{4\pi}{\log|\Lambda|} \quad \text{as } \Lambda\to\mathbb{Z}^2. \tag{2.14}$$

Indeed, the latter is the probability that a particle detaching itself from the critical droplet reaches $\partial\Lambda$ before reattaching itself. This probability is independent of the shape and the location of the critical droplet (as long as Λ is large and the critical droplet is far from $\partial\Lambda$), due to the fact that the free particle moves like a two-dimensional simple random walk, which is recurrent on $\mathbb{Z}^2$. By the reversibility, the reverse motion has the same probability. Combining (2.12–2.14), we get (2.9).

Note that the configuration consisting of an $\ell\times(\ell_c-1)$ quasi-square plus a dimer at distance 1 is an element of $\mathcal{S}$, but is a *dead-end* for the crossover. Indeed, one particle of the dimer must jump back to the droplet and create a protuberance (at cost 0), and the remaining free particle must attach itself next to this protuberance (at gain U) to initiate the motion downhill to the $\ell_c\times\ell_c$ square. Thus, as was announced earlier, we see that $\mathcal{C}subsetneq\mathcal{S}$, contrary to the situation for model (I).

Most of what is described above can be carried over to $\mathbb{Z}^3$, except that it remains an open problem to identify the equivalent of $\mathcal{D}$, i.e., to identify the full set of critical droplets. Fig. 6 shows a set of prototype critical droplets on $\mathbb{Z}^3$. The full set of critical droplets are those that can be obtained from this prototype via a $2U$-path, i.e., a path between two configurations with the same energy that never goes more than $2U$ above this energy. In combinatorial terms, identifying this set amounts to answering the following question about *minimal polyominoes*, i.e., unions of unit cubes in $\mathbb{Z}^3$ that have a given total volume and a minimal surface area:

What minimal polyominoes can be reached from a given minimal polyomino via moves of single unit cubes such that the surface area never exceeds the minimal surface area by more than 2?

Since we lack a full description of $\mathcal{D}$ in $\mathbb{Z}^3$, we also lack knowledge of the asymptotics of $|\mathcal{D}|$ for large Λ. Therefore, we only have bounds for the prefactor K (see Bovier, den Hollander and Nardi [6]).

2.3 Potential-theoretic approach

We give a sketch of the techniques that are used to obtain the fine asymptotics of the average crossover time in Theorem 2.4(a). A key role is played by the notion of capacity between two sets of configurations, in particular, between the stable state and the metastable state.

Define

$$\mathcal{E}(h) = \frac{1}{2} \sum_{\eta,\eta' \in \mathcal{X}} \mu(\eta) c(\eta,\eta') [h(\eta) - h(\eta')]^2, \qquad h\colon\ \mathcal{X} \to [0,1]. \tag{2.15}$$

This is the *Dirichlet form* associated with the dynamics, whose argument is a so-called *potential function* on the configuration space $\mathcal{X}$. Given two non-empty sets $\mathcal{A}, \mathcal{B} \subset \mathcal{X}$, the *capacity* of the pair $\mathcal{A}, \mathcal{B}$ is defined as

$$\mathrm{CAP}(\mathcal{A},\mathcal{B}) = \min_{\substack{h\colon\ \mathcal{X}\to[0,1] \\ h|_{\mathcal{A}} \equiv 1, h|_{\mathcal{B}} \equiv 0}} \mathcal{E}(h), \tag{2.16}$$

where the infimum runs over all potential functions whose restriction to $\mathcal{A}$ and $\mathcal{B}$ equals 1 and 0, respectively. If we think of an electric network with nodes labelled by $\mathcal{X}$ and with conductivities $\mu(\eta)c(\eta,\eta')$ between nodes $\eta, \eta' \in \mathcal{X}$, then $\mathcal{E}(h)$ is the energy produced by an electric current flowing this network when the potential on the nodes is given by h. The capacity is the minimal energy when the nodes of $\mathcal{A}$ are kept at potential 1 and the nodes of $\mathcal{B}$ are kept at potential 0. The minimum in (2.16) is unique, and the minimizer h^* has the interpretation $h^*(\eta) = \mathbb{P}_\eta(\tau_{\mathcal{A}} < \tau_{\mathcal{B}})$.

The key to the fine estimate in (2.4)(a) is the following fact, relating the average crossover time to the capacity. We henceforth focus on Model (II), but the claims apply equally well to model (I).

Proposition 2.5 (Bovier, Eckhoff, Gayrard and Klein [4])
$\mathbb{E}_{\square}(\tau_{\blacksquare}) = [1 + o(1)]/Z\mathrm{CAP}(\square, \blacksquare)$ *as* $\beta \to \infty$.

Thus, to estimate the average crossover time from $\square$ to $\blacksquare$, it suffices to estimate the capacity of the pair $\square, \blacksquare$. This proceeds in several steps.

(1) A crude *a priori estimate* yields that for every $\mathcal{A}, \mathcal{B}$ there exist constants $0 < C_1 < C_2 < \infty$ (depending on $\mathcal{A}, \mathcal{B}$) such that

$$C_1 \leq e^{\beta\Gamma(\mathcal{A},\mathcal{B})} Z\mathrm{CAP}(\mathcal{A},\mathcal{B}) \leq C_2, \tag{2.17}$$

where $\Gamma(\mathcal{A},\mathcal{B})$ is the communication height between $\mathcal{A}$ and $\mathcal{B}$.

(2) With the help of (2.17), it is possible to obtain sharp estimates on the minimizer h^* of (2.16). These estimates show that h^* is exponentially close (in β) to 1 strictly inside the 'Γ-valley' around $\square$ and exponentially close (in β) to 0 strictly inside the 'Γ-valley' around $\blacksquare$. Since the configurations with energy $> \Gamma$ are negligible, because of the Gibbs factor in (2.15), it follows that the sharp asymptotics of $\text{CAP}(\square, \blacksquare) = \mathcal{E}(h^*)$ is determined by the values of h^* *on* and *in the vicinity of* the communication level set $\mathcal{S} = \mathcal{S}(\square, \blacksquare)$.

(3) Due to the above, the variational problem in (2.16) on the full configuration space $\mathcal{X}$ reduces to a variational problem restricted to $\mathcal{S}$ and its vicinity. This *reduced variational problem* has a much simpler structure, and can be understood in terms of the geometry of the configurations that are close to the critical droplet.

(4) For Kawasaki, the reduced variational problem involves the creation of a free particle when the droplet is almost critical, the motion of this free particle towards the droplet, and the way it attaches itself. Since this is a problem about simple random walk travelling between $\partial\Lambda$ and an almost critical droplet somewhere inside Λ, the reduced capacity can be sharply estimated. What is important about (2.16) and its reduced analogue is that upper bounds can be obtained by inserting test functions for h, while lower bounds can be obtained by removing transitions.

The reduced capacity depends on the fine details of the geometry of the critical droplet, which is why it is not possible to compute $K = K(\Lambda, \ell_c)$ in closed form. However, for large Λ the details of the geometry turns out to be only partly relevant, and hence the asymptotics of K can be identified. For Glauber, the reduced variational problem turns out to be zero-dimensional. For Kawasaki, however, it is more difficult, because $\mathcal{S}$ contains plateaus, well and dead-ends.

3 Lecture 3: Crude analysis for large systems at low or positive temperature

In this lecture we move away from finite systems and investigate what happens in large volumes, both at low and at positive temperature. Most of what is described below consists of target theorems and work in progress.

3.1 Large systems at low temperature

• Glauber: For Glauber dynamics, the analogues of the target results to be described below should hold true, but no proof is currently being attempted.

• Kawasaki: Let $\Lambda = \Lambda_\beta$ depend on β such that

$$|\Lambda_\beta| = e^{\Theta\beta}, \qquad \Theta > 0, \tag{3.1}$$

and give Λ_β periodic boundary conditions. Define the *grand-canonical Gibbs measure*

$$\mu(\eta) = \frac{e^{-\beta[H(\eta)+\Delta N(\eta)]}}{Z}, \qquad \eta \in \mathcal{X} = \mathcal{X}_\beta, \tag{3.2}$$

with

$$N(\eta) = \sum_{x\in\Lambda_\beta} \eta(x) \tag{3.3}$$

the number of particles in Λ_β. As before, we think of Λ_β as embedded in an infinite gas reservoir with particle density $e^{-\beta\Delta}$.

Let $\mathcal{R} \subset \mathcal{X}$ denote those configurations where *all* clusters of particles in Λ_β are subcritical, say, are contained in a rectangle of size $(\ell_c - 1) \times (\ell_c - 1)$. The initial configuration $\sigma(0)$ of the dynamics is drawn according to the *conditional* Gibbs measure

$$\mu_{\mathcal{R}}(\eta) = \frac{\mu(\eta)1_{\mathcal{R}}(\eta)}{\mu(\mathcal{R})}, \qquad \eta \in \mathcal{X}_\beta, \tag{3.4}$$

where $\mu(\mathcal{R}) = \sum_{\eta\in\mathcal{R}} \mu(\eta)$. Our goal will be to estimate the first time a critical droplet appears *anywhere* in Λ_β. Note that, because Λ_β has periodic boundary conditions, no particle enters or exits Λ_β at positive times. The equilibrium with the reservoir is needed only at time zero.

In order to have particles at all we must pick $\Theta > \Delta$. We will be interested in the regime

$$\Delta \in (U, 2U), \quad \Theta \in (\Delta, \infty), \quad \beta \to \infty. \tag{3.5}$$

Write $\mathbb{P}_\eta$ to denote the law of the dynamics $(\sigma(t))_{t\geq 0}$ starting from $\sigma(0) = \eta$, and put $\mathbb{P}_{\mu_{\mathcal{R}}} = \sum_{\eta\in\mathcal{R}} \mu_{\mathcal{R}}(\eta)\mathbb{P}_\eta$. Let

$$\tau_{\mathcal{R}^c} = \min\{t \geq 0\colon\ \sigma(t) \notin \mathcal{R}\} \tag{3.6}$$

denote the first time the dynamics exits $\mathcal{R}$.

Conjecture 3.1 (Gaudilliere, den Hollander, Nardi, Olivieri and Scoppola [9])
Suppose that $\ell_c \geq 3$. *If*

$$\Theta \in (\Delta, \Gamma - \Xi) \qquad \textit{with} \qquad \Xi = 2U + (\ell_c - 3)\epsilon, \tag{3.7}$$

then

$$\lim_{\beta\to\infty} \mathbb{P}_{\mu_{\mathcal{R}}}\Big(e^{(\Gamma-\Theta-\delta)\beta} < \tau_{\mathcal{R}^c} < e^{(\Gamma-\Theta+\delta)\beta}\Big) = 1 \qquad \forall \delta > 0. \tag{3.8}$$

Theorem 3.1 is explained as follows. The dynamics locally grows and shrinks subcritical droplets many times until a critical droplet appears somewhere in Λ_β that triggers the crossover. Γ is the *local* grand-canonical *energy of the critical droplet*, which plays the role of the local activation energy for the crossover. Ξ is the *local* grand-canonical *energy needed to evaporate the largest subcritical droplet*, i.e., the cost of shrinking from $(\ell_c - 1) \times \ell_c$ to $(\ell_c - 1) \times (\ell_c - 1)$ and further down to the empty box. Since the particle density is very low, the critical droplet may appear more or less independently anywhere in the box Λ_β. The regime in Theorem (3.7) corresponds to the situation where any subcritical droplet has a tendency to evaporate in a time much smaller than the crossover time. Hence the crossover occurs only when the droplet grows without shrinking, which happens after a time of order $|\Lambda_\beta|^{-1}e^{\Gamma\beta}$, where $|\Lambda_\beta|$ is the *spatial entropy* for the crossover.

The proof of Conjecture 3.1, which is in progress, requires four steps:

(1) Show that, because of the exponentially low density, the lattice gas stays close to the grand-canonical equilibrium over exponentially long time periods, despite the fact that particles collide and locally droplets are formed and desolved.

(2) Show that, because of the exponentially low density, what happens in different local boxes that are far apart but close on the scale of Λ_β is essentially independent.

(3) Show that the dynamics restricted to a single local box is comparable to the dynamics on a finite box that we studied in Lectures 1 and 2.

(4) Show that the local crossover time $e^{\beta\Gamma}$ gets reduced by a factor $|\Lambda_\beta|$ due to the spatial entropy of where the first droplet may appear.

Each of these steps is conceptually involved and highly technical.

If Θ is larger than the threshold $\Gamma - \Xi$, then the crossover time will be smaller than Θ, and the "homogeneous nucleation" behavior in (3.8) will fail. The reason is that the crossover time is now smaller than the time needed to evaporate the largest subcritical droplet, and so the successive attempts to grow a critical droplet typically are no longer made from "local vacuum", but instead from the smallest subcritical droplet whose evaporation time does exceed the crossover time. The analysis of this regime turns out to be rather delicate.

3.2 Large systems at positive temperature

In *equilibrium* statistical physics, for a system that is at a *first-order* phase transition a macroscopically large droplet of one phase inside the other phase takes on the *Wulff shape*, i.e., the droplet minimizes its total surface tension subject to a total volume constraint. This observation, which is over a century old, has been put on a rigorous microscopic basis since only fifteen years or so. For the two-dimensional ferromagnetic nearest-neighbor Ising model at low temperature, Dobrushin, Kotecký and Shlosman [8] proved that a large droplet of the plus-phase inside the minus-phase has the Wulff shape. This result was subsequently extended up to the critical temperature, and its proof was simplified, by Pfister [15], Ioffe [13] and Pisztora [16].

The Wulff construction requires a careful *coarse-graining* analysis. The microscopic phase boundary is approximated on a mesoscopic scale by a polygon consisting of many segments, which decouple on the mesoscopic scale. Each segment contributes to the surface tension in a way that depends on its direction relative to the lattice axes. To handle the fluctuations of the boundary around the polygon, large deviation arguments are required. The polygon tends to a smooth curve in the macroscopic limit, and this curve enters into the *Wulff variational problem*.

To study Wulff droplets in the presence of a stochastic dynamics is part of *non-equilibrium* statistical physics and therefore is quite a different matter. The question of interest is whether *macroscopically large critical droplets for metastable transitions between two phases under a stochastic local dynamics assume the Wulff shape or not*.

In this lecture we return to a large box Λ with an open boundary. We take the density of the infinite gas reservoir to be slightly above that of the gas phase, so that the system is slightly *supersaturated*. We are interested in how the system nucleates, i.e., how it reaches the liquid phase when it starts from the gas phase. In particular, we are interested in determining the shape of the critical droplet that triggers the nucleation and in computing the average time the system needs to create this critical droplet. Our target is to show that, in the limit of *weak supersaturation* when the critical droplet becomes macroscopically large, it scales to the *equilibrium Wulff shape* and appears after a time that scales like the exponential of the *Wulff free energy*. The size of the box is taken to scale in such a way that the critical droplet occupies a finite fraction of the box.

• Glauber:

The only case so far for which the above question has been tackled succesfully in the mathematical physics literature is model (I). It is assumed that $\beta > \beta_c$, the critical inverse temperature at $h = 0$. The system starts in the minus-phase at $h = 0$ (or any distribution that is stochastically lower), the Glauber dynamics is applied for small $h > 0$, and the limit $h \downarrow 0$ is taken. The dynamics will bring the system to equilibrium, close to the plus-phase at $h = 0$, but it needs a long time to do so.

Theorem 3.2 (Schonmann and Shlosman [17])
For $\beta > \beta_c$,

$$\lim_{h\downarrow 0} h \log \mathbb{E}(\tau_{J,h,\beta}) = \frac{W(J,\beta)^2}{12m(J,\beta)}, \tag{3.9}$$

where $\tau_{J,h,\beta}$ is the first time the origin is surrounded by the plus-phase, $W(J,\beta)$ is the total surface tension of the Wulff droplet of unit volume, and $m(J,\beta)$ is the spontaneous magnetization.

In Schonmann and Shlosman [17] it is further proved that the critical droplet typically is not created close to the origin, but rather is *created far away and subsequently invades the origin by growing.*

The idea behind (3.9) is that, in the macroscopic scaling limit, the critical droplet has a length ℓ that maximizes the free energy function

$$f(\ell) = -m(J,\beta)h\ell^2 + W(J,\beta)\ell. \tag{3.10}$$

The maximum is taken at $\ell_{max} = [W(J,\beta)/2m(J,\beta)h]$, giving free energy

$$f(\ell_{max}) = \frac{W(J,\beta)^2}{4m(J,\beta)h}. \tag{3.11}$$

This is the exponential of the time needed to create a droplet at a given location. The actual exponential is *three times smaller*, because the critical droplet may occur anywhere in a space-time cone of this smaller size and invade the origin.

The analysis in Schonmann and Shlosman [17] relies on a range of rather delicate techniques, many of which are specific to the Ising situation. Note that the left-hand side of (3.9) refers to a non-equilibrium quantity, while the right-hand side only contains quantities from equilibrium. This is why the result in (3.9) is deep.

• Kawasaki:

The question we want to address is whether a similar result as in Theorem 3.2 holds for the lattice gas subject to a Kawasaki dynamics. The system starts as an ideal gas at density $\rho > \rho_{gas}(U,\beta)$, where $\rho_{gas}(U,\beta)$ is the density of the gas phase. Thus, at time zero the system undergoes a deep quench from infinite temperature to the subcritical temperature $1/\beta$.

Conjecture 3.3 (Bovier, den Hollander and Messikh [5])
For $\beta > \beta_c$ and C sufficiently large,

$$\lim_{\Delta \uparrow 2U} (2U - \Delta) \log \mathbb{E}(\tau_{U,\Delta,\beta}) = \frac{W(U/2,\beta)^2}{4m(U/2,\beta)}, \tag{3.12}$$

where $\tau_{U,\Delta,\beta}$ is the first time the origin is surrounded by the liquid phase, $\Lambda = \Lambda(N) = (-N/2, N/2]^2 \cap \mathbb{Z}^2$ with $N = C[2U - \Delta]^{-1}$.

For the above choice of N, the Wulff droplet occupies a finite fraction of the box. Thus, nucleation is triggered by a *single* droplet around the origin. The right-hand side of (3.12) is the same as that of (3.11), with J being replaced by $U/2$ because of the link between the Hamiltonians of models (I) and (II) in (1.1). The reason is that, as already observed above, the right-hand side of (3.12) only contains quantities from equilibrium.

A proof is currently being attempted that uses the potential-theoretic techniques developed in Bovier, Eckhoff, Gayrard and Klein [4], but these need to be adapted to deal with large volumes. The hard part is that for large volumes at positive temperature both spatial and temporal entropy need to be controlled. We need to understand the typical way in which the dynamics grows and shrinks large droplets, absorbing and emitting large numbers of particles with the surrounding gas phase in the box and keeping the droplet close to the Wulff shape while doing so.

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