LECTURE 16

Challenges for the future

§ CHALLENGES BEYOND METASTABILITY

> There are several challenges within metastability that as yet remain unsolved, but are potentially within reach of the conceptual and technical machinery described in this course.

In Lectures 7–15 several such challenges were formulated already. This last lecture is devoted to Glauber dynamics in very large and infinite volumes, which offers some further challenges.

> There are also challenges that go beyond metastability and appear not within reach of present day tools.

In this lecture some of these will be addressed as well.

§ LARGE VOLUMES AND SMALL MAGNETIC FIELDS

Consider Glauber dynamics in large volumes and small magnetic fields. The inverse temperature is chosen strictly above the critical inverse temperature of the Ising model on the infinite lattice $\mathbb{Z}^2$ in zero magnetic field.

In the limit as the magnetic field tends to zero, the size of the critical droplet tends to infinity.

> The main idea is that the asymptotic shape of the critical droplet is the Wulff shape from equilibrium statistical physics, i.e., the shape that minimises the integrated surface tension between the minus-phase outside the droplet and the plus-phase inside the droplet.

In what follows we consider volumes that are comparable to the volume of the critical droplet. Later we will see what happens in larger volumes.

1. The Ising-spin Hamiltonian on a finite square box $\Lambda \subset \mathbb{Z}^2$ reads

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

with Λ^* the set of nearest-neighbour edges in Λ, $S = \{-1,+1\}^\Lambda$ and $J, h > 0$, where we use periodic boundary conditions.

The system evolves according to a Metropolis dynamics $(\sigma_t)_{t \geq 0}$ with spin-flip rates

$$c_\beta(\sigma, \sigma^x) = \begin{cases} \mathrm{e}^{-\beta[H(\sigma^x) - H(\sigma)]_+}, & \sigma \in S, x \in \Lambda, \\ 0, & \text{otherwise}, \end{cases}$$

where σ^x is the configuration obtained from σ by flipping the spin at site x. We write $\mathbb{E}_\sigma$ to denote expectation w.r.t. the law of this dynamics starting from $\sigma_0 = \sigma$.

2. We are interested in the metastable behaviour of the system in the limit as $h \downarrow 0$ for fixed $\beta \in (\beta_c, \infty)$, where $\beta_c = \frac{1}{2J}\log(1+\sqrt{2})$ is the critical inverse temperature of the Ising model on $\mathbb{Z}^2$ at $h = 0$. In this limit the critical droplet will be large, namely, it has a linear size of order $1/h$, as we saw in Lecture 7.

3. In order to accommodate this droplet, we pick $\Lambda = \Lambda_h$ with

$$\Lambda_h = \left[-\frac{C}{h}, \frac{C}{h}\right]^2 \cap \mathbb{Z}^2 \qquad \text{with } C \in (0,\infty) \text{ large enough.}$$

As initial configuration we take $\sigma_0 = \boxminus_h$, i.e., all spins in Λ_h are pointing downwards.

§ METASTABLE CROSSOVER TIME

Intuitively, we expect the system to quickly converge to a distribution that is close to the minus-phase of the Ising model on the infinite lattice $\mathbb{Z}^2$ at $h = 0$.

Indeed, since h is small, the barrier for tunnelling towards a distribution that is close to the plus-phase is very high.

We are interested in the metastable crossover time. To that end, let $f\colon S \to \mathbb{R}$ be local, and let $\langle f \rangle_-$ and $\langle f \rangle_+$ be the average of f under the minus-phase, respectively, the plus-phase.

THEOREM 16.1 Shlosman, Schonmann 1998

Fix $\beta \in (\beta_c, \infty)$*. If* f *is a local function, then*

$$\lim_{h \downarrow 0} \mathbb{E}_{\boxminus_h}\Big(f\big(\sigma_{\tau(h;\kappa)}\big)\Big) = \begin{cases} \langle f \rangle_-, & \text{if } \kappa < \kappa_\beta, \\ \langle f \rangle_+, & \text{if } \kappa > \kappa_\beta, \end{cases}$$

where $\tau(h;\kappa) = \exp(\kappa/h)$ *and*

$$\kappa_\beta = \frac{\beta w^*(\beta)^2}{4m^*(\beta)},$$

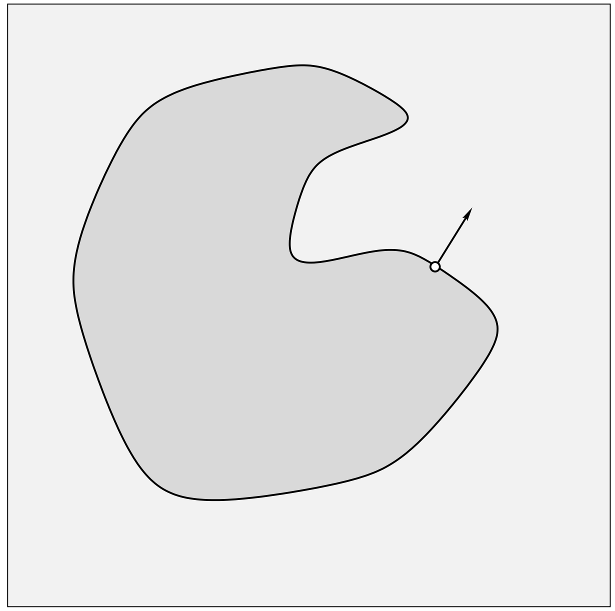
with $m^*(\beta)$ *the spontaneous magnetisation of the plus-phase and* $w^*(\beta)$ *the integrated surface tension of the Wulff droplet of unit volume.*

Theorem 14.1 says that the crossover from the minus-phase to the plus-phase occurs around time

$$\exp(\kappa_\beta / h).$$

What is remarkable is that it relates the crossover time, which is a non-equilibrium quantity, to a certain quotient of the spontaneous magnetisation and the integrated surface tension, which are equilibrium quantities.

A priori there is no reason why the critical droplet should have an equilibrium shape (= Wulff shape).



The surface tension of a droplet equals the integral of the local surface tension over the boundary of the droplet. The local surface tension depends on the direction perpendicular to the boundary.

§ WULFF CONSTRUCTION

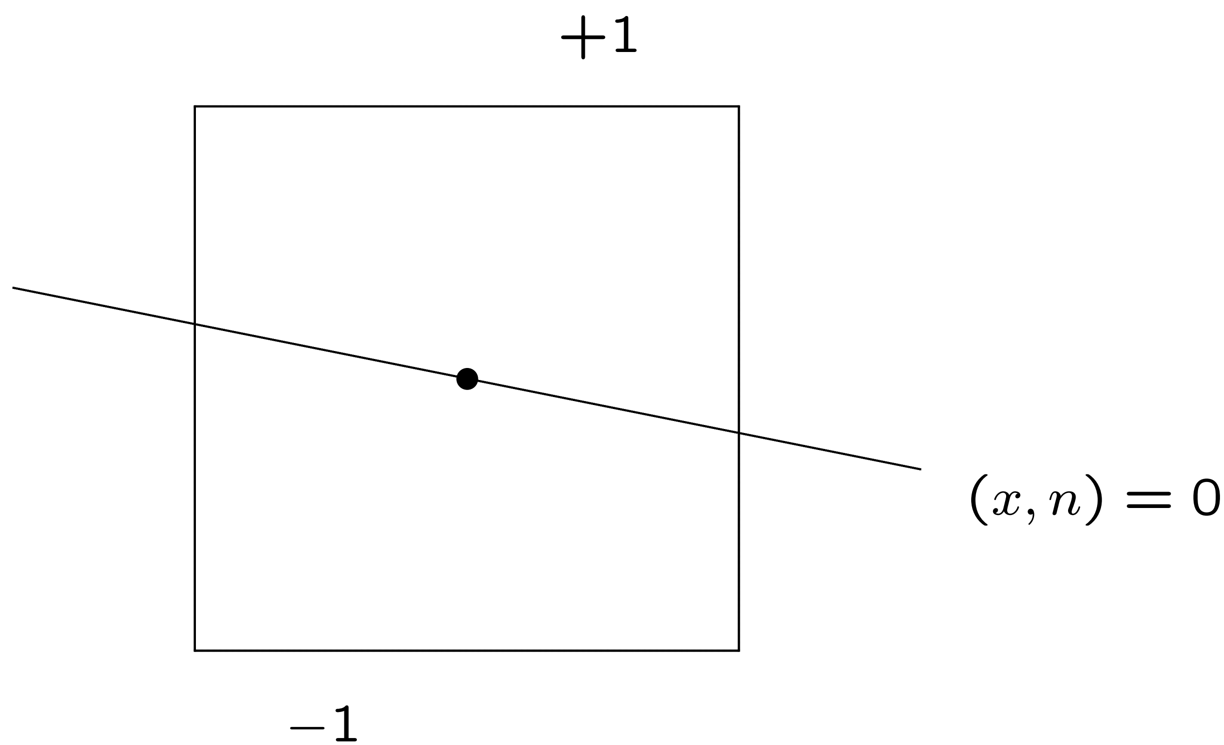
1. Let $\mathcal{S}^1 = \{x \in \mathbb{R}^2 \colon \|x\|_2 = 1\}$ denote the surface of the Euclidean ball of radius 1. The surface tension in the Ising model on $\mathbb{Z}^2$ at $h = 0$ in direction $n \in \mathcal{S}^1$ is defined as

$$T_\beta(n) = -\lim_{\ell \to \infty} \frac{1}{2\beta \|y(\ell)\|_2} \log \left(\frac{Z_{\ell,\sigma(n)}}{Z_{\ell,+}} \right).$$

Here, $y(\ell)$ and $-y(\ell)$ are the points where the straight line $\{x \in \mathbb{R}^2 \colon (x,n) = 0\}$ intersects the boundary of the box $\Lambda^\ell = [-\ell,\ell]^2$, $Z_{\ell,\sigma(n)}$ is the partition sum on $\Lambda^\ell \cap \mathbb{Z}^2$ with the boundary condition $\sigma(n)$ given by

$$\sigma(n)(x) = \begin{cases} +1 & \text{if } (x,n) \geq 0, \\ -1 & \text{if } (x,n) < 0, \end{cases} \qquad x \in \partial\Lambda^\ell,$$

and $Z_{\ell,+}$ is the partition sum with plus boundary condition.



The box Λ^ℓ with opposite boundary conditions on $\partial\Lambda^\ell$ on opposite sides of the line through the origin perpendicular to direction n: plus above and minus below.

2. Let $\mathcal{D}$ denote the set of closed self-avoiding rectifiable curves in $\mathbb{R}^2$ that are the boundary of a bounded region in $\mathbb{R}^2$. For $\gamma \in \mathcal{D}$, define the surface tension along γ as

$$I_\beta(\gamma) = \int_\gamma T_\beta(n_s)\, dn_s,$$

where s parametrises γ according to the Euclidean length measure, and n_s is the unit outward normal vector at the point $s \in \gamma$ (which exists for almost every $s \in \gamma$).

3. For $n \in \mathcal{S}^1$ and $\lambda \in (0, \infty)$, define the region

$$\mathcal{W}_\beta^\lambda(n) = \{x \in \mathbb{R}^2 \colon (x, n) \le \lambda T_\beta(n)\}.$$

For $\lambda \in (0, \infty)$, define the intersection

$$\mathcal{W}_\beta^\lambda = \bigcap_{n \in \mathcal{S}^1} \mathcal{W}_\beta^\lambda(n).$$

The latter region satisfies the scaling relation $\mathcal{W}_\beta^\lambda = \lambda \mathcal{W}_\beta^1$, i.e., its shape stays the same as λ is varied.

The Wulff droplet is defined as the region

$$\mathcal{W}_\beta = \mathcal{W}_\beta^{\lambda(\beta)},$$

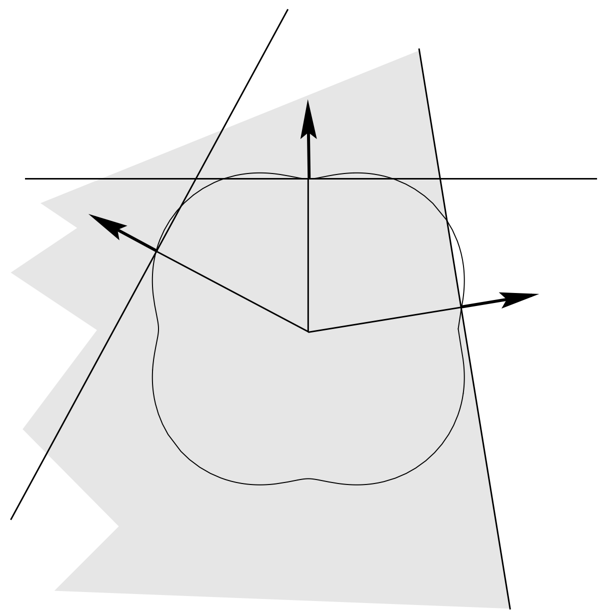
where $\lambda(\beta)$ is chosen such that $\mathcal{W}_\beta$ has volume 1. Clearly, $\mathcal{W}_\beta$ is convex and hence $\partial\mathcal{W}_\beta \in \mathcal{D}$. The integrated surface tension of the Wulff droplet, which is the quantity that appears in THEOREM 16.1, reads

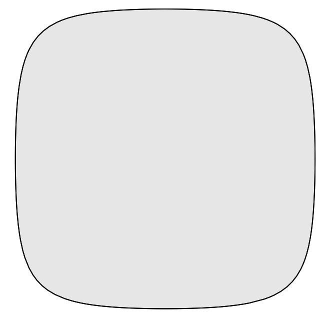
$$w^*(\beta) = I_\beta(\partial\mathcal{W}_\beta).$$

4. It is known that the Wulff droplet is optimal, i.e.,

$$w^*(\beta) \leq I_\beta(\gamma) \quad \forall\, \gamma \in \mathcal{D}\colon \text{vol}(\gamma) = 1,$$

with equality if and only if γ is a translation of $\partial\mathcal{W}_\beta$.





Wulff construction Dobrushin, Kotecký, Shlosman 1992

Left: Polar plot of the function $n \mapsto T_\beta(n)$: three outward directions and three orthogonal tangent lines demark three inward half-spaces (of which only one has been shaded).

Right: The intersection of all the half-spaces gives rise to the Wulff shape (= the inner envelope of the tangent lines). The Wulff droplet is the scaling of the Wulff shape that has unit volume.

§ HEURISTICS

The heuristics behind Theorem 16.1 is as follows. Consider a droplet of the plus-phase inside the minus-phase. Let S be the shape of this droplet and ℓ^2 its volume (i.e., the number of vertices of $\mathbb{Z}^2$ inside).

For large ℓ, the free energy of this droplet is roughly

$$\Phi_S(\ell) = -m^*(\beta)h\ell^2 + w_S(\beta)\ell.$$

The first term is the change of the free energy inside the droplet due to the fact that each minus-spin flipping to a plus-spin lowers the energy by h.

The second term is the change of the free energy due to surface tension $w_S(\beta)$ along the border of the droplet.

The two terms are of the same order of magnitude when ℓ is of order $1/h$. Therefore, putting $\ell = b/h$ and $\Phi_S(\ell) = \phi_S(b)/h$, we get

$$\phi_S(b) = -m^*(\beta)b^2 + w_S(\beta)b.$$

This function takes its maximal value at

$$b_c = \frac{w_S(\beta)}{2m^*(\beta)},$$

reaching the value

$$\phi_S(b_c) = \frac{w_S(\beta)^2}{4m^*(\beta)}.$$

The height of this barrier is minimised by the Wulff shape, i.e., for S with $w_S(\beta) = w^*(\beta)$.

§ INFINITE VOLUME

What happens in infinite volume? A new mechanism of nucleation becomes possible: the critical droplet is created somewhere far from the origin and invades the origin by growing.

Key question: Is this mechanism more efficient than nucleation close to the origin? It turns out that the answer is yes.

Below we look at two metastable regimes:

- small temperatures
- small magnetic fields

We restrict ourselves to presenting the main ideas, and omitting proofs.

§ SMALL TEMPERATURES

The infinite-volume Hamiltonian on $\mathbb{Z}^d$ reads

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

with $\sigma \in S = \{-1, +1\}^{\mathbb{Z}^d}$ and $J, h > 0$. The system follows a Metropolis dynamics $(\sigma_t)_{t \geq 0}$ with spin-flip rates given by

$$c(\sigma, \sigma^x) = \begin{cases} \mathrm{e}^{-\beta[\Delta_x H(\sigma)]_+}, & \sigma \in S,\ x \in \mathbb{Z}^d, \\ 0, & \text{otherwise,} \end{cases}$$

where

$$\Delta_x H(\sigma) = \sigma(x) \Big[\sum_{\substack{y \in \mathbb{Z}^d \\ (x,y) \in (\mathbb{Z}^d)^*}} J\sigma(y) + h \Big].$$

The reason for writing $\Delta_x H(\sigma)$ instead of $H(\sigma^x) - H(\sigma)$ is that H is infinite.

We assume that $h \in (0, dJ)$ with dJ/h non-integer.

THEOREM 16.2

$d = 2$: Dehghanpour, Schonmann 1997

$d \geq 3$: Cerf, Manzo 2013

If f is a local function, then

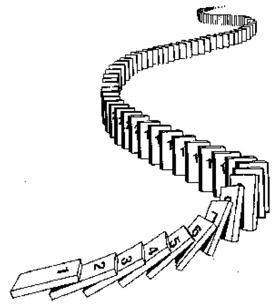
$$\lim_{\beta \to \infty} \mathbb{E}_{\boxminus}\Big(f\left(\sigma_{\tau(\beta;\kappa)}\right)\Big) = \begin{cases} f(\boxminus), & \text{if } \kappa < \kappa_d, \\ f(\boxplus), & \text{if } \kappa > \kappa_d, \end{cases}$$

where $\tau(\beta;\kappa) = \exp(\beta\kappa)$ *and*

$$\kappa_d = \frac{1}{d+1} \sum_{k=1}^{d} \Gamma_k^\star,$$

with $\Gamma_k^\star$ the energy of the critical droplet in k dimensions.

§ HEURISTICS



The heuristics behind Theorem 16.2 is as follows.

1. We know from Lecture 7 that nucleation in a finite box occurs at rate

$$\exp(-\beta\Gamma_d^\star).$$

Denote the speed of growth of a large supercritical droplet by v_d, i.e., the speed at which the faces move outwards.

2. To invade the origin at time t, the droplet must be born inside the space-time cone whose basis is a d-dimensional hypercube with side length $v_d t$ and whose height is t. The critical space-time cone is such that the nucleation rate is of order 1.

3. Writing τ_d for the time when the origin is invaded, we have the relation

$$\tau_d \, (v_d \tau_d)^d \exp(-\beta \Gamma_d^\star) = 1,$$

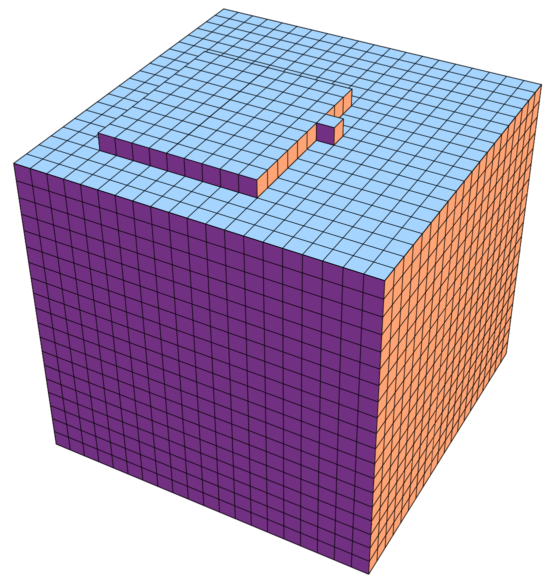
where we ignore terms of order $\exp(o(\beta))$. Since large droplets are approximately parallelepipeds, the dynamics on a face behaves like a $d-1$-dimensional Glauber dynamics, and so the time needed to fill a face is τ_{d-1}. Hence

$$v_d = 1/\tau_{d-1}.$$

4. Combining the above formulas, and putting $\tau_d = \exp(\beta \kappa_d)$, we obtain the recursion relation

$$(d+1)\kappa_d = \Gamma_d^\star + d\kappa_{d-1}.$$

Since $\kappa_0 = 0$, this yields the claimed formula for κ_d.



The factor $\frac{1}{d+1}$ in the formula for κ_d shows that the mechanism of far-away nucleation followed by invasion is faster than the mechanism of close-by nucleation. Thus, the space-time entropy places a crucial role in infinite volume.

§ SMALL MAGNETIC FIELDS

We return to the model on $\mathbb{Z}^2$ with fixed $\beta \in (\beta_c, \infty)$ and $h \downarrow 0$.

THEOREM 16.3 Schonmann, Shlosman 1998

For $d = 2$ the same result as in Theorem 16.1 holds with κ_β replaced by $\frac{1}{3}\kappa_\beta$.

The heuristics behind Theorem 16.3 is the same as for Theorem 16.2.

§ DISCUSSION

1. The proof of Theorem 16.1 is rather long and technical. To obtain control on the growing and shrinking of large droplets, coupling and coarse-graining are needed.

The idea is that microscopic regions where the system changes from the minus-phase to the plus-phase can be approximated on a mesoscopic scale by local pieces of a continuum interface.

2. The extension to $d \geq 3$ of Theorem 16.1 was achieved by Bodineau, Graham, Wouts 2013.

The extension to $d \geq 3$ of Theorem 16.3 is still open.

3. It remains a challenge to obtain a sharper estimate of the crossover time, i.e., to find the function $\beta \mapsto T_d(\beta)$ such that

$$f(\sigma_t) \approx f(\boxminus), \quad t \ll T_d(\beta)\,\mathrm{exp}(\beta\kappa_d),$$
$$f(\sigma_t) \approx f(\boxplus), \quad t \gg T_d(\beta)\,\mathrm{exp}(\beta\kappa_d),$$

as $\beta \to \infty$. This function plays the role of a prefactor.

4. No analogues of Theorems 16.1–16.3 have been proved for Kawasaki dynamics. This is a formidable challenge because Kawasaki dynamics is conservative.

§ POST-NUCLEATION PHASE

In the post-nucleation phase droplets of varying sizes are appearing. Small droplets tend to shrink and be absorbed by large droplets that tend to grow, a phenomenon referred to as Ostwald ripening.

Becker-Döring theory is a phenomenological attempt to capture the size distribution of the droplets as a function of time.

Simulations show that at low densities the average radius of droplets grows like a fractional power of time, with the exponent equal to $\frac{1}{3}$ in $d = 3$.

Post-nucleation growth is not part of metastability theory, which is primarily concerned with pre-nucleation and nucleation phenomena.

Key features such as repeated unsuccessful trials to form a critical droplet are lost.

Potential theory has so far little to say about post-nucleation growth. Consequently, sharp results are hard to get, and fully rely on ad hoc methods.

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