SAPIENZA
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Exit time in presence of multiple metastable states

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Joint work with

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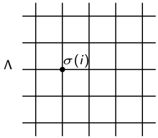
Warwick – January 2016

Summary: first part

Statistical Mechanics Lattice models



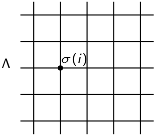
$\Lambda =$ finite square with periodic boundary conditions

$\sigma(i) \in \{1, \ldots, k\}$ spin variable associated with site i

$\Omega = \{1, \ldots, k\}^\Lambda$ configuration space

$\sigma \in \Omega$ configuration

Statistical Mechanics Lattice models



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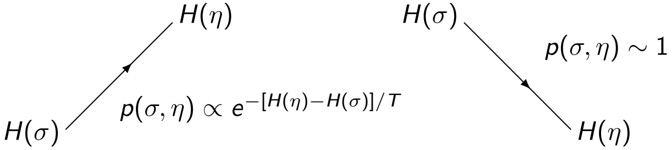
Equilibrium

- $H(\sigma) =$ Hamiltonian
- $\mu(\sigma) = \text{Gibbs measure} = \dfrac{e^{-H(\sigma)/T}}{Z(T)}$
- $Z(T) =$ partition function

Metropolis dynamics: main features

The dynamics is a discrete time dynamics $\sigma_0, \sigma_1, \ldots, \sigma_t, \ldots$ such that

- transitions increasing the energy are inhibited at T small. Consider two configurations σ and η differing at a single site



- single spin–flip dynamics
- detailed balance (reversibility):

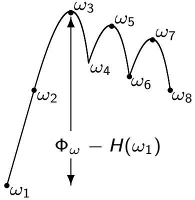
$$p(\sigma,\eta)e^{-H(\sigma)/T} = e^{-H(\eta)/T} p(\eta,\sigma)$$

- detailed balance $\Rightarrow$ the Gibbs measure $\mu(\sigma)$ is stationary

Metastable state definition [Manzo, Nardi, Olivieri, Scoppola JSP 2004]

Height of a path $\omega = \omega_1, \ldots, \omega_n$

$$\Phi_\omega = \max_{i=1,\ldots,n} H(\omega_i)$$



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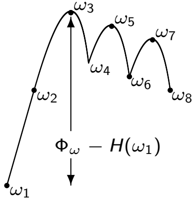

Communication height $\Phi(A, A')$ between $A, A' \subset \Omega$

$$\Phi(A, A') = \min_{\omega: A \to A'} \Phi_\omega$$

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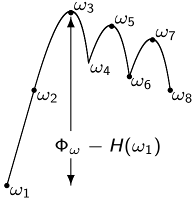
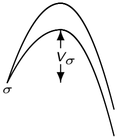


Communication height $\Phi(A, A')$ between $A, A' \subset \Omega$

$$\Phi(A, A') = \min_{\omega: A \to A'} \Phi_\omega$$

Stability level of $\sigma \in \Omega$



$$V_\sigma = \Phi(\sigma, \{\text{states at energy smaller than } \sigma\}) - H(\sigma)$$

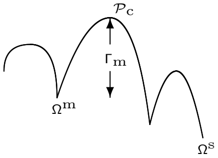
Metastable state definition

Let Ω^{s} be the set of the absolute minima of the Hamiltonian.

Define the **maximal stability level** $\quad \Gamma_{\mathrm{m}} = \max_{\sigma \in \Omega \setminus \Omega^{\mathrm{s}}} V_\sigma > 0$

The set of **metastable** states is $\Omega^{\mathrm{m}} = \{\eta \in \Omega \setminus \Omega^{\mathrm{s}} :\ V_\eta = \Gamma_{\mathrm{m}}\}$.

The set of **critical droplets** $\mathcal{P}_{\mathrm{c}}$ is the set of configurations where the optimal paths from Ω^{m} to Ω^{s} attain the maximal energy level.



Metastable state properties (Olivieri, Scoppola, Ben Arous, Cerf, Catoni, Trouvé, Manzo, Nardi, Bovier, Eckhoff, Gayrard, Klein, den Hollander, Beltrán, Landim, Slowick, Bianchi, Gaudillière, Sohier, C., ...)

Let $\sigma \in \Omega^{\mathrm{m}}$

- for any $\varepsilon > 0$ we have $\lim_{T \to 0} \mathbb{P}_\sigma(e^{(\Gamma_{\mathrm{m}} - \varepsilon)/T} < \tau_{\Omega^{\mathrm{s}}} < e^{(\Gamma_{\mathrm{m}} + \varepsilon)/T}) = 1$
- $\lim_{T \to 0} T \log \mathbb{E}_\sigma(\tau_{\Omega^{\mathrm{s}}}) = \Gamma_{\mathrm{m}}$
- $\lim_{T \to 0} \mathbb{P}_\sigma(\tau_{\mathcal{P}_{\mathrm{c}}} < \tau_{\Omega^{\mathrm{s}}}) = 1$

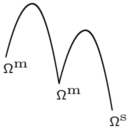
Under suitable hypothesis on the structure of the set $\Omega^{\mathrm{m}} \cup \Omega^{\mathrm{s}}$ you can compute the constant $k > 0$ such that

$$\mathbb{E}_\sigma(\tau_{\Omega^{\mathrm{s}}}) = \frac{1}{k} e^{\Gamma_{\mathrm{m}}/T}[1 + o(1)]$$

Note that k is somehow related to the cardinality of the set of critical droplets (entropy effect).

Comments (on the general results)

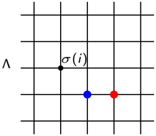
- Not sharp estimates on exit time have been proven first in the case of Metropolis dynamics and recently generalized also to not reversible dynamics.
- General results on sharp estimates on exit time are valid under hypotheses that exclude cases when multiple metastable states are present.

  The case we are interested to: 

- In any case finding out the set of metastable states in a concrete model is often a very difficult task.

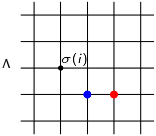
Summary: second part

Blume–Capel model



- $\Lambda =$ finite square with periodic boundary conditions
- $\sigma(i) \in \{-1, 0, +1\}$ spin variable associated with site i
- $h \in \mathbb{R}$ magnetic field and $\lambda \in \mathbb{R}$ chemical potential
- $H(\sigma) = \sum_{\langle ij \rangle} [\sigma(i) - \sigma(j)]^2 - \lambda \sum_i [\sigma(i)]^2 - h \sum_i \sigma(i)$

Blume–Capel model



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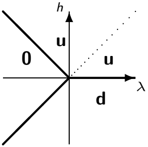
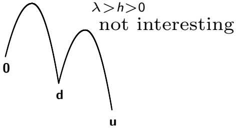
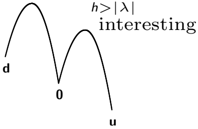
Ground states: $H(\mathbf{u}) = -(h + \lambda)|\Lambda|$, $H(\mathbf{0}) = 0$, and $H(\mathbf{d}) = (h - \lambda)|\Lambda|$







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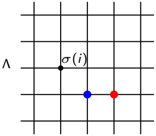

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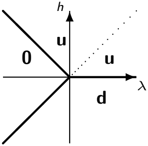
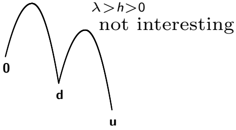
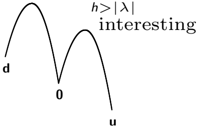






- the candidates $\mathbf{d}$ and $\mathbf{0}$ are metastable states? Can they coexist?
- suppose $\mathbf{d}$ is metastable, does $\mathbf{0}$ have a role in the path from $\mathbf{d}$ to $\mathbf{u}$?

Metropolis dynamics

Let σ_t the configuration at time t:

- chose at random with uniform probability $1/|\Lambda|$ a lattice site and call it i;
- chose with probability $1/2$ one of the two values in

$$\{-1, 0, +1\} \setminus \{\sigma_t(i)\}$$

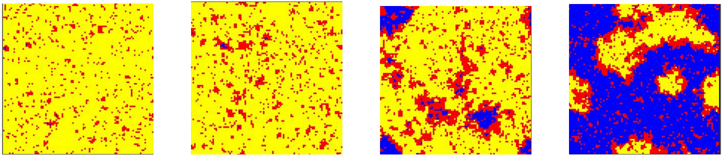
  and call it s;
- flip the spin $\sigma_t(i)$ to s with probability 1 if the energy decreases and with probabilty

$$\exp\{-\Delta H/T\}$$

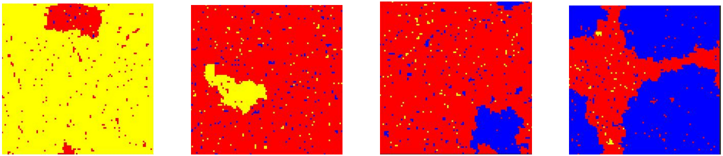
  if the energy increases ($\Delta H > 0$).

Monte Carlo sequences: $\bullet = -1$ $\bullet = 0$ $\bullet = +1$

Parameters: $\Lambda = 100 \times 100$, $h = 0.1$, $\lambda = 0.2$, $T = 1.25$

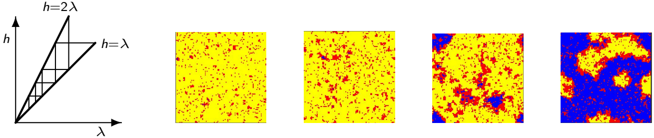


Parameters: $\Lambda = 100 \times 100$, $h = 0.1$, $\lambda = 0.02$, $T = 0.909$

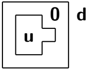


In both cases $\mathbf{d}$ is the unique metastable state: the transition $\mathbf{0} \to \mathbf{u}$ is much faster than the transition $\mathbf{d} \to \mathbf{0}$.

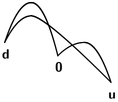
Rigorous results



- $\Omega^{\mathrm{m}} = \{\mathbf{d}\}$

- $\mathcal{P}_{\mathrm{c}} =$  with $\ell_{\mathrm{c}} = \frac{2-h+\lambda}{h}$

- $\Gamma_{\mathrm{m}} = H(\mathcal{P}_{\mathrm{c}}) - H(\mathbf{d}) \sim \frac{8}{h}$ (does not depend on λ)

- Energy landscape: 

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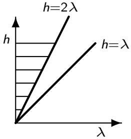
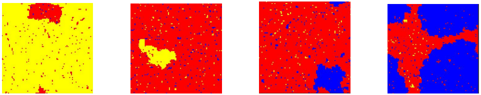
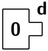
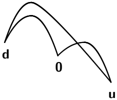


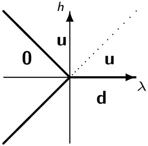


- $\Omega^{\mathrm{m}} = \{\mathbf{d}\}$
- $\mathcal{P}_{\mathrm{c}} =$  with $\ell_{\mathrm{c}} = \frac{2}{h-\lambda}$
- $\Gamma_{\mathrm{m}} = H(\mathcal{P}_{\mathrm{c}}) - H(\mathbf{d}) \sim \frac{4}{h-\lambda}$
- Energy landscape: 

Zero chemical potential Blume–Capel model

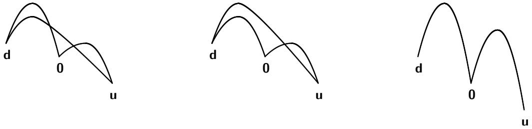
Hamiltonian $H(\sigma) = \sum_{\langle ij \rangle} [\sigma(i) - \sigma(j)]^2 - h \sum_i \sigma(i)$

Ground states:



$H(\mathbf{u}) = -h|\Lambda|,\ H(\mathbf{0}) = 0,\ H(\mathbf{d}) = h|\Lambda|$

Guess:



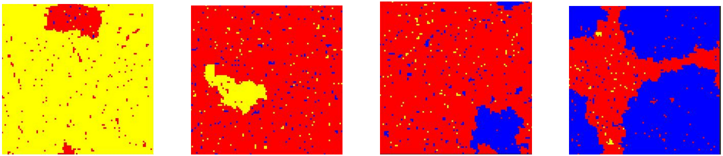
$2\lambda > h > \lambda > 0$ $\quad$ $h > 2\lambda > 0$ $\quad$ $h > \lambda = 0$

Critical droplet: $\ell_c = \lfloor 2/h \rfloor + 1$

$$\Gamma_m = H\Big(\begin{array}{c c c} & \mathbf{d} & \\ \mathbf{d} & \boxed{\mathbf{0}} & \mathbf{d} \\ & \mathbf{d} & \end{array}\Big) - H(\mathbf{d}) = H\Big(\begin{array}{c c c} & \mathbf{0} & \\ \mathbf{0} & \boxed{\mathbf{u}} & \mathbf{0} \\ & \mathbf{0} & \end{array}\Big) - H(\mathbf{0}) \sim \frac{4}{h}$$

Monte Carlo sequences: • $= -1$ • $= 0$ • $= +1$

Parameters: $\Lambda = 100 \times 100$, $h = 0.1$, $\lambda = 0.02$, $T = 0.909$



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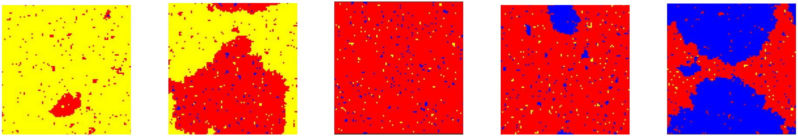
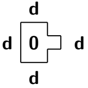
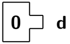


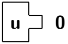
Result to be proven: $\mathbf{d}$ and $\mathbf{0}$ are both metastable: the transitions $\mathbf{0} \to \mathbf{u}$ and $\mathbf{d} \to \mathbf{0}$ take approximately the same time.

Rigorous results

We prove the model dependent results:

1. $\Omega^{\mathrm{s}} = \{\mathbf{u}\}$
2. $\Gamma_{\mathrm{m}} = \max_{\sigma\in\Omega\setminus\Omega^{\mathrm{s}}} V_\sigma = H($ 

$) - H(\mathbf{d}) \equiv \Gamma$
3. $\Omega^{\mathrm{m}} = \{\eta \in \Omega \setminus \Omega^{\mathrm{s}} :\ V_\eta = \Gamma_{\mathrm{m}}\} = \{\mathbf{d}, \mathbf{0}\}$
4. $\mathcal{P}_{\mathrm{c}} =$ 

(critical droplet between **d** and **0**)
5. $\mathcal{Q}_{\mathrm{c}} =$ 

(critical droplet between **0** and **u**)

Then we get that for any $\sigma \in \Omega^{\mathrm{m}}$

- for any $\varepsilon > 0$ we have $\lim_{T\to 0} \mathbb{P}_\sigma\big(e^{(\Gamma-\varepsilon)/T} < \tau_{\mathbf{u}} < e^{(\Gamma+\varepsilon)/T}\big) = 1$
- $\lim_{T\to 0} T \log \mathbb{E}_\sigma(\tau_{\mathbf{u}}) = \Gamma$
- $\lim_{T\to 0} \mathbb{P}_{\mathbf{d}}(\tau_{\mathcal{P}_{\mathrm{c}}} < \tau_{\mathbf{u}}) = 1$ and $\lim_{T\to 0} \mathbb{P}_{\mathbf{0}}(\tau_{\mathcal{Q}_{\mathrm{c}}} < \tau_{\mathbf{u}}) = 1$

Lemma (finding out the metastable states)

Assume $A \subset \Omega \setminus \Omega^{\mathrm{s}}$ and $a \in \mathbb{R}$ are such that

$$\Phi(\eta, \Omega^{\mathrm{s}}) - H(\eta) = a \quad \text{for any } \eta \in A$$

and

$$\Phi(\sigma, \Omega^{\mathrm{s}}) - H(\sigma) < a \quad \text{for any } \sigma \in \Omega \setminus (A \cup \Omega^{\mathrm{s}}) \text{ (recurrence)}$$

Then

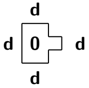
$$\Gamma_{\mathrm{m}} = a \quad \text{and} \quad \Omega^{\mathrm{m}} = A$$

where (recall) $\Gamma_{\mathrm{m}} = \max_{\sigma \in \Omega \setminus \Omega^{\mathrm{s}}} V_\sigma$.

Proof of some of the model dependent ingredients

To prove the model dependent inputs

$$\Gamma_{\mathrm{m}} = \max_{\sigma\in\Omega\setminus\Omega^{\mathrm{s}}} V_\sigma = H\Big($$



$$\Big) - H(\mathbf{d}) \equiv \Gamma$$

and

$$\Omega^{\mathrm{m}} = \{\eta\in\Omega\setminus\Omega^{\mathrm{s}}:\ V_\eta = \Gamma_{\mathrm{m}}\} = \{\mathbf{d},\mathbf{0}\}$$

we have to prove the following:

- $\Phi(\mathbf{d},\mathbf{u}) - H(\mathbf{d}) = \Gamma$
- $\Phi(\mathbf{0},\mathbf{u}) - H(\mathbf{0}) = \Gamma$
- $\Phi(\sigma,\mathbf{u}) - H(\sigma) < \Gamma$ for all $\sigma\in\Omega\setminus\{\mathbf{d},\mathbf{0},\mathbf{u}\}$ (recurrence)

Proof of some of the model dependent ingredients

To prove the model dependent inputs

$$\Gamma_{\mathrm{m}} = \max_{\sigma\in\Omega\setminus\Omega^{\mathrm{s}}} V_\sigma = H\left(\begin{array}{ccc} & \mathbf{d} & \\ \mathbf{d} & \boxed{\mathbf{0}} & \mathbf{d} \\ & \mathbf{d} & \end{array}\right) - H(\mathbf{d}) \equiv \Gamma$$

and

$$\Omega^{\mathrm{m}} = \{\eta\in\Omega\setminus\Omega^{\mathrm{s}} :\ V_\eta = \Gamma_{\mathrm{m}}\} = \{\mathbf{d},\mathbf{0}\}$$

we have to prove the following:

- $\Phi(\mathbf{d},\mathbf{u}) - H(\mathbf{d}) = \Gamma$
- $\Phi(\mathbf{0},\mathbf{u}) - H(\mathbf{0}) = \Gamma$
- $\Phi(\sigma,\mathbf{u}) - H(\sigma) < \Gamma$ for all $\sigma\in\Omega\setminus\{\mathbf{d},\mathbf{0},\mathbf{u}\}$ (recurrence)

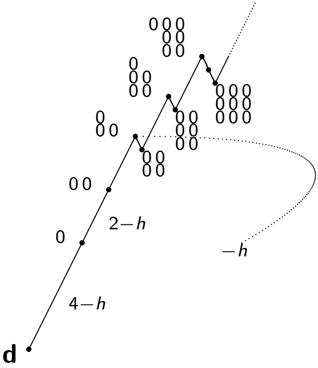
Recurrence is not very difficult but terribly boring. In the sequel I sketch the proof of the first of the three conditions listed above. The second one is similar.

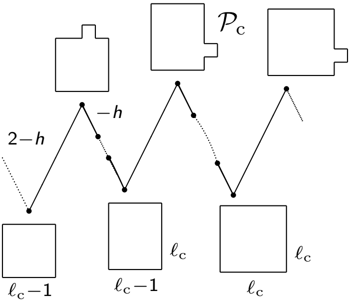
Minmax: upper bound

$$\left.\begin{array}{l}\text{Find a path connecting } \mathbf{d} \text{ to } \mathbf{u} \text{ attaining}\\ \text{its highest energy level at } \mathcal{P}_\mathrm{c}\end{array}\right\} \Rightarrow \Phi(\mathbf{d}, \mathbf{u}) \le H(\mathcal{P}_\mathrm{c})$$

Minmax: upper bound

Find a path connecting **d** to **u** attaining its highest energy level at $\mathcal{P}_c$ $\Bigg\} \Rightarrow \Phi(\mathbf{d},\mathbf{u}) \le H(\mathcal{P}_c)$





Then the path goes down to **0** and the from **0** to **u** in a similar fashion a plus droplet is nucleated inside the sea of zeros.

Minmax: lower bound

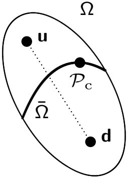
$$\left.\begin{array}{l}\text{Prove that all the paths connecting } \mathbf{d} \text{ to } \mathbf{u}\\ \text{attain an energy level greater than}\\ \text{or equal to } H(\mathcal{P}_c)\end{array}\right\} \Rightarrow \Phi(\mathbf{d}, \mathbf{u}) \geq H(\mathcal{P}_c)$$

Minmax: lower bound

$$\left.\begin{array}{l}\text{Prove that all the paths connecting } \mathbf{d} \text{ to } \mathbf{u}\\ \text{attain an energy level greater than}\\ \text{or equal to } H(\mathcal{P}_c)\end{array}\right\} \Rightarrow \Phi(\mathbf{d},\mathbf{u}) \geq H(\mathcal{P}_c)$$

Strategy (serial dynamics): if there exists $\bar{\Omega} \subset \Omega$ such that

- $\mathcal{P}_c \in \bar{\Omega}$
- all the paths connecting $\mathbf{d}$ to $\mathbf{u}$ necessarily pass through $\bar{\Omega}$
- $\min_{\sigma \in \bar{\Omega}} H(\sigma) = H(\mathcal{P}_c)$



It than follows that all the paths connecting $\mathbf{d}$ to $\mathbf{u}$ attain an energy level greater than or equal to $H(\mathcal{P}_c)$.

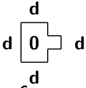
Remark: with this strategy you do not get the model dependent input 4, namely, you do not prove that the maximum along the path is necessarily attained at $\mathcal{P}_c$. To prove that a deeper investigation is needed.

Minmax: lower bound

In two state spin systems (e.g. Ising) life is easier: you have to count the flipped spins. Here you have to count the minus spins that are not flipped:

$$\bar{\Omega} = \text{ set of configurations having } |\Lambda| - [(\ell_\mathrm{c} - 1)\ell_\mathrm{c} + 1] \text{ minus spins}$$

Then

- $\mathcal{P}_\mathrm{c} =$ 

$\in \bar{\Omega} \Leftarrow$ by definition
- paths from **d** to **u** pass through $\bar{\Omega} \Leftarrow$ single spin–flip dynamics (great simplification due to the continuity of the dynamics)

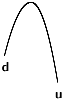
In order to complete the proof of the lower bound one has to show that

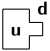
$$\min_{\sigma \in \bar{\Omega}} H(\sigma) = H(\mathcal{P}_\mathrm{c})$$

The analogous of such a result, although not trivial, is less difficult in two state spin systems. In our case the proof is much more delicate due to the presence of three state.

Sharp estimate

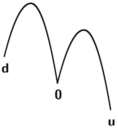
Consider the Ising model with $h > 0$ small (Bovier and Manzo 2002):



$\mathcal{P}_{\mathrm{c}} =$ 

$$\lim_{T \to 0} \frac{\mathbb{E}_{\mathbf{d}}(\tau_{\mathbf{u}})}{e^{\Gamma_{\mathrm{m}}/T}} = \frac{3}{4(2\ell_{\mathrm{c}} - 1)|\Lambda|}$$

For the Blume–Caple model with $\lambda = 0$ we expect (same critical droplets):



$$\lim_{T \to 0} \frac{\mathbb{E}_{\mathbf{d}}(\tau_{\{\mathbf{u},\mathbf{0}\}})}{e^{\Gamma_{\mathrm{m}}/T}} = \lim_{T \to 0} \frac{\mathbb{E}_{\mathbf{0}}(\tau_{\mathbf{u}})}{e^{\Gamma_{\mathrm{m}}/T}} = \frac{3}{4(2\ell_{\mathrm{c}} - 1)|\Lambda|}$$

What can be said about $\mathbb{E}_{\mathbf{d}}(\tau_{\mathbf{u}})$?

Sharp estimate

Since it can be proven that

$$\lim_{T \to 0} \mathbb{P}_{\mathbf{d}}[\tau_{\mathbf{u}} < \tau_{\mathbf{0}}] = 0$$

We expect that the time for the transition $\mathbf{d} \to \mathbf{u}$ is the sum of the time for the transitions $\mathbf{d} \to \mathbf{0}$ and $\mathbf{0} \to \mathbf{u}$.

Sharp estimate

Since it can be proven that

$$\lim_{T \to 0} \mathbb{P}_{\mathbf{d}}[\tau_{\mathbf{u}} < \tau_{\mathbf{0}}] = 0$$

We expect that the time for the transition $\mathbf{d} \to \mathbf{u}$ is the sum of the time for the transitions $\mathbf{d} \to \mathbf{0}$ and $\mathbf{0} \to \mathbf{u}$.

Theorem (Landim, Lemire 8 days ago on arXiv)

For the zero chemical potential Blume–Capel model for h small we have that

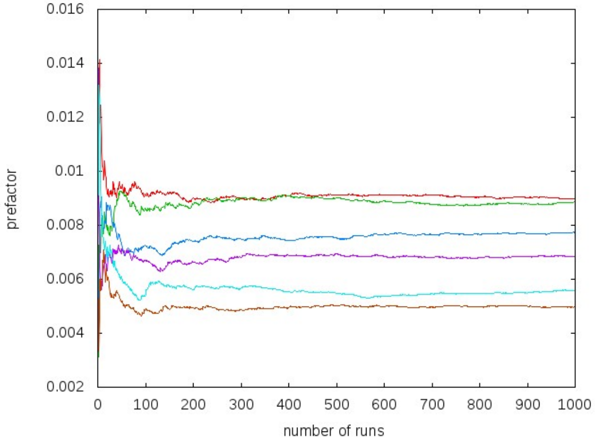
$$\lim_{T \to 0} \frac{\mathbb{E}_{\mathbf{0}}(\tau_{\mathbf{u}})}{e^{\Gamma_{\mathrm{m}}/T}} = \frac{3}{4(2\ell_{\mathrm{c}} - 1)|\Lambda|} \quad \text{and} \quad \lim_{T \to 0} \frac{\mathbb{E}_{\mathbf{d}}(\tau_{\mathbf{u}})}{e^{\Gamma_{\mathrm{m}}/T}} = 2 \times \frac{3}{4(2\ell_{\mathrm{c}} - 1)|\Lambda|}$$

Sharp estimate: numerical check

Prefactor $=$ (averaged exit time from $\mathbf{d}$ to $\mathbf{u}$)/ $\exp\{\Gamma_{\mathrm{m}}/T\}$

Parameters: $\Lambda = 60 \times 60$, $h = 0.8$, $T = 0.4$

Colors for λ: • 0, • 0.001, • 0.01, • 0.02, • 0.04, • 0.06,

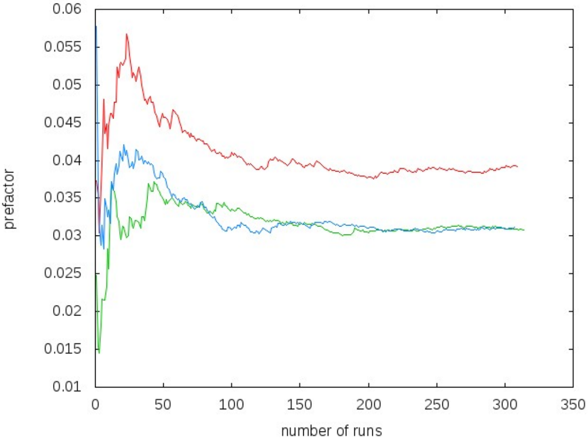


Sharp estimate: numerical check

Prefactor $=$ (averaged exit time from $\mathbf{d}$ to $\mathbf{u}$)/ $\exp\{\Gamma_{\mathrm{m}}/T\}$

Parameters: $\Lambda = 60 \times 60$, $h = 0.8$, $T = 0.27027$

Colors for λ: ● 0, ● 0.01, ● 0.02



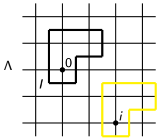
Summary: third part

Metastable states in Statistical Mechanics models

Metastable states in the Blume–Capel model

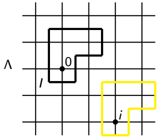
Probabilistic Cellular Automata
- Definition and examples
- Results

Probabilistic Cellular Automata



- $\Lambda =$ finite square with periodic boundary conditions
- $\sigma(i) \in \{1, \dots, k\}$ state variable associated with site i
- $\Omega = \{1, \dots, k\}^\Lambda$ state space, $\sigma \in \Omega$ state
- $I \subset \Lambda$ finite

Probabilistic Cellular Automata



- $\Lambda =$ finite square with periodic boundary conditions
- $\sigma(i) \in \{1, \ldots, k\}$ state variable associated with site i
- $\Omega = \{1, \ldots, k\}^\Lambda$ state space, $\sigma \in \Omega$ state
- $I \subset \Lambda$ finite

- $f_\sigma : \{1, \ldots, k\} \to [0, 1]$ is a probability distribution depending on the state σ restricted to I
- $\Theta_i : \Omega \to \Omega$ shifts a configuration so that the site i is mapped to the origin 0
- Probabilistic Cellular Automaton = Markov chain $\sigma_0, \sigma_1, \ldots, \sigma_t, \ldots$ on Ω with transition matrix

$$p(\sigma, \eta) = \prod_{i \in \Lambda} f_{\Theta_i \sigma}(\eta(i)) \qquad \forall \sigma, \eta \in \Omega$$

Remark: parallel and local character of the evolution; all sites updated at time t looking at the state at time $t-1$.

Reversible Probabilistic Cellular Automata

Assume $\Omega = \{-1,+1\}^{\Lambda}$, I symmetrical with respect to the origin, and

$$f_\sigma(s) = \frac{1}{2}\Big\{1 + s \tanh\Big[\frac{1}{T}\Big(\sum_{j\in I}\sigma(j) + h\Big)\Big]\Big\} \quad \text{for all} \;\; s \in \{-1,+1\}$$

where $T > 0$ and $h \in \mathbb{R}$ are called *temperature* and *magnetic field*.

Reversible Probabilistic Cellular Automata

Assume $\Omega = \{-1,+1\}^\Lambda$, I symmetrical with respect to the origin, and

$$f_\sigma(s) = \frac{1}{2}\Big\{1 + s\tanh\Big[\frac{1}{T}\Big(\sum_{j\in I}\sigma(j) + h\Big)\Big]\Big\} \quad \text{for all} \;\; s\in\{-1,+1\}$$

where $T > 0$ and $h \in \mathbb{R}$ are called *temperature* and *magnetic field*.

Reversibility [Grinstein et. al. PRL 1985, Kozlov, Vasiljev Ad. Prob. 1980]:

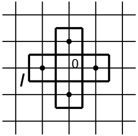
$$G(\sigma) = -h\sum_{i\in\Lambda}\sigma(i) - T\sum_{i\in\Lambda}\log\cosh\Big[\frac{1}{T}\Big(\sum_{j\in i+I}\sigma(j) + h\Big)\Big]$$

- detailed balance: $p(\sigma,\eta)e^{-G(\sigma)/T} = e^{-G(\eta)/T}p(\eta,\sigma)$
- detailed balance $\Rightarrow$ the measure $\exp\{-G(\sigma)/T\}/Z(T)$ is stationary

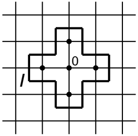
Remark (compare to Metropolis): G depends on T; parallel rule.

Two examples

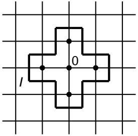
Nearest neighbor model: I = four nearest neighbors of the origin



Cross model: I = four nearest neighbors of the origin plus the origin

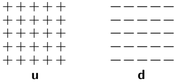


The cross PCA

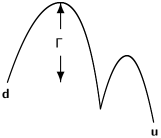


Consider the cross PCA model with positive and small magnetic field $h > 0$.

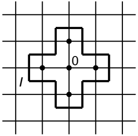
Result:



$\Omega^{\mathrm{s}} = \{\mathbf{u}\}$ and $\Omega^{\mathrm{m}} = \{\mathbf{d}\}$



The cross PCA



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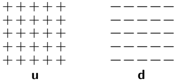

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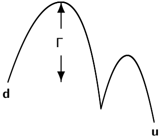
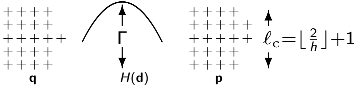


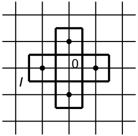
Critical droplet:



and

$$\Gamma = H(\mathbf{q}) + \Delta(\mathbf{q}, \mathbf{p}) - H(\mathbf{d}) \overset{T \to 0}{\sim} \frac{16}{h}$$

The nearest neighbor PCA

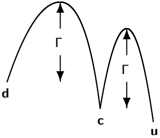


Consider the nearest neighbor PCA model with a positive and small magnetic field $h > 0$.

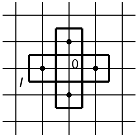
Result: flip–flopping metastable state

$$\underset{\mathbf{u}}{\begin{array}{ccccc} + & + & + & + & + \\ + & + & + & + & + \\ + & + & + & + & + \\ + & + & + & + & + \\ + & + & + & + & + \end{array}} \qquad \underset{\mathbf{d}}{\begin{array}{ccccc} - & - & - & - & - \\ - & - & - & - & - \\ - & - & - & - & - \\ - & - & - & - & - \\ - & - & - & - & - \end{array}} \qquad \underset{\mathbf{c}}{\begin{array}{ccccc} + & - & + & - & + \\ - & + & - & + & - \\ + & - & + & - & + \\ - & + & - & + & - \\ + & - & + & - & + \end{array}}$$

$$\Omega^{\mathrm{s}} = \{\mathbf{u}\}, \Omega^{\mathrm{m}} = \{\mathbf{d}, \mathbf{c}\}$$



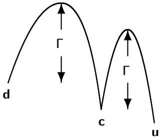
The nearest neighbor PCA



Consider the nearest neighbor PCA model with a positive and small magnetic field $h > 0$.

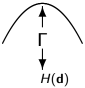
Result: flip–flopping metastable state

$$
\underset{\mathbf{u}}{\begin{array}{c} +++++ \\ +++++ \\ +++++ \\ +++++ \\ +++++ \end{array}}
\qquad
\underset{\mathbf{d}}{\begin{array}{c} ----- \\ ----- \\ ----- \\ ----- \\ ----- \end{array}}
\qquad
\underset{\mathbf{c}}{\begin{array}{c} +-+-+ \\ -+-+- \\ +-+-+ \\ -+-+- \\ +-+-+ \end{array}}
\qquad
\Omega^{\mathrm{s}} = \{\mathbf{u}\}, \Omega^{\mathrm{m}} = \{\mathbf{d},\mathbf{c}\}
$$



Critical droplet in the sea of minuses:

$$
\underset{\mathbf{q}}{\begin{array}{c} +-+- \\ -+-+ \\ +-+- \\ -+-+ \\ +-+- \end{array}}
$$



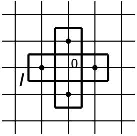
$$
\underset{\mathbf{p}}{\begin{array}{c} -+-+ \\ +-+-+ \\ -+-+ \\ +-+- \\ -+-+ \end{array}}
\qquad
\ell_{\mathrm{c}} = \lfloor \tfrac{2}{h} \rfloor + 1
$$

and

$$
\Gamma = H(\mathbf{q}) + \Delta(\mathbf{q},\mathbf{p}) - H(\mathbf{d}) \overset{T\to 0}{\sim} \frac{8}{h}
$$

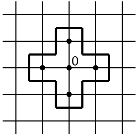
Tuning the self–interaction

PCA nearest neighbor model



$\kappa = 0$

PCA cross model



$\kappa = 1$

Let I be the set of the four nearest neighbors of the origin. Let

$$f_\sigma(s) = \frac{1}{2}\left\{1 + s \tanh\left[\frac{1}{T}\left(\kappa\sigma(0) + \sum_{j \in I} \sigma(j) + h\right)\right]\right\}$$

for $\sigma \in \Omega$, $s \in \{-1, +1\}$ e $\kappa \in [0, 1]$.

The parameter κ tunes the self–interaction: for $\kappa = 0, 1$ we get the nearest neighbor and the cross PCA models.

Close bibliography

[C., Olivieri JSP 1996] "Metastability and nucleation for the Blume-Capel model. Different mechanisms of transition."

[C., Nardi JSP 2003] "Metastability for the Ising model with a parallel dynamics."

[C., Nardi JSP 2013] "Relaxation height in energy landscapes: an application to multiple metastable states."

[C., Nardi, Spitoni AIMI III 2010] "Competitive nucleation in metastable systems."

[Landim, Lemire 2016] "Metastability of the two–dimensional Blume–Capel model with zero chemical potential and small magnetic field."

[Manzo, Nardi, Olivieri, Scoppola JSP 2004] "On the essential features of metastability: tunnelling time and critical configurations."

Bibliography

[Bigelis, C., Lebowitz, Speer PRE 1999] “Critical droplets in metastable probabilistic cellular automata.”

[Bovier et. al. CMP 2002] “Metastability and low lying spectra in reversible Markov chains.”

[Cassandro et. al. JSP 1984] “Metastable behavior of stochastic dynamics: A pathwise approach.”

[C., Lebowitz JSP 1998] “Metastability in the two–dimensional Ising model with free boundary conditions.”

[C., Nardi, Spitoni PRE 2008] “Competitive nucleation in reversible Probabilistic Cellular Automata.”

[C., Nardi, Spitoni JSP 2008] “Metastability for reversible probabilistic cellular automata with self–interaction.”

[Dai Pra, Louis, Roelly ESAIM Probab. Statist. 2002] “Stationary measures and phase transition for a class of probabilistic cellular automata.”

[Derrida 1990] “Dynamical phase transition in spin model and automata,” Fundamental problem in Statistical Mechanics VII, H. van Beijeren, Editor, Elsevier Science Publisher B.V..

Bibliography

[Grinstein et. al. PRL 1985] "Statistical Mechanics of Probabilistic Cellular Automata."

[Isakov CMP 1984] "Nonanalytic features of the first order phase transition in the Ising model."

[Kozlov, Vasiljev Ad. Prob. 1980] "Reversible Markov chain with local interactions," in "Multicomponent random system."

[Neves, Schonmann CMP 1991] "Critical Droplets and Metastability for a Glauber Dynamics at Very Low Temperatures."

[Olivieri, Scoppola JSP 1995] "Markov chains with exponentially small transition probabilities: First exit problem from a general domain. I. The reversible case,"

[Trouvé Annales IHP section B 1996] "Rough large deviation estimates for the optimal convergence speed exponent of generalized simulated annealing algorithms."

Avanzi

Proof of the general Lemma

Assume for simplicity $A = \{\eta\}$ (single metastable state case).

Let $\sigma \neq \eta$ and $\sigma \notin \Omega^{\mathrm{s}}$, then $H(\sigma) > H(\Omega^{\mathrm{s}})$ implies

$$V_\sigma \leq \Phi(\sigma, \Omega^{\mathrm{s}}) - H(\sigma) < a$$

Since $H(\eta) > H(\Omega^{\mathrm{s}})$ we have

$$V_\eta \leq \Phi(\eta, \Omega^{\mathrm{s}}) - H(\eta) = a$$

By absurdity assume $V_\eta < a$:

- there exists $\sigma \neq \eta$ such that $H(\sigma) < H(\eta)$ and $\Phi(\eta, \sigma) - H(\eta) < a$
- there exists a path $\omega^1 : \eta \to \sigma$ such that $\Phi_{\omega^1} - H(\eta) < a$
- if $\sigma \in \Omega^{\mathrm{s}}$ we get a contraddiction
- if $\sigma \notin \Omega^{\mathrm{s}}$, there exists a path $\omega^2 : \sigma \to \Omega^{\mathrm{s}}$ such that $\Phi_{\omega^2} - H(\sigma) < a$,
- since $\Phi_{\omega^1 \omega^2} - H(\eta) < a$ we get a contraddiction

Conclusions:

$$V_\eta = a, V_\sigma < a \text{ for } \sigma \neq \eta \text{ and } \sigma \notin \Omega^{\mathrm{s}} \Rightarrow \Gamma_{\mathrm{m}} = a$$

Lemma

Assume $0 < h < 1$, $\lfloor 2/h \rfloor$ not integer, and $|\Lambda| \geq 49/h^4$.

Pick $\sigma \in \bar{\Omega}$ and let N_σ be the collection of sites i in Λ such that $\sigma(i) \neq -1$.

Then

1. N_σ is not a nearest neighbor connected subset of Λ winding around the torous (recall we assumed periodic boundary conditions)
2. if $\sigma \in \{\text{set of minima of } \bar{\Omega}\}$ then $\sigma(i) = 0$ for all $i \in N_\sigma$
3. $\mathcal{P}_\text{c} \in \{\text{set of minima of } \bar{\Omega}\}$
4. $\min_{\sigma \in \bar{\Omega}} H(\sigma) = H(\mathcal{P}_\text{c})$

Remark: 4 follows from 3 trivially. We have to prove 1 – 3.

Item 1

Pick $\sigma \in \bar{\Omega}$ and let N_σ be the collection of sites i in Λ such that $\sigma(i) \neq -1$. Then N_σ does not wind around the torous.

Proof. Since $h < 1$

$$|N_\sigma| = \ell_c(\ell_c - 1) + 1 \leq \left(\frac{2}{h} + 1\right)\frac{2}{h} + 1 \leq \frac{7}{h^2}$$

The statement follows since we assumed that $|\Lambda|$ is finite but large enough with respect to $1/h$. More precisely we assumed $|\Lambda| \geq 49/h^4$.

Item 2

Pick $\sigma \in \bar{\Omega}$ and let N_σ be the collection of sites i in Λ such that $\sigma(i) \neq -1$. If $\sigma \in$ $\{\text{set of minima of } \bar{\Omega}\}$ then $\sigma(i) = 0$ for all $i \in N_\sigma$.

Proof. Pick $\sigma \in \bar{\Omega}$ and recall $H(\sigma) = \sum_{\langle ij \rangle} [\sigma(i) - \sigma(j)]^2 - h \sum_i \sigma(i)$.

$$\begin{array}{ccccccc}
- & - & - & - & - & - & - \\
- & - & - & - & - & - & - \\
- & 0 & + & - & + & 0 & - \\
- & + & + & - & + & 0 & - \\
- & + & - & - & - & - & - \\
- & - & 0 & 0 & 0 & - & - \\
- & - & - & - & - & - & -
\end{array}$$

Let $\sigma' \in \bar{\Omega}$ obtained by flipping $+ \to 0$ in σ. Then

$$H(\sigma') - H(\sigma) = rh - 3\ell - m \leq rh - (\ell + m)$$

The $+$ unit squares form a polyomino whose perimeter is equal to $\ell + m$ and whose area is r.

By general polyomino properties we have that $(\ell + m)^2 \geq 16r$. Hence

Then $$H(\sigma') - H(\sigma) \leq rh - \sqrt{r}$$

- $H(\sigma') - H(\sigma) \leq 0 \Longleftarrow \sqrt{r} < 4/h$
- $\sqrt{r} < 4/h \Longleftarrow r \leq \ell_c(\ell_c - 1) + 1 < 7/h^2$

Item 3

Pick $\sigma \in \bar{\Omega}$ and let N_σ be the collection of sites i in Λ such that $\sigma(i) \neq -1$. Then $\mathcal{P}_c \in$ set of minima of $\bar{\Omega}$.

Proof. Pick $\sigma \in \{\text{set of minima of } \bar{\Omega}\}$.

$$\begin{array}{ccccccc}
- & - & - & - & - & - & - \\
- & - & - & - & - & - & - \\
- & 0 & 0 & - & 0 & 0 & - \\
- & 0 & 0 & - & 0 & 0 & - \\
- & 0 & - & - & - & - & - \\
- & - & 0 & 0 & 0 & - & - \\
- & - & - & - & - & - & -
\end{array}$$

Recall $H(\sigma) = \sum_{\langle ij \rangle} [\sigma(i) - \sigma(j)]^2 - h \sum_i \sigma(i)$, then

$$H(\sigma) - H(\mathbf{u}) = \text{perimeter of the polyomino} - h[\ell_c(\ell_c - 1) + 1]$$

Hence the configurations in the set of minima of $\bar{\Omega}$ are such that the zeros form a polyomino of area $\ell_c(\ell_c - 1) + 1$ and having minimal perimeter.

From general results on polyominoes we have that the configuration $\mathcal{P}_c$ is an example of such (minimal perimeter) configurations.

Remark: the configuration $\mathcal{P}_c$ is not the unique perimeter minimizer $\Longrightarrow$ we do not have the escape mechanism statement for free!!!!