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Coexisting metastable states in three-state lattice spin systems and Probability Cellular Automata

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Summary

Metastable states

Characteristics of metastable states:

– different from the equilibrium state corresponding to the parameters of the system (temperature, pressure, volume, ...);

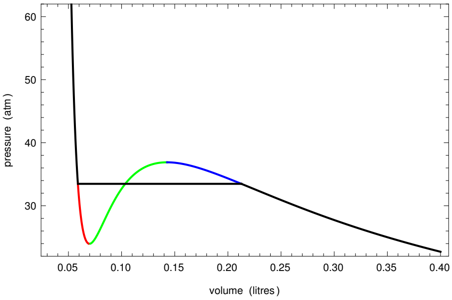
– the life–time of the state is large (infinite): the system exits the metastable state only in presence of external perturbations;

– once the system exits the metastable state and reaches the stable state it will never return back to the metastable state.

The van der Waals theory [1910]

Isotherm of one mole of real gas: $(P + a/V^2)(V - b) = RT$

Oxygen: $a = 1.36\ \ell^2$ atm mol^{-2} and $b = 0.0319\ \ell$ mol^{-1} at $T = 140°$K

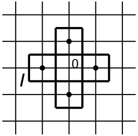


Red: super–heated liquid. Blue: super–saturated vapor.

Rigorous mathematical description? The pathwise approach proposed in [Cassandro, Galves, Olivieri, Vares JSP 1984].

Summary

Nearest Neighbor Probabilistic Cellular Automata



- $\Lambda =$ finite square with periodic boundary conditions
- $\sigma(i) \in \{-1, +1\}$ state variable associated with site i
- $\Omega = \{-1, +1\}^\Lambda$ state space, $\sigma \in \Omega$ state
- I the set of the nearest neighbors of the origin

- $\Theta_i : \Omega \to \Omega$ shifts a configuration so that the site i is mapped to the origin 0
- Markov chain $\sigma_0, \sigma_1, \dots, \sigma_t, \dots$ on Ω with transition matrix

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

where

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

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

Main features

- Parallel and local character of the evolution: all sites updated at time t looking at the state at time $t-1$;
- reversibility:

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

  where

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

- define the *energy cost*

$$\Delta(\sigma,\eta) = -\lim_{T\to 0} T\log p(\sigma,\eta)$$

  then the Wentzel–Friedlin condition is satisfied

$$e^{-[\Delta(\sigma,\eta)-\gamma(T)]/T} \le p(\sigma,\eta) \le e^{-[\Delta(\sigma,\eta)+\gamma(T)]/T}$$

  with $\gamma(T)\to 0$ as $T\to 0$.

Main features

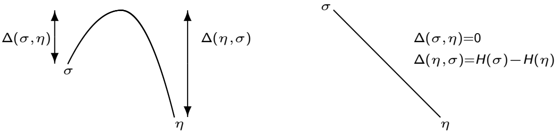
- Define the energy

$$H(\sigma) = \lim_{T \to 0} G(\sigma)$$

and from the detailed balance condition get

$$H(\sigma) + \Delta(\sigma, \eta) = H(\eta) + \Delta(\eta, \sigma)$$

- some possible situations:



- the following notation is compatible with the Metropolis case with:

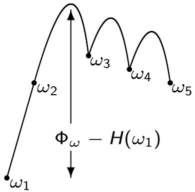
$$\Delta(\sigma, \eta) = \begin{cases} H(\eta) - H(\sigma) & \text{if } H(\eta) > H(\sigma) \\ 0 & \text{if } H(\eta) < H(\sigma) \end{cases}$$

Metastable state definition

[Manzo, Nardi, Olivieri, Scoppola JSP 2004, C., Nardi JSP 2003]

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

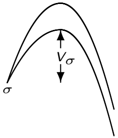
$$\Phi_\omega = \max_{i=1,\ldots,n-1} [H(\omega_i) + \Delta(\omega_i, \omega_{i+1})]$$



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

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

Stability level of $\sigma \in \Omega$



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

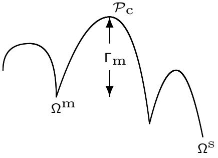
Metastable state definition

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

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

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 necessarily visited by the optimal paths and where the optimal paths from Ω^{m} to Ω^{s} attain the maximal height.



Some properties of the metastable states

[Cassandro, Galves, Olivieri, Vares JSP 1984, Olivieri, Scoppola JSP 1995,

Olivieri, Vares Cambridge University Press 2005, Bovier, den Hollander Springer 2016, **?**]

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

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

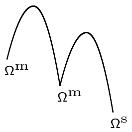
Under suitable hypothesis on the structure of the set $\Omega^{\mathrm{m}} \cup \Omega^{\mathrm{s}}$ you can compute the constant $k > 0$ such that

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

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

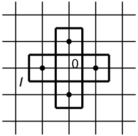
Comments

- Not sharp estimates on exit time have been proven first in the case of Metropolis dynamics and more recently generalized also to not reversible dynamics [C., Nardi, Sohier JSP 2015].
- General results on sharp estimates on exit time are valid under hypotheses that exclude cases when multiple metastable states are present. But the case we were interested to was



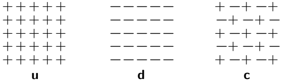
[C., Nardi, Spitoni EPJST 2017, Bet, Jacquier, Nardi JSP 2021].

The nearest neighbor PCA [C., Nardi JSP 2003]

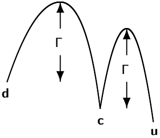


Consider the nearest neighbor PCA model with a positive and small magnetic field $h > 0$.

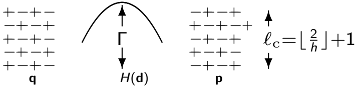
Result: flip–flopping metastable state



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



Critical droplet in the sea of minuses:

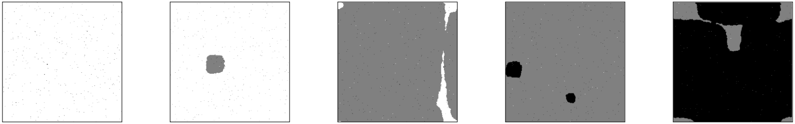


and

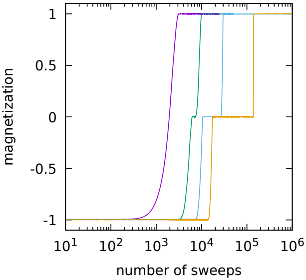
$$\Gamma = H(\mathbf{q}) + \Delta(\mathbf{q},\mathbf{p}) - H(\mathbf{d}) \overset{h\to 0}{\sim} \frac{8}{h}$$

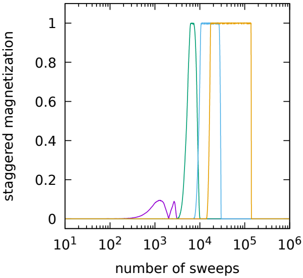
Monte Carlo simulation [?]

Picture: 2×2 tile, white = **d**, gray = **c**, black = **u**, $\Lambda = 512 \times 512$, $h = 0.3$, $1/T = 0.9$, $t = 3.0, 3.6, 6.0, 7.6, 9.6 \times 10^3$ MCS

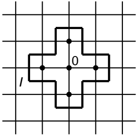


Picture: $\Lambda = 512 \times 512$, $h = 0.3$, $1/T =$ 0.85, 0.90, 0.95, 1.00



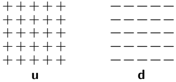


Cross PCA [**?**, C., Nardi, Spitoni JSP 2008]

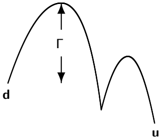


Consider the cross PCA model with positive and small magnetic field $h > 0$.

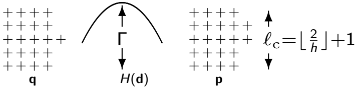
Result:



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



Critical droplet:

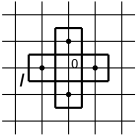


and

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

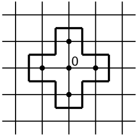
Tuning the self–interaction [C., Nardi, Spitoni PRE 2008]

PCA nearest neighbor model



$\kappa = 0$

PCA with tuned interaction



$\kappa \in (0,1)$

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

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

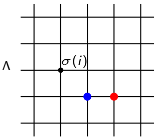
for $\sigma \in \Omega$, $s \in \{-1,+1\}$ e $\kappa \in (0,1)$.

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

Heuristics: reach metastable behavior analogous to that of the Blume–Capel model.

Summary

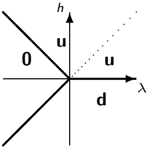
Blume–Capel model

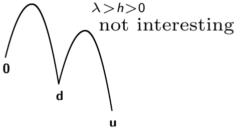


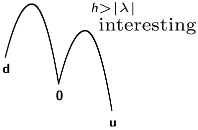
- $\Lambda =$ finite square with periodic boundary conditions
- $\sigma(i) \in \{-1, 0, +1\}$ spin variable associated with site i
- $h \in \mathbb{R}$ magnetic field and $\lambda \in \mathbb{R}$ chemical potential
- $H(\sigma) = \sum_{\langle ij \rangle} [\sigma(i) - \sigma(j)]^2 - \lambda \sum_i [\sigma(i)]^2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

Cost of interfaces: 0 $\langle 00 \rangle, \langle +1+1 \rangle, \langle -1-1 \rangle$; 1 $\langle +10 \rangle, \langle -10 \rangle$; 4 $\langle +1-1 \rangle$

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







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

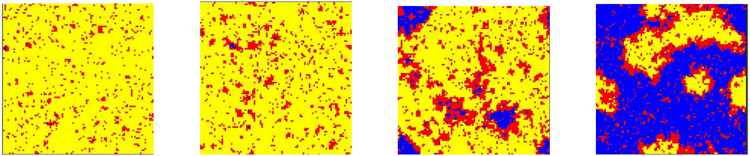
Metropolis dynamics

Let σ_t the configuration at time t:

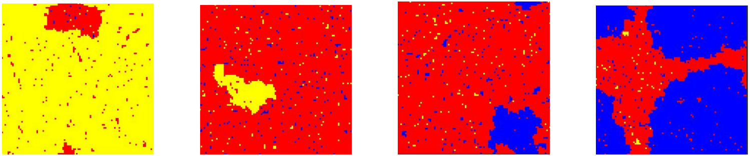
- chose at random with uniform probability $1/|\Lambda|$ a lattice site and call it i;
- chose with probability $1/2$ one of the two values in
$$\{-1, 0, +1\} \setminus \{\sigma_t(i)\}$$
  and call it s;
- flip the spin $\sigma_t(i)$ to s with probability 1 if the energy decreases and with probability
$$\exp\{-\Delta H/T\}$$
  if the energy increases ($\Delta H > 0$).

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

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

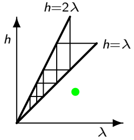


Parameters: $\Lambda = 100 \times 100$, $h = 0.1$, $\lambda = 0.02$, $T = 0.909$

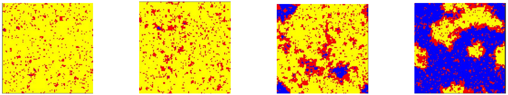


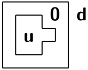
In both cases $\mathbf{d}$ is the unique metastable state: the transition $\mathbf{0} \to \mathbf{u}$ is much faster than the transition $\mathbf{d} \to \mathbf{0}$.

Rigorous results [C., Olivieri JSP 1996]

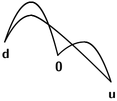


- Simulations done for $h < \lambda$, but similar behavior

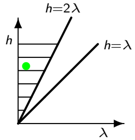


- $\Omega^{\mathrm{m}} = \{\mathbf{d}\}$
- $\mathcal{P}_{\mathrm{c}} =$  with $\ell_{\mathrm{c}} = \frac{2-h+\lambda}{h}$

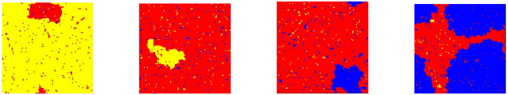
- $\Gamma_{\mathrm{m}} = H(\mathcal{P}_{\mathrm{c}}) - H(\mathbf{d}) \sim \frac{8}{h}$ (does not depend on λ)
- Energy landscape:



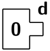
Rigorous results [C., Olivieri JSP 1996]



- Simulations done for $h > \lambda$

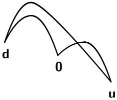


- $\Omega^{\mathrm{m}} = \{\mathbf{d}\}$

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

- $\Gamma_{\mathrm{m}} = H(\mathcal{P}_{\mathrm{c}}) - H(\mathbf{d}) \sim \frac{4}{h-\lambda}$

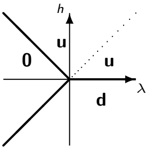
- Energy landscape:



Zero chemical potential Blume–Capel model

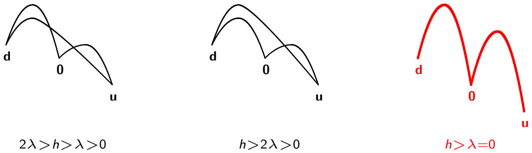
Hamiltonian $H(\sigma) = \sum_{\langle ij \rangle} [\sigma(i) - \sigma(j)]^2 - h \sum_i \sigma(i)$

Ground states:



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

Guess:

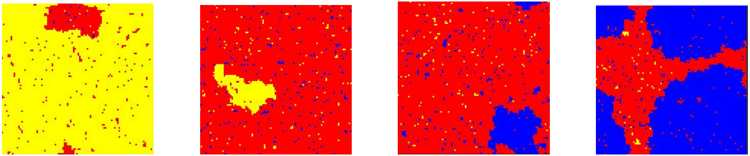


Critical droplet: $\ell_{\rm c} = \lfloor 2/h \rfloor + 1$

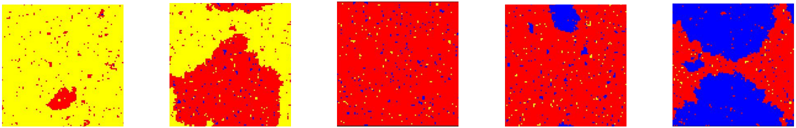
$$\Gamma_{\rm m} = H\left(\mathbf{d}\ \boxed{\mathbf{0}}\ \mathbf{d}\right) - H(\mathbf{d}) = H\left(\mathbf{0}\ \boxed{\mathbf{u}}\ \mathbf{0}\right) - H(\mathbf{0}) \sim \frac{4}{h}$$

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

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



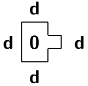
Parameters: $\Lambda = 100 \times 100,\ h = 0.1,\ \lambda = 0,\ T = 0.909$

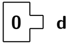


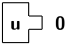
Result to be proven: $\mathbf{d}$ and $\mathbf{0}$ are both metastable: the transitions $\mathbf{0} \to \mathbf{u}$ and $\mathbf{d} \to \mathbf{0}$ take approximatively the same time.

Rigorous results [C., Nardi JSP 2013]

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. $\mathcal{Q}_{\mathrm{c}} =$ 

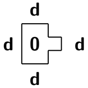
(critical droplet between **0** and **u**)

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

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

Proof of some of the model dependent ingredients

To prove the model dependent inputs

$$\Gamma_{\rm m} = \max_{\sigma\in\Omega\setminus\Omega^{\rm s}} V_\sigma = H($$  $$) - H(\mathbf{d}) \equiv \Gamma$$

and

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

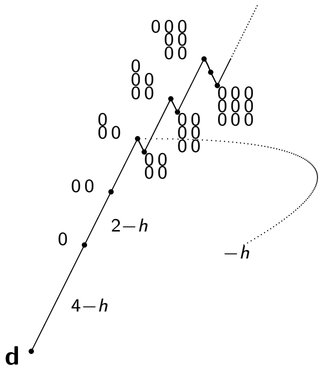
we have to prove the following:

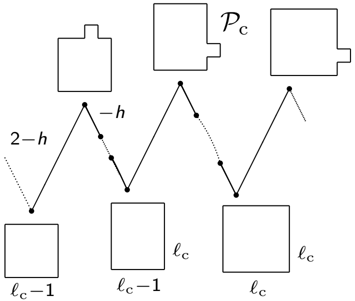
- $\Phi(\mathbf{d}, \mathbf{u}) - H(\mathbf{d}) = \Gamma$
- $\Phi(\mathbf{0}, \mathbf{u}) - H(\mathbf{0}) = \Gamma$
- $\Phi(\sigma, \mathbf{u}) - H(\sigma) < \Gamma$ for all $\sigma \in \Omega \setminus \{\mathbf{d}, \mathbf{0}, \mathbf{u}\}$ (recurrence)

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

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





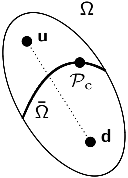
Then the path goes down to **0** and the from **0** to **u** in a similar fashion a plus droplet is nucleated inside the sea of zeros.

Minmax: lower bound

Prove that all the paths connecting **d** to **u** attain an energy level greater than or equal to $H(\mathcal{P}_c)$ $\Big\} \Rightarrow \Phi(\mathbf{d},\mathbf{u}) \geq H(\mathcal{P}_c)$

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

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

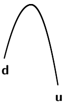


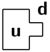
It than follows that all the paths connecting **d** to **u** attain an energy level greater than or equal to $H(\mathcal{P}_c)$.

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.

Sharp estimate

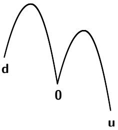
Consider the Ising model with $h > 0$ small [?]:



$\mathcal{P}_c =$ 

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

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



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

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

Sharp estimate [?, C., Nardi, Spitoni EPJST 2017, C., Nardi, Spitoni Lect. Notes Comp. Sc. 2016, Bet, Jacquier, Nardi JSP 2021]

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 $\mathbf{0} \to \mathbf{u}$.

Indeed,

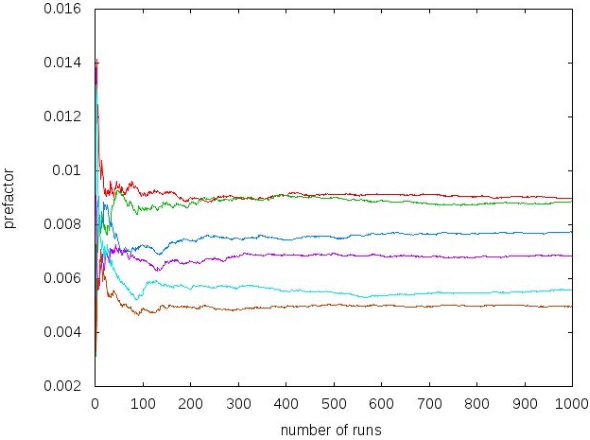
$$\lim_{T \to 0} \frac{\mathbb{E}_{\mathbf{0}}(\tau_{\mathbf{u}})}{e^{\Gamma_{\mathrm{m}}/T}} = \frac{3}{4(2\ell_{\mathrm{c}} - 1)|\Lambda|} \quad \text{and} \quad \lim_{T \to 0} \frac{\mathbb{E}_{\mathbf{d}}(\tau_{\mathbf{u}})}{e^{\Gamma_{\mathrm{m}}/T}} = 2 \times \frac{3}{4(2\ell_{\mathrm{c}} - 1)|\Lambda|}$$

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,

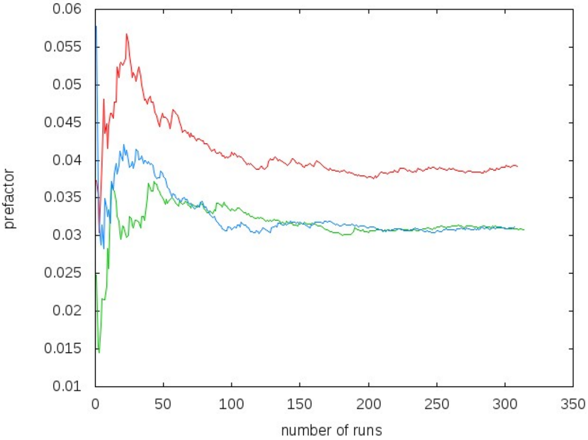


Sharp estimate: numerical check

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



Conclusions and next steps

Description of the pathwise approach to metastability valid for Probabilistic Cellular Automata and Statistical Mechanics spin systems.

Results for particular models: nearest neighbors PCA and cross PCA. Effect of the self–interaction.

Metastable behavior of the Blume–Capel model: connection with PCA.

Future steps:

- studying the effect of different (not periodic) boundary conditions;
- Blume–Capel model with conserved (Kawasaki) dynamics.

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