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

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Summary

Introduction

Nearest neighbor Probabilistic Cellular Automata

Metastable states in the Blume–Capel model

Conclusions and next steps
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: \(a = 1.36 \ \ell^2 \text{ atm mol}^{-2}\) and \(b = 0.0319 \ \ell \ \text{ mol}^{-1}\) at \(T = 140^\circ\text{K}\)


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

Introduction

Nearest neighbor Probabilistic Cellular Automata
  Definition of the model
  Definition of metastable states
  Some properties of the metastable states
  Results

Metastable states in the Blume–Capel model

Conclusions and next steps
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 $\sigma_0, \sigma_1, \ldots, \sigma_t, \ldots$ on $\Omega$ with transition matrix

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

where

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

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
  \[
  G(\sigma) = -h \sum_{i \in \Lambda} \sigma(i) - T \sum_{i \in \Lambda} \log \cosh \left[ \frac{1}{T} \left( \sum_{j \in i + I} \sigma(j) + h \right) \right]
  \]
- define the energy cost
  \[ \Delta(\sigma, \eta) = - \lim_{T \to 0} T \log p(\sigma, \eta) \]
  then the Wentzel–Friedlin condition is satisfied
  \[ e^{-[\Delta(\sigma, \eta) - \gamma(T)]/T} \leq p(\sigma, \eta) \leq e^{-[\Delta(\sigma, \eta) + \gamma(T)]/T} \]
  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:

\[ \Delta(\sigma, \eta) = 0 \]
\[ \Delta(\eta, \sigma) = H(\sigma) - H(\eta) \]

• 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 $\Omega^s$ be the set of the absolute minima of the Hamiltonian.

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

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

The set of critical droplets $\mathcal{P}_c$ is the set of configurations necessarily visited by the optimal paths and where the optimal paths from $\Omega^m$ to $\Omega^s$ attain the maximal height.
Some properties of the metastable states

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

Let $\sigma \in \Omega^m$

- for any $\varepsilon > 0$ we have $\lim_{T \to 0} P(\sigma(e^{(\Gamma_m - \varepsilon)/T} < \tau_{\Omega^s} < e^{(\Gamma_m + \varepsilon)/T}) = 1$
- $\lim_{T \to 0} T \log E(\tau_{\Omega^s}) = \Gamma_m$
- $\lim_{T \to 0} P(\tau_P < \tau_{\Omega^s}) = 1$

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

$$E(\tau_{\Omega^s}) = \frac{1}{k} e^{\Gamma_m/T} [1 + o(1)]$$

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

\[ \Omega^m \]

\[ \Omega^m \]

\[ \Omega^s \]

[C., Nardi, Spitoni EPJST 2017, Bet, Jacquier, Nardi JSP 2021].
Consider the nearest neighbor PCA model with a positive and small magnetic field $h > 0$.

Result: flip–flopping metastable state

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

Critical droplet in the sea of minuses:

$$\Gamma = H(q) + \Delta(q, p) - H(d) \xrightarrow{h \to 0} \frac{8}{h}$$
Monte Carlo simulation [?]  

Picture: 2 × 2 tile, white = d, gray = c, black = u, Λ = 512 × 512, 
h = 0.3, 1/T = 0.9, t = 3.0, 3.6, 6.0, 7.6, 9.6 × 10³ MCS

Picture: Λ = 512 × 512, h = 0.3, 1/T = 0.85, 0.90, 0.95, 1.00
Consider the cross PCA model with positive and small magnetic field $h > 0$.

Result:

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

Critical droplet:

$$\Gamma = H(q) + \Delta(q, p) - H(d) \sim 0 \frac{16}{h}$$
Tuning the self–interaction \cite{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

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

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

The parameter \( \kappa \) 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

Introduction

Nearest neighbor Probabilistic Cellular Automata

Metastable states in the Blume–Capel model
  The Blume–Capel model
  Metastability in presence of a single metastable state
  Metastability in presence of multiple metastable states
  Sharp estimates on the exit time

Conclusions and next steps
Blume–Capel model

- $\Lambda = \text{finite square with periodic boundary conditions}$
- $\sigma(i) \in \{-1, 0, +1\}$ 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: $H(u) = -(h + \lambda)|\Lambda|$, $H(0) = 0$, and $H(d) = (h - \lambda)|\Lambda|$

- 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 $\sigma_t$ 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: \( \bullet = -1 \quad \bullet = 0 \quad \bullet = +1 \)

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 \( d \) is the unique metastable state: the transition \( 0 \rightarrow u \) is much faster than the transition \( d \rightarrow 0 \).
Rigorous results [C., Olivieri JSP 1996]

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

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

- $\mathcal{P}_c = \begin{bmatrix} 0 & d \\ u & 0 \end{bmatrix}$ with $\ell_c = \frac{2-h+\lambda}{h}$

- $\Gamma_m = H(\mathcal{P}_c) - H(d) \sim \frac{8}{h}$ (does not depend on $\lambda$)

- Energy landscape:
Rigorous results [C., Olivieri JSP 1996]

- Simulations done for $h > \lambda$

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

- $\mathcal{P}_c = \begin{array}{c} 0 \\ d \end{array}$ with $\ell_c = \frac{2}{h-\lambda}$

- $\Gamma_m = H(\mathcal{P}_c) - H(d) \sim \frac{4}{h-\lambda}$

- 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:

\[
H(u) = -h|\Lambda|, \quad H(0) = 0, \quad H(d) = h|\Lambda|
\]

Guess:

\[
2\lambda > h > \lambda > 0 \quad h > 2\lambda > 0 \quad h > \lambda = 0
\]

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

\[
\Gamma_m = H(\begin{array}{c} d \\ 0 \\ d \end{array}) - H(d) = H(\begin{array}{c} 0 \\ u \\ 0 \end{array}) - H(0) \sim \frac{4}{h}
\]
Monte Carlo sequences \( \bullet = -1 \quad \bullet = 0 \quad \bullet = +1 \)

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

Result to be proven: \( d \) and \( 0 \) are both metastable: the transitions \( 0 \to u \) and \( d \to 0 \) take approximatively the same time.
Rigorous results [C., Nardi JSP 2013]

We prove the model dependent results:

1. \( \Omega^s = \{u\} \)

2. \( \Gamma_m = \max_{\sigma \in \Omega \setminus \Omega^s} V_\sigma = H \left( d \begin{array}{c} d \\ d \end{array} \right) - H(d) \equiv \Gamma \)

3. \( \Omega^m = \{\eta \in \Omega \setminus \Omega^s : V_\eta = \Gamma_m\} = \{d, 0\} \)

4. \( P_c = \begin{array}{c} 0 \\ d \end{array} \) (critical droplet between \(d\) and \(0\))

5. \( Q_c = \begin{array}{c} u \\ 0 \end{array} \) (critical droplet between \(0\) and \(u\))

Then we get that for any \(\sigma \in \Omega^m\)

- for any \(\varepsilon > 0\) we have \(\lim_{T \to 0} \mathbb{P}_\sigma (e^{(\Gamma-\varepsilon)/T} < \tau_u < e^{(\Gamma+\varepsilon)/T}) = 1\)

- \(\lim_{T \to 0} T \log \mathbb{E}_\sigma (\tau_u) = \Gamma\)

- \(\lim_{T \to 0} \mathbb{P}_d (\tau_{P_c} < \tau_u) = 1\) and \(\lim_{T \to 0} \mathbb{P}_0 (\tau_{Q_c} < \tau_u) = 1\)
Proof of some of the model dependent ingredients

To prove the model dependent inputs

\[
\Gamma_m = \max_{\sigma \in \Omega \setminus \Omega^s} V_\sigma = H(\begin{array}{c} d \\ d \\ 0 \end{array}) - H(d) \equiv \Gamma
\]

and

\[
\Omega^m = \{ \eta \in \Omega \setminus \Omega^s : V_\eta = \Gamma_m \} = \{d, 0\}
\]

we have to prove the following:

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

\[
\Phi(d, u) \leq H(P_c)
\]

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 \( H(\mathcal{P}_c) \)

\[
\Rightarrow \Phi(d, u) \geq H(\mathcal{P}_c)
\]

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 [?]:

$$\mathcal{P}_c = \begin{array}{c} u \end{array}^d$$

$$\lim_{T \to 0} \frac{\mathbb{E}_d(\tau_u)}{e^{\Gamma_m/T}} = \frac{3}{4(2\ell_c - 1)|\Lambda|}$$

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

$$\lim_{T \to 0} \frac{\mathbb{E}_d(\tau_{\{u,0\}})}{e^{\Gamma_m/T}} = \lim_{T \to 0} \frac{\mathbb{E}_0(\tau_u)}{e^{\Gamma_m/T}} = \frac{3}{4(2\ell_c - 1)|\Lambda|}$$

What can be said about $\mathbb{E}_d(\tau_u)$?
Since it can be proven that

$$\lim_{T \to 0} P_d[\tau_u < \tau_0] = 0$$

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

Indeed,

$$\lim_{T \to 0} \frac{E_0(\tau_u)}{e^{\Gamma_m/T}} = \frac{3}{4(2\ell_c - 1)|\Lambda|}$$

and

$$\lim_{T \to 0} \frac{E_d(\tau_u)}{e^{\Gamma_m/T}} = 2 \times \frac{3}{4(2\ell_c - 1)|\Lambda|}$$
Sharp estimate: numerical check

Prefactor = \( \frac{\text{averaged exit time from } d \text{ to } u}{\exp\frac{\Gamma_m}{T}} \)

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

Colors for \( \lambda \):  
- 0,  
- 0.001,  
- 0.01,  
- 0.02,  
- 0.04,  
- 0.06,  

![Graph showing prefactor over number of runs for different colors representing \( \lambda \) values.]
Sharp estimate: numerical check

Prefactor = (averaged exit time from $d$ to $u$)/ $\exp\{\Gamma_m/T\}$

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

Colors for $\lambda$: • 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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