Second Workshop on Random Dynamical Systems

Bielefeld, 17-19 Nov 2008

Coupling in potential wells: from average to pointwise estimates of metastable times

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Work supported by the Germany Israeli Foundation

November 17, 2008

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Outline

Motivation

The RFCW model

- The model and the dynamics.
- Energy landscape and metastability.
- Metastable time: results.

Potential theory approach

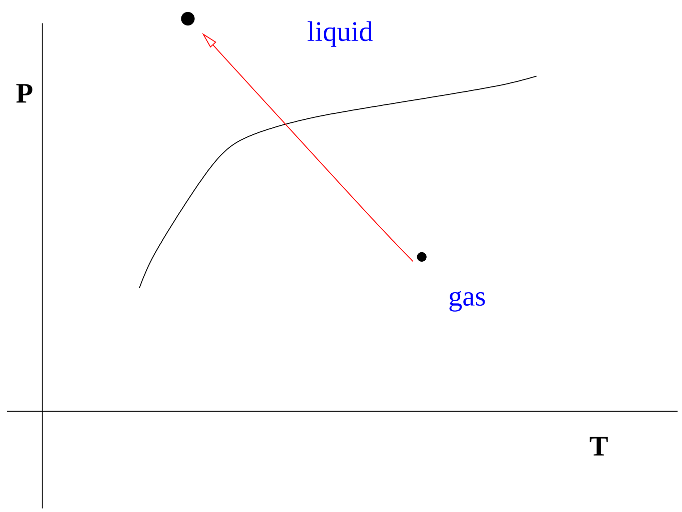
- Preliminary tools: metastable time and capacities.
- Two variational principles for capacities.
- Application to the RFCW model.

From average to pointwise estimates

- Heuristics and results.
- Coupling in potential wells.

Motivation

Metastability is a common phenomenon of non linear dynamics, related to first order phase transition.

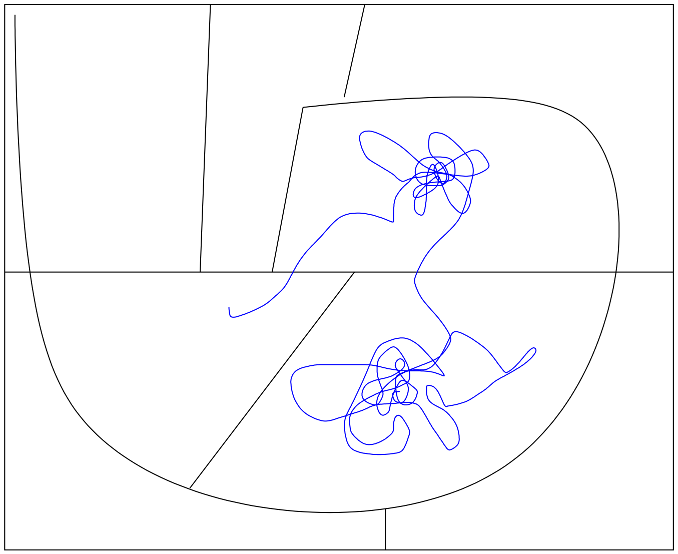


If the parameters of the system changes along the line of the first order phase transition, *the system moves from one metastable state to the new equilibrium*.

Two main properties characterizing the metastability are:

1. The existence of quasi-invariant subspaces S_i.
2. The presence of multiple, separated time scales:

- on a short time scale, every S_i reaches a local equilibrium
- on a longer metastable time scale the system moves from S_i to S_j.



The Random Field Curie-Weiss (RFCW) model

- System of N particles described by configurations $\sigma = \{\sigma_i\}_{i=1}^N \in \{-1, 1\}^N$.

- The energy of a configuration is specified by the random Hamiltonian

$$H_N(\sigma) = -\frac{1}{2N} \sum_{i,j=1}^{N} \sigma_i \sigma_j - \sum_{i=1}^{N} h_i \sigma_i$$

$\boldsymbol{h_i}$, $i \in \mathbb{N}$ are i.i.d. (**continuous**) random variables called external fields.

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- At the equilibrium the system is described by the probability Gibbs measure

$$\boldsymbol{\mu_N(\sigma) = \frac{e^{-\beta H_N(\sigma)}}{Z_N}}$$

Glauber dynamics

- Consider a discrete time **Glauber dynamics** for the RCFW model. This is a Markov chain on $\{-1,1\}^N$ **reversible w.r.t.** μ_N.

  Generator: $(Lf)(\sigma) = \sum_{i=1}^{N} p(\sigma,\sigma^i)(f(\sigma^i) - f(\sigma))$

  where
  $$p(\sigma,\sigma^i) = \frac{1}{N} e^{-\beta[H_N(\sigma^i) - H_N(\sigma)]_+}$$
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- The dynamics follows the direction of lower energy, but the system can be trapped in a local minimum for long time before arriving to the global one. *How long will it take the system to escape from local minima?*

Energy landscape

Macroscopic parameter:

Define the magnetization $\boldsymbol{m_N(\sigma) = \frac{1}{N}\sum_{i=1}^{N}\sigma_i}$ taking value on $\Gamma_N = \{-1, -1+2/N, \ldots, +1\}$

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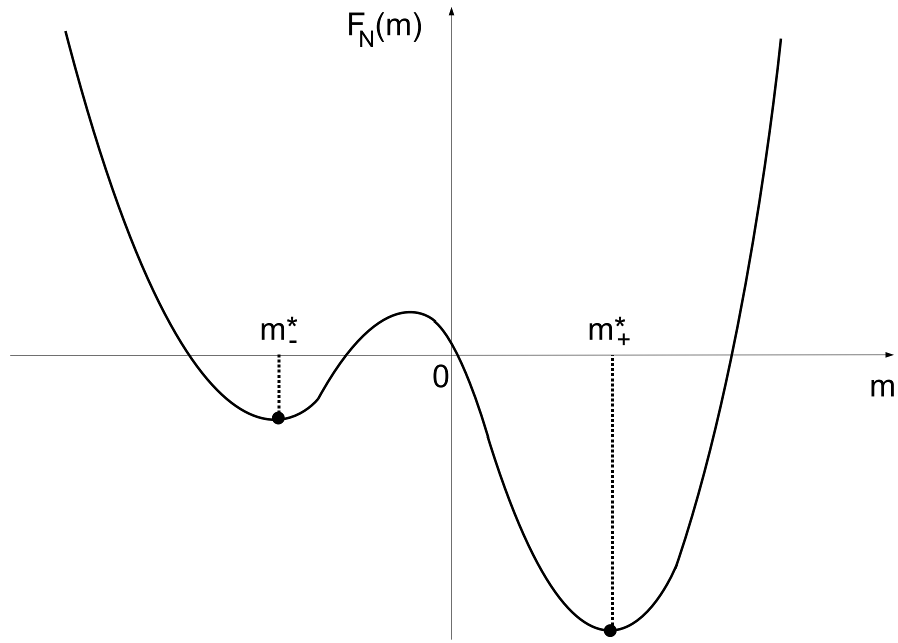
A simple case: $h =$ constant

- $H_N(\sigma) = -\frac{N}{2} m_N(\sigma)^2 - h m_N(\sigma) \Longrightarrow$ the dynamics just depends on $m_N(\sigma)$.

- the induced measure on Γ_N: $Q_N(m) \equiv \mu_N(m_N(\sigma) = m) = \frac{e^{-N\beta F_N(m)}}{Z_N}$ where $F_N(m)$ is the free energy.

- The critical points of $F_N(m)$ satisfy $m^* = \tanh(\beta(h + m^*))$.

A simple example: $h =$ constant



Remark 1. *When $h =$ constant, the induced process $m(\sigma(t))$ is Markovian. In particular, it is a nearest-neighbors RW on Γ_N reversible w.r.t. Q_N. The analysis of the metastability can then be reduced to the macroscopic setting.*

General case: h_i's i.i.d. continuous random variables

The Hamiltonian does not depend only on $m(\sigma)$, but:

- Using sharp large deviation estimates, we get

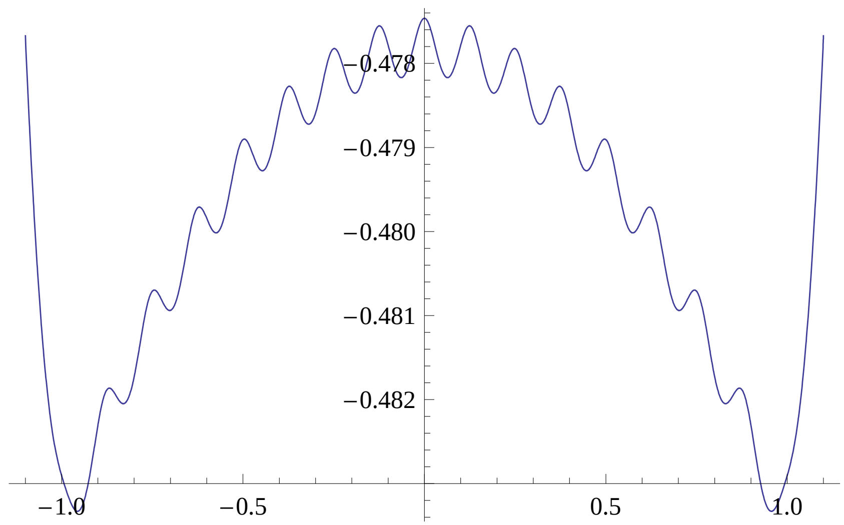
$$\mathcal{Q}_N(m) = K_N(m)\frac{e^{-N\beta F_N(m)}}{Z_N}\left(1 + o(1)\right),$$

  where $F_N(m)$ is the free energy.

- Asymptotically and $\mathbb{P}_h$-a.s, the critical points of F_N are solutions of

$$m^* = \mathbb{E}_h \tanh(\beta(m^* + h_i))$$

General case: h_i's i.i.d. continuous random variables



From now on, we will assume β and the distribution of the fields $\{h_i\}_{i=1}^N$, such that there exist at least two minima of $F_N(m)$.

Main question

- Let m^* be a local minimum and consider the set of "deeper" local minima

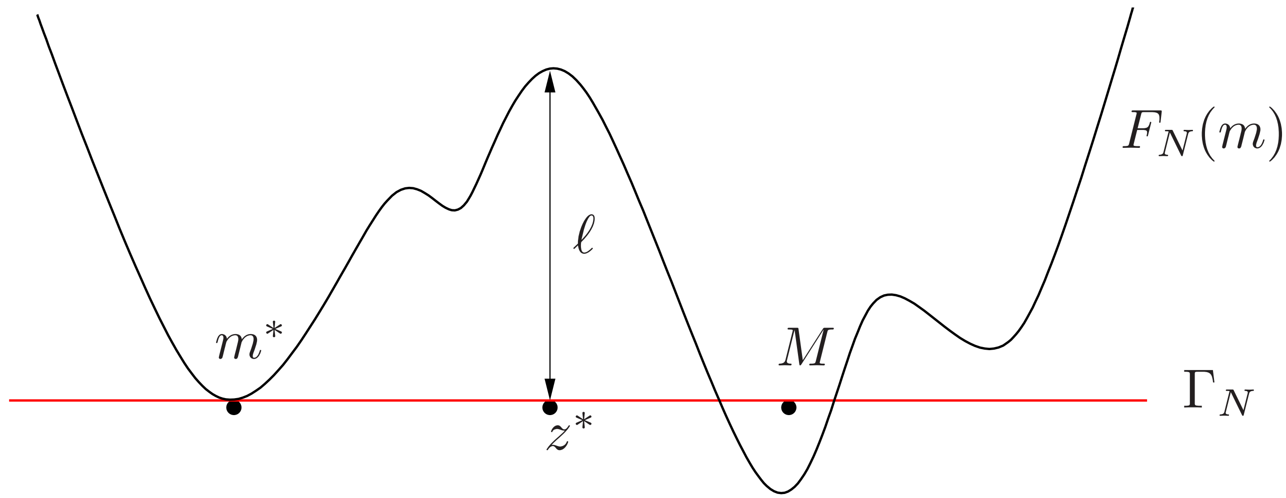
$$M = \{m : F_N(m) \leq F_N(m^*)\}.$$

- For any $A \subset \Gamma_N$, let $S[A] = \{\sigma \in S_N : m_N(\sigma) \in A\}$.
  Then define the metastable exit time:

$$\tau_{S[M]} = \inf\{t > 0 | \sigma(t) \in S[M]\}\,.$$

What can we say about $\mathbb{E}_{\boldsymbol{\sigma}} \boldsymbol{\tau}_{S[M]}$ for $\boldsymbol{\sigma} \in S[m^*]$?

Example of energy landscape



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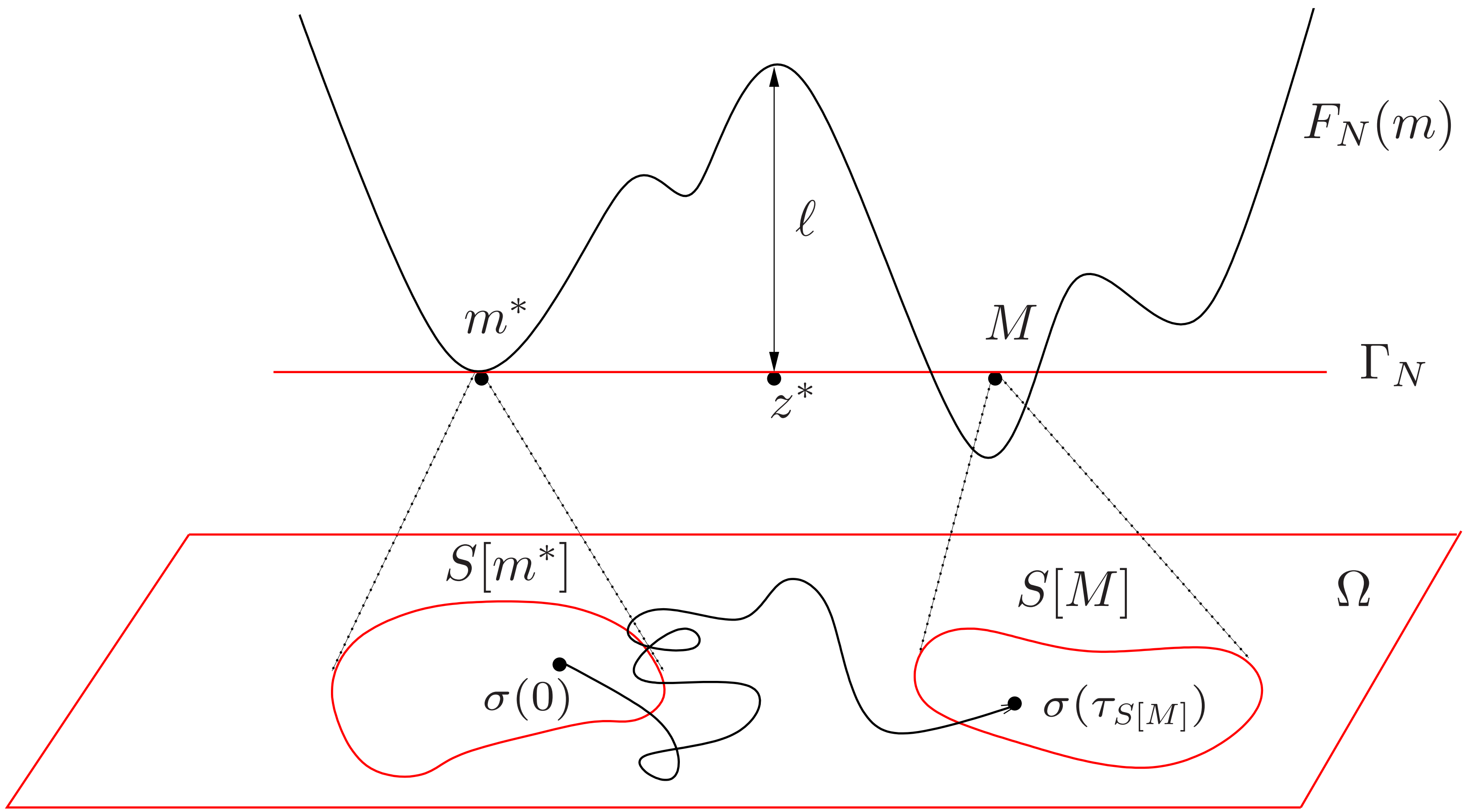

Mean metastable time

Following the potential theory approach:

THM 1. [B., Bovier, Ioffe] *Let $\boldsymbol{m^*}$ be a local minimum of F_N and let $\boldsymbol{z^*}$ be the minimax between m^* from M. Then, $\mathbb{P}_h$-a.s.,*

$$\mathbb{E}_{\boldsymbol{\nu}} \boldsymbol{\tau}_{\boldsymbol{S}[\boldsymbol{M}]} = \boldsymbol{c}(\boldsymbol{m}^*, \boldsymbol{z}^*)\, \boldsymbol{e}^{\boldsymbol{\beta N}\left(\boldsymbol{F_N}(\boldsymbol{z}^*) - \boldsymbol{F_N}(\boldsymbol{m}^*)\right)} (1 + o(1)) \ ,$$

where ν is a probability measure on $S[m^*]$ and $c(m^*, z^*)$ is the prefactor (explicit formula).

Potential theory approach

Preliminary tools:

$A, B \subset \{-1,1\}^N$, $A \cap B = \emptyset$;

$L = P - \mathbb{1}$ generator of the dynamics

Equilibrium potential, $h_{A,B} : \{-1,1\}^N \mapsto \mathbb{R}$, is the solution of

Dirichlet problem
$$\begin{cases} (Lh_{A,B})(\sigma) = 0 & \text{if } \sigma \notin A \cup B \\ h_{A,B}(\sigma) = 1 & \text{if } \sigma \in A \\ h_{A,B}(\sigma) = 0 & \text{if } \sigma \in B \end{cases}$$

Probabilistic interpretation: if $\sigma \notin A \cup B$ then $\boxed{h_{A,B}(\sigma) = \mathbb{P}_\sigma[\tau_A < \tau_B]}$

$\Longrightarrow$ formula for the mean metastable time from A to B, i.e.

for a suitable probability measure $\boldsymbol{\nu}$ on A (last exit measure):

$$\mathbb{E}_\nu \tau_B \equiv \sum_{\sigma \in A} \nu(\sigma) \mathbb{E}_\sigma \tau_B = \frac{1}{\mathrm{cap}(A,B)} \mu_N(h_{A,B})$$

where $\mathbf{cap}(A,B)$ is the capacity of the capacitor A, B.

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More explicitly:

$$\nu(\sigma) = \frac{\mu(\sigma)\mathbb{P}_\sigma[\tau_B < \tau_A]}{\mathrm{cap}(A,B)}; \qquad \mathrm{cap}(A,B) = \sum_{\sigma \in A} \mu(\sigma)\mathbb{P}_\sigma[\tau_B < \tau_A]$$

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Thus we need

- precise control of capacities.
- some rough control of the equilibrium potential.

Variational principle I

Let $\Phi(f)$ be the *Dirichlet form* of f associated to L, i.e $\Phi(f) = \langle Lf, f \rangle_{\mu_N}$.
By the Dirichlet principle,

$$\mathbf{cap}(\boldsymbol{A}, \boldsymbol{B}) = \inf_{\boldsymbol{h} \in \boldsymbol{\mathcal{H}}_{\boldsymbol{A},\boldsymbol{B}}} \boldsymbol{\Phi}(\boldsymbol{h}) \,,$$

and the unique minimizer is given by the harmonic function $h_{A,B}$.

Any test function in $\mathcal{H}_{A,B}$ provides an upper bound on capacities
$\longrightarrow$ **the goal is to find an approximated harmonic function.**

Variational principle II

Let f be a non-negative cycle free unit flow from A to B, and $\mathbb{P}^f$ be the law on paths $\mathcal{X} : A \to B$ induced by a stopped Markov chain driven by f.
Let $\mathcal{X} = (a_0, a_1, \ldots, a_{|\mathcal{X}|})$.

By the variational principle due to **Berman and Konsowa [1990]**,

$$\mathbf{cap}(A,B) = \sup_{f \in \mathbb{U}_{A,B}} \mathbb{E}^f \left[\sum_{\ell=0}^{|\mathcal{X}|-1} \frac{f(a_\ell, a_{\ell+1})}{\mu(a_\ell) p(a_\ell, a_{\ell+1})} \right]^{-1},$$

and the maximizer is given by the harmonic flow.

Any flow in $\mathbb{U}_{A,B}$ provides a lower bound on capacities
$\longrightarrow$ **the goal is to find an approximated harmonic flow.**

RFCW model: Coarse graining

- $I_k, k \in \{1, \dots, n\}$: partition of the support of h.
- $\Lambda_k = \{i \in \{1, \dots, N\} : h_i \in I_k\}$: random partition of the set $\{1, \dots, N\}$.

Order parameters: $m_k(\sigma) = \frac{1}{N} \sum_{i \in \Lambda_k} \sigma_i \,, \quad \boldsymbol{m}(\sigma) = (m_k(\sigma))_{k=1}^n$

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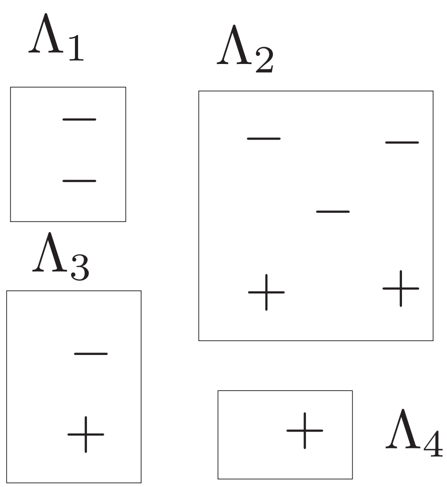
Example:



$$N = 10, \;\; n = 4$$

$$\boldsymbol{m}(\sigma) = \left(-\tfrac{1}{5}, -\tfrac{1}{10}, \tfrac{1}{10}, 0\right)$$

$$m(\sigma) = \sum_{i=1}^{n} m_i(\sigma) = -\tfrac{1}{5}$$

$\Longrightarrow$ Rewrite the Hamiltonian as

$$H_N(\sigma) = -NE(\boldsymbol{m}(\sigma)) + \sum_{k=1}^{n} \sum_{i \in \Lambda_k} \sigma_i \tilde{h}_i$$

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$$H_N(\sigma) = -N E(\boldsymbol{m}(\sigma)) + \sum_{k=1}^{n} \sum_{i \in \Lambda_k} \sigma_i \tilde{h}_i$$

- $E(\boldsymbol{m}) = \frac{1}{2}\left(\sum_{k=1}^{n} m_k\right)^2 + \sum_{k=1}^{n} \bar{h}_k m_k$

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Strategy: Analyze the metastable behavior of the model as a perturbation of the model: $H_N(\sigma) = -NE(\boldsymbol{m}(\sigma))$.

In conclusion:

Let $A = S[m^*]$ and $B = S[M]$. Then:

- $\mathbb{P}_h$-a.s. and for every fixed $n \in \mathbb{N}$, it holds

$$\mathrm{cap}(A, B) = K(\boldsymbol{z}^*, n)\frac{e^{-\beta N F_N(z^*)}}{Z_N}(1 + O(\epsilon))$$

- Using super-harmonic functions techniques, we get

$$\mu_N(h_{A,B}) = K(m^*)\frac{e^{-\beta N F_N(m^*)}}{Z_N}(1 + o(1))$$

Altogether, taking $\boldsymbol{n}$ large enough, we get

$$\mathbb{E}_{\boldsymbol{\nu}}\boldsymbol{\tau}_{\boldsymbol{B}} = \boldsymbol{K}(\boldsymbol{m}^*, \boldsymbol{z}^*)\, \boldsymbol{e}^{\boldsymbol{\beta N}\left(\boldsymbol{F_N}(\boldsymbol{z}^*) - \boldsymbol{F_N}(\boldsymbol{m}^*)\right)}(\mathbf{1} + \boldsymbol{o}(\mathbf{1}))$$

From average to pointwise estimates

Questions:

- Does the metastable time really depend on the *last exit measure* ν?
- Under which conditions can we deduce *pointwise estimates*?
- Can we say something about the *distribution*?

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Previous results:

(1) P. Mathieu, P. Picco (JSP, 1998) [binary distribution]

(2) A. Bovier, M. Eckhoff, V. Gayrard, M. Klein (PTRF, 2001) [discrete finite distribution]

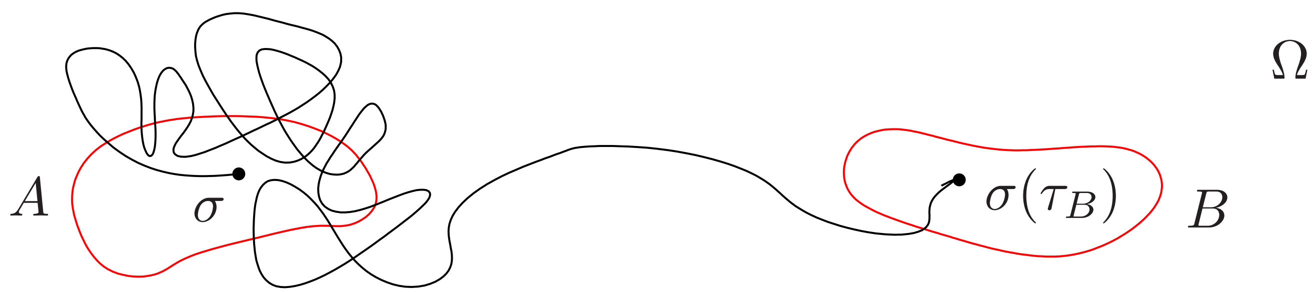
(3) A. Bovier, F. Manzo (JSP, 2002) [Ising model in the low-temperature limit]

Heuristics:

The time spent in the starting well before reaching B is much larger then the mixing time of the dynamics conditioned to stay in the well. Thus we infer

$$\mathbb{E}_\sigma \tau_B \sim \mathbb{E}_\nu \tau_B \,, \quad \forall \sigma \in A$$

After the system is mixed, the return times to A are i.i.d. random variables, and the number of returns to A is geometric. Provided that the mixing time is small enough respect to $\mathbb{E}_\nu \tau_B$, the metastable time is expected to be exponential.



Main result

Consider the RFCW model with continuous random fields.

With the same notation introduced before, it holds the following:

THM 2. [BBI, 2008] $\mathbb{P}_h$-*a.s., for all* $n \geq n_0$ *and for all* $\sigma, \eta \in S[\boldsymbol{m}^*]$,

$$\mathbb{E}_{\boldsymbol{\sigma}} \boldsymbol{\tau}_{\boldsymbol{S}[\boldsymbol{M}]} = \mathbb{E}_{\boldsymbol{\eta}} \boldsymbol{\tau}_{\boldsymbol{S}[\boldsymbol{M}]} (\mathbf{1} + \boldsymbol{o}(\mathbf{1})).$$

In particular, for all $\sigma \in S[\boldsymbol{m}^*]$, $\mathbb{E}_{\boldsymbol{\sigma}} \boldsymbol{\tau}_{\boldsymbol{S}[\boldsymbol{M}]} = \mathbb{E}_{\boldsymbol{\nu}} \boldsymbol{\tau}_{\boldsymbol{S}[\boldsymbol{M}]} (\mathbf{1} + \boldsymbol{o}(\mathbf{1}))$

Consequences

- Sharp estimates on the metastable time between any two minima.

Corollary 1. *Let $\boldsymbol{m}_1$ and $\boldsymbol{m}_2$ be two minima of $F_N(\boldsymbol{m})$, let $\boldsymbol{z}^*$ be the minmax between them. Assume $F_N(\boldsymbol{m}_1) \geq F_N(\boldsymbol{m}_2)$.*
Then P_h-a.s., for all $\sigma \in S[\boldsymbol{m}_1]$,

$$\mathbb{E}_\sigma \tau_{S[\boldsymbol{m}_2]} = c(\boldsymbol{m}_1, \boldsymbol{m}_2) e^{\beta N (F_N(\boldsymbol{m}_1) - F_N(\boldsymbol{m}_2))} (1 + o(1))$$

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- Distribution of the metastable time: *work in progress.*

Coupling in potential wells

D.A. Levin, M. Luczak, Y. Peres (arXiv:0712.0790).

The authors use coupling techniques to estimate the mixing time of the restricted dynamics in the standard CW model (for $h = 0$ and $\beta > 1$).

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Generalization to the RFCW model. A simple case

Assume that fields take only finitely many values, i.e. $h_i \in \mathcal{A} = \{a_1, \dots, a_n\}$.

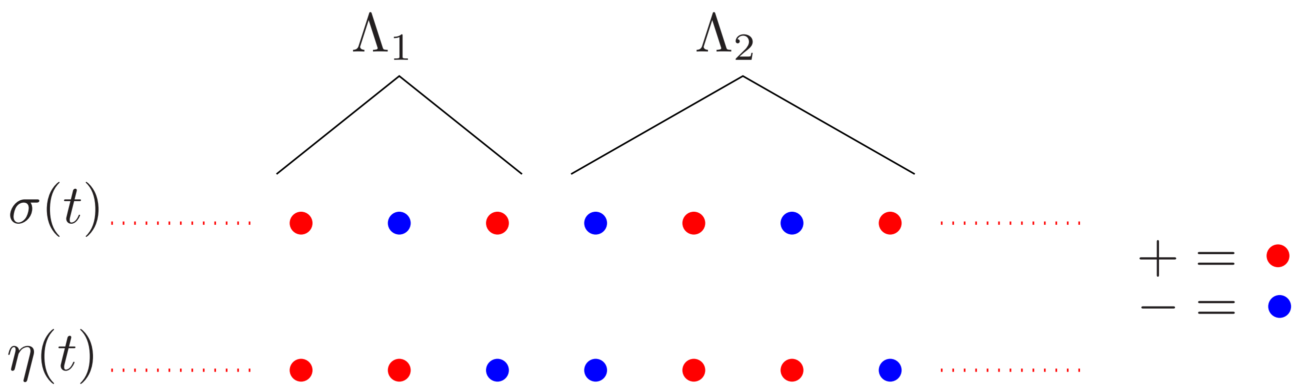
Define as before $\boldsymbol{m}(\sigma) = (m_1(\sigma), \dots, m_n(\sigma))$ and recall that

$$H_N(\sigma) = H_N(\boldsymbol{m}(\sigma)) = -(\sum_{i=1}^{n} m_i(\sigma))^2 - \sum_{i=1}^{n} a_i m_i$$

$\Longrightarrow$ *the microscopic dynamics only depends on the mesoscopic variables* $\boldsymbol{m}$.

Construction of the coupling: a simple case

Let $\boldsymbol{\sigma}$, $\boldsymbol{\eta} \in \boldsymbol{S}[\boldsymbol{m}^*]$ and assume that at time t, $\boldsymbol{m}(\sigma(t)) = \boldsymbol{m}(\eta(t))$.



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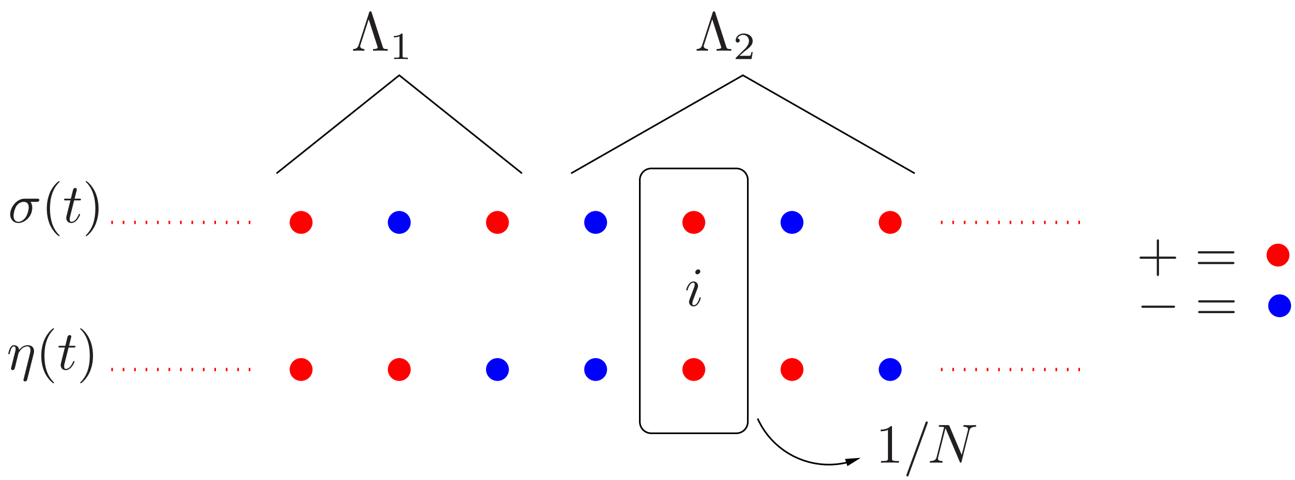

Choose a particle i u.a.r. (with prob$= 1/N$).

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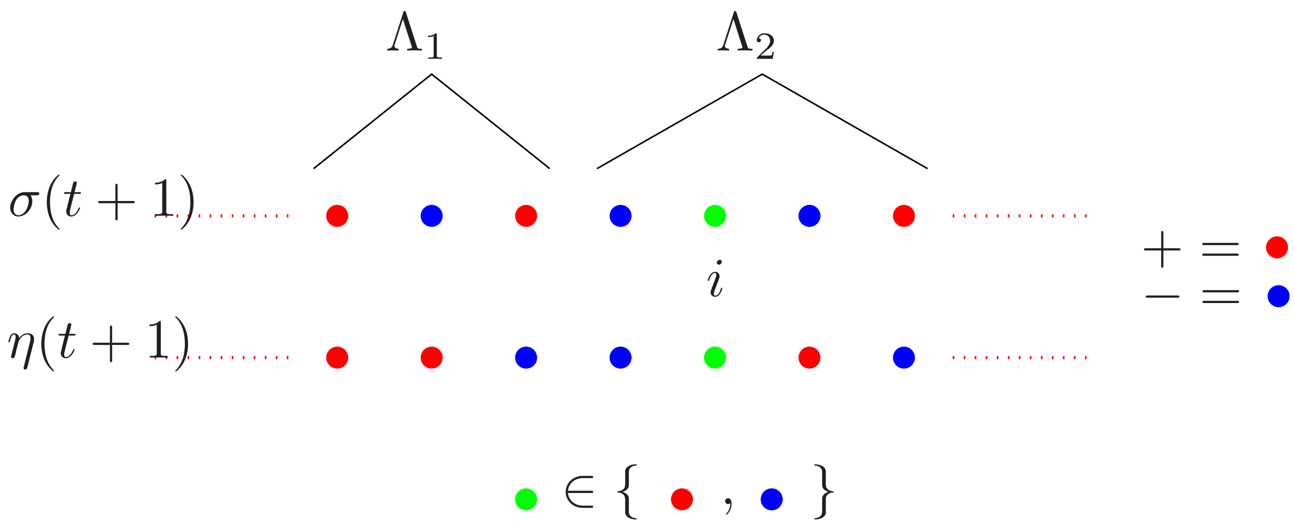

If $\sigma_i(t) = \eta_i(t) \implies \sigma_i(t+1) = \eta_i(t+1)$ with probability one.

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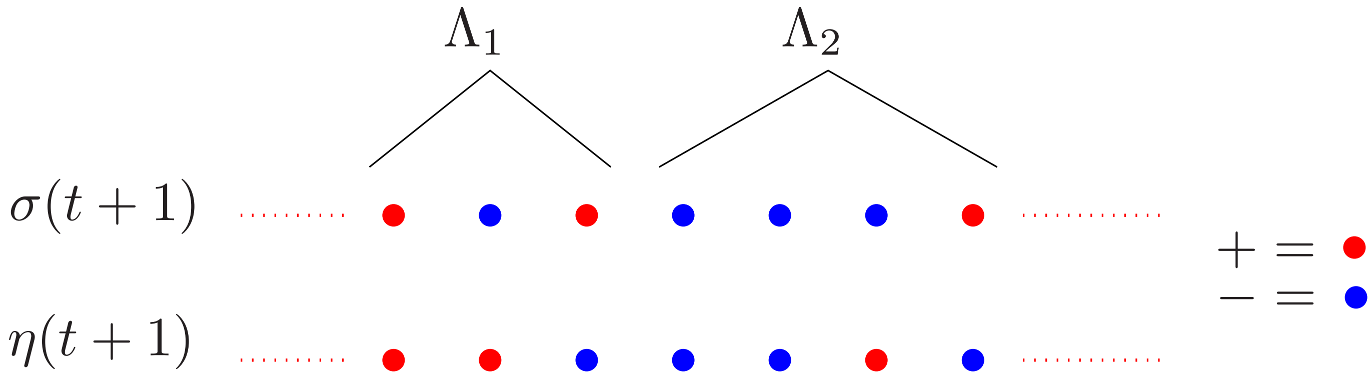

For example, update to $\sigma_i(t+1) = \eta_i(t+1) = -$ with probability

$$p(\sigma(t), \sigma^{i,-}(t)) = p(\eta(t), \eta^{i,-}(t))$$

Construction of the coupling: a simple case

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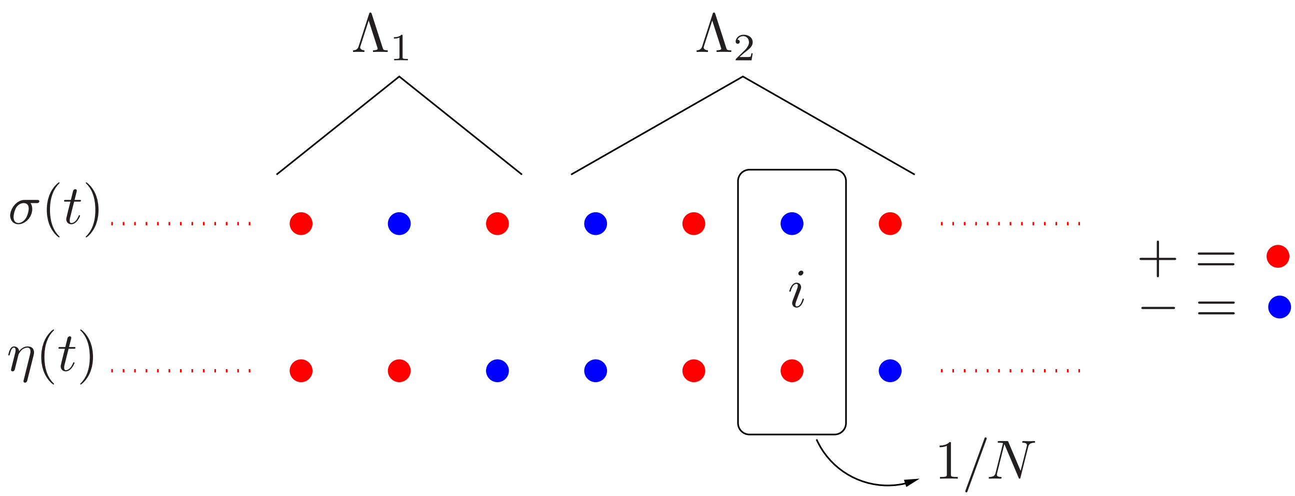

If $\sigma_i(t) \neq \eta_i(t) \implies$

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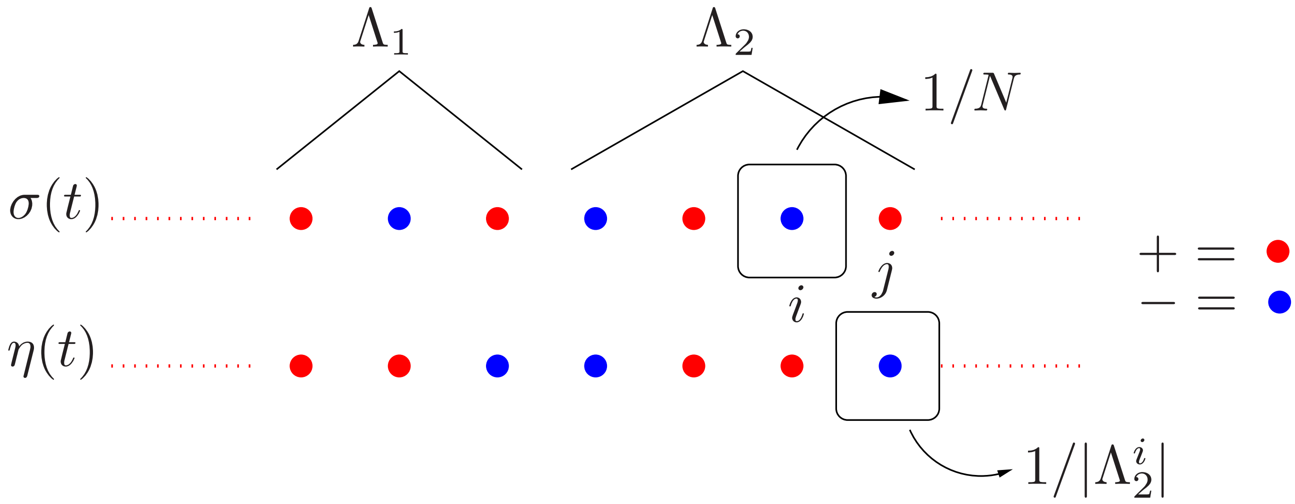

Choose, u.a.r, a particle j s.t. $i, j \in \Lambda_k$ and $\sigma_i(t) = \eta_j(t)$.

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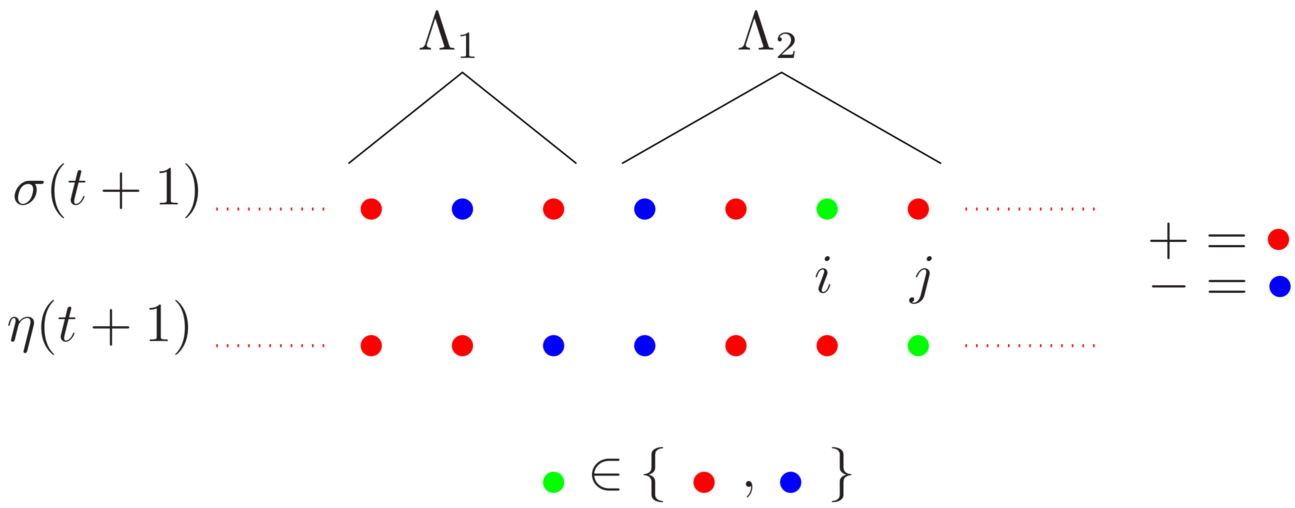

Then let $\sigma_i(t+1) = \eta_j(t+1)$ with probability one.

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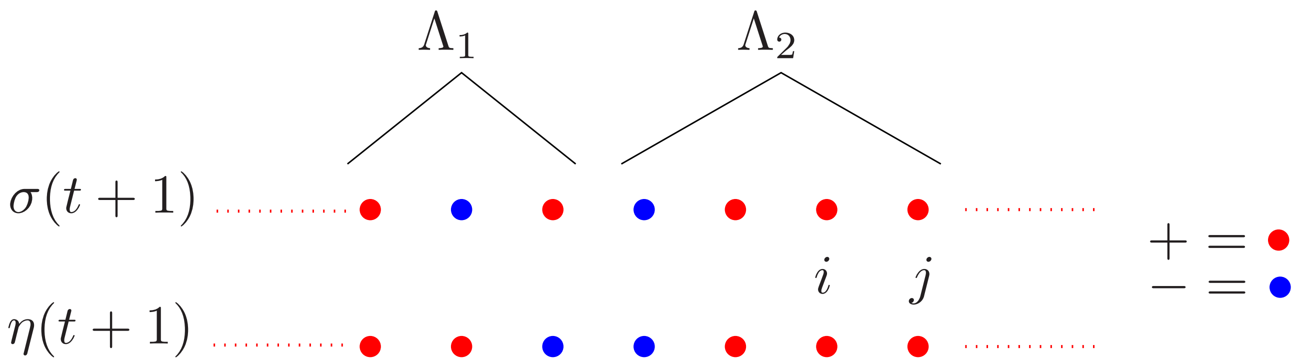

For example, update to $\sigma_i(t+1) = \eta_j(t+1) = +$ with probability

$$p(\sigma(t), \sigma^{i,+}(t)) = p(\eta(t), \eta^{j,+}(t))$$

Notice that along the coupling, $d(\sigma(t), \eta(t))$ never increases.

In particular

$$\mathbb{E}(d(\sigma(t), \eta(t))) \leq N e^{-ct/N}$$

which implies that the processes $\sigma(t)$ and $\eta(t)$ couple in time of order $N \log N$.

Idea: Extend this coupling to the general case (continuous random fields) using the many returns of the dynamics to $S[\boldsymbol{m}^*]$ before hitting $S[M]$.

Extended coupling

- Let h_i's i.i.d continuous variables.
- Fix $n \in \mathbb{N}$ large enough, and define $\boldsymbol{m}(\sigma)$ as usually.

Notice that the dynamics depends on the specific choice of $i \in \Lambda_k$ where the configuration is updated, and not only from Λ_k as before.

On the other hand, the variation of the h_i's in any Λ_k is of order $\epsilon = c/n$.
Then for all $\sigma, \eta \in S[\boldsymbol{m}]$ and $i, j \in \Lambda_k$,

$$|p(\sigma, \sigma^i) - p(\eta, \eta^j)| \leq \epsilon$$

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- Let V_i, $i \in \mathbb{N}$, i.i.d. random variables, s.t.

$$\mathbb{P}(\boldsymbol{V_i} = \mathbf{1}) = \mathbf{1} - \mathbb{P}(\boldsymbol{V_i} = \mathbf{0}) = \mathbf{1} - \boldsymbol{\epsilon}.$$

Construction of the coupling: general case

Let $\sigma, \eta \in S[\boldsymbol{m}^*]$ and proceed as before, unless $\sigma_i(t) \neq \eta_i(t) \implies$ choose a particle j s.t. $i, j \in \Lambda_k$ and $\sigma_i(t) = \eta_j(t)$, and toss a coin corresponding to a variable $V_{i(t)}$.

- if $V_{i(t)} = 1$, then let $\sigma_i(t+1) = \eta_j(t+1)$ with probability one.
- if $V_{i(t)} = 0$, then let $\sigma_i(t+1) \neq \eta_j(t+1)$ with probability one (suitable choice of rates).

Warning: it may happens that $\boldsymbol{m}(\sigma(t)) \neq \boldsymbol{m}(\eta(t))$ for some t.

How to proceed?

- Stop the coupling and let the dynamics $\sigma(t)$ run until the first hitting time in $S[\boldsymbol{m}^*]$.

- Make a second attempt of coupling between $\sigma(\tau_{S[\boldsymbol{m}^*]})$ and η, proceeding as before.

- Do this iteratively until the stopping time

$$\boldsymbol{T} := \boldsymbol{\tau}^{\boldsymbol{\sigma}}_{\boldsymbol{S}[\boldsymbol{M}]} \wedge \boldsymbol{\tau}^{\boldsymbol{\eta}}_{\boldsymbol{S}[\boldsymbol{M}]}$$

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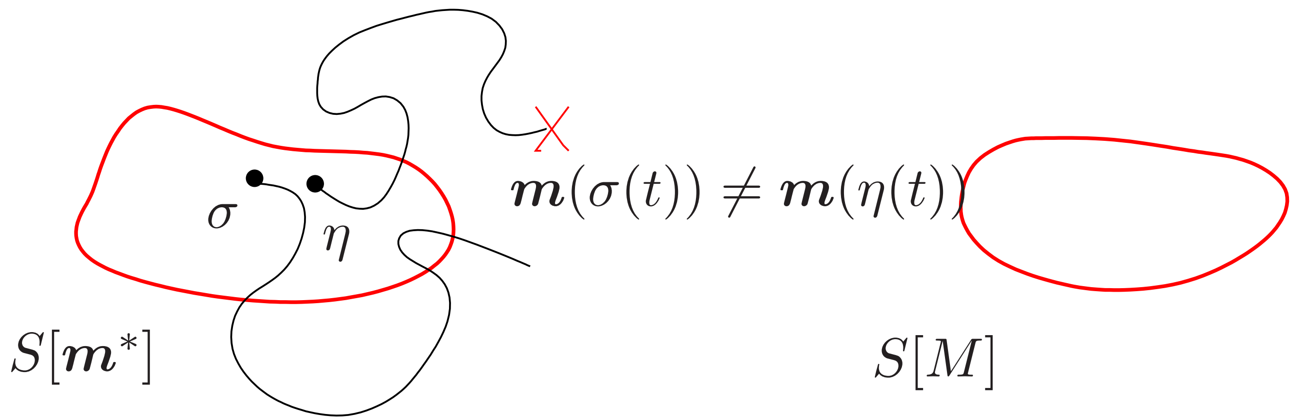

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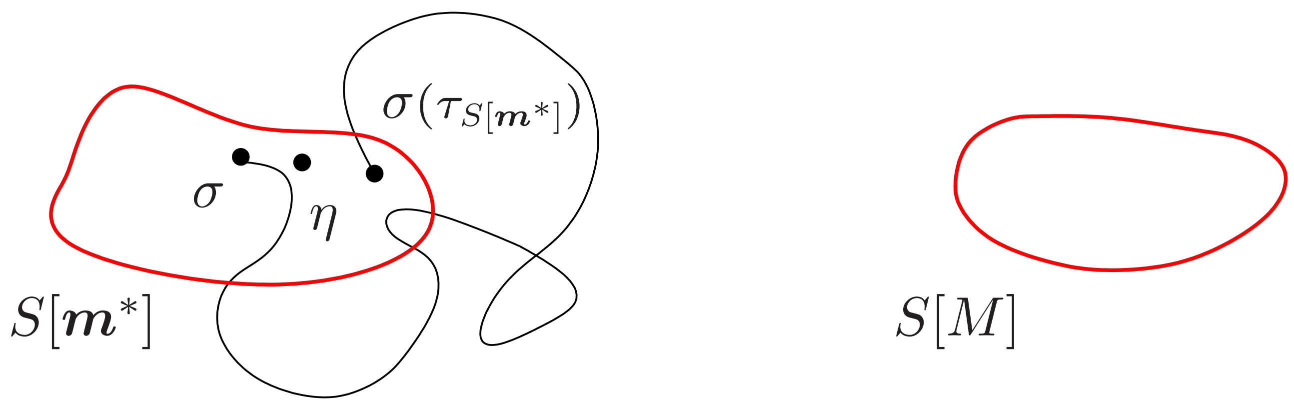

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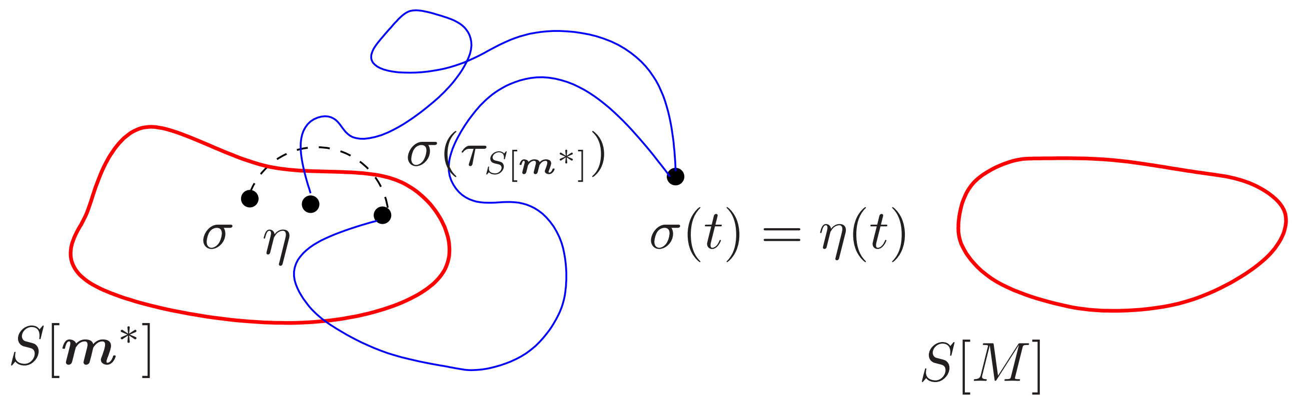

Good and bad events

- If $\boldsymbol{\tau_{\text{coup}} \ll T \implies \mathbb{E}_\sigma \tau_{S[M]} = \mathbb{E}_\eta \tau_{S[M]}(1 + o(1))}$

- The probability of the event $E = \{\tau_{\text{coup}} \ll T\}$ is estimated from below by the probability of an event $F \subset E$.

- Due to the particular construction of the coupling, F is defined as intersection of independent events. Their probability can then be easily computed.

- For all n large enough, $\mathbb{P}(E) \xrightarrow{N \uparrow \infty} 1$. This concludes the proof.

Thank you for your attention!