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

Alessandra Bianchi
(in collaboration with A. Bovier and D. Ioffe)

Work supported by the Germany Israeli Foundation

November 17, 2008
Outline

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The RFCW model

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- Energy landscape and metastability.
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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*. 
Motivation

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 model and the dynamics

**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

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

$h_i, i \in \mathbb{N}$ are i.i.d. (continuous) random variables called external fields.
The model and the dynamics

**The Random Field Curie-Weiss (RFCW) model**

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

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

  $$\mu_N(\sigma) = \frac{e^{-\beta H_N(\sigma)}}{Z_N}$$
The model and the dynamics

**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. \(\mu_N\).

**Generator:**

\[
(Lf)(\sigma) = \sum_{i=1}^{N} p(\sigma, \sigma^i) (f(\sigma^i) - f(\sigma))
\]

where

\[
p(\sigma, \sigma^i) = \frac{1}{N} e^{-\beta[H_N(\sigma^i) - H_N(\sigma)]_+}
\]

are the **Metropolis transition probabilities**.
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. \( \mu_N \).

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

where

\[
p(\sigma, \sigma^i) = \frac{1}{N} e^{-\beta[H_N(\sigma^i) - H_N(\sigma) + \beta]} + \text{Metropolis transition probabilities.}
\]

• 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 and metastability

**Energy landscape**

**Macroscopic parameter:**
Define the magnetization
\[ m_N(\sigma) = \frac{1}{N} \sum_{i=1}^{N} \sigma_i \]
taking value on
\[ \Gamma_N = \{-1, -1 + 2/N, \ldots, +1\} \]
Energy landscape and metastability

Energy landscape

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

A simple case: \( h = \) constant

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

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

- The critical points of \( F_N(m) \) satisfy \( m^* = \tanh(\beta(h + m^*)) \).
A simple example: \( h = \text{constant} \)

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

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
  
  $$ Q_N(m) = K_N(m) \frac{e^{-N\beta F_N(m)}}{Z_N} (1 + o(1)) , $$

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

- Asymptotically and $\mathbb{P}_h$-a.s, the critical points of $F_N$ are solutions of
  
  $$ m^* = \mathbb{E}_h \tanh(\beta (m^* + h_i)) $$
Energy landscape and metastability

General case: $h_i$’s i.i.d. continuous random variables

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

Second Workshop on Random Dynamical Systems, Bielefeld, 17-19 Nov. 2008
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 \( \mathbb{E}_\sigma\tau_{S[M]} \) for \( \sigma \in S[m^*] \)?
Metastable time: results

Example of energy landscape
Metastable time: results

Example of energy landscape
Mean metastable time

Following the potential theory approach:

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

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

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

Potential theory approach

Preliminary tools:

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

\( L = P - I \) generator of the dynamics

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

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

Probabilistic interpretation: if \( \sigma \notin A \cup B \) then

\[
h_{A,B}(\sigma) = \mathbb{P}_\sigma[\tau_A < \tau_B]
\]

\( \implies \) formula for the mean metastable time from \( A \) to \( B \), i.e.
Preliminary tools

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

$$E_{\nu} \tau_B \equiv \sum_{\sigma \in A} \nu(\sigma) E_{\sigma} \tau_B = \frac{1}{\text{cap}(A,B)} \mu_N(h_{A,B})$$

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

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

More explicitly:

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

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More explicitly:

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Thus we need

- precise control of capacities.
- some rough control of the equilibrium potential.
Two variational principles for capacities

**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*,

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

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*

$\rightarrow$ 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],

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

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.
Application to the RFCW model

RFCW model: Coarse graining

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

Order parameters:

\[
m_k(\sigma) = \frac{1}{N} \sum_{i \in \Lambda_k} \sigma_i, \quad \mathbf{m}(\sigma) = (m_k(\sigma))_{k=1}^n
\]
Application to the RFCW model

**RFCW model: Coarse graining**

- $I_k, k \in \{1, \ldots, n\}$: partition of the support of $h$.
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**Order parameters:**

\[ m_k(\sigma) = \frac{1}{N} \sum_{i \in \Lambda_k} \sigma_i, \quad m(\sigma) = (m_k(\sigma))_{k=1}^n \]

**Example:**

\[
\begin{array}{ccc}
| & | & |
\end{array}
\begin{array}{ccc}
| & | & |
\end{array}
\begin{array}{ccc}
| & | & |
\end{array}
\begin{array}{ccc}
| & | & |
\end{array}
\]

\[
\begin{array}{ccc}
- & - & - \\
- & - & - \\
- & + & + \\
+ & + & + \\
\end{array}
\]

$N = 10, \ n = 4$

\[
m(\sigma) = (-\frac{1}{5}, -\frac{1}{10}, \frac{1}{10}, 0)
\]

\[
m(\sigma) = \sum_{i=1}^n m_i(\sigma) = -\frac{1}{5}
\]
Application to the RFCW model

⇒ Rewrite the Hamiltonian as

\[ H_N(\sigma) = -NE(m(\sigma)) + \sum_{k=1}^{n} \sum_{i \in \Lambda_k} \sigma_i \tilde{h}_i \]
Application to the RFCW model

⇒ Rewrite the Hamiltonian as

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

• \( E(m) = \frac{1}{2} (\sum_{k=1}^{n} m_k)^2 + \sum_{k=1}^{n} \tilde{h}_k m_k \)
Application to the RFCW model

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Application to the RFCW model

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

- $E(m) = \frac{1}{2} (\sum_{k=1}^{n} m_k)^2 + \sum_{k=1}^{n} \bar{h}_k m_k$
- $\tilde{h}_i = h_i - \bar{h}_k, i \in \Lambda_k$. Note $|\tilde{h}_i| \leq c/n \equiv \epsilon$
Application to the RFCW model

⇒ Rewrite the Hamiltonian as

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

• \(E(m) = \frac{1}{2} (\sum_{k=1}^{n} m_k)^2 + \sum_{k=1}^{n} \tilde{h}_k m_k\)

• \(\tilde{h}_i = h_i - \bar{h}_k, i \in \Lambda_k\). Note \(|\tilde{h}_i| \leq c/n \equiv \epsilon\)

Strategy: Analyze the metastable behavior of the model as a perturbation of the model: \(H_N(\sigma) = -NE(m(\sigma))\).
Application to the RFCW model

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

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

- Using super-harmonic functions techniques, we get

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

Altogether, taking $n$ large enough, we get

$$\mathbb{E}_\nu \tau_B = K(m^*, z^*) e^{\beta N (F_N(z^*) - F_N(m^*))} (1 + o(1))$$
Heuristics and results

From average to pointwise estimates

Questions:

• Does the metastable time really depend on the last exit measure \( \nu \)?

• Under which conditions can we deduce pointwise estimates?

• Can we say something about the distribution?
Heuristics and results

From average to pointwise estimates

Questions:

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

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 and results

Heuristics:
The time spent in the starting well before reaching $B$ is much larger than 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] \( \mathbb{P}_h \text{-a.s.}, \) for all \( n \geq n_0 \) and for all \( \sigma, \eta \in S[m^*] \),

\[
\mathbb{E}_\sigma \tau_{S[M]} = \mathbb{E}_\eta \tau_{S[M]} (1 + o(1)).
\]

In particular, for all \( \sigma \in S[m^*] \), \( \mathbb{E}_\sigma \tau_{S[M]} = \mathbb{E}_\nu \tau_{S[M]} (1 + o(1)) \)
Heuristics and results

Consequences

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

**Corollary 1.** Let \( m_1 \) and \( m_2 \) be two minima of \( F_N(m) \), let \( z^* \) be the minmax between them. Assume \( F_N(m_1) \geq F_N(m_2) \).

Then \( P_h \)-a.s., for all \( \sigma \in S[m_1] \),

\[
\mathbb{E}_{\sigma \tau_{S[m_2]}} = c(m_1, m_2) e^{\beta N (F_N(m_1) - F_N(m_2))} (1 + o(1))
\]
Heuristics and results

Consequences

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

**Corollary 1.** Let $m_1$ and $m_2$ be two minima of $F_N(m)$, let $z^*$ be the minmax between them. Assume $F_N(m_1) \geq F_N(m_2)$. Then $P_h$-a.s., for all $\sigma \in S[m_1],$

$$\mathbb{E}_\sigma \tau_{S[m_2]} = c(m_1, m_2)e^{\beta N(F_N(m_1)-F_N(m_2))}(1 + o(1)).$$

• **Distribution** of the metastable time: work in progress.
Coupling in potential wells


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

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Generalization to the RFCW model. A simple case
Assume that fields take only finitely many values, i.e. \(h_i \in \mathcal{A} = \{a_1, \ldots, a_n\}\). Define as before \(m(\sigma) = (m_1(\sigma), \ldots, m_n(\sigma))\) and recall that

\[
H_N(\sigma) = H_N(m(\sigma)) = -\left(\sum_{i=1}^{n} m_i(\sigma)\right)^2 - \sum_{i=1}^{n} a_i m_i
\]

\(\Rightarrow\) the microscopic dynamics only depends on the mesoscopic variables \(m\).
Coupling in potential wells

Construction of the coupling: a simple case

Let $\sigma, \eta \in S[m^*]$ and assume that at time $t$, $m(\sigma(t)) = m(\eta(t))$.
Coupling in potential wells

Construction of the coupling: a simple case

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

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

Construction of the coupling: a simple case

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

$$\sigma(t + 1) = \Lambda_1$$
$$\eta(t + 1) = \Lambda_2$$

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

Construction of the coupling: a simple case

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

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

\[
p(\sigma(t), \sigma^i,-(t)) = p(\eta(t), \eta^i,-(t))
\]
Coupling in potential wells

Construction of the coupling: a simple case

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

If $\sigma_i(t) \neq \eta_i(t) \implies$
Coupling in potential wells

Construction of the coupling: a simple case

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

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

Construction of the coupling: a simple case

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

\[
\begin{array}{c}
\sigma(t+1) & \Lambda_1 & \eta(t+1) \\
\Lambda_2 & \Lambda_2 \\
i & j & + = \bullet \\
\end{array}
\]

\( \in \{ \bullet, \bullet, \bullet \} \)

Then let \( \sigma_i(t+1) = \eta_j(t+1) \) with probability one.
Coupling in potential wells

Construction of the coupling: a simple case

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

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

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

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

In particular

\[
\mathbb{E}(d(\sigma(t), \eta(t))) \leq Ne^{-ct/N}
\]

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 \( S[m^*] \) before hitting \( S[M] \).
Coupling in potential wells

Extended coupling

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

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

$$|p(\sigma, \sigma^i) - p(\eta, \eta^j)| \leq \epsilon$$
Coupling in potential wells

**Extended coupling**

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- Fix $n \in \mathbb{N}$ large enough, and define $m(\sigma)$ as usually.

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On the other hand, the variation of the $h_i$'s in any $\Lambda_k$ is of order $\epsilon = c/n$.

Then for all $\sigma, \eta \in S[m]$ and $i, j \in \Lambda_k$,

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

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

$$\mathbb{P}(V_i = 1) = 1 - \mathbb{P}(V_i = 0) = 1 - \epsilon.$$
Coupling in potential wells

Construction of the coupling: general case

Let $\sigma, \eta \in S[m^*]$ 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 happen that $m(\sigma(t)) \neq m(\eta(t))$ for some $t$. 
Coupling in potential wells

How to proceed?

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

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

• Do this iteratively until the stopping time

$$T := \tau_{S[M]}^\sigma \wedge \tau_{S[M]}^\eta$$
Coupling in potential wells

How to proceed?

\[ S[m^*] \]

\[ S[M] \]
Coupling in potential wells

How to proceed?

\[ S[m^*] \quad \times \quad m(\sigma(t)) \neq m(\eta(t)) \quad S[M] \]
Coupling in potential wells

How to proceed?

$S[m^*] \rightarrow \sigma(\tau S[m^*]) \rightarrow S[M]$
Coupling in potential wells

How to proceed?

\[
\sigma(t) = \eta(t)
\]
Coupling in potential wells

Good and bad events

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

• 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!