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Quasi-stationary measures and metastability

Alessandra Bianchi
Department of Mathematics, University of Padova

in collaboration with A. Gaudillière (Marseille)

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Outline

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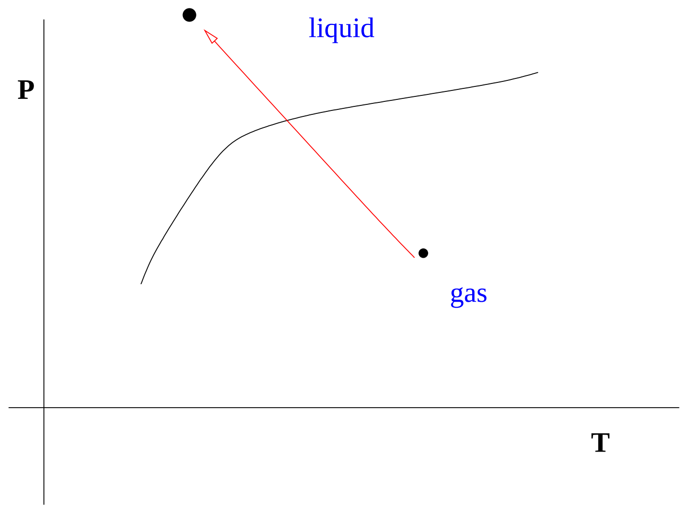
   - Markovian models.
   - Metastable state: restricted ensemble and quasi stationary measure
2. Exit time: law and sharp average estimates
   - Exponential law of the exit time.
   - Sharp estimates on average exit time and relaxation time.
   - Example: Curie-Weiss model.
3. Escape from metastability
   - Soft measures as generalization of quasi-stationary measures.
   - Transition times and mixing time asymptotics.

Metastable systems

Metastability is a common dynamical phenomenon related to *first order phase transition*.



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

Main features: This transition takes a long time, while the system stays in an apparent equilibrium.

Rigorous description

Due to the work of Lebowitz & Penrose (*J. Stat. Phys.*, **3**, 1971):

"We shall characterize metastable thermodynamic states by the following properties:

(a) only one thermodynamic phase is present,
(b) a system that starts in this state is likely to take a long time to get out,
(c) once the system has gotten out, it is unlikely to return. "

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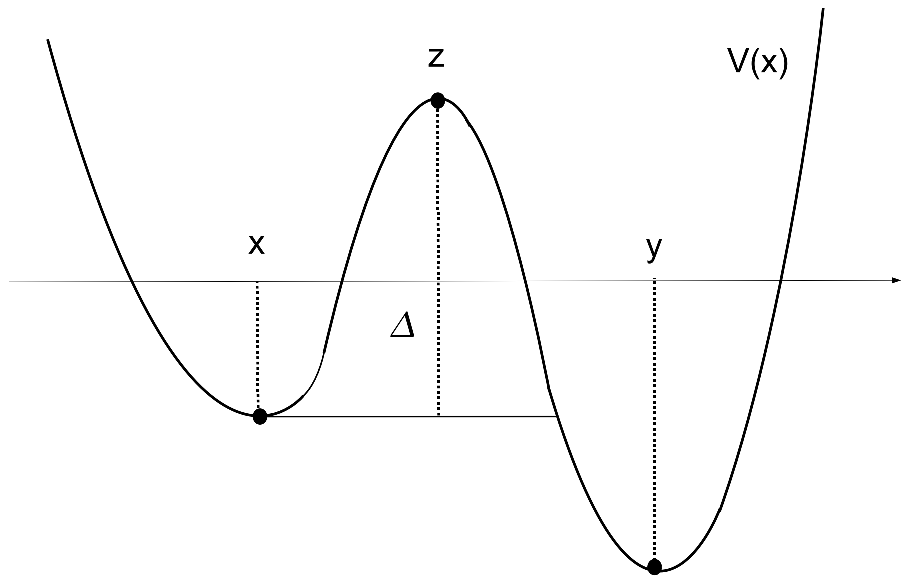
one phase of metastable state $\longrightarrow$ region $\mathcal{R} \subset \mathcal{X}$ of the phase space
metastable state $\longrightarrow$ $\mu_{\mathcal{R}} = \mu(\cdot|\mathcal{R})$, the restricted ensemble.

Main question: Show properties (b) and (c) by analyzing the exit time from $\mathcal{R}$: $\mathcal{T}_{\mathcal{R}^c}$.

Metastability in stochastic dynamics

Previous results and techniques

A simple example: Let $X_t \in \mathbb{R}$ solution of $\qquad dX_t = -V'(X_t) + \sqrt{2\varepsilon}\, dW_t$



- Large deviations techniques [Freidlin, Wentzell ('84)]:

$$(1) \quad \lim_{\varepsilon\to 0} \varepsilon \log \mathbb{E}_x \mathcal{T}_y = \Delta \qquad (2) \quad \lim_{\varepsilon\to 0} \mathbb{P}_x \left(\frac{\mathcal{T}_y}{\mathbb{E}_x \mathcal{T}_y} > t \right) = e^{-t}$$

- Pathwise approach[Cassandro, Galves, Olivieri, Vares ('84)]:
  It focuses on typical trajectories and exponential law of the exit time.
  By LD techniques, it provides (1)-(2). Developed and generalized in many ways: [Neves, Schonmann ('92)], [Ben Arous, Cerf ('96)], [Schonmann, Shlosman ('98)], [Gaudillière, Olivieri, Scoppola ('05)].

- Potential theoretic approach [Bovier, Eckhoff, Gayrard, Klein ('01-'04)]:
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Our main goal: *Give a different description of metastable state and find simple hypotheses to get sharp estimates on the average exit time and prove its exponential law.*

Markovian Models

Markov process $X = (X_t)_{t\in\mathbb{R}}$ on a finite set $\mathcal{X}$ with generator

$$\mathcal{L}f(x) = \sum_{y\in\mathcal{X}} p(x,y)(f(y) - f(x))$$

For $\mathcal{R} \subset \mathcal{X}$ metastable set, let $X_{\mathcal{R}}$ ($X_{\mathcal{R}^c}$) be the reflected process on $\mathcal{R}$ ($\mathcal{R}^c$).
Assume:

1) X *irreducible* and *reversible* w.r.t μ;
2) $X_{\mathcal{R}}$, $X_{\mathcal{R}^c}$ *irreducible* $\longrightarrow$ *reversible* w.r.t. $\mu_{\mathcal{R}}$ and $\mu_{\mathcal{R}^c}$.

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- Consider the sub-Markovian kernel on $\mathcal{R}$

$$r^*(x,y) = p(x,y), \quad \text{for all } x,y \in \mathcal{R}$$

and let $\quad e_{\mathcal{R}}(x) = \sum_{y\notin\mathcal{R}} p(x,y) \quad$ (escape probability from $\mathcal{R}$).

Quasi-stationary measure

From Perron-Frobenius Theorem and Darroch & Seneta('62):

- $\exists$ a measure $\mu^*_{\mathcal{R}}$ on $\mathcal{R}$, called **quasi stationary measure** defined as

$$\mu^*_{\mathcal{R}}(y) = \lim_{t\to\infty} \mathbb{P}_x(X(t) = y | \mathcal{T}_{\mathcal{R}^c} > t) \qquad \text{Yaglom limit}$$

- Moreover $\exists \phi^* > 0$ s.t.

1. $\mu^*_{\mathcal{R}} r^* = (1-\phi^*)\mu^*_{\mathcal{R}}$ $\longrightarrow$ left eigenvector
2. $\mathbb{P}_{\mu^*_{\mathcal{R}}}(\mathcal{T}_{\mathcal{R}^c} > t) = e^{-\phi^* t}$ $\longrightarrow$ exponential law
3. $\mathbb{E}_{\mu^*_{\mathcal{R}}}(\mathcal{T}_{\mathcal{R}^c})^{-1} = \phi^* = \mu^*_{\mathcal{R}}(e_{\mathcal{R}})$ $\longrightarrow$ exponential rate .

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- Choose $\mu^*_{\mathcal{R}}$ instead of $\mu_{\mathcal{R}}$ in order to describe the metastable state.

Advantages and disadvantages.

- $\mu^*_{\mathcal{R}}$ immediately provides the exponential law of $\mathcal{T}_{\mathcal{R}}$, that in general is hard to deduce.
- $\mu^*_{\mathcal{R}}$ is not explicitly given, then preventing from getting quantitative estimates.

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Question: Are $\mu_{\mathcal{R}}^*$ and $\mu_{\mathcal{R}}$ very different?

Let $\gamma_{\mathcal{R}}$ be the spectral gap of $X_{\mathcal{R}}$ and define $\boldsymbol{\varepsilon_{\mathcal{R}} := \frac{\phi^*}{\gamma_{\mathcal{R}}}}$.

Proposition 1. *If $\varepsilon_{\mathcal{R}} < 1$, then*

$$\left\| \frac{\mu_{\mathcal{R}}^*}{\mu_{\mathcal{R}}} - 1 \right\|_{\mathcal{R},2}^2 \leq \frac{\varepsilon_{\mathcal{R}}}{1 - \varepsilon_{\mathcal{R}}}$$

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Remark. *Note that $\varepsilon_{\mathcal{R}} = \gamma_{\mathcal{R}}^{-1} / \mathbb{E}_{\mu^*_{\mathcal{R}}}(\mathcal{T}_{\mathcal{R}^c})$.*

For metastable systems, we expect $\varepsilon_{\mathcal{R}} \ll 1$ with some parameter of the system (e.g. size of the system $\to \infty$, $T \to 0$)

Exponential law of the exit time

Assume that $\varepsilon_{\mathcal{R}} \to 0$ and let $S_{\mathcal{R}} := \frac{1}{\gamma^*_{\mathcal{R}}} \ln \frac{2}{\delta(1-\delta)\zeta_{\mathcal{R}}}$ (local mixing time), with $\zeta_{\mathcal{R}} := \min_{x\in\mathcal{R}}\{{\mu^*_{\mathcal{R}}}^2(x)/\mu_{\mathcal{R}}(x)\}$, $\gamma^*_{\mathcal{R}}$ the spectral gap of r^*, and $\delta = O(\varepsilon_{\mathcal{R}})$.

THM 1. [Exponential law] *If $S_{\mathcal{R}} \cdot \phi^* = o(1)$ as $\varepsilon_{\mathcal{R}} \to 0$, then*

$$1) \quad \mathbb{E}_{\mu_{\mathcal{R}}}(\mathcal{T}_{\mathcal{R}^c}) = {\phi^*}^{-1}(1 + o(1))$$

$$2) \quad \mathbb{P}_{\mu_{\mathcal{R}}}(\mathcal{T}_{\mathcal{R}^c} > t \cdot {\phi^*}^{-1}) = e^{-t}(1 + o(1))$$

Remark. *In fact we can prove much more. We can consider general initial measure ν, and get exact corrective terms which are matching in the regime $S_{\mathcal{R}} \cdot \phi^* = o(1)$.*

Sharp average estimates

Recall that:

If $A, B \subset \mathcal{X}$, $A \cap B = \emptyset \implies \text{cap}(A, B) = \sum_{a \in A} \mu(a)\mathbb{P}_a(\tau_A^+ > \tau_B^+)$.

As shown in a series of papers by Bovier, Eckhoff, Gayrard & Klein ('01-'04), *capacities enter in the computation of the average exit time from A to B.*

Main advantage of capacities, is that they satisfy a two-sided variational principle

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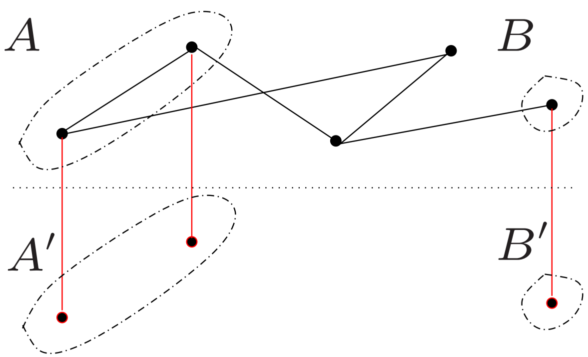
Generalized capacities
For $k, \lambda > 0$, define an extended system $\mathcal{X}' = \mathcal{X} \cup A' \cup B'$, A', B' copies of A, B.



$$c'(x, y) = c(x, y) = \mu(x)p(x, y)$$

$$c'(a, a') = k\mu(a)$$

$$c'(b, b') = \lambda\mu(b)$$

Definition ($\boldsymbol{k}, \boldsymbol{\lambda}$**-capacities**): $\text{cap}_{\boldsymbol{k}}^{\boldsymbol{\lambda}}(\boldsymbol{A}, \boldsymbol{B}) = \text{cap}(\boldsymbol{A}', \boldsymbol{B}')$.

When $\lambda = +\infty \longrightarrow B = B'$ and $\text{cap}_k^{\infty}(A, B) = \text{cap}_k(A, B)$.
In particular $\text{cap}_{\infty}^{\infty}(A, B) = \text{cap}(A, B)$.

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THM 2. [Mean exit time] *If $S_{\mathcal{R}} \cdot \phi^* = o(1)$ as $\varepsilon_{\mathcal{R}} \to 0$, and choosing $\phi^* \ll k \ll \gamma_{\mathcal{R}}$,*

$$\phi^{*-1} = \frac{\mu(\mathcal{R})}{\text{cap}_k(\mathcal{R},\mathcal{R}^c)}(1 + o(1))$$

Definition (k, λ-capacities): $\quad \text{cap}_k^{\lambda}(A, B) = \text{cap}(A', B')$.

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THM 3. [relaxation time] *If $S_{\mathcal{R}} \cdot \phi^* = o(1)$ and $S_{\mathcal{R}^c} \cdot \phi^{c*} = o(1)$ with $\varepsilon_{\mathcal{R}}, \varepsilon_{\mathcal{R}^c} \to 0$, and choosing $\phi^* \ll k \ll \gamma_{\mathcal{R}}$ and $\phi^{c*} \ll \lambda \ll \gamma_{\mathcal{R}^c}$, then*

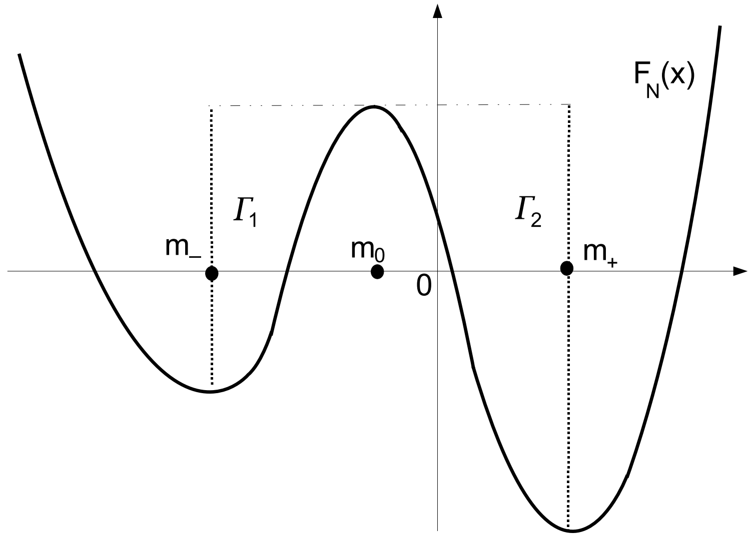
$$\mathcal{T}_{rel} \equiv \frac{1}{\gamma} = \frac{\mu(\mathcal{R})\mu(\mathcal{R}^c)}{\text{cap}_k^{\lambda}(\mathcal{R}, \mathcal{R}^c)}(1 + o(1))$$

A simple example: the Curie-Weiss model

Let $m \in \Gamma = \{-1, -1 + \frac{2}{N}, \ldots, 1\}$ (magnetization) a 1D-parameter

Let $\mu(m) \propto e^{-\beta N F_N(m)}$ the Gibbs measure on Γ and consider a dynamics reversible w.r.t. μ with transition rates $p(m, m^{\pm}) \propto e^{-\beta N \nabla_{\pm} F_N}$.

For some values of the parameters



Let $\mathcal{R} = \{\sigma \in \mathcal{X} : m_N(\sigma) \leq m_0\}$.

Questions:

1. Law and average of $\mathcal{T}_{\mathcal{R}^c}$ w.r.t. $\mu_{\mathcal{R}}$?
2. Relaxation time?

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We want to show that $\boldsymbol{\varepsilon_{\mathcal{R}}, \varepsilon_{\mathcal{R}^c} \xrightarrow[N\to\infty]{} 0}$ and $\boldsymbol{S_{\mathcal{R}} \cdot \phi^* = o(1)}$, $\boldsymbol{S_{\mathcal{R}^c} \cdot \phi^{c*} = o(1)}$.

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   and similarly $\phi^{c*} \leq e^{-\beta N \Gamma_2}$, with $\Gamma_1 < \Gamma 2$.

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2. ${\gamma_{\mathcal{R}}}^{-1} \leq \mathcal{T}^{\mathcal{R}}_{mix} \leq c(\beta) N^{3/2}$ $\longleftarrow$ argument used in [Levin,Luczak, Peres ('10)] .

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3. With the above estimates we get easily $S_{\mathcal{R}}, S_{\mathcal{R}^c} \leq c(\beta) N^3$.

$\longrightarrow$ Then the required hypotheses follow.

Second step: compute the capacities

We make use of the two-side variational principle over the capacities.
Test functions and flows are provided by the 1D process over the magnetizations, where capacities can be computed explicitly.

Then, for all $\phi^*_{\mathcal{R}} \ll k \ll \gamma_{\mathcal{R}}$ and $\phi^*_{\mathcal{R}^c} \ll \lambda \ll \gamma_{\mathcal{R}^c}$

1. $\text{cap}_k(\mathcal{R}, \mathcal{R}^c) = \frac{1}{Z_N} \cdot \frac{1}{\sqrt{\pi N}} c(m_0) e^{-\beta N f_N(m_0)}(1 + o(1))$,

2. $\text{cap}_k^{\lambda}(\mathcal{R}, \mathcal{R}^c) = \frac{1}{Z_N} \cdot \frac{1}{2\sqrt{\pi N}} c(m_0) e^{-\beta N f_N(m_0)}(1 + o(1))$,

where $c(m_0) = \sqrt{(1 - {m_0}^2)|f''_N(m_0)|}$.

The result

From Theorems 1.,2. and 3., it holds

(i) $\mathcal{T}_{\mathcal{R}^c}$ has asymptotic exponential law w.r.t. $\mu_{\mathcal{R}}$ with mean

$$\mathbb{E}_{\mu_{\mathcal{R}}}(\mathcal{T}_{\mathcal{R}^c}) = \frac{\pi N}{\beta c(m_0)c(m_-)} e^{\beta N \Gamma_1}(1 + o(1))$$

(ii) The relaxation time γ^{-1} is given by

$$\gamma^{-1} = \frac{2\pi N}{\beta c(m_0)c(m_-)} e^{\beta N \Gamma_1}(1 + o(1))$$

Soft measure and escape from metastability

Recall property (c) of Lebowitz & Penrose:

"once the system has gotten out, it is unlikely to return "

What does it mean "to get out" from $\mathcal{R}$? Exit from $\mathcal{R}$?
When the system just exited $\mathcal{R}$, the probabilities to go back to $\mathcal{R}$ or proceed in $\mathcal{R}^C$ are equal, and (c) fails.

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Main Idea

If the dynamics spends in $\mathcal{R}^c$ a time $\geq S_{\mathcal{R}^c}$ (local mixing in $\mathcal{R}^c$) then it is close to $\mu^*_{\mathcal{R}^c}$.

$$\Longrightarrow$$

Define the "true escape from $\mathcal{R}$" as the first time that the "dynamics on $\mathcal{R}$" makes an excursion in $\mathcal{R}^c$ of order $\geq S_{\mathcal{R}^c}$.

Formally:

- For any $\lambda > 0$ and $\sigma_\lambda \sim \exp(\lambda)$ indep. of X, sub-Markovian kernel on $\mathcal{R}$:

$$\boldsymbol{r}^*_{\boldsymbol{\lambda}}(\boldsymbol{x},\boldsymbol{y}) = \mathbb{P}_{\boldsymbol{x}}(\boldsymbol{X}(\boldsymbol{\tau}^+_{\mathcal{R}}) = \boldsymbol{y}, \boldsymbol{L}_{\mathcal{R}^c}(\boldsymbol{\tau}^+_{\mathcal{R}}) \le \boldsymbol{\sigma}_{\boldsymbol{\lambda}})$$

where L_A = local time in $A \subset \mathcal{X}$ and G_A its right-continuous inverse.

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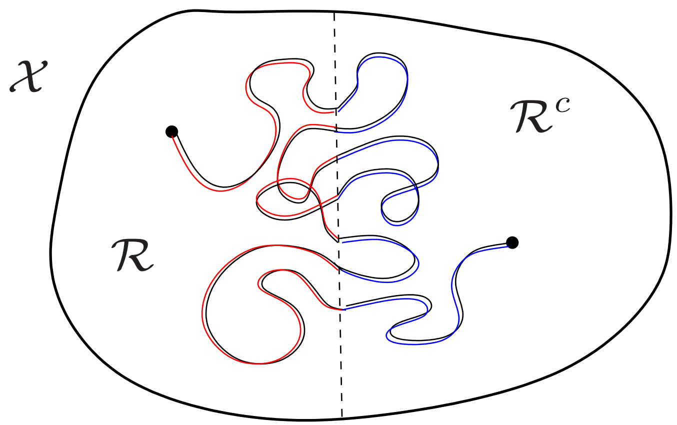
- Define the transition time: $\mathcal{T}_{\mathcal{R}^c,\lambda} = L_{\mathcal{R}}(G_{\mathcal{R}^c}(\sigma_\lambda))$



σ_λ = length of blue-path

$G_{\mathcal{R}^c}(\sigma_\lambda)$ = length of black-path

$\mathcal{T}_{\mathcal{R}^c,\lambda}$ = length of red-path

By similar arguments to those used for the analysis of r^*, we define the **soft measure** $\boldsymbol{\mu^*_{\mathcal{R},\lambda}}$ on $\mathcal{R}$ as

$$\mu^*_{\mathcal{R},\lambda}(y) = \lim_{t\to\infty} \mathbb{P}_x(X(G_{\mathcal{R}}(t)) = y | \mathcal{T}_{\mathcal{R}^c,\lambda} > t)$$

It turns out that $\exists \phi^*_\lambda > 0$ *s.t.*

1. $\mu^*_{\mathcal{R},\lambda} r^*_\lambda = (1 - \phi^*_\lambda)\mu^*_{\mathcal{R},\lambda}$ $\longrightarrow$ *left eigenvector*
2. $\mathbb{P}_{\mu^*_{\mathcal{R},\lambda}}(\mathcal{T}_{\mathcal{R}^c,\lambda} > t) = e^{-\phi^*_\lambda t}$ $\longrightarrow$ *exponential law*
3. $\mathbb{E}_{\mu^*_{\mathcal{R},\lambda}}(\mathcal{T}_{\mathcal{R}^c,\lambda})^{-1} = \phi^*_\lambda = \mu^*_{\mathcal{R},\lambda}(e_{\mathcal{R},\lambda})$ $\longrightarrow$ *average time*

Remark 1. $\mu^*_{\mathcal{R},\lambda}$ *is continuous interpolation between* $\mu_{\mathcal{R}} = \mu^*_{\mathcal{R},0}$ *and* $\mu^*_{\mathcal{R}} = \mu^*_{\mathcal{R},\infty}$.

Remark 2. The same construction can be done for the dynamics on $\mathcal{R}^c$: For $k > 0$ and taking a time ($\mathcal{R}$)-excursion bound of $\sigma_k \sim \exp(k)$, we construct $\mu^*_{\mathcal{R}^c,k}$.

Transition time and mixing time

THM 4. *All the results proved for* $\mathcal{T}_{\mathcal{R}^c}$ *and* ϕ^**, hold for* $\mathcal{T}_{\mathcal{R}^c,\lambda}$ *and* ϕ^*_λ *under analogous hypotheses (*$\varepsilon_\mathcal{R} \ll 1$ *and* $S_{\mathcal{R},\lambda} \cdot \phi^*_\lambda = o(1)$ *as* $\varepsilon_\mathcal{R} \to 0$*).*
In particular:

1. $\mathcal{T}_{\mathcal{R}^c,\lambda}$ *has asymptotic exponential law w.r.t.* $\mu_\mathcal{R}$*, with rate* ϕ^*_λ
2. ϕ^*_λ *satisfied sharp asymptotics expressed in term of capacity*

Transition time and mixing time

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2. ϕ^*_λ *satisfied sharp asymptotics expressed in term of capacity*

From 1. *and* 2.

$$\mathbb{E}_{\mu_{\mathcal{R}}}(\mathcal{T}_{\mathcal{R}^c,\lambda}) = {\phi^*_\lambda}^{-1}(1+o(1)) = \frac{\mu(\mathcal{R})}{\text{cap}_k^\lambda(\mathcal{R},\mathcal{R}^c)}(1+o(1))$$

Moreover, the truly escape from $\mathcal{R}$ is given by the time $G_{\mathcal{R}^c}(\sigma_\lambda)$, (*first excursion* $\sim \sigma_\lambda$) for $\lambda = O(S^{-1}_{\mathcal{R}^c,0})$. Indeed it holds, for all $x \in \mathcal{X}$,

$$\begin{cases} \|\mathbb{P}_x(X(G_{\mathcal{R}^c}(\sigma_\lambda)) = \cdot\,) - \mu_{\mathcal{R}^c}\|_{\mathsf{TV}} \leq \lambda S_{\mathcal{R}^c,0} + o(1) \\ \\ \|\mathbb{P}_x(X(G_{\mathcal{R}^c}(\sigma_\lambda)) = \cdot\,) - \mu\|_{\mathsf{TV}} \leq \mu(\mathcal{R}) + \lambda S_{\mathcal{R}^c,0} + o(1) \end{cases}$$

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THM 5. [mixing time] *If* $S_{\mathcal{R}} \cdot \phi^* = o(1)$ *and* $S_{\mathcal{R}^c} \cdot \phi^{c*} = o(1)$ *as* $\varepsilon_{\mathcal{R}}, \varepsilon_{\mathcal{R}^c} \to 0$, *and taking* $\lambda = O(S^{-1}_{\mathcal{R}^c,0})$,

$$\boxed{\mathcal{T}_{mix} \leq \frac{4}{\gamma}\left(\frac{1-\mu(\mathcal{R})}{1-2\mu(\mathcal{R})}\right)(1+o(1))}$$

Transition and mixing time of the Curie-Weiss model:

Recall that we get:

- $\mathcal{T}_{\mathcal{R}^c}$ has exponential law w.r.t. $\mu_{\mathcal{R}}$;
- $\mathbb{E}_{\mu_{\mathcal{R}}}(\mathcal{T}_{\mathcal{R}^c}) = \frac{\pi N}{\beta c(m_0)c(m_-)} e^{\beta N \Gamma_1}(1+o(1))\,;$
- $\gamma^{-1} = \frac{2\pi N}{\beta c(m_0)c(m_-)} e^{\beta N \Gamma_1}(1+o(1))\,.$

By Theorem 6., with no need of further computations, it holds:

(i) $\mathcal{T}_{\mathcal{R}^c,\lambda}$ has exponential law w.r.t. $\mu_{\mathcal{R}}$, with mean

$$\mathbb{E}_{\mu_{\mathcal{R}}}(\mathcal{T}_{\mathcal{R}^c,\lambda}) = \frac{2\pi N}{\beta c(m_0)c(m_-)} e^{\beta N \Gamma_1}(1+o(1))$$

(ii) The mixing time $\mathcal{T}_{mix}$ is bounded as

$$\gamma^{-1} \le \mathcal{T}_{mix} \le \frac{8\pi N}{\beta c(m_0)c(m_-)} e^{\beta N \Gamma_1}(1+o(1)) = 4\gamma^{-1}(1+o(1))$$

Thank you for your attention!