

Eyring-Kramers law for the underdamped Langevin process

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In collaboration with Seungwoo Lee, Insuk Seo (Seoul National University)

Minisymposium "Echantillonnage et métastabilité II" (June 5, 2025)

1 Motivation

2 Eyring-Kramers law in the elliptic and reversible setting

- Potential theory
- Scheme of proof

3 Eyring-Kramers law in a non-reversible and non-elliptic setting

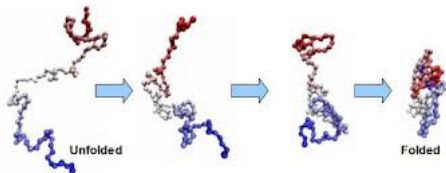
- Extension of the potential theory
- Scheme of proof

Motivation

- **Molecular dynamics:** *Biology, Chemistry, Material science and applications in Nuclear physics.*

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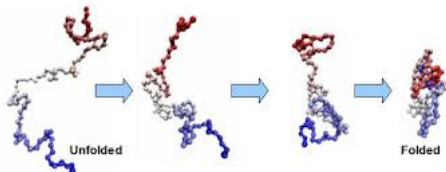
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- **Examples:**



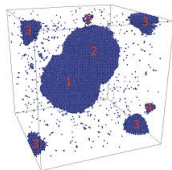
Folding of a protein

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- **Examples:**



Folding of a protein



Liquid-solid phase transition

Underdamped Langevin process

Consider N particles with unitary mass described by their *position* $q_t = (q_t^1; \dots; q_t^N) \in \mathbb{R}^{3N}$ and *velocity* $p_t = (p_t^1; \dots; p_t^N) \in \mathbb{R}^{3N}$ **at a constant temperature** $\beta > 0$.

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Newton equation + Thermostat:

$$\begin{cases} dq_t = p_t dt; \\ dp_t = -\nabla U(q_t) dt - \beta p_t dt + \sqrt{\beta} dB_t \end{cases}$$

where

- $U : \mathbb{R}^{3N} \rightarrow \mathbb{R}$ is the *interaction potential*,
- $\beta > 0$ is the *friction coefficient*,
- $(B_t)_{t \geq 0}$ is the **Brownian motion** accounting for the random thermal fluctuations.

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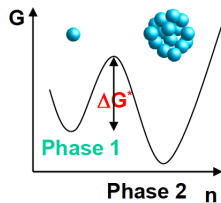
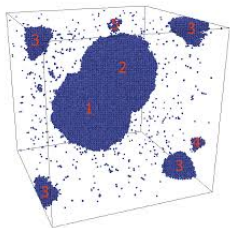
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Numerical sampling : Approach $(\tilde{q}_{n\Delta t}; \tilde{p}_{n\Delta t})$ using a numerical scheme

$$\tilde{q}_{(n+1)\Delta t}; \tilde{p}_{(n+1)\Delta t} = \Phi_{\Delta t}(\tilde{q}_{n\Delta t}; \tilde{p}_{n\Delta t})$$

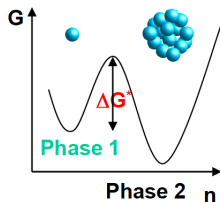
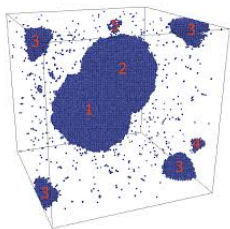
where Δt is the timestep.

Metastability



Let τ be the transition time **Phase 1** / **Phase 2**.

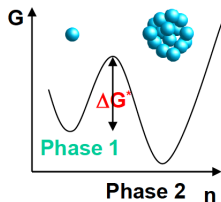
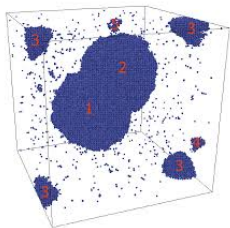
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Let τ be the transition time **Phase 1** / **Phase 2**.

- **Metastability** : The **transition** timescale ($\tau \sim 10^6$ s) is much higher than the **microscopic fluctuations** timescale ($\Delta t \sim 10^{-15}$ s).

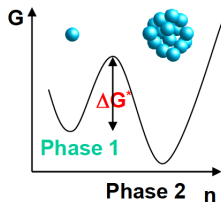
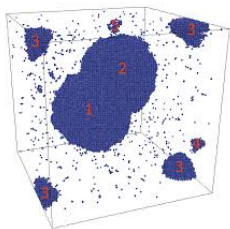
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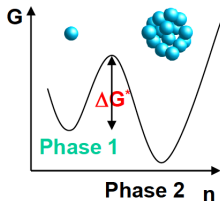
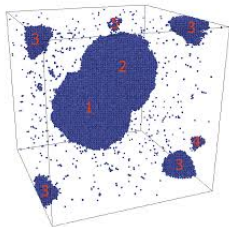
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- Sample the phase transition **Phase 1** / **Phase 2** = Sample a **rare event** of the evolution of the system.

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Question : What is the exact asymptotic of the average transition time when β is small?

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Equilibrium potential

Let M, S be bounded C^2 sets of \mathbb{R}^n .



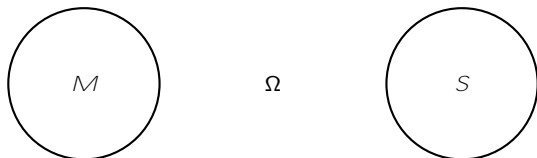
The *equilibrium potential* $h_{M;S}$ is defined as the solution to

$$\begin{cases} \Delta h_{M;S}(x) = 0; & x \in \Omega; \\ h_{M;S}(x) = 1; & x \in \partial M; \\ h_{M;S}(x) = 0; & x \in \partial S; \end{cases}$$

where $L = \Delta$.

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where $L = \Delta$.

Interpretation:

- 1 Metal plates attached to a battery imposing a constant voltage,
- 2 $h_{M;S}$ is the electrostatic potential at equilibrium on Ω .

Probabilistic representation

Let $(X_t)_{t \geq 0}$ be the **overdamped Langevin process** in \mathbb{R}^n solution to

$$dX_t = -\nabla U(X_t)dt + \sqrt{\frac{\rho}{2}} dB_t ;$$

which infinitesimal generator is L .

Let $\tau_C := \inf\{t > 0 : X_t \notin C\}$, then

$$h_{M;S}(x) = P_x(\tau_M < \tau_S) :$$

Probabilistic representation

Let $(X_t)_{t \geq 0}$ be the **overdamped Langevin process** in \mathbb{R}^n solution to

$$dX_t = -r U(X_t)dt + \sqrt{\frac{\rho}{2}} dB_t ;$$

which infinitesimal generator is L .

Let $\tau_C := \inf\{t > 0 : X_t \notin C\}$, then

$$h_{M;S}(x) = P_x(\tau_M < \tau_S) ;$$

Invariant measure: The process $(X_t)_{t \geq 0}$ admits the Gibbs invariant probability distribution:

$$d\mu(x) = \frac{1}{Z} e^{-U(x)} dx ;$$

where Z is the normalizing constant.

Equilibrium measure

The *equilibrium measure* is defined as:

$$\mu_{M;S}(dx) = r \int_M h_{M;S} \cdot n_M(x) \, dx ;$$

where \int_M is the surface measure, n_M is the unitary inward normal vector on ∂M .

The *capacity* is defined as:

$$\text{cap}(M; S) = \int_{\partial M} \mu_{M;S}(dx) ;$$

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$$\text{cap}(M; S) = \int_{\partial M} \mu_{M;S}(dx) ;$$

By the divergence theorem,

$$\text{cap}(M; S) = \int_{\Omega} r h_{M;S}(x)^2 (dx) ;$$

Equilibrium measure

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$$\text{cap}(M; S) = \int_{\partial M} \mu_{M;S}(dx) ;$$

By the divergence theorem,

$$\text{cap}(M; S) = \int_{\Omega} |\nabla h_{M;S}(x)|^2 dx ;$$

Interpretation:

- 1 $\mu_{M;S}$ is the *distribution of charge* at the surface of M ,
- 2 $\text{cap}(M; S)$ is the *total charge* on the plate M .
- 3 $\text{cap}(M; S)$ is also equal to the *total electrostatic energy* on Ω .

Identity

Let f be a smooth function in \mathbb{R}^n vanishing on ∂S . Then,

$$\begin{aligned}
 \int_{\partial M} f(x) \nu_{M;S}(dx) &= \int_{\mathbb{R}^n} f(x) \nu_{M;S} \cdot n_M(x) \, dx \\
 &= \int_{\Omega} f(x) \underbrace{\nu_{M;S}(x)}_{=0} \, dx + \int_{\Omega} f(x) \nu_{M;S}(x) \, dx \\
 &= \int_{\mathbb{R}^n} h_{M;S}(x) (\nu_{M;S}(x)) \, dx :
 \end{aligned}$$

Identity

Let f be a smooth function in \mathbb{R}^n vanishing on ∂S . Then,

$$\begin{aligned} \int_{\partial M} f(x) \, h_{M;S}(x) \, dx &= \int_{\partial M} f(x) \, r \, h_{M;S}(x) \, n_M(x) \, dx \\ &= \int_{\Omega} f(x) \, \underbrace{L h_{M;S}(x)}_{=0} \, dx + \int_{\Omega} r f(x) \, r h_{M;S}(x) \, dx \\ &= \int_{\mathbb{R}^n} h_{M;S}(x) \, (L f(x)) \, dx : \end{aligned}$$

Defining $f(x) = E_x[S]$, there exists a probability measure $\mu_{M;S}$ on ∂M such that

$$\int_{\partial M} E_x[S] \, \mu_{M;S}(dx) = \frac{1}{\text{cap}(M;S)} \int_{\mathbb{R}^n} h_{M;S}(x) \, dx ;$$

since $L f = 1$.

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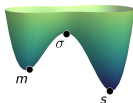
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Eyring-Kramers law

Assumption : U is a C^2 Morse function.



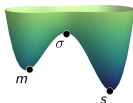
Double well potential.

Let $M = B(m; \epsilon)$ and $S = B(s; \epsilon)$.

Eyring-Kramers law: Asymptotics of $E_m[S]$ when $\epsilon \rightarrow 0$?

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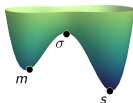
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Proof idea: [Bovier-Eckhoff-Gaynard-Klein, JEMS, 2004]

$$\int_M E_x[S]_{M;S}(\mathrm{d}x) = \frac{1}{\mathrm{cap}(M;S)} \int_{\mathbb{R}^n} h_{M;S}(x) \mathrm{d}x :$$

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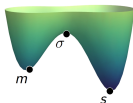
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$$\mathbb{E}_x[S]_{M;S} = \frac{1}{\text{cap}(M;S)} \int_{\mathbb{R}^n} h_{M;S}(x) \, (dx) :$$

For $x \in M$, $E_x[S] \sim E_m[S]$:

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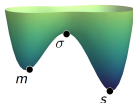
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$$\int_M E_x[S] \mu_{M;S}(dx) = \frac{1}{\text{cap}(M;S)} \int_{\mathbb{R}^n} h_{M;S}(x) \mu(dx) :$$

- 1 For $x \in M$, $E_x[S] \sim E_m[S]$:
- 2 $h_{M;S}(x) \sim 1_{\text{first well}(x)}$:

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Proof idea: [Bovier-Eckhoff-Gaynard-Klein, JEMS, 2004]

$$\mathbb{R}^n \int_M E_x[S] \mathbb{1}_{M;S}(dx) = \frac{1}{\text{cap}(M;S)} \int_{\mathbb{R}^n} h_{M;S}(x) \mathbb{1}_M(dx) :$$

1 For $x \in M$, $E_x[S] \sim E_m[S]$:

2 $h_{M;S}(x) \sim \mathbb{1}_{\text{first well}(x)}$:

3 **Dirichlet principle:**

$$\text{cap}(M;S) = \inf_{f \in C^1(\mathbb{R}^n)} \int_{\mathbb{R}^n} |\nabla f(x)|^2 e^{-U(x)} dx ; \quad f = 1 \text{ on } M; f = 0 \text{ on } S :$$

Capacity computation

Let $\beta = \frac{\rho}{\log(1+\rho)}$. Define

$$\beta(x) = \frac{1}{\int_{\mathbb{R}} e^{-\frac{1}{2}t^2} dt} \int_{hx; e_1^i} e^{-\frac{1}{2}t^2} dt;$$

which is solution to the **linearized operator** $\beta = H x r + \Delta$ when $x \rightarrow \infty$.

Capacity computation

Let $\rho = \frac{1}{\log(1-\epsilon)}$. Define

$$p(x) = \frac{1}{\int_{\mathbb{R}} e^{-\frac{1}{2}t^2} dt} \int_{hx; e_1^i}^Z e^{-\frac{1}{2}t^2} dt;$$

which is solution to the **linearized operator** $\mathcal{L} = H x r + \Delta$ when $x' = \dots$. Let f be the test function satisfying

where the colored zones are connected components of $fU(x) = U(x) + \rho^2 g$.

Eyring-Kramers law

Theorem (Overdamped Langevin process)

Let H^m (resp. H) be the Hessian of U on m (resp. s). Then,

$$E_m(\tau) = (1 + o(1)) \frac{2}{|\lambda_1|} \sqrt{\frac{\det H}{\det H^m}} \exp \left(\frac{U(s) - U(m)}{\epsilon} \right);$$

where λ_1 is the unique negative eigenvalue of H .

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where λ_1 is the unique negative eigenvalue of H .

This law was extended in [Lee-Seo, PTRF, 2021] for **elliptic and non-reversible** diffusion processes satisfying

$$dX_t = (r U(X_t) + \nabla \cdot (X_t)) dt + \sqrt{\beta} dB_t;$$

such that for all $x \in \mathbb{R}^n$,

$$r U(x) - \nabla \cdot (x) = 0; \quad (r \nabla \cdot)(x) = 0;$$

Remarks:

- τ remains invariant,
- λ_1 is replaced by the unique negative eigenvalue λ_1 of $H + DL$,
- β does not satisfy the same boundary conditions.

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Non-elliptic and non-reversible setting

Consider the **underdamped Langevin process**

$$\begin{cases} dq_t = p_t dt; \\ dp_t = -r U(q_t) dt - p_t dt + \sqrt{\frac{\rho}{2}} dB_t; \end{cases}$$

Its infinitesimal generator is the **kinetic Fokker-Planck operator**

$$L = \frac{\rho}{2} \frac{\partial^2}{\partial p^2} + p \frac{\partial}{\partial q} - r U(q) \frac{\partial}{\partial p}$$

Non-elliptic and non-reversible setting

Consider the **underdamped Langevin process**

$$\begin{cases} dq_t = p_t dt; \\ dp_t = -\gamma U(q_t) dt - p_t dt + \sqrt{2\gamma} dB_t; \end{cases}$$

Its infinitesimal generator is the **kinetic Fokker-Planck operator**

$$\mathcal{L} = \gamma p \partial_q + \partial_p \left(-\gamma U(q) - p \right) + \gamma \partial_p^2$$

Its invariant measure is given by

$$d\mu(q; p) = \frac{1}{Z} e^{-V(q; p)} dq dp;$$

where $V(q; p) = \gamma U(q) + \frac{p^2}{2\gamma}$ and Z is the normalizing factor.

Notation: Let

$$M = B((m; 0); \gamma); \quad S = B((s; 0); \gamma):$$

Capacity

Difficulties:

L is not reversible.

The equilibrium measure, thus the capacity are ill-defined because of the non-ellipticity.

The [Dirichlet principle](#) is an open question with recent advancements [Albritton-Armstrong-Mourrat-Novack, 2025].

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Idea inspired from [Bovier-den Hollander, 2015], [Lee-Seo, PTRF, 2021] Let f be a smooth function in \mathbb{R}^n satisfying $f = 1$ on ∂M and $f = 0$ on ∂S . By integration by parts (to be justified),

$$\text{cap}(M; S) = \int_{\mathbb{R}^{2n}} h_{M; S}(x) (L^* f(x)) (dx);$$

where L^* is the adjoint of L on (dx) , i.e.

$$L^* = h(p; r, q) + h(r, U(q); r, p) \quad h(p; r, p) + \quad p :$$

Potential theory

Equilibrium measure: We show the existence of a non-negative measure $\mu_{M;S}$ on \mathcal{M} such that for all smooth test functions satisfying $f = 0$ on ∂S ,

$$\int_{\mathbb{R}^{2n}} h_{M;S}(x) (\Delta f(x)) \, (dx) = \int_{\mathcal{M}} f(x) \mu_{M;S}(dx) :$$

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Capacity: Additionally, if $f = 1$ on ∂M ,

$$\text{cap}(M;S) = \int_{\mathbb{R}^{2n}} h_{M;S}(x) (\Delta f(x)) \, (dx) :$$

It is independent of the choice of f .

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It is independent of the choice of f .

The first step of the proof then consists in showing that

$$\int_{\partial M} E_x[S] \mu_{M;S}(dx) = \frac{1}{\text{cap}(M;S)} \int_{\mathbb{R}^{2n}} h_{M;S}(x) \, (dx) ;$$

where $\mu_{M;S} = \mu_{M;S} = \text{cap}(M;S)$.

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Consider the process $X_t^i = (q_t^i; p_t^i)$ $t \geq 0$

$$\begin{cases} dq_t^i = p_t^i dt - r U(q_t^i) dt + \sqrt{\frac{p}{2}} dB_t^i; \\ dp_t^i = -r U(q_t^i) dt - p_t^i dt + \sqrt{\frac{p}{2}} dB_t^i \end{cases}$$

where $(B_t)_{t \geq 0}$, $(\tilde{B}_t)_{t \geq 0}$ are independent Brownian motions.

Its infinitesimal generator L_i is given by

$$L_i = L - hr U(q); r q^i + \dots q^i$$

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Properties:

The process $(X_t^i)_{t \geq 0}$ is **elliptic and non-reversible**,

Its invariant measure is also .

Scheme of proof

Consider the process $X_t^i = (q_t^i ; p_t^i)$ on

$$\begin{cases} dq_t^i &= p_t^i dt - r U(q_t^i) dt + \sqrt{\frac{p}{2}} dB_t^i \\ dp_t^i &= -r U(q_t^i) dt - p_t^i dt + \sqrt{\frac{p}{2}} dB_t^i \end{cases}$$

where $(B_t)_{t \geq 0}$, $(\tilde{B}_t)_{t \geq 0}$ are independent Brownian motions.

Its infinitesimal generator $L_{i, \epsilon}$ is given by

$$L_{i, \epsilon} = L_{i, \epsilon} \left(\frac{1}{\epsilon} \left(\frac{p}{2} \frac{\partial^2}{\partial p^2} + \frac{\partial}{\partial p} \right) + \frac{1}{\epsilon} \left(\frac{p}{2} \frac{\partial^2}{\partial q^2} + \frac{\partial}{\partial q} \right) \right)$$

Properties:

The process $(X_t^i)_{t \geq 0}$ is **elliptic and non-reversible**,

Its invariant measure is also $\mu_{i, \epsilon}$.

As a result,

$$\int_{\mathbb{R}^{2n}} \mathbb{E}_x [\mathbb{1}_M] \mu_{i, \epsilon}(dx) = \frac{1}{\text{cap}_\epsilon(M; S)} \int_{\mathbb{R}^{2n}} \mathbb{1}_M h_{M; S}^i(x) \mu_{i, \epsilon}(dx);$$

Objective: Take the limit $\epsilon \rightarrow 0$.

Scheme of proof

$$\int_{\mathbb{R}^{2n}} \mathbb{E}_x[\tilde{h}_{M;S}^{\tilde{s}}] \tilde{h}_{M;S}^{\tilde{s}}(dx) = \frac{1}{\text{cap}_M(M;S)} \int_{\mathbb{R}^{2n}} \tilde{h}_{M;S}^{\tilde{s}}(x) P_x(\tilde{s} \in M) (dx);$$

Objective: Take $\tilde{s} = 0$ and then $M = 1$.

Scheme of proof

$$\int_{\mathbb{M}} \mathbb{E}_x[\hat{M}]_{M;S} (dx) = \frac{1}{\text{cap}_0(M;S)} \int_{\mathbb{R}^{2n}} h_{M;S}^i(x) P_x(\hat{M}) (dx);$$

Objective: Take $\epsilon > 0$ and then $M \geq 1$.

For any smooth function f such that $f = 0$ on $\partial\mathbb{S}$,

$$\int_{\mathbb{M}} f(x)_{M;S} (dx) = \int_{\mathbb{R}^{2n}} h_{M;S}^i(x) (L_{\epsilon} f(x)) (dx)$$

$$\stackrel{\epsilon > 0}{\geq} \int_{\mathbb{R}^{2n}} h_{M;S}^i(x) (L f(x)) (dx):$$

By Riesz{Markov{Kakutani representation theorem, there exists a probability measure $\mu_{M;S}$ such that

$$\int_{\mathbb{M}} f(x)_{M;S} (dx) = \int_{\mathbb{R}^{2n}} f(x) \mu_{M;S} (dx)$$

In particular, $\text{cap}_0(M;S) \leq \int_{\mathbb{R}^{2n}} \mu_{M;S} (dx)$.

Scheme of proof

$$\int_{\mathbb{M}} \mathbb{E}_x [S^{\wedge M}]_{M;S} (dx) = \frac{1}{\text{cap}_0(M;S)} \int_{\mathbb{R}^{2n}} h_{M;S}^{\dot{}}(x) P_x(S^{\wedge M}) (dx);$$

Objective: Take $\epsilon > 0$ and then $M \gg 1$.

For any smooth function f such that $f = 0$ on $\partial\mathbb{S}$,

$$\int_{\mathbb{M}} f(x)_{M;S} (dx) = \int_{\mathbb{R}^{2n}} h_{M;S}^{\dot{}}(x) (L_{\dot{}} f(x)) (dx)$$

$$\stackrel{!}{=} \int_{\mathbb{R}^{2n}} h_{M;S}^{\dot{}}(x) (L f(x)) (dx):$$

By Riesz{Markov{Kakutani representation theorem, there exists a probability measure $\mu_{M;S}$ such that

$$\int_{\mathbb{M}} f(x)_{M;S} (dx) = \int_{\mathbb{R}^{2n}} f(x) \mu_{M;S} (dx)$$

In particular, $\text{cap}_0(M;S) \leq \int_{\mathbb{R}^{2n}} \mu_{M;S} (dx)$.

Additionally, by studying the trajectories,

$$\sup_{x \in \mathbb{M}} \mathbb{E}_x [S^{\wedge M}] \leq \mathbb{E}_x [S^{\wedge M}] \leq 0:$$

Scheme of proof

$$\int_{\mathbb{M}} \mathbb{E}_x [S^{\wedge M}]_{M;S} (dx) = \frac{1}{\text{cap}_M(M;S)} \int_{\mathbb{R}^{2n}} h_{M;S}^{\dot{}}(x) P_x(S^{\wedge M}) (dx);$$

Objective: Take $\epsilon > 0$ and then $M \gg 1$.

For any smooth function f such that $f = 0$ on $\partial\mathbb{S}$,

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By Riesz (Markov-Kakutani representation theorem), there exists a probability measure $\mu_{M;S}$ such that

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In particular, $\text{cap}_M(M;S) \leq \text{cap}(M;S)$.

Additionally, by studying the trajectories,

$$\sup_{x \in \mathbb{M}} \mathbb{E}_x [S^{\wedge M}] \leq \mathbb{E}_x [S^{\wedge M}] \leq 0:$$

Finally,

$$\int_{\mathbb{M}} \mathbb{E}_x [S^{\wedge M}]_{M;S} (dx) = \frac{1}{\text{cap}(M;S)} \int_{\mathbb{R}^{2n}} h_{M;S}^{\dot{}}(x) P_x(S^{\wedge M}) (dx):$$

Taking $M \gg 1$ concludes the first step of the proof.

Scheme of proof

Secondary steps of the proof:

- 1 By [Golse-Imbert-Mouhot-Vasseur, Ann. Pisa, 2019], we deduce that for $x \geq M$,

$$E_x[S] \sim E_{(m;0)}[S] :$$

Scheme of proof

Secondary steps of the proof:

- 1 By [Golse-Imbert-Mouhot-Vasseur, Ann. Pisa, 2019], we deduce that for $x \in M$,

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- 2

$$h_{M;S}(x) \sim 1_{\text{first well}(x)} :$$

Scheme of proof

Secondary steps of the proof:

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$$h_{M;S}(x) \sim 1_{\text{first well}(x)} :$$

- 3 By choosing $f = \mathbb{1}$ in a neighborhood of ∂M and multiply by a cutoff function to satisfy the boundary conditions,

$$\text{cap}(M; S) = [1 + o(1)] \frac{1}{Z} \frac{(2\pi)^{n/2}}{2} \int \frac{1}{\det H_U} e^{-U(x)} dx :$$

Low-lying spectrum

Theorem (Underdamped Langevin process)

$$E_m(s) = (1 + o(1)) \frac{2^{-r}}{\lambda_1} \frac{\sqrt{\det H}}{\det H^m} \exp \left(\frac{U(x) - U(m)}{\hbar} \right);$$

where λ_1 is the unique negative eigenvalue of the matrix $\begin{pmatrix} H & O_n \\ O_n & I_n \end{pmatrix} \in \mathbb{R}^{2n \times 2n}$.

Remark: The low-lying spectrum was also studied when $\hbar \neq 0$ in [Hérau-Hitrik- Sjöstrand, AIHP, 2008], [Bony-Le Peutrec-Michel, JEMS, 2024] using semi-classical analysis techniques.

Open questions

Many questions remain...

Formalizing **Potential theory** tools (work in progress)

- Expression of the equilibrium measure and the capacity.
- Well-definition of the electrostatic energy.
- Dirichlet principle.

Extension of Eyring-Kramers law to **general forces**

- Elliptic setting with non Gibbs invariant measure.
- Non-elliptic setting with non Gibbs invariant measure.

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Thank you for your attention!