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)

Motivation

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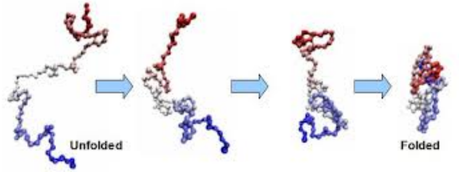

Folding of a protein

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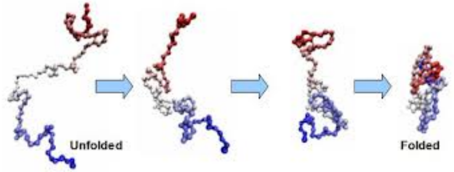

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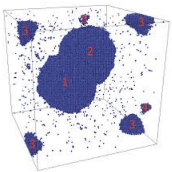

Liquid-solid phase transition

Underdamped Langevin process

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

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Newton equation + **Thermostat**:

$$\begin{cases} \mathrm{d}q_t = p_t \mathrm{d}t, \\ \mathrm{d}p_t = -\nabla U(q_t)\mathrm{d}t - \gamma p_t \mathrm{d}t + \sqrt{2\gamma\epsilon}\,\mathrm{d}B_t \end{cases}$$

where

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

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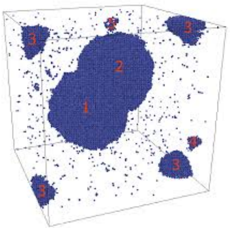
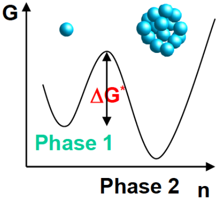
Numerical sampling : Approach $(\tilde{q}_{n\Delta t}, \tilde{p}_{n\Delta t})$ using a numerical scheme

$$\left(\tilde{q}_{(n+1)\Delta t}, \tilde{p}_{(n+1)\Delta t}\right) = \Phi_{\Delta_t}\left(\tilde{q}_{n\Delta t}, \tilde{p}_{n\Delta t}\right)$$

where Δt is the timestep.

Metastability





Let τ be the transition time **Phase 1** $\rightarrow$ **Phase 2**.

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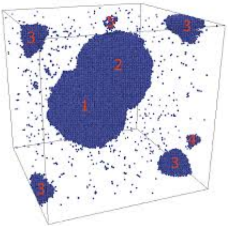

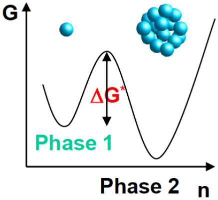

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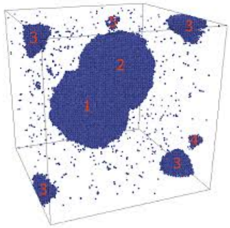

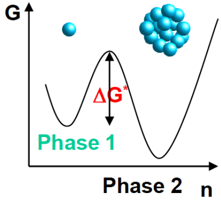

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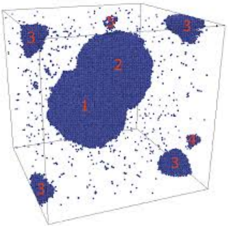

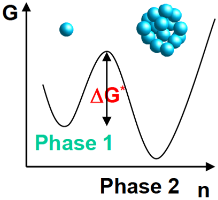

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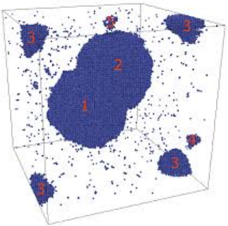

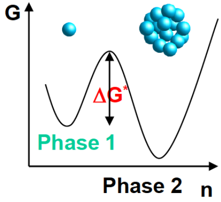

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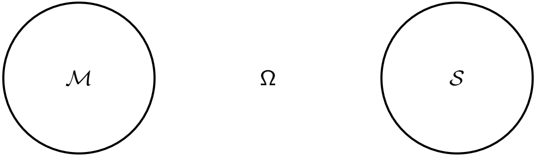
Question : What is the exact asymptotic of the average transition time when ϵ is small?

Equilibrium potential

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



The *equilibrium potential* $h^{\epsilon}_{\mathcal{M},\,\mathcal{S}}$ is defined as the solution to

$$\begin{cases} \mathcal{L}_\epsilon \, h^{\epsilon}_{\mathcal{M},\,\mathcal{S}}(x) = 0, & x \in \Omega \,, \\ \quad\; h^{\epsilon}_{\mathcal{M},\,\mathcal{S}}(x) = 1, & x \in \partial\mathcal{M} \,, \\ \quad\; h^{\epsilon}_{\mathcal{M},\,\mathcal{S}}(x) = 0, & x \in \partial\mathcal{S} \,, \end{cases}$$

where $\mathcal{L}_\epsilon = -\nabla U \cdot \nabla + \epsilon\Delta$.

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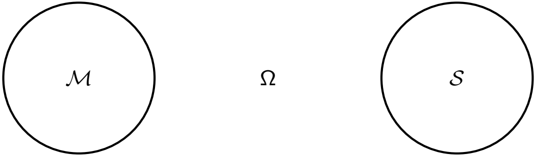

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where $\mathcal{L}_\epsilon = -\nabla U \cdot \nabla + \epsilon\Delta$.

Interpretation:

1. Metal plates attached to a battery imposing a constant voltage,
2. $h^{\epsilon}_{\mathcal{M},\mathcal{S}}$ is the electrostatic potential at equilibrium on Ω.

Probabilistic representation

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

$$\mathrm{d}X_t^\epsilon = -\nabla U(X_t^\epsilon)\mathrm{d}t + \sqrt{2\epsilon}\mathrm{d}B_t \ ,$$

which infinitesimal generator is $\mathcal{L}_\epsilon$.

Let $\tau_{\mathcal{C}}^\epsilon := \inf\{t > 0 : X_t^\epsilon \in \mathcal{C}\}$, then

$$h_{\mathcal{M},\mathcal{S}}^\epsilon(x) = \mathbb{P}_x(\tau_{\mathcal{M}}^\epsilon < \tau_{\mathcal{S}}^\epsilon) \ .$$

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

$$\mathrm{d}\mu_\epsilon(x) = \frac{1}{Z_\epsilon}\mathrm{e}^{-U(x)/\epsilon}\mathrm{d}x\,,$$

where Z_ϵ is the normalizing constant.

Equilibrium measure

The *equilibrium measure* is defined as:

$$\nu^{\epsilon}_{\mathcal{M},\,\mathcal{S}}(\mathrm{d}x) = \epsilon \nabla h^{\epsilon}_{\mathcal{M},\,\mathcal{S}} \cdot n_{\mathcal{M}}(x)\,\sigma(\mathrm{d}x)\;,$$

where σ is the surface measure, $n_{\mathcal{M}}$ is the unitary inward normal vector on $\partial\mathcal{M}$.

The *capacity* is defined as:

$$\mathrm{cap}_{\epsilon}(\mathcal{M},\,\mathcal{S}) = \int_{\partial\mathcal{M}} \nu^{\epsilon}_{\mathcal{M},\,\mathcal{S}}(\mathrm{d}x)\;.$$

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Interpretation:

1. $\nu^{\epsilon}_{\mathcal{M},\,\mathcal{S}}$ is the *distribution of charge* at the surface of $\mathcal{M}$,
2. $\mathrm{cap}_{\epsilon}(\mathcal{M},\,\mathcal{S})$ is the *total charge* on the plate $\mathcal{M}$.
3. $\mathrm{cap}_{\epsilon}(\mathcal{M},\,\mathcal{S})$ is also equal to the *total electrostatic energy* on Ω.

Identity

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

$$
\begin{aligned}
\int_{\partial\mathcal{M}} f(x)\,\nu^{\epsilon}_{\mathcal{M},\mathcal{S}}(\mathrm{d}x) &= \int_{\partial\mathcal{M}} f(x)\,\nabla h^{\epsilon}_{\mathcal{M},\mathcal{S}}\cdot n_{\mathcal{M}}(x)\,\sigma(\mathrm{d}x) \\
&= \int_{\Omega} f(x)\,\underbrace{\mathcal{L}_{\epsilon} h^{\epsilon}_{\mathcal{M},\mathcal{S}}(x)}_{=0}\,\mu_{\epsilon}(\mathrm{d}x) + \int_{\Omega} \nabla f(x)\cdot\nabla h^{\epsilon}_{\mathcal{M},\mathcal{S}}(x)\,\mu_{\epsilon}(\mathrm{d}x) \\
&= \int_{\mathbb{R}^n} h^{\epsilon}_{\mathcal{M},\mathcal{S}}(x)\,(-\mathcal{L}_{\epsilon} f(x))\,\mu_{\epsilon}(\mathrm{d}x)\,.
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$$

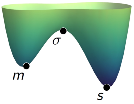
Defining $f(x)=\mathbb{E}_x[\tau^{\epsilon}_{\mathcal{S}}]$, there exists a probability measure $\theta^{\epsilon}_{\mathcal{M},\,\mathcal{S}}$ on $\partial\mathcal{M}$ such that

$$
\int_{\partial\mathcal{M}} \mathbb{E}_x[\tau^{\epsilon}_{\mathcal{S}}]\,\theta^{\epsilon}_{\mathcal{M},\,\mathcal{S}}(\mathrm{d}x) = \frac{1}{\mathrm{cap}_{\epsilon}(\mathcal{M},\,\mathcal{S})}\int_{\mathbb{R}^n} h^{\epsilon}_{\mathcal{M},\,\mathcal{S}}(x)\,\mu_{\epsilon}(\mathrm{d}x)\ ,
$$

since $\mathcal{L}_{\epsilon} f = -1$.

Eyring-Kramers law

Assumption : U is a $\mathcal{C}^2$ Morse function.



Double well potential.

Let $\mathcal{M} = \mathrm{B}(m, \epsilon)$ and $\mathcal{S} = \mathrm{B}(s, \epsilon)$.

Eyring-Kramers law: Asymptotics of $\mathbb{E}_m[\tau_{\mathcal{S}}^{\epsilon}]$ when $\epsilon \to 0$?

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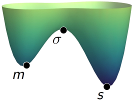

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Proof idea: [Bovier-Eckhoff-Gayrard-Klein, JEMS, 2004]

$$\boxed{\int_{\partial\mathcal{M}} \mathbb{E}_x[\tau_{\mathcal{S}}^{\epsilon}]\, \theta_{\mathcal{M},\,\mathcal{S}}^{\epsilon}(\mathrm{d}x) = \frac{1}{\mathrm{cap}_{\epsilon}(\mathcal{M},\mathcal{S})} \int_{\mathbb{R}^n} h_{\mathcal{M},\,\mathcal{S}}^{\epsilon}(x)\, \mu_{\epsilon}(\mathrm{d}x)\ .}$$

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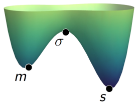

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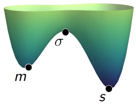

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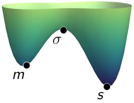

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2. $h_{\mathcal{M},\,\mathcal{S}}^{\epsilon}(x) \simeq \mathbb{1}_{\text{first well}(x)}$.
3. **Dirichlet principle**:

$$\mathrm{cap}_{\epsilon}(\mathcal{M},\, \mathcal{S}) = \epsilon \inf\left\{ \int_{\mathbb{R}^{2d}} |\nabla f(x)|^2 \mathrm{e}^{-U(x)/\epsilon} \mathrm{d}x\,, \quad f = 1 \text{ on } \partial\mathcal{M},\ f = 0 \text{ on } \partial\mathcal{S} \right\}.$$

Capacity computation

Let $\delta = \sqrt{\epsilon \log(1/\epsilon)}$. Define

$$\widehat{f}(x) = \frac{1}{\int_{-\delta}^{\delta} \mathrm{e}^{-\frac{\lambda_1^\sigma}{2\epsilon} t^2} \mathrm{d}t} \int_{-\delta}^{\langle x,\, e_1 \rangle} \mathrm{e}^{-\frac{\lambda_1^\sigma}{2\epsilon} t^2} \mathrm{d}t \,,$$

which is solution to the **linearized operator** $\widehat{\mathcal{L}} = -\mathbb{H}^\sigma x \cdot \nabla + \epsilon \Delta$ when $x \simeq \sigma$.

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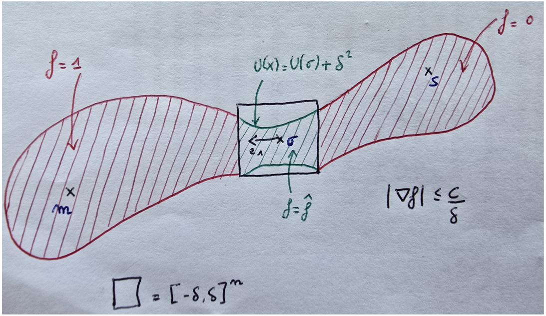

where the colored zones are connected components of $\{U(x) \leq U(\sigma) + \delta^2\}$.

Eyring-Kramers law

Theorem (Overdamped Langevin process)

Let $\mathbb{H}^m$ (resp. $\mathbb{H}^\sigma$) be the Hessian of U on m (resp. σ). Then,

$$\mathbb{E}_m(\tau_{\mathcal{S}}^\epsilon) = (1 + o_\epsilon(1)) \frac{2\pi}{\lambda_1^\sigma} \sqrt{\frac{-\det \mathbb{H}^\sigma}{\det \mathbb{H}^m}} \exp\left(\frac{U(\sigma) - U(m)}{\epsilon}\right),$$

where $-\lambda_1^\sigma$ is the unique negative eigenvalue of $\mathbb{H}^\sigma$.

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where $-\lambda_1^\sigma$ *is the unique negative eigenvalue of* $\mathbb{H}^\sigma$*.*

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

$$\mathrm{d}X_t^\epsilon = -(\nabla U(X_t^\epsilon) + \ell(X_t^\epsilon))\mathrm{d}t + \sqrt{2\epsilon}\mathrm{d}B_t \ ,$$

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

$$\nabla U(x) \cdot \ell(x) = 0, \qquad (\nabla \cdot \ell)(x) = 0 \ .$$

Remarks:

- μ_ϵ remains invariant,
- -λ_1^σ is replaced by the unique negative eigenvalue $-\mu_1^\sigma$ of $\mathbb{H}^\sigma + D\mathbb{L}^\sigma$,
- $\widehat{f}$ does not satisfy the same boundary conditions.

Non-elliptic and non-reversible setting

Consider the **underdamped Langevin process**

$$\begin{cases} \mathrm{d}q_t^\epsilon = p_t^\epsilon \mathrm{d}t, \\ \mathrm{d}p_t^\epsilon = -\nabla U(q_t^\epsilon)\mathrm{d}t - \gamma p_t^\epsilon \mathrm{d}t + \sqrt{2\gamma\epsilon}\mathrm{d}B_t. \end{cases}$$

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

$$\mathcal{L}_\epsilon = \langle p, \nabla_q \rangle - \langle \nabla U(q), \nabla_p \rangle - \gamma \langle p, \nabla_p \rangle + \epsilon \Delta_p.$$

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$$\mathcal{L}_\epsilon = \langle p, \nabla_q \rangle - \langle \nabla U(q), \nabla_p \rangle - \gamma \langle p, \nabla_p \rangle + \epsilon \Delta_p.$$

Its invariant measure is given by

$$\mathrm{d}\mu_\epsilon(q, p) = \frac{1}{Z_\epsilon} \mathrm{e}^{-V(q, p)/\epsilon} \mathrm{d}q\mathrm{d}p \ ,$$

where $V(q, p) = U(q) + |p|^2/2$ and Z_ϵ is the normalizing factor.

Notation: Let

$$\mathcal{M} = \mathrm{B}((m, 0), \epsilon), \qquad \mathcal{S} = \mathrm{B}((s, 0), \epsilon) \ .$$

Capacity

Difficulties:

1. $\mathcal{L}_\epsilon$ is not reversible.
2. The **equilibrium measure**, thus the **capacity** are ill-defined because of the non-ellipticity.
3. 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 $\partial\mathcal{M}$ and $f = 0$ on $\partial\mathcal{S}$. By **integration by parts** (to be justified),

$$\mathrm{cap}_\epsilon(\mathcal{M}, \mathcal{S}) = \int_{\mathbb{R}^{2n}} h^\epsilon_{\mathcal{M},\mathcal{S}}(x)\,(-\mathcal{L}^*_\epsilon f(x))\,\mu_\epsilon(\mathrm{d}x)\ ,$$

where $\mathcal{L}^*_\epsilon$ is the adjoint of $\mathcal{L}_\epsilon$ on $\mu_\epsilon(\mathrm{d}x)$, i.e.

$$\mathcal{L}^*_\epsilon = -\langle p, \nabla_q\rangle + \langle \nabla U(q), \nabla_p\rangle - \gamma\langle p, \nabla_p\rangle + \epsilon\Delta_p\ .$$

Potential theory

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

$$\int_{\mathbb{R}^{2n}} h^{\epsilon}_{\mathcal{M},\,\mathcal{S}}(x)\,(-\mathcal{L}^{*}_{\epsilon} f(x))\,\mu_{\epsilon}(\mathrm{d}x) = \int_{\partial\mathcal{M}} f(x)\,\nu^{\epsilon}_{\mathcal{M},\,\mathcal{S}}(\mathrm{d}x)\,.$$

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Capacity: Additionally, if $f = 1$ on $\partial\mathcal{M}$,

$$\mathrm{cap}_{\epsilon}(\mathcal{M},\,\mathcal{S}) = \int_{\mathbb{R}^{2n}} h^{\epsilon}_{\mathcal{M},\,\mathcal{S}}(x)\,(-\mathcal{L}^{*}_{\epsilon} f(x))\,\mu_{\epsilon}(\mathrm{d}x)\,.$$

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It is **independent** of the choice of f.

The first step of the proof then consists in showing that

$$\int_{\partial\mathcal{M}} \mathbb{E}_{x}[\tau^{\epsilon}_{\mathcal{S}}]\,\theta^{\epsilon}_{\mathcal{M},\,\mathcal{S}}(\mathrm{d}x) = \frac{1}{\mathrm{cap}_{\epsilon}(\mathcal{M},\,\mathcal{S})}\int_{\mathbb{R}^{2n}} h^{\epsilon}_{\mathcal{M},\,\mathcal{S}}(x)\,\mu_{\epsilon}(\mathrm{d}x)\,,$$

where $\theta^{\epsilon}_{\mathcal{M},\,\mathcal{S}} = \nu^{\epsilon}_{\mathcal{M},\,\mathcal{S}}/\mathrm{cap}_{\epsilon}(\mathcal{M},\,\mathcal{S})$.

Scheme of proof

Consider the process $(X_t^{\epsilon,\,\alpha} = (q_t^{\epsilon,\,\alpha},\, p_t^{\epsilon,\,\alpha}))_{t\geq 0}$

$$\begin{cases} \mathrm{d}q_t^{\epsilon,\,\alpha} = p_t^{\epsilon,\,\alpha}\mathrm{d}t - \alpha\nabla U(q_t^{\epsilon,\,\alpha})\mathrm{d}t + \sqrt{2\alpha\epsilon}\mathrm{d}\tilde{B}_t, \\ \mathrm{d}p_t^{\epsilon,\,\alpha} = -\nabla U(q_t^{\epsilon,\,\alpha})\mathrm{d}t - \gamma p_t^{\epsilon,\,\alpha}\mathrm{d}t + \sqrt{2\gamma\epsilon}\mathrm{d}B_t \end{cases}$$

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

Its infinitesimal generator $\mathcal{L}_{\epsilon,\,\alpha}$ is given by

$$\mathcal{L}_{\epsilon,\,\alpha} = \mathcal{L}_\epsilon - \alpha\langle\nabla U(q),\, \nabla_q\rangle + \alpha\epsilon\Delta_q.$$

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Properties:

- The process $(X_t^{\epsilon,\,\alpha})_{t\geq 0}$ is **elliptic and non-reversible**,
- Its invariant measure is also μ_ϵ.

Scheme of proof

Consider the process $(X_t^{\epsilon,\alpha} = (q_t^{\epsilon,\alpha}, p_t^{\epsilon,\alpha}))_{t\geq 0}$

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- The process $(X_t^{\epsilon,\alpha})_{t\geq 0}$ is **elliptic and non-reversible**,
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As a result,

$$\int_{\partial\mathcal{M}} \mathbb{E}_x[\tau_{\mathcal{S}}^{\epsilon,\alpha}]\,\theta_{\mathcal{M},\mathcal{S}}^{\epsilon,\alpha}(\mathrm{d}x) = \frac{1}{\mathrm{cap}_{\epsilon,\alpha}(\mathcal{M},\mathcal{S})}\int_{\mathbb{R}^{2n}} h_{\mathcal{M},\mathcal{S}}^{\epsilon,\alpha}(x)\,\mu_\epsilon(\mathrm{d}x)\,,$$

Objective: Take the limit $\alpha \to 0$.

Scheme of proof

$$\int_{\partial\mathcal{M}} \mathbb{E}_x[\tau_{\mathcal{S}}^{\epsilon,\,\alpha} \wedge M]\, \theta_{\mathcal{M},\,\mathcal{S}}^{\epsilon,\,\alpha}(\mathrm{d}x) = \frac{1}{\mathrm{cap}_{\epsilon,\,\alpha}(\mathcal{M},\,\mathcal{S})} \int_{\mathbb{R}^{2n}} h_{\mathcal{M},\,\mathcal{S}}^{\epsilon,\,\alpha}(x)\, \mathbb{P}_x(\tau_{\mathcal{S}}^{\epsilon,\,\alpha} \leq M)\, \mu_\epsilon(\mathrm{d}x)\ ,$$

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$$\int_{\partial\mathcal{M}} \mathbb{E}_x[\tau_{\mathcal{S}}^{\epsilon,\,\alpha} \wedge M]\, \theta_{\mathcal{M},\,\mathcal{S}}^{\epsilon,\,\alpha}(\mathrm{d}x) = \frac{1}{\mathrm{cap}_{\epsilon,\,\alpha}(\mathcal{M},\,\mathcal{S})} \int_{\mathbb{R}^{2n}} h_{\mathcal{M},\,\mathcal{S}}^{\epsilon,\,\alpha}(x)\, \mathbb{P}_x(\tau_{\mathcal{S}}^{\epsilon,\,\alpha} \leq M)\, \mu_\epsilon(\mathrm{d}x) ,$$

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

$$\begin{aligned}\int_{\partial\mathcal{M}} f(x)\, \theta_{\mathcal{M},\,\mathcal{S}}^{\epsilon,\,\alpha}(\mathrm{d}x) &= \int_{\mathbb{R}^{2n}} h_{\mathcal{M},\,\mathcal{S}}^{\epsilon,\,\alpha}(x)\, (-\mathcal{L}_{\epsilon,\,\alpha}^{*} f(x))\mu_\epsilon(\mathrm{d}x) \\ &\underset{\alpha\to 0}{\longrightarrow} \int_{\mathbb{R}^{2n}} h_{\mathcal{M},\,\mathcal{S}}^{\epsilon}(x)\, (-\mathcal{L}_{\epsilon}^{*} f(x))\mu_\epsilon(\mathrm{d}x).\end{aligned}$$

By **Riesz–Markov–Kakutani representation theorem**, there exists a probability measure $\theta_{\mathcal{M},\,\mathcal{S}}^{\epsilon}$ such that

$$\theta_{\mathcal{M},\,\mathcal{S}}^{\epsilon,\,\alpha} \underset{\alpha\to 0}{\longrightarrow} \theta_{\mathcal{M},\,\mathcal{S}}^{\epsilon} .$$

In particular, $\mathrm{cap}_{\epsilon,\,\alpha}(\mathcal{M},\,\mathcal{S}) \underset{\alpha\to 0}{\longrightarrow} \mathrm{cap}_{\epsilon}(\mathcal{M},\,\mathcal{S})$.

Scheme of proof

$$\int_{\partial\mathcal{M}} \mathbb{E}_x[\tau_{\mathcal{S}}^{\epsilon,\,\alpha} \wedge M]\, \theta_{\mathcal{M},\,\mathcal{S}}^{\epsilon,\,\alpha}(\mathrm{d}x) = \frac{1}{\mathrm{cap}_{\epsilon,\,\alpha}(\mathcal{M},\,\mathcal{S})} \int_{\mathbb{R}^{2n}} h_{\mathcal{M},\,\mathcal{S}}^{\epsilon,\,\alpha}(x)\, \mathbb{P}_x(\tau_{\mathcal{S}}^{\epsilon,\,\alpha} \le M)\, \mu_\epsilon(\mathrm{d}x)\ ,$$

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In particular, $\mathrm{cap}_{\epsilon,\,\alpha}(\mathcal{M},\,\mathcal{S}) \underset{\alpha\to 0}{\longrightarrow} \mathrm{cap}_{\epsilon}(\mathcal{M},\,\mathcal{S})$.

Additionally, by studying the trajectories,

$$\sup_{x\in\partial\mathcal{M}} \left|\mathbb{E}_x[\tau_{\mathcal{S}}^{\epsilon,\,\alpha} \wedge M] - \mathbb{E}_x[\tau_{\mathcal{S}}^{\epsilon} \wedge M]\right| \underset{\alpha\to 0}{\longrightarrow} 0\ .$$

Scheme of proof

$$\int_{\partial\mathcal{M}} \mathbb{E}_x[\tau_{\mathcal{S}}^{\epsilon,\,\alpha} \wedge M]\, \theta_{\mathcal{M},\,\mathcal{S}}^{\epsilon,\,\alpha}(\mathrm{d}x) = \frac{1}{\mathrm{cap}_{\epsilon,\,\alpha}(\mathcal{M},\,\mathcal{S})} \int_{\mathbb{R}^{2n}} h_{\mathcal{M},\,\mathcal{S}}^{\epsilon,\,\alpha}(x)\, \mathbb{P}_x(\tau_{\mathcal{S}}^{\epsilon,\,\alpha} \leq M)\, \mu_\epsilon(\mathrm{d}x)\ ,$$

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In particular, $\mathrm{cap}_{\epsilon,\,\alpha}(\mathcal{M},\,\mathcal{S}) \xrightarrow[\alpha\to 0]{} \mathrm{cap}_{\epsilon}(\mathcal{M},\,\mathcal{S})$.

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Finally,

$$\int_{\partial\mathcal{M}} \mathbb{E}_x[\tau_{\mathcal{S}}^{\epsilon} \wedge M]\, \theta_{\mathcal{M},\,\mathcal{S}}^{\epsilon}(\mathrm{d}x) = \frac{1}{\mathrm{cap}_{\epsilon}(\mathcal{M},\,\mathcal{S})} \int_{\mathbb{R}^{2n}} h_{\mathcal{M},\,\mathcal{S}}^{\epsilon}(x)\, \mathbb{P}_x(\tau_{\mathcal{S}}^{\epsilon} \leq M)\, \mu_\epsilon(\mathrm{d}x)\ .$$

Taking $M \to \infty$ 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 $x \in \partial\mathcal{M}$,

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$$h^{\epsilon}_{\mathcal{M},\,\mathcal{S}}(x) \simeq \mathbb{1}_{\text{first well}(x)} \,.$$

3. By choosing $f_\epsilon = \widehat{f_\epsilon}$ in a neighborhood of σ and multiply by a cutoff function to satisfy the boundary conditions,

$$\mathrm{cap}_\epsilon(\mathcal{M},\,\mathcal{S}) = [1 + o_\epsilon(1)]\,\frac{1}{Z_\epsilon}\,\frac{(2\pi\epsilon)^{n/2}}{2\pi}\,\frac{\mu_1^\sigma}{\sqrt{-\det \mathbb{H}_U^\sigma}}\,e^{-U(\sigma)/\epsilon}.$$

Low-lying spectrum

Theorem (Underdamped Langevin process)

$$\mathbb{E}_m(\tau_{\mathcal{S}}) = (1 + o_\epsilon(1))\frac{2\pi}{\mu_1^\sigma}\sqrt{\frac{-\det \mathbb{H}^\sigma}{\det \mathbb{H}^m}}\exp\left(\frac{U(\sigma) - U(m)}{\epsilon}\right),$$

where $-\mu_1^\sigma$ *is the unique negative eigenvalue of the matrix* $\begin{pmatrix} \mathbb{H}^\sigma & \mathbb{O}_n \\ \mathbb{O}_n & \mathbb{I}_n \end{pmatrix}\begin{pmatrix} \mathbb{O}_n & \mathbb{I}_n \\ -\mathbb{I}_n & \gamma\mathbb{I}_n \end{pmatrix} \in \mathbb{R}^{2n\times 2n}$.

Remark: The low-lying spectrum was also studied when $\epsilon \to 0$ 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!