Sharp spectral asymptotics for reversible diffusions trapped in moving domains

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Setting: overdamped Langevin dynamics

We work with the SDE

$$\mathrm{d}X_t^\beta = -\nabla V(X_t^\beta)\,\mathrm{d}t + \sqrt{2\beta^{-1}}\,\mathrm{d}W_t, \tag{1}$$

Assume $V : \mathbb{R}^d \to \mathbb{R}$ is smooth and **Morse**, $V(x) = c|x|^2 > 0$ outside a compact set $\mathcal{K} \subset \mathbb{R}^d$.
Then, X_t^β is reversible and ergodic with respect to the Gibbs measure

$$\mathrm{d}\mu(x) = \mathcal{Z}_\beta^{-1}\mathrm{e}^{-\beta V(x)}\,\mathrm{d}x.$$

Used in computationalstatistical physics/molecular dynamics, where X_t^β: nuclear positions, V: interatomic potential, $\beta = 1/(k_{\mathrm{B}}T)$: inverse temperature.
For smooth bounded $\Omega \subset \mathbb{R}^d$, the Dirichlet generator

$$\mathcal{L}_\beta = -\nabla V \cdot \nabla + \frac{1}{\beta}\Delta.$$

with domain $H_0^1(\Omega,\mu) \cap H^2(\Omega,\mu)$ is self-adjoint on $L^2(\Omega,\mu)$, with compact resolvent and spectrum:

$$\cdots \leq -\lambda_{2,\beta}(\Omega) < -\lambda_{1,\beta}(\Omega) < 0$$

Local approach to metastability

We consider metastable domains $\Omega \subset \mathbb{R}^d$, where a **local equilibrium** is reached quickly after which the exit time is large.
Notion of local equilibrium: **quasistationary distributions**.

Definition

Denote $\tau_\Omega = \inf \left\{ t \geq 0 \middle| X_t^\beta \notin \Omega \right\}$. A QSD for X_t^β on Ω is a probability measure $\nu \in \mathcal{P}_1(\Omega)$ such that for all $A \in \mathcal{B}(\Omega)$

$$\mathbb{P}^\nu \left(X_t^\beta \in A \middle| \tau_\Omega > t \right) = \nu(A)$$

Metastability of Ω is related to **separation of timescales**: fast relaxation to/slow exit from the local equilibrium ν.

Metastable exit event: link with the Dirichlet spectrum

Proposition (Le Bris, Lelièvre, Luskin, Perez 2012 [14])

Let $(\lambda_{1,\beta}, u_{1,\beta})$ be the principal Dirichlet eigenpair of $-\mathcal{L}_\beta$ in Ω, i.e.

$$\lambda_{1,\beta} = \inf_{u \in H^1_{0,\mu}(\Omega)} \frac{\langle -\mathcal{L}_\beta u, u\rangle_{L^2_\mu(\Omega)}}{\|u\|^2_{L^2_\mu(\Omega)}} = \frac{1}{\beta} \frac{\int_\Omega |\nabla u_{1,\beta}|^2 \mathrm{e}^{-\beta V}}{\int_\Omega u_{1,\beta}^2 \mathrm{e}^{-\beta V}}, \tag{2}$$

and choose $u_{1,\beta} > 0$ on Ω. Then

$$\nu(A) = \frac{\int_A u_{1,\beta}\, \mathrm{e}^{-\beta V}}{\int_\Omega u_{1,\beta}\, \mathrm{e}^{-\beta V}} \tag{3}$$

is the unique QSD for X_t^β on Ω. Moreover, the exit time τ_Ω is exponentially distributed from ν and independent from the exit point:

$$\mathbb{E}^\nu \left[\varphi(X^\beta_{\tau_\Omega}) \mathbb{1}_{\tau_\Omega > t}\right] = \mathrm{e}^{-\lambda_{1,\beta}} \mathbb{E}^\nu \left[\varphi(X^\beta_{\tau_\Omega})\right]. \tag{4}$$

The **exit rate** (slow time scale) from the QSD is given by the principal **Dirichlet** eigenvalue $\lambda_{1,\beta}$.

Decorrelation inside the state

Let $\lambda_{2,\beta}$ be the second Dirichlet eigenvalue of $-\mathcal{L}_\beta$ in Ω.

Theorem (Le Bris, Lelièvre, Luskin, Perez 2012 [14])

Assume $\rho_0 \ll \mu|_\Omega$, *write* $\mu_t = \mathrm{Law}\left(X_t^\beta \middle| \tau_\Omega > t\right)$. *Then,* $\exists (C_1, C_2)(\beta, \rho_0)$*:*

$$\|\mu_t - \nu\|_{\mathrm{TV}} \leq C_1 \mathrm{e}^{-(\lambda_{2,\beta} - \lambda_{1,\beta})t},$$

$$\sup_{\|f\|_\infty \leq 1} \left| \mathbb{E}^{\mu_t}\left[f(X^\beta_{\tau_\Omega}, \tau_\Omega)\right] - \mathbb{E}^{\nu}\left[f(X^\beta_{\tau_\Omega}, \tau_\Omega)\right] \right| \leq C_2 \mathrm{e}^{-(\lambda_{2,\beta} - \lambda_{1,\beta})t}.$$

The **relaxation rate** to the QSD (fast time scale) is at least as large as the spectral gap $\lambda_{2,\beta} - \lambda_{1,\beta}$ of the Dirichlet generator $\mathcal{L}_\beta$.

A spectral optimization problem

Question: how to make Ω as locally metastable as possible ? Maximize separation of timescales.

$$J_\beta(\Omega) = \frac{\lambda_{2,\beta}(\Omega) - \lambda_{1,\beta}(\Omega)}{\lambda_{1,\beta}(\Omega)}.$$

Make exit time from the QSD $\gg$ decorrelation time to the QSD.
Objective: define highly locally metastable states $(\Omega_i)_{i\in\mathbb{N}}$ in $\mathbb{R}^d$.
Motivation:

- Accurate approximate state-to-state dynamics via renewal processes [3]/jump processes.
- Efficient algorithms to sample long trajectories (Parallel replica methods [22, 20]).
- The case $V = 0$ has been studied in the shape optimization litterature, e.g. the Payne–Polyá–Weinberger conjecture [19, 4].

Shape gradient descent

Isolated Dirichlet eigenvalues of $\mathcal{L}_\beta$ are **shape-differentiable**:

Proposition (B., Lelièvre, Stoltz, 2024 (in preparation))

The map

$$\begin{cases} \mathcal{W}^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d) \to \mathbb{R} \\ \theta \mapsto \lambda_{k,\beta}((\theta+\mathrm{Id})\Omega) \end{cases}$$

is continuously Fréchet-differentiable at 0*, with:*

$$\mathrm{d}\lambda_{k,\beta}(\Omega_0)\xi = -\frac{1}{\beta}\int_{\partial\Omega_0}\left(\frac{\partial u_{k,\beta}(\Omega_0)}{\partial \mathrm{n}}\right)^2 (\xi\cdot\mathrm{n})\,\mathrm{e}^{-\beta V}\,\mathrm{d}\sigma,\quad \forall \xi\in\mathcal{W}^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d),$$

where σ *denotes the surface measure on* $\partial\Omega_0$*, and* n *the outward surface normal to* Ω_0*.*

Proof of the case $V=0$ by Henrot transfers to the $L^2(\Omega,\mu)$ setting.
Algorithm: iterate

$$\Omega\mapsto(\mathrm{Id}+\eta_k\nabla J_\beta(\Omega))\Omega,\quad \nabla J_\beta(\Omega) = -\frac{\mathrm{n}}{\beta}\left[\frac{1}{\lambda_{1,\beta}}\left(\frac{\partial u_{2,\beta}}{\partial\mathrm{n}}\right)^2 - \frac{\lambda_{2,\beta}}{\lambda_{1,\beta}^2}\left(\frac{\partial u_{1,\beta}}{\partial\mathrm{n}}\right)^2\right](\Omega)$$

Local shape optimization around a minimum

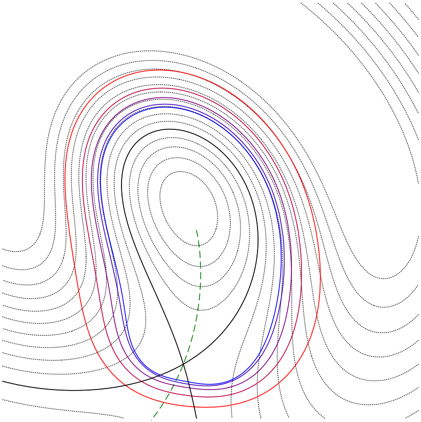

Figure: Optimized domains for $\beta \to \infty$

Asymptotic optimization in the low-temperature limit

For realistic problems, $d \gg 1$, so solving $-\mathcal{L}_\beta u = \lambda u$ is not possible.
Idea: Family of domains $(\Omega_\beta)_{\beta>0}$ parametrized by low-dimensional α, compute asymptotically optimal α as $\beta \to \infty$.
Choice: parameter $\alpha = (\alpha^{(i)})_{0\leq i<N}$ will be the signed distance of the boundary to the critical points on the scale $\beta^{-\frac{1}{2}}$:

$$\alpha^{(i)} = \lim_{\beta\to\infty} \sqrt{\beta}\sigma(\partial\Omega_\beta, z_i),$$

where $(z_i)_{0\leq i<N}$ are the critical points. We say z_i is **far** from the boundary if $\alpha^{(i)} = +\infty$, and **close** to the boundary if $\alpha^{(i)} < +\infty$.
Goal: compute the spectral asymptotics of $\lambda_1(\Omega_\beta), \lambda_2(\Omega_\beta)$ in the limit $\beta \to 0$, and optimize the asymptotic behavior of the ratio $\lambda_2(\Omega_\beta)/\lambda_1(\Omega_\beta)$ w.r.t. α.
Standard choice: Ω is the bassin of attraction of a single minimum z_0.
Corresponds to $\alpha^{(0)} = +\infty$, $\alpha^{(i)} = 0$ for $1 \leq i < N$.
Problem in spectral asymptotics **with moving boundary**.

Mathematical approaches to the exit problem and metastability

- **Large deviations:** (Friedlin & Wentzell): first mathematical proof of Ahrennius' law [23]
- **Potential theory for Markov processes:** (Bovier, Eckhoff & al.) first general sharp estimates of low-lying eigenvalues (Eyring–Kramers formulæ) [6, 7]
- **Semiclassical analysis, Witten Laplacians:** (Hellfer, Sjöstrand, Nier & al.): spectral point of view [21, 11, 12, 10]
- **Numerical analysis for accelerated dynamics:** (Nier, Lelièvre & al.) Hyperdynamics [17], TAD/KMC [8, 16], rigorous Eyring–Kramers transition rates.
- **Recent developments:** non-reversible diffusions [5, 13, 15], entropic barriers [18, 9], non-Markovian setting [1, 2]

And many more...

Geometric assumptions

Suppose $\Omega_\beta \subset \mathcal{K}_0$ compact for all $\beta > 0$.
$(z_i)_{0\leq i<N}$: critical points of V in $\mathcal{K}_0$
$(\nu_j^{(i)}, v_j^{(i)})_{j=1,\dots,d}$ eigendecomposition of $\nabla^2 V(z_i)$, $U^{(i)}$ eigenrotation.
Assume there exist $\delta, \gamma : \mathbb{R}_+ \to \mathbb{R}_+$ such that:

$$\begin{cases} \sqrt{\beta}\delta(\beta) \xrightarrow{\beta\to\infty} +\infty, \\ \delta(\beta) \xrightarrow{\beta\to\infty} 0, \\ \sqrt{\beta}\gamma(\beta) \xrightarrow{\beta\to\infty} 0, \\ \mathcal{O}_i^-(\beta) \subseteq B(z_i, \delta(\beta)) \cap \Omega_\beta \subseteq \mathcal{O}_i^+(\beta), \end{cases} \tag{5}$$

where

$$\mathcal{O}_i^{\pm}(\beta) = z_i + B(0, \delta(\beta)) \cap E^{(i)}\left(\frac{\alpha^{(i)}}{\sqrt{\beta}} \pm \gamma(\beta)\right), \tag{6}$$

$$E^{(i)}(\alpha) = U^{(i)}\left[(-\infty, \alpha) \times \mathbb{R}^{d-1}\right]. \tag{7}$$

Parametrization: local geometry of the boundary around critical points

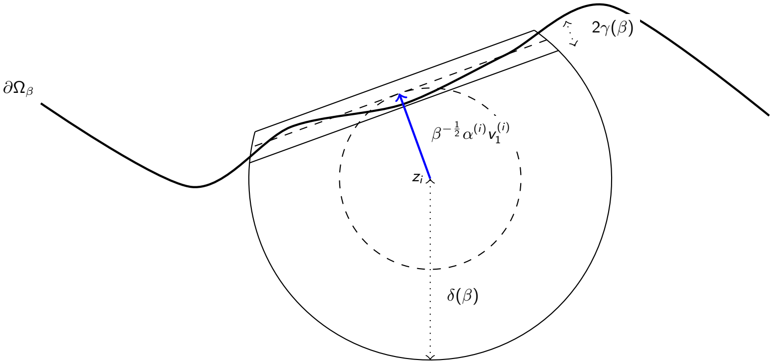

Figure: The local geometry of Ω_β in the neighborhood of a critical point z_i which is close to the boundary. The relevant length scales are $\gamma(\beta) \ll \beta^{-\frac{1}{2}} \ll \delta(\beta) \ll 1$.

Domains whose boundaries are **perpendicular to minimum energy paths**.

Harmonic approximation of the Dirichlet spectrum

Theorem (B., Lelièvre, Stoltz 2024 (in preparation))

Let $k \in \mathbb{N}^*$. Then:

$$\lim_{\beta \to \infty} \lambda_{k,\beta}(\Omega_\beta) = \lambda^{\mathrm{H}}_{k,\alpha},$$

where $\lambda^{\mathrm{H}}_{k,\alpha}$ is the k-th eigenvalue of a certain operator $-\mathcal{L}^{\mathrm{H}}_\alpha$, which can be computed easily.

Crucially, the limit $\lambda^{\mathrm{H}}_{k,\alpha}$ is **explicit** in terms of a 1D-eigenvalue.
Example: one minimum z_0 and order-one saddle points $z_1, \dots, z_m$.

$$\lambda_1(\Omega_\beta) \xrightarrow{\beta\to\infty} 0, \quad \lambda_2(\Omega_\beta) \xrightarrow{\beta\to\infty} \min\left[\nu_1^{(0)}, \min_{i=1,\dots,m} |\nu_1^{(i)}| \mu_{0,\alpha^{(i)}\sqrt{|\nu_1^{(i)}|/2}}\right] =: \lambda^{\mathrm{H}}_{2,\alpha}$$

$\nu_1^{(i)} =$ bottom eigenvalue of $\nabla V^2(z_i)$.
$1/\mu_{0,\theta} =$ metastable exit time from $(-\infty, \theta)$ for $\mathrm{d}Y_t = -Y_t\,\mathrm{d}t + \mathrm{d}B_t$.

Idea of proof (upper bound, à la CFKS [12])

1. Idea: take local harmonic models around each z_i $\mathrm{d}X_t^{\beta,(i)} = -\frac{\nabla^2 V(z_i)}{2}(X_t^{\beta,(i)} - z_i)\,\mathrm{d}t + \sqrt{2\beta^{-1}}\,\mathrm{d}W_t^{(i)}$ killed on hyperplane $\Pi_{\beta,\alpha}^{(i)} := \{(x-z_i)^\intercal v_1^{(i)} = \beta^{-\frac{1}{2}}\alpha^{(i)}\}$.
2. Work with Witten Laplacian on $L^2(\Omega)$, with form domain $H_0^1(\Omega)$:
$$H_\beta := -\mathrm{e}^{-\beta V/2}\mathcal{L}_\beta \mathrm{e}^{\beta V/2} = \frac{\beta}{4}|\nabla V|^2 - \frac{\Delta V}{2} - \frac{1}{\beta}\Delta,$$
locally approximated by
$$H_{\beta,\alpha}^{(i)} := \beta(x-z_i)^\intercal \frac{\nabla^2 V(z_i)^2}{4}(x-z_i) - \frac{\Delta V(z_i)}{2} - \frac{1}{\beta}\Delta$$
with Dirichlet b.c. on $\Pi_{\beta,\alpha}^{(i)}$.
3. Take k first eigenvectors of $\bigoplus_i H_{\beta,\alpha}^{(i)}$, and take localized quasimodes $\left(\chi_\beta^{(i_j)}\psi_{n_j,\beta,\alpha}^{(i_j)}\right)_{1\le j\le k}$, using cutoff functions $\chi_\beta^{(i)}$ supported on $B(z_i,\delta(\beta))$.
4. Shift boundary condition by small $\rho > 0$ to ensure $\chi_\beta\psi_{n,\beta,\alpha-\rho}^{(i)} \in H_0^1(\Omega_\beta)$.
5. Use IMS formula + Courant–Fischer to show $\lambda_{k,\beta}(\Omega_\beta) \le \lambda_{k,\alpha-\rho}^{\mathrm{H}}$, take $\rho \to 0$ using analytic perturbation theory on the $H_{\beta,\alpha-\rho}^{(i)}$.

Idea of proof (lower bound)

1. Construct smooth extended domain $\Omega_\beta \subset \Omega_\beta^\rho$ such that $B(z_i,\delta(\beta)) \cap \Omega_\beta^\rho = B(z_i,\delta(\beta)) \cap E^{(i)}\left(\frac{\alpha^{(i)}+\rho}{\sqrt{\beta}}\right)$ for each $0 \leq i < N$.
2. Take u orthogonal to each of the $\left(\chi_\beta^{(i_j)}\psi_{n_j,\beta,\alpha+\rho}^{(i_j)}\right)_{1\leq j\leq k-1}$ in $L^2(\Omega_\beta^\rho)$.
3. Since $u\chi_\beta^{(i_j)}$ is orthogonal to $\psi_{n_j,\beta,\alpha+\rho}^{(i_j)}$ in $L^2\left(E^{(i_j)}\left(\frac{\alpha^{(i_j)}+\rho}{\sqrt{\beta}}\right)\right)$, use Courant–Fischer on $H_{\beta,\alpha+\rho}^{(i_j)}$.
4. Using Courant–Fischer again, deduce $\lambda_{k,\beta}(\Omega_\beta) \leq \lambda_{k,\beta}(\Omega_\beta^\rho) \leq \lambda_{k,\alpha+\rho}^{\mathrm{H}}$.

Finer asymptotics: setting and notations

Assume z_0 is the unique local minimum of V in all the Ω_β, and define its bassin of attraction:

$$\mathcal{A}(z_0) = \left\{ x_0 \in \mathbb{R}^d \,\middle|\, \lim_{t\to\infty} x_t = z_0 \right\},$$

where $x_t' = -\nabla V(x_t)$. The low-lying saddle points are given by

$$I_{\min} = \underset{\substack{1\leq i<N_1 \\ z_i\in\partial\mathcal{A}(z_0)}}{\operatorname{Argmin}} V(z_i), \quad V^* = \min_{\substack{1\leq i<N_1 \\ z_i\in\partial\mathcal{A}(z_0)}} V(z_i). \tag{8}$$

Assume also that the domains contain enough of the energy well

$$\left[\mathcal{A}(z_0) \cap \{V < V^* + C_V\delta(\beta)^2\}\right] \setminus \bigcup_{i\in I_{\min}} B(z_i, \delta(\beta)) \subset \Omega_\beta$$

Illustration around a 2D well

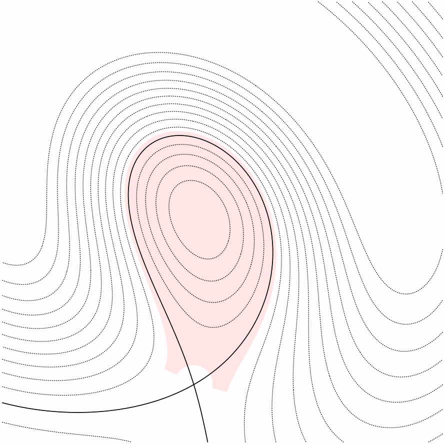

Figure: The boundary cannot cross the shaded region.

Finer asymptotics for $\lambda_1(\Omega_\beta)$

Modified Eyring–Kramers formula:

Theorem (B., Lelièvre, Stoltz 2024 (in preparation))

Let $0 < \epsilon < 1$. Under the previous assumptions, there exists $c > 0$ so that the following estimate holds in the limit $\beta \to +\infty$:

$$\lambda_{1,\beta} = \mathrm{e}^{-\beta(V^* - V(z_0))} \left[\sum_{i \in I_{\min}} \frac{|\nu_1^{(i)}|}{2\pi \Phi\left(|\nu_1^{(i)}|^{\frac{1}{2}} \alpha^{(i)}\right)} \sqrt{\frac{\det \nabla^2 V(z_0)}{|\det \nabla^2 V(z_i)|}} \left(1 + \mathcal{O}(\varepsilon_i(\beta))\right) \right], \tag{9}$$

where $\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} \mathrm{e}^{-\frac{t^2}{2}} \, \mathrm{d}t$, and

$$\varepsilon_i(\beta) = \begin{cases} \beta^{\epsilon - 1}, & \alpha^{(i)} = +\infty, \\ \sqrt{\beta}\gamma(\beta), & \alpha^{(i)} \in \mathbb{R}. \end{cases} \tag{10}$$

Asymptotic optimization of the boundary position

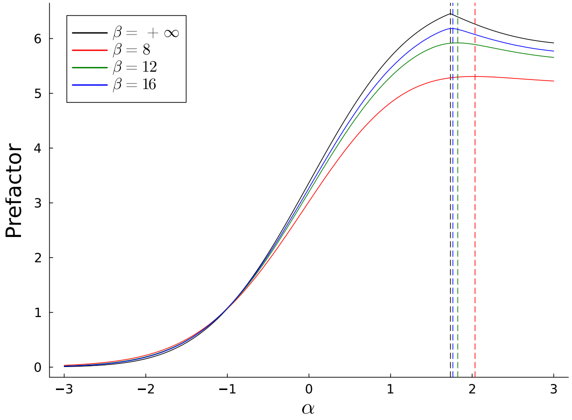

Figure: $\mathrm{e}^{-\beta(V^* - V(z_0))} J_\beta(\Omega_\beta)$ as a function of α. The semiclassical prescription is asymptotically optimal.

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