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**. X_t^β is reversible and ergodic with respect to the Gibbs measure

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

In computational statistical physics/molecular dynamics
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:

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

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 $\frac{\mathrm{d}\mu_0}{\mathrm{d}\mu} \in L^2(\Omega, \mu)$, *where* $X_0^\beta \sim \mu_0$, *write* $\mu_t = \mathrm{Law}\left(X_t^\beta \middle| \tau_\Omega > t\right)$.
Then, $\exists (C_1, C_2)(\beta, \mu_0)$*:*

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

$$\sup_{\|f\|_\infty \leq 1} \left| \mathbb{E}^{\mu_0}\left[f(X_{\tau_\Omega}^\beta, \tau_\Omega - t) \middle| \tau_\Omega > t \right] - \mathbb{E}^\nu \left[f(X_{\tau_\Omega}^\beta, \tau_\Omega) \right] \right| \leq C_2 \mathrm{e}^{-(\lambda_{2,\beta} - \lambda_{1,\beta})t}.$$

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 [23, 21]).
- The case $V = 0$ has been studied in the shape optimization litterature, e.g. the Payne–Polyá–Weinberger conjecture [20, 4].

Shape gradient descent

Isolated Dirichlet eigenvalues of $\mathcal{L}_\beta$ are **shape-differentiable**. Assume $\lambda_{k,\beta}(\Omega_0)$ is simple.

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.

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

Local shape optimization around a potential well

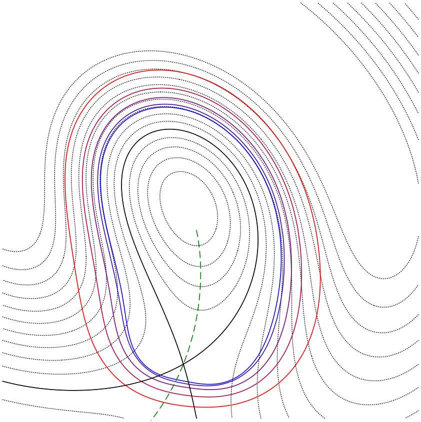

Figure: Optimized domains for increasing β.

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: Take a family of domains $(\Omega_\beta)_{\beta>0}$. The spectrum is sensitive to a $\alpha \in \mathbb{R}^N$ with $N \ll d$ as $\beta \to \infty$. Find asymptotically optimal α as $\beta \to \infty$.
Parameter: $\alpha = (\alpha^{(i)})_{0\leq i<N}$ is signed distance of critical points to the boundary on the scale $\beta^{-\frac{1}{2}}$:

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

where $(z_i)_{0\leq i<N}$ are the critical points (assume this limit exists).
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.
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 [24]
- **Potential theory for Markov processes:** first general sharp estimates of low-lying eigenvalues (Eyring–Kramers formulæ) [6, 7]
- **Semiclassical analysis, Witten Laplacians:**: spectral point of view [22, 11, 12, 10]
- **Numerical analysis for accelerated dynamics:** Hyperdynamics [18], TAD/KMC [8, 17], rigorous Eyring–Kramers transition rates.
- **Recent developments:** non-reversible diffusions [5, 13, 15], entropic barriers [19, 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 $\mathcal{K}_0$
Fix $(\nu_j^{(i)}, v_j^{(i)})_{j=1,\dots,d}$ eigendecomposition of $\nabla^2 V(z_i)$, $U^{(i)}$ eigenrotation.
Assume $\nu_1^{(i)} < 0$ if $\mathrm{Ind}(z_i) = 1$, and 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

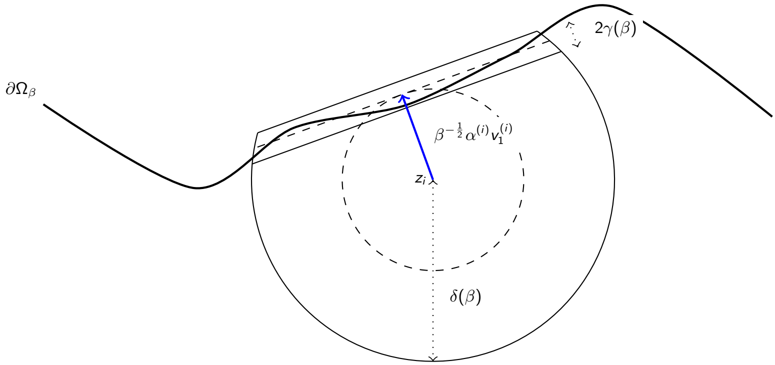

Figure: The local geometry of Ω_β in the neighborhood of a critical point z_i which is close to the boundary. The relevant length scales are $\gamma(\beta) \ll \beta^{-\frac{1}{2}} \ll \delta(\beta) \ll 1$.

Around saddle points close to the boundary, domains are asymptotically **orthogonal to the minimum energy path**.

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 an explicit operator $-\mathcal{L}^{\mathrm{H}}_{\alpha}$, the harmonic approximation.

Example of a single minimum z_0 and order-one saddle points $z_1, \dots, z_{N-1}$.

$$\lambda_1(\Omega_\beta) \xrightarrow{\beta\to\infty} 0, \quad \lambda_2(\Omega_\beta) \xrightarrow{\beta\to\infty} \min\left[\nu_1^{(0)}, \min_{0<i<N} |\nu_1^{(i)}| \left(\mu_{0,\alpha^{(i)}\sqrt{|\nu_1^{(i)}|/2}} + \frac{1}{2}\right)\right]$$

$\mu_{0,\theta}$ ground-state energy of harmonic oscillator $\frac{1}{2}(x^2 - \partial_x^2)$ with Dirichlet boundary conditions on $(-\infty, \theta)$.

Idea of proof à la CFKS [12]: harmonic quasimodes

1. Work with Schrödinger-like Witten Laplacian, self-adjoint operator 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

$$H^{(i)}_{\beta,\alpha} := \beta(x-z_i)^\intercal \frac{\nabla^2 V(z_i)^2}{4}(x-z_i) - \frac{\Delta V(z_i)}{2} - \frac{1}{\beta}\Delta$$

   with Dirichlet boundary condition on $z_i + B(0,\delta(\beta)) \cap E^{(i)}\left(\frac{\alpha^{(i)}}{\sqrt{\beta}} \pm \gamma(\beta)\right)$.
   Denote $\left(\lambda^{(i)}_{n,\beta,\alpha}, \psi^{(i)}_{n,\beta,\alpha}\right)$ its n-th eigenpair. Note $\lambda^{(i)}_{n,\beta,\alpha}$ is constant w.r.t. β.
2. The k-th first eigenvectors of $\bigoplus_i H^{(i)}_{\beta,\alpha}$ can be seen as a family $\left(\psi^{(i_j)}_{n_j,\beta,\alpha}\right)_{j=1,\dots,k}$, with $\psi^{(i_j)}_{n_j,\beta,\alpha}$ fastly decaying away from z_{i_j}.
3. Consider quasimodes $\left(\chi^{(i_j)}_\beta \psi^{(i_j)}_{n_j,\beta,\alpha}\right)_{j=1,\dots,k}$ with $\mathbb{1}_{B(z_i,\frac{1}{2}\delta(\beta))} \le \chi^{(i)}_\beta \le \mathbb{1}_{B(z_i,\delta(\beta))}$ smooth.

Idea of proof (estimates)

1. Shift boundary condition inward by $\rho/\sqrt{\beta} > 0$: for β large enough, each $\psi^{(i)}_{n,\beta,\alpha-\rho}$ is in the form domain $H^1_0(\Omega_\beta)$.
2. Standard arguments and Courant–Fischer Min-Max give upper bound $\lambda_{k,\beta}(\Omega_\beta) \leq \lambda^{\mathrm{H}}_{k,\alpha-\rho}$, and perturbation theory allows to take $\rho \to 0$.
3. Construct smooth extended domain $\Omega_\beta \subset \Omega^\rho_\beta$ such that $B(z_i, \delta(\beta)) \cap \Omega^\rho_\beta = B(z_i, \delta(\beta)) \cap E^{(i)}\left(\frac{\alpha^{(i)}+\rho}{\sqrt{\beta}}\right)$ for each $0 \leq i < N$.
4. Take u orthogonal to each of the $\left(\chi^{(i_j)}_\beta \psi^{(i_j)}_{n_j,\beta,\alpha+\rho}\right)_{1\leq j\leq k-1}$ in $L^2(\Omega^\rho_\beta)$, so that $u\chi^{(i_j)}_\beta$ is orthogonal to $\psi^{(i_j)}_{n_j,\beta,\alpha+\rho}$ in $L^2\left(E^{(i_j)}\left(\frac{\alpha^{(i_j)}+\rho}{\sqrt{\beta}}\right)\right)$ for each j.
5. Standard arguments using IMS formula and Courant–Fischer Max-Min give $\lambda_{k,\beta}(\Omega^\rho_\beta) \leq \lambda^{\mathrm{H}}_{k,\alpha+\rho}$.
6. Domain monotonicity gives $\lambda_{k,\beta}(\Omega_\beta) \leq \lambda^{\mathrm{H}}_{k,\alpha+\rho}$, take $\rho \to 0$.

Finer asymptotics: additional assumptions

Harmonic approximation only
says $\#\{\text{small eigenvalues}\} = \#\{\text{local minima far from the boundary}\}$.

- Assume z_0 is the unique local minimum of V far from the boundary 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 index-one saddle points are:

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

- Assume that the domains contain enough of the energy well around z_0:

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

Energy well assumption

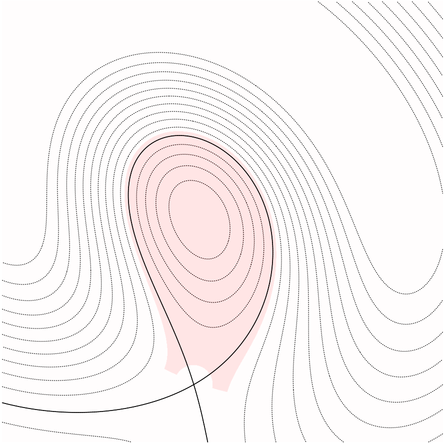

Figure: The boundary cannot cross the shaded region.

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 $\varepsilon_i(\beta)$ decays polynomially in β.

Construction of a more precise quasimode, see [7, 16]

Quasimode for $u_{1,\beta}$

$$\psi_\beta = \frac{1}{Z_\beta}\left[\eta_\beta + \sum_{i\in I_{\min}} \chi_\beta^{(i)}\left(\varphi_\beta^{(i)} - \eta_\beta\right)\right], \tag{10}$$

where $\eta_\beta = \eta\left(\frac{V(x)-V^*}{C_\eta\,\delta(\beta)^2}\right)\mathbb{1}_{\mathcal{A}(z_0)}(x)$ is a rough energy cutoff, and, as before, $\mathbb{1}_{B(z_i,\frac{1}{2}\delta(\beta))} \le \chi_\beta^{(i)} \le \mathbb{1}_{B(z_i,\delta(\beta))}$ is smooth.
Local approximation:

$$\varphi_\beta^{(i)}(x) = \frac{\displaystyle\int_{(x-z_i)^\intercal v_1^{(i)}}^{+\infty} \mathrm{e}^{-\beta\frac{|\nu_1^{(i)}|}{2}t^2}\xi_\beta^{(i)}(t)\,\mathrm{d}t}{\displaystyle\int_{-\infty}^{+\infty} \mathrm{e}^{-\beta\frac{|\nu_1^{(i)}|}{2}t^2}\xi_\beta^{(i)}(t)\,\mathrm{d}t}, \tag{11}$$

with $\mathbb{1}_{(-C_\xi\delta(\beta),\alpha^{(i)}/\sqrt{\beta}-2\gamma(\beta))} \le \xi_\beta^{(i)} \le \mathbb{1}_{(-2C_\xi\delta(\beta),\alpha^{(i)}/\sqrt{\beta}-\gamma(\beta))}$ is smooth.

Construction near a low-energy saddle point

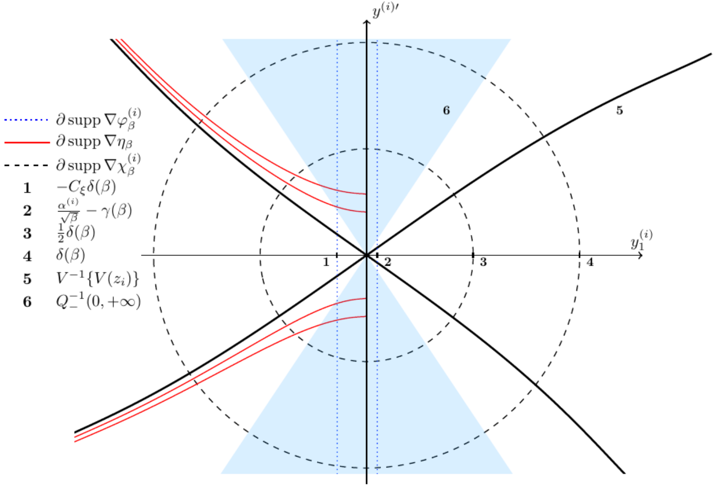

Figure: Construction of the quasimode close to the boundary.

Idea of proof of Eyring–Kramers formula.

Tune C_ξ, C_η to ensure $\psi_\beta \in H_0^1 \cap H^2(\Omega_\beta, \mu)$ for β large enough. Project ψ_β using the spectral projector π_β associated with $\lambda_{1,\beta}$.

$$\varphi \mapsto \frac{1}{2i\pi} \oint_\Gamma (\mathcal{L}_\beta + z)^{-1} \varphi \, \mathrm{d}z.$$

Easy to show, using harmonic limit to isolate $\lambda_{1,\beta}$ from the rest of the spectrum, that

$$\begin{cases} \|(1-\pi_\beta)\psi_\beta\|_{L^2_\mu(\Omega_\beta)} = \mathcal{O}(\|\mathcal{L}_\beta \psi_\beta\|_{L^2_\mu(\Omega_\beta)}), \\ \|\nabla \pi_\beta \psi_\beta\|^2_{L^2_\mu(\Omega_\beta)} = \|\nabla \psi_\beta\|^2_{L^2_\mu(\Omega_\beta)} + \mathcal{O}\left(\|\mathcal{L}_\beta \psi_\beta\|^2_{L^2_\mu(\Omega_\beta)}\right). \end{cases} \tag{12}$$

Using a Laplace method adapted to moving domains, we estimate $\|\nabla \psi_\beta\|^2_{L^2_\mu(\Omega_\beta)}$, and show $\|\mathcal{L}_\beta \psi_\beta\|_{L^2_\mu(\Omega_\beta)} \ll \|\nabla \psi_\beta\|_{L^2_\mu(\Omega_\beta)}$. Allows to compute sharp asymptotics for

$$\lambda_{1,\beta}(\Omega_\beta) = \frac{\|\nabla \pi_\beta \psi_\beta\|^2_{L^2_\mu(\Omega_\beta)}}{\|\pi_\beta \psi_\beta\|^2_{L^2_\mu(\Omega_\beta)}}.$$

Asymptotic optimization of the boundary position

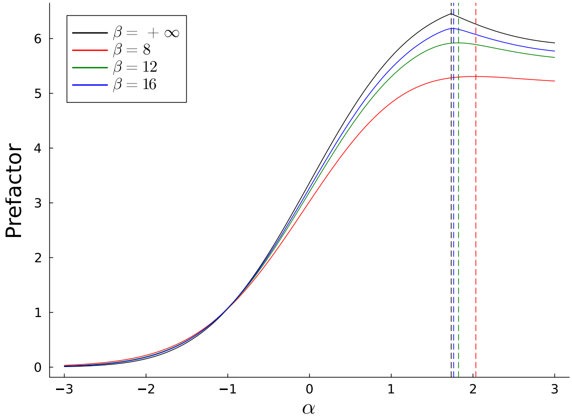

Figure: Blow-up of the transition $\mathrm{e}^{-\beta(V^*-V(z_0))}J_\beta(\Omega_\beta)$ as a function of α. The semiclassical prescription is asymptotically optimal.

- Extension to Riemannian setting / multiple wells.
- Moving generalized saddle points.
- More general asymptotic geometries.
- Asymptotic shape optimization in the entropic case.

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