Spectre basse température du générateur OL tué au bord d'un domaine mouvant.

Noé Blassel

October 11, 2023

1 Setting

The problem Let $V:\mathbb{R}^d\to\mathbb{R}$ be a C^∞ function. The overdamped Langevin dynamics

$$dX_t = -\nabla V(X_t) dt + \sqrt{\frac{2}{\beta}} dW_t,$$

The measure

$$\mu(\mathrm{d}x) = \mathrm{e}^{-\beta V(x)} \,\mathrm{d}x,$$

The generator

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

We consider a family

$$(\Omega_{\beta})_{\beta \geq 0}$$

of open, smooth, bounded, connected domains.

Assumptions.

• The domains are non-increasing

$$\beta_1 > \beta_2 \implies \Omega_{\beta_1} \subseteq \Omega_{\beta_2}.$$

- The potential V is a \mathcal{C}^{∞} Morse function $\overline{\Omega_0}$, such that $z_0 \in \Omega_0$ is the unique local minimum.
- The z_1, \dots, z_m are all the order-1 saddle points of V in $\overline{\Omega_0}$.
- The critical points $(z_i)_{i=0,\dots,m}$ adhere to all the domains:

$$z_i \in \overline{\Omega}_\beta \, \forall 0 \le i \le m, \, \forall \beta \ge 0.$$

Define, for $i = 0, \dots, m$

$$\varepsilon_{\beta}^{(i)} = d(z_i, \partial \Omega_{\beta}) = \inf_{x \in \mathbb{R}^d \setminus \Omega_{\beta}} |x - z_i|.$$

The assumption that the Ω_{β} are non-increasing implies that, $\beta \mapsto \varepsilon_{\beta}^{(i)}$ is also non-increasing for all i. We distinguish three regimes.

- The subcritical case $\lim_{\beta \to \infty} \sqrt{\beta} \varepsilon_{\beta}^{(i)} = 0$.
- The **critical** case $\lim_{\beta \to \infty} \sqrt{\beta} \varepsilon_{\beta}^{(i)} = \alpha > 0$.

Motiver les dénominations

• The supercritical case $\lim_{\beta \to \infty} \sqrt{\beta} \varepsilon_{\beta}^{(i)} = +\infty$.

We then make the following further assumptions:

• (coreset) There exists r > 0 such that

$$\varepsilon_{\beta}^{(0)} > r$$
.

the

pour i=1,...,m • (spill out in unstable direction) In the (sub)critical case, $\varepsilon_{\beta}^{(i)} \to 0$ as $\beta \to \infty$. Denoting then by $v_1^{(i)}$ an eigenvector of $\nabla^2 V(z_i)$ associated with the unique negative eigenvalue, we assume that $v_1^{(i)} \sim n_{\partial\Omega_{\beta}}(x_{\beta})$ in the sense of essential convergence, for any $(x_{\beta})_{\beta \geq 0} \in \prod_{\beta > 0} \partial\Omega_{\beta}$ such that $\varepsilon_{\beta}^{(i)} = |x_{\beta} - z^{(i)}|$.

It is helpful to think loosely of Ω_{β} as a positive temperature perturbation of the bassin of attraction of z_0 for the steepest-descent dynamics $\dot{X} = -\nabla V(X)$.

Nommer les hypothèses

We define

$$\lambda_{1,\beta} \leq \lambda_{2,\beta} \leq \cdots$$

the sequence of eigenvalues of $-\mathcal{L}_{\beta}$ on the domain $H_0^1 \cap H^2(\Omega_{\beta}; \mu) \subset L_{\mu}^2$, for which it is self-adjoint with pure point spectrum.

We first aim to extend the harmonic approximation (CKFS 11.1) to the case with Dirichlet boundary and temperature-dependent domain. More precisely, we aim to show that, for all integers $k \geq 1$,

$$\lambda_{k,\beta} = \lambda_k^{\text{harm}} + o(\beta^{-1}), \, \beta \to \infty,$$

where by λ_k^{harm} we denote the k-th eigenvalue of some temperature-independent operator (4) whose spectrum can be computed explicitly.

This operator is obtained by considering local approximations around each critical point z_i , which are harmonic oscillators whose realization depends on the behavior of $\sqrt{\beta}\varepsilon_{\beta}^{(i)}$. Hence we define the following model spaces.

Definition 1. • In the subcritical case:

$$S^{(i)} = (-\infty, 0) \times \mathbb{R}^{d-1}.$$

• In the critical case:

$$S^{(i)} = (-\infty, \alpha) \times \mathbb{R}^{d-1}, \ \alpha > 0.$$

• In the supercritical case:

$$S^{(i)} = \mathbb{R}^d.$$

2 Tools

In this section we collect definitions and useful lemmas.

\Omega ou \Omega_\beta ?

Witten Laplacian.

Here we consider an open domain $\Omega \subseteq \mathbb{R}^d$, and $V : \mathbb{R}^d \to \mathbb{R}$ a smooth potential.

Definition 2. The Witten Laplacian is the following operator

$$H_{\beta} = U_{\beta} - \Delta, \qquad U_{\beta} = \frac{\beta^2}{4} |\nabla V|^2 - \frac{\beta}{2} \Delta V,$$
 (1)

with domain $D(H_{\beta}) = H_0^1 \cap H^2(\Omega) \subset L^2(\Omega)$.

The interest of considering this operator is that one can relate the spectral properties of \mathcal{L}_{β} to those of H_{β} , which acts on a flat L^2 space. Consider the unitary transformation $U: L^2(\Omega) \to L^2_{\mu}(\Omega), \ u \to \mathrm{e}^{\beta V/2}u$, with $U^*: L^2_{\mu}(\Omega) \to L^2(\Omega), \ U^*v = \mathrm{e}^{-\beta V/2}v$. The conjugate of \mathcal{L}_{β} is then an operator on $L^2(\Omega)$ which ressembles a Schrödinger operator:

$$U^*(-\mathcal{L}_{\beta})U = e^{-\beta V/2} \left(\nabla V \cdot \nabla - \frac{1}{\beta} \Delta \right) e^{\beta V/2}$$

$$= e^{-\beta V/2} \left(\nabla V \cdot -\frac{1}{\beta} \operatorname{div} \right) \nabla e^{\beta V/2}$$

$$= e^{-\beta V/2} \left(\nabla V \cdot -\frac{1}{\beta} \operatorname{div} \right) \left[e^{\beta V/2} \nabla + \frac{\beta}{2} \nabla V e^{\beta V/2} \right]$$

$$= \nabla V \cdot \left[\nabla + \frac{\beta}{2} \nabla V \right] - \frac{1}{2} \nabla V \cdot \nabla - \frac{1}{\beta} \Delta - \frac{\beta}{4} |\nabla V|^2 - \frac{1}{2} \nabla V \cdot \nabla - \frac{1}{2} \Delta V$$

$$= \frac{1}{2} (\frac{\beta}{2} |\nabla V|^2 - \Delta V) - \frac{1}{\beta} \Delta$$

$$= \frac{1}{\beta} H_{\beta}.$$

Therefore, the spectrum of $-\mathcal{L}_{\beta}$ is related to that of H_{β} via

$$\sigma(H_{\beta}) = \beta \sigma(-\mathcal{L}_{\beta}).$$

We denote by

$$Q_{\beta}(u) = \langle U_{\beta}u, u \rangle + \|\nabla u\|^2 \tag{2}$$

the quadratic form associated to the Witten Laplacian, with domain $H_0^1(\Omega_\beta)$.

Local harmonic approximation.

The potential part of H_{β} , given by $\frac{1}{2} \left(\beta^2 \frac{|\nabla V|^2}{2} - \beta \Delta V \right)$, has wells around each critical point of V. Furthermore, these wells are separated by increasing barriers as $\beta \to \infty$, which motivates the study of local harmonic approximations of H_{β} around each critical point of V. To that effect, we define:

$$\Sigma^{(i)} = \frac{1}{2} \text{Hess} \left(\frac{1}{4} |\nabla V|^2 \right) (z_i) = \frac{1}{2} \left[\frac{1}{2} D^3 V \nabla V + \frac{1}{2} \left(\text{Hess } V \right)^2 \right] (z_i) = \frac{1}{4} \left(\text{Hess } V \right)^2 (z_i),$$

and let

$$\sigma(\text{Hess }V(z_i)) = \{\nu_1^{(i)} \le \nu_2^{(i)} \le \dots \le \nu_d^{(i)}\}$$

denote the eigenvalues of $\operatorname{Hess} V$ at z_i , with

the associated orthonormal eigenbasis, which induces a unitary transformation on L^2 via

$$\mathcal{U}^{(i)}f(x) = f\left(U^{(i)}x\right), \quad \mathcal{U}^{(i)*}f(x) = f\left(U^{(i)\mathsf{T}}x\right).$$

Since the critical points are non-degenerate, $\nu_j^{(i)} \neq 0$ for all $1 \leq j \leq d$, $0 \leq i \leq k$, and $\nu_1^i < 0$ if and only if $i \geq 1$. Suppose $z_i \in \partial \Omega$ for some $i \geq 1$. In this case, assume that $\nu_1^{(i)}$ is the outward normal to Ω at z_i ,

Preciser hypothese – convergence de $v_1^{(i)}$ vers $n_{\partial\Omega_{\beta}}(e_{\beta}(z^{(i)}))$ où $|x - e_{\beta}(x)| = d(x, \partial\Omega_{\beta})$ ("on dépasse dans la direction instable")

and introduce the half-space

We define local harmonic approximations to H_{β} around each critical point:

$$H_{\beta}^{(i)} = -\Delta + \beta^2 (x - z_i)^{\mathsf{T}} \Sigma^{(i)} (x - z_i) - \beta \frac{\Delta V(z_i)}{2},$$

and the shifted harmonic oscillators:

$$K^{(i)} = -\Delta + x^{\mathsf{T}} \Lambda^{(i)} x - \frac{\Delta V(z_i)}{2}.$$

By dilation $D_{\lambda}f(x) = \lambda^{d/2}f(\lambda x)$, translation $T_bf(x) = f(x-b)$ and orthogonal change of coordinates $\mathcal{U}^{(i)}$, $H_{\beta}^{(i)}$ acting sur $L^2(\Omega)$ is unitarily equivalent to $\beta K^{(i)}$ acting on $L^2(\sqrt{\beta}U^{(i)}(\Omega - z_i))$:

$$H_{\beta}^{(i)} = D_{\beta^{1/2}} \mathcal{U}^{(i)} T_{\beta^{1/2} z_i} \left(\beta K^{(i)} \right) T_{-\beta^{1/2} z_i} \mathcal{U}^{(i)*} D_{\beta^{-1/2}}.$$

Spectra of the harmonic oscillators.

The advantage of working with the harmonic oscillators $K^{(i)}$ is that the eigendecomposition By $\sigma(K^{(i)})$, we denote the spectrum of the Dirichlet realization of the harmonic oscillator $K^{(i)}$ on $S^{(i)}$, which are (almost) analytically known.

The supercritical case $S^{(i)} = \mathbb{R}^d$.

In this case, the spectrum is given by

$$\sigma(K^{(i)}) = \left\{ \frac{1}{2} \sum_{j=1}^{d} \left(|\nu_j^{(i)}| (2n_j + 1) - \nu_j^{(i)} \right), \quad n \in \mathbb{N}^d \right\}.$$

For i = 0, $\nu_j^{(i)} = |\nu_j^{(i)}|$, hence

$$\sigma(K^{(0)}) = \left\{ \sum_{j=1}^{d} \nu_j^{(i)} n_j, \quad n \in \mathbb{N}^d \right\} \ni 0.$$

For $i \ge 1$, $\nu_1^{(i)} = -|\nu_1^{(i)}|$ and $\nu_j^{(i)} = |\nu_j^{(i)}|, \ j \ge 2$, thus

$$\sigma(K^{(i)}) = \left\{ |\nu_1^{(i)}|(n_1+1) + \sum_{j=2}^d \nu_j^{(i)} n_j, \quad n \in \mathbb{N}^d \right\}, \quad i \ge 1.$$

The bottom of the latter spectrum is given by $|\nu_1^{(i)}|$. For simplicity, we will denote, for a multi-index $n \in \mathbb{N}^d$,

$$\nu_n^{(i)} = \sum_{i=1}^d |\nu_j^{(i)}| n_j + \mathbb{1}_{\nu_1^{(i)} < 0} \text{ | \n_1^{(i)}| }$$

and $\psi_n^{(i)}$ the corresponding eigenfunction (which, up to a phase, we assume to be real-valued). Then, $\psi_n^{(i)}$ can be written as a product of ...

$$\psi_n^{(i)}(x) = \prod_{j=1}^d \left(\frac{|\nu_j^{(i)}|}{2}\right)^{\frac{1}{4}} \psi_{n_j} \left(\sqrt{\frac{|\nu_j^{(i)}|}{2}} x_j\right)$$
(3)

into a product of elementary eigenfunctions, where for $k \in \mathbb{N}$, we denote

$$\psi_k(x) = \frac{1}{\sqrt{2^k k! \sqrt{\pi}}} e^{-\frac{x^2}{2}} H_k(x),$$

with H_k being the k-th Hermite polynomial. The function ψ_k is an eigenstate for the canonical harmonic oscillator $\frac{1}{2}(x^2 - \partial^2)$.

The subcritical case $S^{(i)} = (-\infty, 0) \times \mathbb{R}^{d-1}$.

The difference in this case is that the oscillator corresponding to the unstable direction is restricted to the half-space $(-\infty,0)$. Its eigenstates correspond to the odd eigenstates of the harmonic oscillator on the full space. The spectrum is thus given, for i > 1, by

$$\sigma(K^{(i)}) = \left\{ |\nu_1^{(i)}|(2n_1 + 2) + \sum_{j=2}^d \nu_j^{(i)} n_j, \quad n \in \mathbb{N}^d \right\}$$

In this case, the bottom of the spectrum is given by

$$\min\{2|\nu_1^{(i)}|,\nu_2^{(i)}\}.$$

The eigenfunctions are identical to the restriction of (3) to the half-space, up to a $\sqrt{2}$ factor to account for L^2 normalization. avec n_1 remplacé par 2n_1+1

The critical case $S^{(i)} = (-\infty, \alpha) \times \mathbb{R}^{d-1}$.

In this case, the spectrum of the oscillator corresponding to the unstable direction, restricted to the half-space $(-\infty, \alpha)$, is not analytically known. Nevertheless, we denote for $k \in \mathbb{N}$

$$(\lambda_k^{\alpha}, \psi_k^{\alpha})$$

the k-th eigenpair for the Dirichlet realization of the harmonic oscillator $\frac{1}{2}(x^2 - \partial^2)$ on $(-\infty, \alpha)$.

monique. (critère de Molchanov)

Elaborer sur propriétés spectrales, idem pour on a le fait que le spectre est discret.

The spectrum is then given, for $i \geq 1$, by

$$\sigma(K^{(i)}) = \left\{ |\nu_1^{(i)}| (2\lambda_{n_1}^{\alpha} - \frac{1}{2}) + \sum_{j=2}^d \nu_j^{(i)} n_j, \quad n \in \mathbb{N}^d \right\},\,$$

while the eigenstates are given by

$$\psi_n^{(i)}(x) = \left(\frac{|\nu_1^{(i)}|}{2}\right)^{\frac{1}{4}} \psi_{n_j}^{\alpha} \left(\sqrt{\frac{|\nu_1^{(i)}|}{2}} x_1\right) \prod_{j=2}^d \left(\frac{|\nu_j^{(i)}|}{2}\right)^{\frac{1}{4}} \psi_{n_j} \left(\sqrt{\frac{|\nu_j^{(i)}|}{2}} x_j\right).$$

In each of the three cases, we denote by $\lambda_k^{(i)}$ the k-th eigenvalue of $K^{(i)}$ acting on $S^{(i)}$. In the case of an eigenvalue λ which occurs multiple times (that is, such that multiple d-uplets $n \in \mathbb{N}^d$ correspond to λ), we convene that we count λ with multiplicity, using the ordering induced by the lexicographic order on \mathbb{N}^d .

Global harmonic approximation.

We consider the following operator

$$K = \bigoplus_{i=0}^{m} K^{(i)}, \quad \mathcal{D}(K) = H_0^1 \cap H^2 \left(\prod_{i=0}^{m} S^{(i)} \right),$$
 (4)

with spectrum

$$\sigma(K) = \bigcup_{i=0}^{m} \sigma(K^{(i)}).$$

We denote by $(\lambda_k^{\text{harm}}, \psi_k^{\text{harm}})$ the k-th smallest eigenpair of K. We count eigenvalues with multiplicity, defering first to the ordering on 0, \cdots , m, then to the ordering of eigenvalues of each $K^{(i)}$ to order multiple eigenvalues.

We also define the maps $k: \mathbb{N}^* \to \mathbb{N}^*, i: \mathbb{N}^* \to \{0, \dots, m\}$ such that

$$\lambda_n^{\text{harm}} = \lambda_{k_n}^{(i_n)}.$$

Definition of the harmonic quasimodes.

We now give the definition of rough quasimodes for H_{β} . We fix $n \in \mathbb{N}^*$, and define

$$\widetilde{\psi}_{\beta,n}(x) = \beta^{\frac{d}{4}} \chi_{\beta}^{(i_n)}(x) \psi_{k_n}^{(i_n)}(\sqrt{\beta} U^{(i_n)}(x - z_i)), \tag{5}$$

where $\chi_{\beta}^{(i_n)}$ is a C_c^{∞} cutoff function whose specific definition depends on $S^{(i_n)}$.

The supercritical case $S^{(i_n)} = \mathbb{R}^d$.

The subcritical case $S^{(i_n)} = (-\infty, 0) \times \mathbb{R}^{d-1}$.

The critical case $S^{(i_n)} = (-\infty, \alpha) \times \mathbb{R}^{d-1}$.

Various lemmas.

The following lemma expresses the monotonicity of eigenvalues with respect to the domain of the operator.

Lemma 1. Let $\mathcal{H}_1 \subset \mathcal{H}_2$ be separable Hilbert spaces such that the positive unbounded operator A with domain D_1 (respectively D_2) is self-adjoint in \mathcal{H}_1 (respectively \mathcal{H}_2), with $D_1 \subset D_2$. Denote $0 \leq \lambda_1(D_i) \leq \lambda_2(D_i) \leq \ldots$ the sequence of ordered eigenvalues (counted with multiplicity) below the essential spectrum for the realization of A on D_i .

Then, $\lambda_k(D_1) \geq \lambda_k(D_2)$ whenever these two eigenvalues exist.

Proof. By the Courant–Fischer Min-Max principle (we write, for $u, v \in \mathcal{H}_1$, $\langle u, v \rangle_{\mathcal{H}_1} = \langle u, v \rangle_{\mathcal{H}_2}$):

$$\lambda_k(D_i) = \inf_{\substack{V \subset D_i \\ \dim V = k}} \sup_{u \in V \setminus \{0\}} \frac{\langle Au, u \rangle_{\mathcal{H}_2}}{\|u\|_{\mathcal{H}_2}^2}.$$

The claimed result follows immediately since

$$\{V \subset D_1 \mid \dim V = k\} \subset \{V \subset D_2 \mid \dim V = k\},\,$$

so that the inf is taken over a smaller set in the expression for $\lambda_k(D_1)$.

Corollary 1. The map $\beta \mapsto \lambda_{k,\beta}$ is non-decreasing for all k, since $\beta \mapsto H_0^1 \cap H^2(\Omega_\beta; \mu)$ is non-increasing. Non —> pour le spectre de K(i) sur un domaine qui croit?

A key technical tool is the following formula, which allows to decompose Schrödinger operators as sums of localized terms, at the cost of an error term involving gradients of cutoff functions.

Lemma 2. Let $\Omega \subset \mathbb{R}^d$ be an open set, and $(\chi_i)_{i=1,...,m}$ be a partition of unity on Ω , in the sense that

$$\sum_{i=1}^{m} \chi_i^2 = \mathbb{1}_{\Omega}, \quad \chi_i \in C^2(\Omega) \quad \forall 1 \le i \le m.$$

Let also $H = U - \Delta$ be the Schrödinger Hamiltonian operator acting on $H_0^1 \cap H^2(\Omega) \subset L^2(\Omega)$. Then the following identity holds:

$$H = \sum_{i=1}^{m} \chi_i H \chi_i - \sum_{i=1}^{m} |\nabla \chi_i|^2.$$
 (6)

Writing $Q(u) = \langle Hu, u \rangle = \langle Uu, u \rangle + ||\nabla u||^2$, we also have the following identity for any $u \in H_0^1(\Omega)$:

$$Q(u) = \sum_{i=1}^{m} Q(\chi_i u) - \||\nabla \chi_i| u\|^2.$$
 (7)

Proof. We compute the following commutator in two ways:

$$\begin{split} [\chi_i, [\chi_i, H]] &= \chi_i^2 H - 2\chi_i H \chi_i + H \chi_i^2, \\ [\chi_i, [\chi_i, H]] &= - [\chi_i, [\chi_i, \Delta]] \\ &= - [\chi_i, \chi_i \Delta - \Delta \chi_i] \\ &= - [\chi_i, -2\nabla \chi_i \cdot \nabla - (\Delta \chi_i)] \\ &= 2 [\chi_i, \nabla \chi_i \cdot \nabla] \\ &= 2 \left(\chi_i \nabla \chi_i \cdot \nabla - \chi_i \nabla \chi_i \cdot \nabla - |\nabla \chi_i|^2 \right) \\ &= -2 |\nabla \chi_i|^2. \end{split}$$

Summing in the first equality over i, we obtain

$$\sum_{i=1}^{m} (\chi_i^2 H + H \chi_i^2 - 2\chi_i H \chi_i) = -2 \sum_{i=1}^{m} |\nabla \chi_i|^2,$$

which gives the required conclusion upon using $\sum_i \chi_i^2 = \mathbbm{1}_\Omega$ and rearranging terms.

The quadratic form of the IMS formula follows by density since for any $\varphi \in \mathcal{C}^{\infty}_{c}(\Omega)$,

$$Q(\varphi) = \langle H\varphi, \varphi \rangle = \sum_{i=1}^m \langle \chi H\chi \varphi, \varphi \rangle - \langle |\nabla \chi_i|^2 \varphi, \varphi \rangle = \sum_{i=1}^m \langle H\chi_i \varphi, \chi_i \varphi \rangle - \langle |\nabla \chi_i| \varphi, |\nabla \chi_i| \varphi \rangle,$$

which is the claimed identity for φ .

3 The 1D case

As a first step we consider the case d = 1:

$$\Omega_{\beta} = (a_{\beta}, b_{\beta}).$$

Then V has at most three critical points in Ω_0 , say $a_{\beta} \leq z_1 < z_0 < z_2 \leq b_{\beta}$ for all β , thus $\varepsilon_{\beta}^{(1)} = z_1 - a_{\beta}$ and $\varepsilon_{\beta}^{(2)} = b_{\beta} - z_2$. We use the notation $\kappa_i = V''(z_i)$.

3.1 Coarse estimates of the full spectrum through a harmonic approximation.

We have the following result which identifies the first-order asymptotics of the spectrum of $-\mathcal{L}_{\beta}$.

Theorem 1. For all $n \in \mathbb{N}^*$, we have the convergence

$$\lim_{\beta \to \infty} \lambda_{n,\beta} = \lambda_n^{\text{harm}} + o(1)$$

Before giving the proof, we give the following definition of approximate eigenfunctions of

Definition 3 (Harmonic quasimodes). For $n \in \mathbb{N}^d$, we set

$$\widetilde{\psi}_{\beta,n}(x) = \frac{\chi_{\beta}^{(i_n)}(x)\psi_{k_n}^{(i_n)}(\sqrt{\beta}(x-z_i))}{\|\chi_{\beta}^{(i_n)}\psi_{k_n}^{(i_n)}(\sqrt{\beta}(\cdot-z_i))\|}.$$

The definition of the cutoff function $\chi_{\beta}^{(i)}$ depends on the nature of the critical point z_i . In the following, $0 < \alpha < \frac{1}{6}$ is a parameter we are free to fix.

If i = 1 or 2, we may assume in the following that z_i is the rightmost saddle point, the leftmost case being symmetrical.

- In the supercritical case $\sqrt{\beta}\varepsilon_{\beta}^{(i)} \to \infty$, we choose $\chi_{\beta}^{(i)}$ such that $0 \le \chi_{\beta}^{(i)} \le 1$, $\chi_{\beta}^{(i)} \equiv 1$ on $(z_i (\varepsilon_{\beta}^{(i)} \wedge \beta^{\alpha \frac{1}{2}})/2, z_i + (\varepsilon_{\beta}^{(i)} \wedge \beta^{\alpha \frac{1}{2}})/2)$, and $\chi_{\beta}^{(i)} \equiv 0$ outside $(z_i \varepsilon_{\beta}^{(i)} \wedge \beta^{\alpha \frac{1}{2}}, z_i + \varepsilon_{\beta}^{(i)} \wedge \beta^{\alpha \frac{1}{2}})$.
- In the subcritical case $\sqrt{\beta}\varepsilon_{\beta}^{(i)} \to 0$, we choose $\chi_{\beta}^{(i)} \equiv 1$ on $(z_i \beta^{\alpha \frac{1}{2}}/2, z_i)$, $\chi_{\beta}^{(i)} \equiv 0$ outside $(z_i \beta^{\alpha \frac{1}{2}}, z_i)$. Attention IMS avec \chi discontinu, ou alors garder des \chi réguliers.
 In the critical case $\sqrt{\beta}\varepsilon_{\beta}^{(i)} \to c > 0$, we choose $\chi_{\beta}^{(i)} \equiv 1$ on $(z_i \beta^{\alpha \frac{1}{2}}/2, z_i + \beta^{\alpha \frac{1}{$
- $\varepsilon_{\beta}^{(i)}$, $\chi_{\beta}^{(i)} \equiv 0$ outside $(z_i \beta^{\alpha \frac{1}{2}}, z_i + \varepsilon_{\beta}^{(i)})$

Note that by construction, each $\widetilde{\psi}_{\beta,n}$ has support in $\overline{\Omega}_{\beta}$ and satisfies the Dirichlet boundary conditions on $\partial\Omega_{\beta}$.

Lemma 3 (Exponential bounds). We have the following estimates for any $n, m \geq 1$.

$$\exists C_1, C_2, \beta_0 > 0: \quad \left| \langle \widetilde{\psi}_{\beta,n}, \widetilde{\psi}_{\beta,m} \rangle - \delta_{nm} \right| \le C_1 e^{-C_2 \beta^{1+2\alpha}}, \, \forall \, \beta > \beta_0. \tag{8}$$

(9)

(10)

Proof. We start by proving (8). If $i_n \neq i_m$, the statement is void since the quasimodes have disjoint support for $\beta > 0$ large enough. Thus we convene that we fix $i := i_n = i_m = i$, and thus it suffices to estimate

$$\langle \chi_{\beta}^{(i)} \psi_n^{(i)}(\sqrt{\beta}(\cdot - z_i)), \chi_{\beta}^{(i)} \psi_m^{(i)}(\sqrt{\beta}(\cdot - z_i)) \rangle.$$

Changing variables with $y = \sqrt{\beta}(x - z_i)$, this equals

$$\beta^{-\frac{1}{4}}\langle \eta^{(i)}\psi_n^{(i)}, \eta^{(i)}\psi_m^{(i)}\rangle,$$

where $\eta^{(i)}(y) = \chi_{\beta}^{(i)}(x)$.

Observe, examining the definition of the cutoff functions, that $\eta^{(i)} \equiv 1$ on $B_{S^{(i)}}(0,\beta^{\alpha+\frac{1}{2}}/2)$, and $\eta^{(i)} \equiv 0$ outside $B_{S^{(i)}}(0,\beta^{\alpha+\frac{1}{2}})$, where we recall the definition nition of the model space $S^{(i)}$ 1

raffiner definition du cutoff dans le cas critique pour garantir cette condi-

Then, in $L^2(S^{(i)})$, we write

$$\langle \eta^{(i)} \psi_n^{(i)}, \eta^{(i)} \psi_m^{(i)} \rangle = \langle \psi_n^{(i)}, \psi_m^{(i)} \rangle + \langle (1 - \eta^{(i)}) \psi_n^{(i)}, (1 - \eta^{(i)}) \psi_m^{(i)} \rangle + 2 \langle (1 - \eta^{(i)}) \psi_n^{(i)}, \psi_m^{(i)} \rangle$$

The first term is δ_{nm} , by definition of the harmonic eigenmodes on $S^{(i)}$. We then proceed to bound:

$$\left| \langle (1 - \eta^{(i)}) \psi_n^{(i)}, (1 - \eta^{(i)}) \psi_m^{(i)} \rangle + 2 \langle (1 - \eta^{(i)}) \psi_n^{(i)}, \psi_m^{(i)} \rangle \right| \leq \int_{S^{(i)}} \left((1 - \eta^{(i)})^2 + 2(1 - \eta^{(i)}) \right) \left| \psi_n^{(i)} \psi_m^{(i)} \right|$$

$$\leq 3 \int\limits_{S^{(i)}\backslash B(0,\beta^{\alpha+\frac{1}{2}}/2)} |\psi_m^{(i)}\psi_n^{(i)}|.$$

Using the form (3) of the $\psi_m^{(i)}$ as a product of a polynomial and a Gaussian kernel, a tail bound allows us to deduce the claim (8), upon absorbing the polynomial terms inside the exponential.

Là il faudrait des estimations sur la décroissance des fonctions propres pour le cas $S^{(i)} = (-\infty, c)...$

Lemma 4. Fix, $\beta > 0$, $0 \le i \le 2$ and $u \in L^2(\Omega_\beta)$. There exists C > 0 and $\beta_0 > 0$ such that, for all $\beta > \beta_0$, the following estimate holds:

$$\|(H_{\beta} - H_{\beta}^{(i)})\chi_{\beta}^{(i)}u\| \le C\beta^{3\alpha + \frac{1}{2}} \|\chi_{\beta}^{(i)}u\| = o(\beta)\|\chi_{\beta}^{(i)}u\|. \tag{11}$$

Proof. Since $H_{\beta} - H_{\beta}^{(i)}$ is a multiplication operator, it is enough to uniformly bound

$$U_{\beta} - \beta^2 (x - z_i)^{\mathsf{T}} \Sigma^{(i)} (x - z_i) - \beta \frac{\Delta V(z_i)}{2}$$

on supp $\chi_{\beta}^{(i)}$. In turn, this is given by the sum of two contributions:

$$\beta^2 \left(\frac{|\nabla V|^2}{4} - (x - z_i)^{\mathsf{T}} \Sigma^{(i)} (x - z_i) \right) - \frac{\beta}{2} (\Delta V - \Delta V(z_i)).$$

Recall that, in each case, supp $\chi_{\beta}^{(i)}$ is a closed interval containing z_i , contained in $B(z_i, \beta^{\alpha - \frac{1}{2}})$ for β large enough. Thus, there exists $\beta_0 > 0, C > 0$ depending only on V and i such that for all $\beta > \beta_0$ and every $x \in \text{supp } \chi_{\beta}^{(i)}$,

$$\left| \frac{|\nabla V|^2}{4} - (x - z_i)^\mathsf{T} \Sigma^{(i)} (x - z_i) \right| < C\beta^{3\alpha - \frac{3}{2}},$$

where we use a second-order Taylor bound. Similarly, we treat the Laplacian term by a first-order Taylor bound, yielding,

$$|\Delta V - \Delta V(z_i)| \le C\beta^{2\alpha - 1}.$$

In turn, we get that

$$\|(H_{\beta} - H_{\beta}^{(i)})\chi_{\beta}^{(i)}u\| \le C \max\{\beta^{3\alpha + \frac{1}{2}}, \beta^{2\alpha}\}\|\chi_{\beta}^{(i)}u\|,$$

which yields the desired bound, and which is small with respect to β since $0 < \alpha < \frac{1}{6}$.

Proof of Theorem 1. Step 1: Upper bound.

Fix $n \geq 1$. We consider the family $(\widetilde{\psi}_{\beta,j})_{j=1,\dots,n}$. The quasi-orthogonality estimate (8) implies the Gram matrix $(\langle \widetilde{\psi}_{\beta,j}, \widetilde{\psi}_{\beta,k} \rangle)_{1 \leq j,k \leq n}$ is non-singular, hence the $\widetilde{\psi}_{\beta,j}$ span a *n*-dimensional subspace of $H_0^1(\Omega_\beta) \cap H^2(\Omega_\beta)$. By the Max-Min Courant-Fischer principle, it suffices to show that, for all $u \in \text{Span}(\widetilde{\psi}_{\beta,j}, 1 \leq$

$$Q_{\beta}(u) \leq (\beta \lambda_n^{\text{harm}} + o(\beta)) \|u\|^2$$

Indeed, we will have shown that

$$\max_{\substack{E\subset H^1_0\cap H^2(\Omega_\beta)\\ \text{dim }E=n\\ }} \min_{u\in E} \frac{Q_\beta(u)}{\|u\|^2} \leq (\beta \lambda_n^{\text{harm}} + \mathrm{o}(\beta)):$$

which implies

$$\overline{\lim}_{\beta \to \infty} \beta^{-1} \lambda_{\beta,n} = \lambda_n^{\text{harm}}.$$

We start with $u = \chi_{\beta}^{(i_j)} \psi_{k_j}^{(i_j)} (\sqrt{\beta} (\cdot - z_{i_j})) =: \chi \psi$. Firstly, we write:

$$Q_{\beta}(u) = \langle H_{\beta}\chi\psi, \chi\psi\rangle = \langle H_{\beta}^{(i_j)}\chi\psi, \chi\psi\rangle + \langle (H_{\beta} - H_{\beta}^{(i_j)})\chi\psi, \chi\psi\rangle.$$

By a Cauchy–Schwarz inequality and the bound (11), we estimate the rightmost term by

$$\left| \langle (H_{\beta} - H_{\beta}^{(i_j)}) \chi \psi, \chi \psi \rangle \right| \le C e^{3\alpha + \frac{1}{2}} \| \chi \psi \|^2.$$

We next proceed to use the IMS formula in its quadratic form (7) to write

$$Q^{(i_j)}(\chi\psi) = \langle H_\beta^{(i_j)}\chi\psi,\chi\psi\rangle = \langle H_\beta^{(i_j)}\psi,\psi\rangle - \sum_{\substack{i=1\\i\neq i_j}}^3 \langle H_\beta^{(i_j)}\chi_\beta^{(i)}\psi,\chi_\beta^{(i)}\psi\rangle + \sum_{i=1}^3 \left\||\nabla\chi_\beta^{(i)}|\psi\right\|^2,$$

where we define $\chi_{\beta}^{(3)} = \sqrt{\mathbbm{1}_{\Omega_{\beta}} - \sum_{i=0}^{2} \chi_{\beta}^{(i)2}}$.

We have $\langle H_{\beta}^{(i_j)} \psi, \psi \rangle = \beta \lambda_{k_j}^{(i_j)} \|\psi\|^2 \leq \beta \lambda_n^{\text{harm}} \|\psi\|^2$. Due to the exponential decay of ψ away from z_i , one can show that the other terms are exponentially small.

Compléter le lemme 3 avec les estimations et préciser.

For general u, the bound follows from the quasi-orthogonality estimate (8)idem

Thus,

$$\underline{\lim}_{\beta \to \infty} \beta^{-1} \lambda_{n,\beta} \le \lambda_n^{\text{harm}}.$$

Step 2: Lower bound.

This time, we use the Min-Max version of the Courant-Fischer principle. Namely, it suffices to show that, for any $u \in \text{Span}(\psi_{\beta,j}, 1 \leq j \leq n-1)^{\intercal}$,

$$Q_{\beta}(u) \ge (\beta \lambda_n^{\text{harm}} + o(\beta)) ||u||^2.$$

Since the $\widetilde{\psi}_{\beta,j}$ are linearly independent as $\beta \to \infty$, we will have shown

$$\min_{\substack{E \subset H_0^1 \cap H^2(\Omega_\beta) \\ \dim E = n-1}} \max_{u \in E^{\mathsf{T}}} \frac{Q_\beta(u)}{\|u\|^2} \ge \beta \lambda_n^{\mathrm{harm}} + \mathrm{o}(\beta),$$

which entails

$$\underline{\lim}_{\beta \to \infty} \beta^{-1} \lambda_{n,\beta} \ge \lambda_n^{\text{harm}}.$$

Hence, let u be orthogonal to $\widetilde{\psi}_{\beta,j}$ for every $1 \leq j \leq n-1$. We compute $Q_{\beta}(u)$ using the IMS formula:

$$Q_{\beta}(u) = \sum_{i=0}^{3} Q_{\beta}(\chi_{\beta}^{(i)}u) - \||\nabla \chi_{\beta}^{(i)}|u\|^{2}.$$

Note that we are free to assume that, for some C > 0,

$$\|\nabla \chi_{\beta}^{(i)}\|_{\infty} \le C\beta^{\frac{1}{2}-\alpha}.$$

Thus,

$$Q_{\beta}(u) \ge \sum_{i=0}^{3} Q_{\beta}(\chi_{\beta}^{(i)}u) + C\beta^{1-2\alpha} \|u\|^{2} = \sum_{i=0}^{3} Q_{\beta}(\chi_{\beta}^{(i)}u) + o(\beta) \|u\|^{2}.$$

On estime $Q_{\beta}(\chi_{\beta}^{(3)}u)$. Notons que supp $\chi_{\beta}^{(3)}\subset\bigcup_{i=0}^2B_{\Omega_{\beta}}(z_i,\beta^{\alpha-\frac{1}{2}}/2)$.

Minorer ce terme en utilisant la croissance quadratique de U_{β} en dehors de voisinages des z_i s (sinon il y a plus de points critiques!) (il faut aussi controller la contribution du Laplacien, qui est négligeable)

Remplacer $Q_{\beta}(\chi_{\beta}^{(i)}u)$ par $Q_{\beta}^{(i)}(\chi_{\beta}^{(i)})$.

3.2 Finer estimates of the smallest eigenvalue.

Discuss WKB solutions with moving boundaries?