Low-temperature asymptotics of the Dirichlet spectrum for a Fokker-Planck operator in temperature-dependent domain.

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Contents

1 Setting

We consider a potential function, $V : \mathbb{R}^d \to \mathbb{R}$, which we assume to be smooth. We are interested in understanding the behavior of metastable exit and relaxation times for the overdamped Langevin dynamics

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

when the trajectories of the process are conditioned to remaining inside a potential well for a long time. The full unconditionned process (1) is ergodic for the Gibbs measure

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

We associate with this probability measure the weighted Sobolev spaces, defined, for $\Omega \subset \mathbb{R}^d$ any open domain by:

$$L^2_\mu(\Omega) = \left\{u : \int_\Omega u^2\,d\mu < +\infty\right\}, \qquad H^k_\mu(\Omega) = \{u \in L^2_\mu(\Omega) :\, \partial^\alpha u \in L^2_\mu(\Omega),\, \forall\,|\alpha| \le k\}, \tag{2}$$

where ∂^α denotes the weak differentation operator associated to a multi-index α. Finally let $H^k_{0,\mu}(\Omega)$ denote the $H^k(\Omega)$ norm-closure of $\mathcal{C}^\infty_c(\Omega)$.

The infinitesimal generator for the dynamics is defined by the differential operator:

$$-\mathcal{L}_\beta u = \nabla V \cdot \nabla u - \frac{1}{\beta}\Delta u =,\, u \in \mathcal{C}_c^\infty(\mathbb{R}^d). \tag{3}$$

The problem we consider here is that of computing low-temperature spectral asymptotics for the Dirichlet problem associated with the generator, for a domain which depends on the inverse temperature β. To this effect, we consider a non-increasing family of open, bounded, simply connected domains

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

and consider, for $\beta > 0$, the spectrum of Dirichlet realization $-\mathcal{L}_\beta^D$, whose domain is $H^1_{0,\mu} \cap H^2_\mu(\Omega_\beta) \subset L^2_\mu(\Omega_\beta)$, and whose action is defined formally by (3). The operator $-\mathcal{L}_\beta^D$ is known to be self-adjoint, with compact resolvent, so that its spectrum is comprised of a sequence of non-negative, isolated eigenvalues of finite multiplicity, thus tending to $+\infty$.

$$0 \geq \lambda_{1,\beta} \leq \lambda_{2,\beta} \leq \cdots \leq \lambda_{N,\beta} \underset{N\to\infty}{\longrightarrow} +\infty.$$

Furthermore, since Ω_β is bounded for all β, one can show that the first eigenvalue is simple and strictly positive, so that $0 < \lambda_{1,\beta} < \lambda_{2,\beta}$, with $\dim\ker(-\mathcal{L}_\beta - \lambda_{1,\beta}) = 1$.

1.1 Hypotheses on V and the domains Ω_β.

We are specifically interested in studying the case in which all the domains encompass one potential well of V, which furthermore contain every saddle point connecting it to some other well in their closure. Loosely, one should think of Ω_β as a positive temperature outward perturbation of the bassin of attraction attached to the bottom of the well for the steepest descent dynamics

$$\dot{X} = -\nabla V(X). \tag{4}$$

We formalize the setting using the following assumptions:

i) The potential V is a $\mathcal{C}^\infty$ Morse function on $\overline{\Omega}_0$, such that $z_0 \in \Omega_0$ is the unique (local and global) minimum of V on $\overline{\Omega}_0$.

ii) Define the bassin of attraction for z_0 as the set

$$\mathbf{B} = \left\{ x \in \mathbb{R}^d : \lim_{t\to\infty} \phi_t(x) = z_0 \right\}, \tag{5}$$

where $(\phi_t)_{t\geq 0}$ is the flow associated with the steepest descent dynamics (4), and

$$\Omega_\infty = \bigcap_{\beta\geq 0} \Omega_\beta.$$

Assume that $\mathbf{B} \subset \overline{\Omega}_\infty$.

probablement pas nécessaire tant qu'on contient le puits $\{f < \min_i V(z_i)\}$

iii) For all $\beta > 0$, the boundaries $\partial\Omega_\beta$ are C^1 submanifolds of $\mathbb{R}^d$, and the domains non-increasing:

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

iv) For all $z \in \overline{\Omega}_0$ such that z is a order-one saddle point of V, $z \in \overline{\mathbf{B}}$.

v) We denote by $\mathrm{n}_\beta : \partial\Omega_\beta \to \mathbb{R}^d$ the outward normal to Ω_β. We assume:

$$\forall\, \beta > 0,\, \forall\, x \in \partial\Omega_\beta, \mathrm{n}_\beta \cdot \nabla V(x) \leq 0. \tag{6}$$

v) $\implies$ ii)

Let us make a few informal comments about these hypotheses. Assumption i) expresses the fact that we specialize our study to the one-well setting, where the well is attached to the minimum x_0. Combined with ii), it implies that there exists $\varepsilon_0 > 0$ such that for all $\beta > 0$, a coreset $B(z_0, \varepsilon_0)$ is strictly contained in Ω_β. The standard numerical practice is to take the basin of attraction $\mathbf{B}$ as a definition of the well, and thus as a metastable domain, independently of β. We can of course recover this case by setting $\Omega_\beta = \mathbf{B}$ for all $\beta > 0$. Assumption ii) expresses the fact that every domain indeed contains the well $\mathbf{B}$, while iii) expresses the fact that the domains contract as the temperature decreases. Assumption iv) guarantees that any first-order saddle point is associated with an exit from $\mathbf{B}$, and indeed by ii) that all such exits are in $\overline{\Omega}_\beta$, for any $\beta > 0$. Finally, v) expresses the fact that the steepest descent-dynamics "spills out" at the boundary of the domain.

Defricher ce qu'il faut prouver/ Formaliser/ mettre dans un lemme

Let $z_0, \cdots, z_{m+r}$ denote the critical points of V in $\overline{\Omega}_\infty$, where $z_1, \cdots, z_m$ are the order-one saddle points. By assumption i) all these critical points are non-degenerate, by which we mean that the eigenvalues

$$\sigma(\operatorname{Hess} V(z_i)) = \{\nu_1^{(i)} \le \nu_2^{(i)} \le \cdots \le \nu_d^{(i)}\} \tag{7}$$

of the Hessian of V at z_i are non-zero for all i, with

$$U^{(i)} = \begin{pmatrix} v_1^{(i)} & \cdots & v_d^{(i)} \end{pmatrix}, \quad \operatorname{diag}(\nu_1^{(i)}, \cdots, \nu_d^{(i)}) = U^{(i)\intercal}\Sigma^{(i)}U^{(i)}. \tag{8}$$

the associated orthonormal eigenbasis. Our analysis of the smallest eigenvalue is heavily inspired by the quasimodal construction performed in [2]. For this reason, we will make the following assumption on the local geometry of the domains around each order-one saddle point, which furthermore fixes the orientation convention for the eigenvector $v_1^{(i)}$, which points towards $\partial\Omega_\beta$.

We assume that, there exists a positive number $\delta > 0$ and functions $\delta^{(i)} : \mathbb{R}_+^* \to \mathbb{R}_+$ such that the domain Ω_β contains a box neighborhood of the saddle point, which furthermore touches the boundary in the unstable direction:

$$R_\beta^{(i)} = z_i + U^{(i)\intercal}\left[(-\delta, \delta^{(i)}(\beta) \wedge \delta) \times (-\delta, \delta)^{d-1}\right] \subset \Omega_\beta, \quad z_i + \delta^{(i)}(\beta)v_1^{(i)} \in \partial\Omega_\beta \text{ if } \delta^{(i)} < \delta\ ,\ \forall\, \beta > 0. \tag{9}$$

Dessins...

Note that, for $\delta^{(i)} < \delta$, $d(z_i, \partial\Omega_\beta^{(i)}) = \delta^{(i)}(\beta)$ and $\partial\Omega_\beta$ is tangent to $z_i + \delta^{(i)}(\beta)v_1^{(i)\perp}$. The assumption that the Ω_β are non-increasing implies that, $\beta \mapsto \delta^{(i)}(\beta)$ is also non-increasing for all i. We will use the following terminology to distinguish between different scalings

- If $\lim\limits_{\beta\to\infty} \sqrt{\beta}\delta^{(i)}(\beta) = 0$, we say that z_i is a **subcritical** saddle-point.
- If $\lim\limits_{\beta\to\infty} \sqrt{\beta}\delta^{(i)}(\beta) = \alpha \left|\nu_1^{(i)}\right|^{-\frac{1}{2}} > 0$, it is a **critical** saddle-point.
- If $\lim\limits_{\beta\to\infty} \sqrt{\beta}\delta^{(i)}(\beta) = +\infty$, it is a **supercritical** saddle-point.

Note that $\left(\beta\left|\nu_1^{(i)}\right|\right)^{-\frac{1}{2}}$ is the standard deviation of the Gaussian approximation to $x \mapsto \mathrm{e}^{\beta V(z_i + x v_1^{(i)})}$, which motivates this choice of terminology. In the case in which z_i is not an order-one saddle point, we still assume that Ω_β contains a box neighborhood of z_i, uniformly in the temperature:

$$R^{(i)} = z_i + U^{(i)}(-\delta, \delta)^d \subset \Omega_\beta \quad \forall\, \beta > 0. \tag{10}$$

(the case $i = 0$ follows directly from assumptions i and ii).

En fait cette hypothese est seulement nécessaire pour avoir l'approximation harmonique , a terme, organiser/nommer hypotheses + les invoquer au moment d'énoncer les théorèmes

2 Coarse asymptotics of the spectrum using the harmonic approximation

We first aim to extend the harmonic approximation [1, Theorem 11.1] to the case of a temperature-dependent Dirichlet boundary condition. More precisely, we aim to show that, for all integers $k \geq 1$,

$$\lambda_{k,\beta} = \lambda_k^H + e(\beta),\, e(\beta) \overset{\beta\to\infty}{\to} 0,$$

where by λ_k^H we denote the k-th eigenvalue of some temperature-independent operator (13), the harmonic approximation to the Witten Laplacian, whose spectrum can be computed easily.

2.1 Definition of the harmonic approximation

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:*

$$S^{(i)} = (-\infty, \alpha_i) \times \mathbb{R}^{d-1},\, \alpha_i = \frac{\alpha}{\sqrt{|\nu_1^{(i)}|}} > 0.$$

- *In the supercritical case:*

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

Local harmonic models.
The potential part of $H_\beta = U_\beta - \Delta$, given by $U_\beta = \frac{1}{2}\left(\beta^2\frac{|\nabla V|^2}{2} - \beta\Delta V\right)$, 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:

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

and let

$$\sigma(\mathrm{Hess}\,V(z_i)) = \{\nu_1^{(i)} \leq \nu_2^{(i)} \leq \cdots \leq \nu_d^{(i)}\}$$

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

$$U^{(i)} = \begin{pmatrix} v_1^{(i)} & \cdots & v_d^{(i)} \end{pmatrix}, \quad U^{(i)\intercal}\Sigma^{(i)}U^{(i)} = \frac{1}{4}\mathrm{diag}\left[\left(\nu_j^{(i)}\right)^2, 1 \leq j \leq d\right] = \Lambda^{(i)}$$

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

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

Since the critical points are non-degenerate, $\nu_j^{(i)} \neq 0$ for all $1 \leq j \leq d$, $0 \leq i \leq m+r$, and $\nu_1^i < 0$ if and only if $i \geq 1$.

We define local harmonic approximations to H_β around each critical point:

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

and the shifted harmonic oscillators:

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

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

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

2.2 Spectra of the local oscillators.

The advantage of working with the harmonic approximations $K^{(i)}$ is that their eigendecompositions can be written in terms of those of one-dimensional harmonic oscillators, which are either analytically known or easy to compute. By $\sigma(K^{(i)})$, we denote the spectrum of the Dirichlet realization of the harmonic oscillator $K^{(i)}$ on $L^2(S^{(i)})$.

As a first step, we note the following result, which ensures that the $K^{(i)}$ have pure point spectra.

Lemma 1. *The operator $K^{(i)}$ with domain $H_0^1 \cap H^2(S^{(i)})$ is self-adjoint with compact resolvent.*

Proof. The assumption that z_i is a non-degenerate critical point implies the case $S^{(i)} = \mathbb{R}^d$ by a standard result on Schrödinger operators (see [3, Theorem 12. ...]), as

$$W^{(i)}(x) := x^\intercal \Lambda^{(i)} x - \frac{\Delta V(z_i)}{2}, \underset{|x|\to\infty}{\longrightarrow} +\infty.$$

Thus it is enough to treat the case $S^{(i)} = (-\infty, \alpha) \times \mathbb{R}^{d-1}$, for some $\alpha \geq 0$.

We start with the case $d = 1$. For a function $f \in L^2(\mathbb{R})$, we will use the notation

$$\iota_\alpha f(x) = f(2\alpha - x)$$

for the reflection of f across $\partial S^{(i)} = \{x = \alpha\}$. We consider now the Schrödinger operator on $L^2(\mathbb{R})$ obtained by reflecting the potential through $\partial S^{(i)}$:

$$\widetilde{K}^{(i)} = -\Delta + W^{(i)} \mathbb{1}_{x \leq \alpha} + \iota_\alpha W^{(i)} \mathbb{1}_{x > \alpha} = -\Delta + \widetilde{W}^{(i)}.$$

Since $\widetilde{W}^{(i)}(x) \overset{|x|\to+\infty}{\longrightarrow} +\infty$, the operator $\widetilde{K}^{(i)}$ is self-adjoint with compact resolvent. Thus $\sigma(\widetilde{K}^{(i)})$ consists of a sequence of isolated eigenvalues of finite multiplicity tending to $+\infty$.

The claim is implied by the inclusion $\sigma(K^{(i)}) \subset \sigma(\widetilde{K}^{(i)})$, which is equivalent to the reverse inclusion of resolvent sets. Let $\lambda \in \mathbb{C} \setminus \sigma(\widetilde{K}^{(i)})$, and $f \in L^2(S^{(i)})$. We define $\widetilde{u} \in H^2(\mathbb{R})$ as the λ-resolvent of $\widetilde{K}^{(i)}$ applied to the odd reflection of f along $\partial S^{(i)}$:

$$\widetilde{f}(x) = f \mathbb{1}_{x \leq \alpha} - \iota_\alpha f \mathbb{1}_{x > \alpha}, \qquad (\lambda - \widetilde{K}^{(i)}) \widetilde{u} = \widetilde{f}, \qquad \|\widetilde{u}\|_{L^2(\mathbb{R})} \leq C_\lambda \|\widetilde{f}\|_{L^2(\mathbb{R})},$$

for some $C_\lambda > 0$ independent of f. It is simple to check, by symmetry of the potential, that the commutation relation $\iota_\alpha \widetilde{K}^{(i)} = \widetilde{K}^{(i)} \iota_\alpha$ holds. Thus, applying ι_α on both sides of the resolvent equation, we get

$$(\lambda - \widetilde{K}^{(i)}) \iota_\alpha \widetilde{u} = \iota_\alpha \widetilde{f} = -\widetilde{f}.$$

It follows that $\iota_\alpha \widetilde{u} = -\widetilde{u}$, which straightforwardly implies, since $\widetilde{u} \in H^2(\mathbb{R}) \hookrightarrow C^{1,1/2}(\mathbb{R})$, that $\widetilde{u}(\alpha) = 0$. Thus, $u = \widetilde{u}|_{S^{(i)}}$ belongs to $H_0^1 \cap H^2(S^{(i)})$, and $(\lambda - K^{(i)}) u = f$. Furthermore, we have

$$\|u\|_{L^2(S^{(i)})} \leq \|\widetilde{u}\|_{L^2(\mathbb{R}^d)} \leq C_\lambda \|\widetilde{f}\|_{L^2(\mathbb{R}^d)} = 2C_\lambda \|f\|_{L^2(S^{(i)})},$$

which shows, since f was arbitrary, that $\lambda \in \mathbb{C} \setminus \sigma(K^{(i)})$, and concludes the proof for $d = 1$.

For a general $d \geq 2$, we notice that we can construct a complete orthonormal basis set for $L^2(S^{(i)})$, consisting of eigenvectors for $K^{(i)}$, which is nothing more than the tensor basis generated from the orthonormal eigenbases of each of the one-dimensional harmonic oscillators:

$$K_j^{(i)} = -\partial_x^2 + \frac{\nu_j^{(i)2}}{4} x^2, \quad D(K_1^{(i)}) = H_0^1 \cap H^2((-\infty, \alpha)), \quad D(K_j^{(i)}) = H^2(\mathbb{R}),\, j \geq 2.$$

The basis thus obtained is orthonormal in $L^2(S^{(i)})$, complete, and consists of eigenvectors for $K^{(i)}$ associated with real eigenvalues of finite multiplicity. It follows that $K^{(i)}$ is self-adjoint with compact resolvent. $\square$

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

In this case, the spectrum is given by

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

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

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

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

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

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

$$\psi_n^{(i)}(x) = \prod_{j=1}^{d} \left(\frac{|\nu_j^{(i)}|}{2} \right)^{\frac{1}{4}} \psi_{n_j} \left(\sqrt{\frac{|\nu_j^{(i)}|}{2}} x_j \right) \tag{11}$$

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

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

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

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 $i \geq 1$, 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

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

The eigenfunctions have the same product form as (11), but are restricted to the half-space, and only the odd modes contribute in the x_1 direction. The factor $\sqrt{2}$ accounts for L^2 normalization.

$$\psi_n^{(i)}(x) = \mathbb{1}_{S^{(i)}}(x)\sqrt{2} \left(\frac{|\nu_1^{(i)}|}{2} \right)^{\frac{1}{4}} \psi_{2n_1+1} \left(\sqrt{\frac{|\nu_1^{(i)}|}{2}} x_1 \right) \prod_{j=2}^{d} \left(\frac{|\nu_j^{(i)}|}{2} \right)^{\frac{1}{4}} \psi_{n_j} \left(\sqrt{\frac{|\nu_j^{(i)}|}{2}} x_j \right) \tag{12}$$

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

In this case, the spectrum of the oscillator corresponding to the unstable direction, restricted to the half-space $(-\infty, \alpha_i)$, is not analytically known.

Nevertheless, we denote for $k \in \mathbb{N}$

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

the k-th $L^2(S^{(i)})$-normalized eigenpair for the Dirichlet realization of the harmonic oscillator $\frac{1}{2}\left(x^2 - \partial^2\right)$ on $(-\infty, \alpha/\sqrt{2})$.

A double-check..

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

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

the lowest eigenvalue is

$$|\nu_1^{(i)}| \left(\lambda_1^\alpha + \frac{1}{2} \right),$$

and the eigenstates are given by

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

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 enumeration induced by the lexicographic order on $\mathbb{N}^d$.

Global harmonic approximation.

We consider the following operator

$$K = \bigoplus_{i=0}^{m} K^{(i)}, \quad \mathcal{D}(K) = H_0^1 \cap H^2 \left(\prod_{i=0}^{m} S^{(i)} \right), \tag{13}$$

with spectrum

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

We denote by $(\lambda_k^{\mathrm{H}}, \psi_k^{\mathrm{H}})$ the k-th smallest eigenpair of K. We count eigenvalues with multiplicity, defering first to the ordering on $1, \cdots, m$, then to the ordering of eigenvalues of each $K^{(i)}$ to order multiple eigenvalues.

We also define the maps $k : \mathbb{N}^* \to \mathbb{N}^*$, $i : \mathbb{N}^* \to \{1, \dots, m\}$ such that

$$\lambda_n^{\mathrm{H}} = \lambda_{k_n}^{(i_n)}.$$

En fait, on pourrait facilement étendre la définition à tous les points critiques, si on suppose qu'aucun ne franchit la frontière quand β bouge (la preuve du théorème d'approximation harmonique ne devrait pas changer)

2.3 Definition of the harmonic quasimodes.

We now give the definition of rough quasimodes for H_β, which are given by localizing exact modes for the $K_\beta^{(i)}$ in the neighborhood of each critical point, to ensure the Dirichlet boundary conditions are met and the harmonic approximation is valid. More precisely, we fix $n \in \mathbb{N}^*$, and define

$$\widetilde{\psi}_{\beta,n}(x) = \frac{\beta^{\frac{d}{4}}}{Z_{\beta,n}} \left[\chi_\beta^{(i_n)} \psi_{k_n}^{(i_n)}\right] (\sqrt{\beta} U^{(i_n)\intercal}(x - z_{i_n})), \quad \|\widetilde{\psi}_{\beta,n}\|_{L^2(\Omega_\beta)} = 1, \tag{14}$$

where $\chi_\beta^{(i_n)}$ is a $\mathcal{C}_c^\infty$ cutoff function whose specific definition depends on $S^{(i_n)}$, and $Z_{\beta,n}$ is a normalization constant. We recall the definition of the box neighborhoods (10) and (9). Let us fix once and for all a reference cutoff function

$$\chi \in \mathcal{C}_c^\infty(-1,1), \quad \chi \equiv 1 \text{ in } (-1/2, 1/2), \quad 0 \le \chi \le 1. \tag{15}$$

Thus, $\operatorname{supp} \chi' \subset (-1,-1/2) \cap (1/2,1)$, and we may furthermore require that $\|\chi'\|_\infty \le 3$.

Now, we set

$$\chi_\beta^{(i)}(y) = \eta_\beta^{(i)}(y_1) \prod_{k=2}^{d} \chi(\beta^{-r} y_d), \tag{16}$$

for some small parameter $0 < r < \frac{1}{2}$ we fix later on.

au final il faudra le fixer

We set $\eta_\beta^{(i)}(y_1) = \chi(\beta^{-r} y_1)$ if $y_1 \le 0$, and otherwise we define $\eta_\beta^{(i)}$ according to the nature of $S^{(i)}$.

- In the supercritical case $\sqrt{\beta}\delta^{(i)}(\beta) \to \infty$, we choose $\eta_\beta^{(i)}(y_1) = \chi\left(\left[\sqrt{\beta}\delta^{(i)}(\beta) \wedge \beta^r\right]^{-1} y_1\right)$ for $y_1 > 0$.
- In the (sub)critical case $\sqrt{\beta}\delta^{(i)}(\beta) \to \alpha \ge 0$, we set $\varepsilon^{(i)}(\beta) = |\alpha - \sqrt{\beta}\delta^{(i)}(\beta)| \to 0$, and choose a smooth $\eta_\beta^{(i)}$ such that $\eta_\beta^{(i)} \equiv 1$ on $[0, \alpha - 2(\varepsilon^{(i)}(\beta) \vee \beta^{-s})]$, $\eta_\beta^{(i)} \equiv 0$ on $[\alpha - (\varepsilon^{(i)}(\beta) \vee \beta^{-s}), +\infty)$, and $0 \le \eta_\beta^{(i)} \le 1$, where $\frac{1}{2} < s < 1$ is a parameter we fix later on.

In the following lemma, we

Lemma 2 (Localization estimate)**.** *We have the following localization estimate. For any $n \in \mathbb{N}$, there exists $\beta_0, C > 0$ such that, for all $\beta > \beta_0$, the following estimate holds:*

$$\|(1 - \chi_\beta^{(i)}) \tag{17}$$

We note that, by construction, each quasimode (14) is in $H^1_0 \cap H^2(R^{(i)}_\beta)$ for β large enough

Ici, dans le cas critique il faut une hypothèse technique $\sqrt{\beta}\delta^{(i)}(\beta) \downarrow \alpha_i$?

Let us also denote the complementary cutoff function

$$\chi_\beta^{(m+1)} = \sqrt{\mathbb{1}_{\Omega_\beta} - \sum_{i=0}^{m} \chi_\beta^{(i)2}}. \tag{18}$$

2.4 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 $-\mathcal{L}_\beta$.

Lemma 3 (Localization estimates)**.** *There exists positive constants $c, \beta_0 > 0$ such that, for all $\beta > \beta_0$ and any integers $n, m \in \{0, \cdots, m\}$, the following estimates hold:*

$$\left|\langle \widetilde{\psi}_{\beta,n}, \widetilde{\psi}_{\beta,m}\rangle - \delta_{nm}\right| \leq \mathrm{e}^{-c\beta^{1+2r}}, \tag{19}$$

$$\tag{20}$$

$$\tag{21}$$

$$\tag{22}$$

Proof. We start by proving (19). If $i_n \neq i_m$, the statement is void since the quasimodes have disjoint support for β 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 of the model space $S^{(i)}$ 1. 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:

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

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

Since (11) expresses $\psi_m^{(i)}$ as the product of a polynomial with a Gaussian function, a tail bound allows us to deduce the claim (19), upon absorbing the polynomial terms inside the exponential.

Ajouter cas $S^{(i)} = (-\infty, \alpha_i)$ avec Agmon + réecrire en dimension d.

□

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:*

$$\|(H_\beta - H_\beta^{(i)})\chi_\beta^{(i)} u\| \le C\beta^{3\alpha+\frac{1}{2}} \|\chi_\beta^{(i)} u\| = \mathrm{o}(\beta)\|\chi_\beta^{(i)} u\|. \tag{23}$$

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

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

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

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

Recall that, in each case, $\operatorname{supp} \chi_\beta^{(i)}$ 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 $x \in \operatorname{supp} \chi_\beta^{(i)}$,

$$\left| \frac{|\nabla V|^2}{4} - (x - z_i)^\intercal \Sigma^{(i)} (x - z_i) \right| < C_1 \beta^{3\alpha - \frac{3}{2}},$$

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

$$|\Delta V - \Delta V(z_i)| \le C_2 \beta^{\alpha - \frac{1}{2}}.$$

In turn, we get that

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

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

□

Proof of Theorem **??**. **Step 1:** Upper bound.
Fix $n \ge 1$. We consider the family $(\widetilde{\psi}_{\beta,j})_{j=1,\dots,n}$. The quasi-orthogonality estimate (19) implies the Gram matrix $\left(\langle \widetilde{\psi}_{\beta,j}, \widetilde{\psi}_{\beta,k} \rangle \right)_{1 \le j,k \le n}$ is non-singular, hence the $\widetilde{\psi}_{\beta,j}$ span a n-dimensional subspace of $H_0^1(\Omega_\beta) \cap H^2(\Omega_\beta)$. It suffices to show that, for all $u \in \operatorname{Span}(\widetilde{\psi}_{\beta,j},\, 1 \le j \le n)$,

$$Q_\beta(u) \le (\beta \lambda_n^{\mathrm{H}} + \mathrm{o}(\beta))\|u\|^2,$$

which implies

$$\overline{\lim_{\beta\to\infty}}\, \beta^{-1} \lambda_{\beta,n} \le \lambda_n^{\mathrm{H}}$$

by the Max-Min Courant–Fischer principle.

We start with $u = \chi_\beta^{(i_j)} \psi_{k_j}^{(i_j)}(\sqrt{\beta} U^{(i_j)\intercal}(\cdot - z_{i_j}))$. For simplicity, we write, recalling the definition of the harmonic quasimodes (14), $u = \chi^{(i)}\psi$, where $\chi^{(i)} = \chi_\beta^{(i_j)}$ is the cutoff function supported around $z_i = z_{i_j}$, and ψ is an L^2-normalized eigenfunction of the harmonic oscillator $H_\beta^{(i)}$ around z_i. We then have:

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

By a Cauchy–Schwarz inequality and the bound (23), we estimate the rightmost term by

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

. We treat the other term using the IMS formula (29), which gives

$$\langle H_\beta^{(i)}\chi^{(i)}\psi,\chi^{(i)}\psi\rangle = \langle H_\beta^{(i)}\psi,\psi\rangle - \sum_{\substack{i=0\\ j\neq i}}^{m+1}\left[\langle H_\beta^{(i)}\chi_\beta^{(j)}\psi,\chi_\beta^{(j)}\psi\rangle - \left\||\nabla\chi_\beta^{(j)}|\psi\right\|^2\right] + \left\||\nabla\chi^{(i)}|\psi\right\|^2,$$

where we recall the definition of $\chi_\beta^{(m+1)}$ (18).

We have $\langle H_\beta^{(i)}\psi,\psi\rangle = \beta\lambda_k^{(i)}\|\psi\|^2 \le \beta\lambda_n^{\mathrm{H}}\|\psi\|^2$, by definition of the harmonic modes. Since $\|\psi\|^2 = \|u\|^2 + 2\langle\chi^{(i)}\psi,(1-\chi^{(i)})\psi\rangle + \|(1-\chi^{(i)})\psi\|^2$, we are left to show that

$$2\beta\langle\chi^{(i)}\psi,(1-\chi^{(i)})\psi\rangle+\beta\|(1-\chi^{(i)})\psi\|^2 - \sum_{\substack{i=0\\ j\neq i}}^{m+1}\left[\langle H_\beta^{(i)}\chi_\beta^{(j)}\psi,\chi_\beta^{(j)}\psi\rangle - \left\||\nabla\chi_\beta^{(j)}|\psi\right\|^2\right] + \left\||\nabla\chi^{(i)}|\psi\right\|^2 = \mathrm{o}(\beta)\|u\|^2. \tag{24}$$

In fact, since $\|u\|^2 = \|\chi^{(i)}\psi\|^2 \le \|\psi\|^2 = 1$, it is enough to show that each of the terms comprising the sum are $\mathrm{o}(\beta)$.

By a Cauchy-Schwartz inequality, we write

$$|\langle\chi^{(i)}\psi,(1-\chi^{(i)})\psi\rangle| \le \|\chi^{(i)}\psi\|\|(1-\chi^{(i)})\psi\| \le \|(1-\chi^{(i)})\psi\|,$$

which shows that the two leftmost terms in (24) are small, owing to

estimation 1

We treat the terms

$$\langle H_\beta^{(i)}\chi_\beta^{(j)}\psi,\chi_\beta^{(j)}\psi\rangle,\quad j\neq i$$

using

Decay of eigenmodes in H^2 away from z_i

To treat the terms of the form $\||\nabla\chi^{(j)}|\psi\|^2$, we separate depending on the nature of z_i

Case z_i is a supercritical saddle point or z_i is not a saddle point In this case,

Case z_i (sub)critical saddle point We note that for $j\neq i$, $\chi^{(j)}\psi$ is supported away from z_i, and thus we may bound $\langle H_\beta^{(i)}\chi_\beta^{(j)}\psi,\chi_\beta^{(j)}\psi\rangle$ by an exponentially small quantity in β. Similarly, a uniform bound $|\nabla_\chi\beta^{(j)}| \le C\beta$ yields an exponential bound on $\|\chi_\beta^{(j)}\psi\|^2$.

Furthermore, each term inside the sum is small with respect to β, owing to the exponential decay of ψ away from z_i.

revenir mettre les estimées dans le bon lemme et préciser

. 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 (19)

idem

Thus,

$$\overline{\lim_{\beta\to\infty}}\,\beta^{-1}\lambda_{n,\beta} \le \lambda_n^H.$$

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 $u\in\mathrm{Span}(\widetilde{\psi}_{\beta,j}, 1\le j\le n-1)^\perp$,

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

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

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

which entails

$$\varliminf_{\beta \to \infty} \beta^{-1} \lambda_{n,\beta} \geq \lambda_n^{\mathrm{H}}.$$

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

$$Q_\beta(u) = \sum_{i=0}^{m+1} Q_\beta(\chi_\beta^{(i)} u) - \| |\nabla \chi_\beta^{(i)}| u\|^2.$$

For the terms $0 \leq i \leq m$, we have

$$Q_\beta(\chi_\beta^{(i)} u) - \langle H_\beta^{(i)} \chi_\beta^{(i)} u, \chi_\beta^{(i)} \rangle = \langle (H_\beta - H_\beta^{(i)}) \chi_\beta^{(i)} uj, \chi_\beta^{(i)} u \rangle = o(\beta) \|u\|^2, \tag{25}$$

using the Taylor bound (23). On the other hand, the assumption that u is orthogonal to the $\widetilde{\psi}_{\beta,k}$ for $1 \leq k \leq n-1$ implies that $\chi_\beta^{(i_k)} u$ is orthogonal to the $\psi_{\beta,k_k}^{(i_k)}$, so that the Courant-Fischer principle applied to $H_\beta^{(i)}$ implies

□

3 Finer asymptotics for the first eigenvalue.

In this section, we analyze the finer behavior of $\lambda_{\beta,1}$.

Strategy

- Using a simple Gaussian quasi-mode supported in a neighborhood of the unique minimum z_0, it is easy to see that $\lambda_{\beta,1} < \mathrm{e}^{-\beta c}$ for some $c > 0$ and β large enough. Thus, $\operatorname{Ran} \pi_{[0,c/\beta)} = 1$ for β small enough. By similar arguments, one shows that $\operatorname{Ran} \pi_{[0,c/\beta)}^{(1)} = m$ (now this is the spectral projector for the Witten Laplacian on 1-forms)
- Next, one constructs a quasi-mode for $u_{1,\beta}$, the first eigenvector of $\mathcal{L}_\beta$. It is defined in the vicinity $R_\beta^(i)$ of the saddle point, where $y = \sqrt{\beta} U^{(i)\intercal}(x - z_i)$, by

$$\widetilde{u}(y) = \frac{\int_{-\delta}^{y_1} \chi(t) \mathrm{e}^{-\beta |\nu_1^{(i)}| t^2/2} \, \mathrm{d}t}{\int_{-\delta}^{\delta^{(i)}(\beta)} \chi(t) \mathrm{e}^{-\beta |\nu_1^{(i)}| t^2/2} \, \mathrm{d}t},$$

  where χ is an appropriate cutoff function, and defined to be 1 inside the well, and properly extended at the boundary.

  This is the construction of [2], which only requires a slight adaptation here for the critical case. Since these only depend on y_1, they respect the tangential Dirichlet boundary conditions and so can serve as a quasimode on 1-forms.
- Passing to the Witten representation, we get a first (upper) estimate for the first eigenvalue using a Laplace method.
- Using the form $H_\beta = d^* d$, one can estimate the singular value of the linear map d : $\operatorname{Ran} \pi_{[0,c/\beta)} \to \operatorname{Ran} \pi_{[0,c/\beta)}^1$, which is the square of the smallest eigenvalue.

3.1 Construction of the quasimode.

3.2 Estimate using Laplace method

3.3 Estimation of the singular values

4 Technical tools

In this section we collect various definitions and lemmata.

Witten Laplacian.

Instead of studying the spectral asymptotics of the generator $-\mathcal{L}_\beta$, it is useful to perform the following change a variables.

Definition 2. *The Witten Laplacian is the differential operator*

$$H_\beta = U_\beta - \Delta, \qquad U_\beta = \frac{\beta^2}{4}|\nabla V|^2 - \frac{\beta}{2}\Delta V, \tag{26}$$

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 $\mathcal{L}_\beta$ 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 $\mathcal{L}_\beta$ is then an operator on $L^2(\Omega)$ which ressembles a Schrödinger operator:

$$\begin{aligned}
U^*(-\mathcal{L}_\beta)U &= \mathrm{e}^{-\beta V/2}\left(\nabla V \cdot \nabla - \frac{1}{\beta}\Delta\right)\mathrm{e}^{\beta V/2} \\
&= \mathrm{e}^{-\beta V/2}\left(\nabla V \cdot -\frac{1}{\beta}\mathrm{div}\right)\nabla \mathrm{e}^{\beta V/2} \\
&= \mathrm{e}^{-\beta V/2}\left(\nabla V \cdot -\frac{1}{\beta}\mathrm{div}\right)\left[\mathrm{e}^{\beta V/2}\nabla + \frac{\beta}{2}\nabla V \mathrm{e}^{\beta V/2}\right] \\
&= \nabla V \cdot \left[\nabla + \frac{\beta}{2}\nabla V\right] - \frac{1}{2}\nabla V \cdot \nabla - \frac{1}{\beta}\Delta - \frac{\beta}{4}|\nabla V|^2 - \frac{1}{2}\nabla V \cdot \nabla - \frac{1}{2}\Delta V \\
&= \frac{1}{2}(\frac{\beta}{2}|\nabla V|^2 - \Delta V) - \frac{1}{\beta}\Delta \\
&= \frac{1}{\beta}H_\beta.
\end{aligned}$$

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

$$Q_\beta(u) = \langle U_\beta u, u\rangle + \|\nabla u\|^2 \tag{27}$$

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

Various lemmas.

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

Lemma 5. *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 $0 \leq \lambda_1(D_i) \leq \lambda_2(D_i) \leq \dots$ 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 $u, v \in \mathcal{H}_1$, $\langle u, v\rangle_{\mathcal{H}_1} = \langle u, v\rangle_{\mathcal{H}_2}$):

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

The claimed result follows immediately since

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

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 $\beta \mapsto \ H^1_0 \cap \ H^2(\Omega_\beta; \mu)$ is non-increasing.*

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 6. *Let $\Omega \subset \mathbb{R}^d$ be an open set, and $(\chi_i)_{i=1,\dots,m}$ 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 $H^1_0 \cap H^2(\Omega) \subset L^2(\Omega)$. Then the following identity holds:

$$H = \sum_{i=1}^m \chi_i H \chi_i - \sum_{i=1}^m |\nabla\chi_i|^2. \tag{28}$$

Writing $Q(u) = \langle Hu, u\rangle = \langle Uu, u\rangle + \|\nabla u\|^2$, we also have the following identity for any $u \in H^1_0(\Omega)$:

$$Q(u) = \sum_{i=1}^m Q(\chi_i u) - \||\nabla\chi_i| u\|^2. \tag{29}$$

Proof. We compute the following commutator in two ways:

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

Summing in the first equality over i, we obtain

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

which gives the required conclusion upon using $\sum_i \chi_i^2 = \mathbb{1}_\Omega$ 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. □

In the following $(\mathcal{H}, \langle\cdot\rangle)$ is a general Hilbert space, $\|\cdot\|$ the associated norm, and P is a self-adjoint unbounded operator on $\mathcal{H}$ with domain $\mathcal{D}(P)$. We denote by π the projection-valued measure given by the spectral theorem, and denote $\pi_\lambda = \pi_{\{\lambda\}}$ for $\lambda \in \mathbb{R}$. We also denote the quadratic form defined for $u \in \mathcal{D}(P)$ by $Q(u) = \langle Pu, u\rangle$,with domain $\mathcal{D}(Q)$.

Lemma 7 (Abstract estimates for quasimodes)**.** *Let $z \in \mathbb{C} \setminus \sigma(P)$, and $u \in \mathcal{H}$ such that $\|u\| = 1$. The role of u is that of an approximate eigenvector for P, or quasimode.*

i) We have the identity

$$\|(z - P)^{-1}\|_{\mathcal{B}(\mathcal{H})} = \mathrm{d}(z, \sigma(P))^{-1} \tag{30}$$

ii) Let $u \in \mathcal{D}(P)$, $\|u\| = 1$, and $\mu \in \mathbb{C}$. Then

$$\|(P - \mu)u\| \leq \varepsilon \implies \exists \lambda \in \sigma(P),\ |\mu - \lambda| \leq \varepsilon. \tag{31}$$

iii) Assume furthermore that λ is an isolated eigenvalue of P: $\sigma(P) \cap B(\lambda, \delta) = \{\lambda\}$ for some $\delta > 2\varepsilon$. Then,

$$\|u - \pi_\lambda u\| \leq \frac{2\varepsilon}{\delta}, \tag{32}$$

where in this case π_λ is the orthogonal projector onto the eigenspace $\ker(P - \lambda)$ *associated with the eigenvalue λ.*

iv) Assume furthermore that P is non-negative, that is $Q(u) \geq 0$ for all $u \in \mathcal{D}(Q)$ then, for $u \in \mathcal{D}(P)$ with $\|u\| = 1$ and $b > 0$, we have

$$\|\pi_{[b,+\infty)} u\|^2 \leq \frac{Q(u)}{b}. \tag{33}$$

Proof. i) This is a simple corollary of the spectral theorem, see

ii) Assume without loss of generality $\mu \notin \sigma(P)$, otherwise the statement is void. Then $1 = \|u\| \leq \|(P - \mu)^{-1}\|_{\mathcal{B}(\mathcal{H})}\|(P - \mu)u\|$, whence $\mathrm{d}(\mu, \sigma(P)) \leq \|(P - \mu)u\|$ by i).

iii) We consider the operator $P_\lambda = P - \lambda\pi_\lambda$. Acting on $\mathcal{H}_\lambda = \ker(P - \lambda)^\perp$ with domain $\mathcal{D}(P) \cap \mathcal{H}_\lambda$, P_λ is a self-adjoint operator with spectrum $\sigma(P_\lambda) = \sigma(P) \setminus \{\lambda\}$, and therefore $d(\lambda, \sigma(P_\lambda)) > \delta$, which implies $\|(P_\lambda - \lambda)^{-1}\|_{\mathcal{B}(\mathcal{H}_\lambda)} \leq \frac{1}{\delta}$ by i). Noticing that $\|u\| = \|u\|_{\mathcal{H}_\lambda}$ for all $u \in \mathcal{H}_\lambda$, and $\pi_\lambda u - u \in \mathcal{H}_\lambda$, we compute:

$$\begin{aligned}
\|\pi_\lambda u - u\| &= \|\pi_\lambda u - u\|_{\mathcal{H}_\lambda} \\
&\leq \|(P_\lambda - \lambda)^{-1}\|_{\mathcal{B}(\mathcal{H}_\lambda)} \|(P_\lambda - \lambda)(\pi_\lambda u - u)\| \\
&\leq \frac{1}{\delta}\|(P_\lambda - \lambda)(\pi_\lambda u - u)\| \\
&= \frac{1}{\delta}\|(P - \lambda\pi_\lambda - \lambda)(\pi_\lambda u - u)\| \\
&= \frac{1}{\delta}\|P\pi_\lambda u - Pu - \lambda\pi_\lambda^2 u + \lambda\pi_\lambda u - \lambda\pi_\lambda u + \lambda u\| \\
&= \frac{1}{\delta}\|P\pi_\lambda u - Pu - \lambda\pi_\lambda u + \lambda u + \mu u - \mu u\| \\
&\leq \frac{1}{\delta}\left(\|(P - \lambda)\pi_\lambda u\| + \|\mu u - Pu\| + |\lambda - \mu|\|u\|\right) \\
&\leq \frac{2\varepsilon}{\delta}\|u\| = \frac{2\varepsilon}{\delta}.
\end{aligned}$$

In the last line, we use that $(P - \lambda)\pi_\lambda = 0$ by definition of π_λ, and that $\|(\lambda - \mu)u\| = |\lambda - \mu|\|u\| \leq \varepsilon$ by ii).

iv) The spectral theorem yields a probability measure $\mu_u : A \mapsto \langle \pi_A u, u\rangle$ on $\mathbb{R}_+$. Let $U \sim \mu_u$. Applying Markov's inequality, we get:

$$\|\pi_{[b,+\infty)} u\|^2 = \mathbb{P}(U \geq b) \leq \frac{\mathbb{E}[U]}{b} = \frac{1}{b}\int_0^\infty \langle \lambda \,\mathrm{d}\pi_\lambda u, u\rangle = \frac{1}{b}\langle Pu, u\rangle = \frac{Q(u)}{b}. \tag{34}$$

□

The following result is a version of Laplace's method in which the asymptotic concerns both the integrand and the domain of integration.

Lemma 8. *We consider a family of Borel sets $\{A_\lambda\}_{\lambda\geq 0}$ of $\mathbb{R}^d$, and two functions f and g. We are interested in computing the leading-order asymptotics as $\lambda \to +\infty$ of quantities of the form*

$$I_\lambda = \int_{A_\lambda} \mathrm{e}^{-\lambda f(x)} g(x)\,\mathrm{d}x.$$

Assume:

i) The function f is $\mathcal{C}^2$ and has a unique non-degenerate global and local minimum x_0 in $\mathbb{R}^d$.

ii) The unique local and global minimum x_0 belongs to $\overline{A}_\lambda$ for all $\lambda \geq 0$.

iii) The function g is in $C^0 \cap L^1(\mathbb{R}^d)$, and $g(x_0) \neq 0$.

iv) The sequence $\sqrt{\lambda}(A_\lambda - x_0)$ converges to a Borel set:

$$\bigcap_{\lambda\geq 0}\bigcup_{\mu\geq\lambda} \sqrt{\lambda}(A_\mu - x_0) = \bigcup_{\lambda\geq 0}\bigcap_{\mu\geq\lambda} \sqrt{\lambda}(A_\mu - x_0) = A_\infty \in \mathcal{B}(\mathbb{R}^d),$$

which furthermore has a negligible boundary: $|\partial A_\infty| = 0$.

Then, the following asymptotic equivalent holds:

$$I_\lambda \underset{\lambda\to\infty}{\sim} \mathrm{e}^{-\lambda f(x_0)} g(x_0) \left(\frac{2\pi}{\lambda}\right)^{\frac{d}{2}} \left|\det \nabla^2 f(x_0)\right|^{-\frac{1}{2}} \mathbb{P}\left(\xi \in A_\infty\right), \quad \xi \sim \mathcal{N}\left(0, \nabla^2 f(x_0)^{-1}\right) \tag{35}$$

hypothese ou argument supplementaire car $f(x) \to f(x_0)$ peut-être pb quand $x \to \infty$

Proof. Upon replacing f by $f - f(x_0)$, changing g to $g/g(x_0)$ and x to $x - x_0$, we may assume without loss of generality that $x_0 = 0$, with $f(0) = 0$ and $\nabla f(0) = 0$, that $H = \nabla^2 f(0)$ is positive definite and that $g(0) = 1$.

Let $0 < \varepsilon < \varepsilon_0$, such that $H - \varepsilon_0 I$ is positive definite. By assumptions i and iii, and using a Taylor expansion, there exists $\delta > 0$ such that for all $|x| < \delta$.

$$\left|f(x) - \frac{1}{2}x^\intercal Hx\right| < \frac{\varepsilon}{2}|x|^2, \quad |g(x) - 1| \leq \varepsilon,$$

By assumptions iii and ii we are also free to assume that, $f(x) > \eta$ for $|x| \geq \delta$ and some $\eta > 0$.

Writing I_λ as the sum of a local term and a remainder,

$$I_\lambda = \int_{A_\lambda \cap B(0,\delta)} \mathrm{e}^{-\lambda f(x)} g(x)\,\mathrm{d}x + \int_{A_\lambda \setminus B(0,\delta)} \mathrm{e}^{-\lambda f(x)} g(x)\,\mathrm{d}x, \tag{36}$$

we note that we can bound the remainder term by a quantity which is exponentially small with respect to λ:

$$\left|\int_{A_\lambda \setminus B(0,\delta)} \mathrm{e}^{-\lambda f(x)} g(x)\,\mathrm{d}x\right| \leq \mathrm{e}^{-\lambda\eta}\|g\|_{L^1(\mathbb{R}^d)}.$$

Next, we bound the local term from above:

$$\int_{A_\lambda \cap B(0,\delta)} \mathrm{e}^{-\lambda f(x)} g(x)\,\mathrm{d}x \le (1+\varepsilon) \int_{A_\lambda \cap B(0,\delta)} \mathrm{e}^{-\frac{\lambda}{2} x^\intercal (H-\varepsilon I) x}\,\mathrm{d}x \le (1+\varepsilon) \int_{A_\lambda} \mathrm{e}^{-\frac{\lambda}{2} x^\intercal (H-\varepsilon I) x}\,\mathrm{d}x.$$

Using $y = \sqrt{\lambda} x$, we obtain

$$\int_{A_\lambda} \mathrm{e}^{-\frac{\lambda}{2} x^\intercal (H-\varepsilon I) x}\,\mathrm{d}x = \lambda^{-\frac{d}{2}} \int_{\sqrt{\lambda} A_\lambda} \mathrm{e}^{-\frac{1}{2} y^\intercal (H-\varepsilon I) y}\,\mathrm{d}y = \left(\frac{2\pi}{\lambda}\right)^{\frac{d}{2}} |\det{(H-\varepsilon I)}|^{-\frac{1}{2}} \mathbb{P}(\xi_\varepsilon \in \sqrt{\lambda} A_\lambda),$$

where $\xi_\varepsilon \sim \mathcal{N}(0, (H-\varepsilon I)^{-1})$. Denote

$$C_\varepsilon = (1+\varepsilon)\,(2\pi)^{\frac{d}{2}}\,|\det{(H-\varepsilon I)}|^{-\frac{1}{2}}.$$

Then, we get

$$\varlimsup_{\lambda\to\infty} \lambda^{\frac{d}{2}} I_\lambda \le \varlimsup_{\lambda\to\infty} \lambda^{\frac{d}{2}} \mathrm{e}^{-\lambda\eta} \|g\|_{L^1} + C_\varepsilon \mathbb{P}(\xi_\varepsilon \in \sqrt{\lambda} A_\lambda) = C_\varepsilon \mathbb{P}(\xi_\varepsilon \in A_\infty),$$

since assumption iv is equivalent to the Lebesgue almost-everywhere convergence of $\mathbb{1}_{\sqrt{\lambda}(A_\lambda - x_0)}$ to $\mathbb{1}_{A_\infty}$. Since $\xi_\varepsilon \xrightarrow[\varepsilon\to 0]{\mathcal{L}} \xi \sim \mathcal{N}(0, H^{-1})$ and $|\partial A_\infty| = 0$, the Portmanteau lemma together with $C_\varepsilon \xrightarrow{\varepsilon\to 0} C = (2\pi)^{\frac{d}{2}} |\det H|^{-\frac{1}{2}}$ yields the desired upper bound upon taking the limit $\varepsilon \to 0$.

For the lower bound, we write similarly

$$\int_{A_\lambda \cap B(0,\delta)} \mathrm{e}^{-\lambda f(x)} g(x)\,\mathrm{d}x \ge (1-\varepsilon) \int_{A_\lambda \cap B(0,\delta)} \mathrm{e}^{-\frac{\lambda}{2} x^\intercal (H+\varepsilon I) x}\,\mathrm{d}x,$$

whereby an identical argument yields

$$\varliminf_{\lambda\to\infty} \lambda^{\frac{d}{2}} I_\lambda \ge \varliminf_{\lambda\to\infty} \lambda^{\frac{d}{2}} \mathrm{e}^{-\lambda\eta} \|g\|_{L^1} + C'_\varepsilon \mathbb{P}\left(\xi'_\varepsilon \in \left[\sqrt{\lambda} A_\lambda \cap B(0, \sqrt{\lambda}\delta)\right]\right) = C'_\varepsilon \mathbb{P}(\xi'_\varepsilon \in A_\infty),$$

where this time $\xi'_\varepsilon \sim \mathcal{N}(0, (H+\varepsilon I)^{-1})$, $C'_\varepsilon = (1-\varepsilon)(2\pi)^{\frac{d}{2}} |\det(H+\varepsilon I)|^{-\frac{1}{2}}$, and where we used the almost-everywhere convergence $\mathbb{1}_{\sqrt{\lambda} A_\lambda} \mathbb{1}_{B(0,\sqrt{\lambda}\delta)} \xrightarrow{\lambda\to\infty} \mathbb{1}_{A_\infty}$. Using the convergence in distribution $\xi'_\varepsilon \xrightarrow[\varepsilon\to 0]{\mathcal{L}} \xi$ with the Portmanteau lemma once again, and the convergence $C'_\varepsilon \to C$, we finally get

$$C\mathbb{P}(\xi \in A_\infty) \le \varliminf_{\lambda\to\infty} \lambda^{\frac{d}{2}} I_\lambda \le \varlimsup_{\lambda\to\infty} \lambda^{\frac{d}{2}} I_\lambda \le C\mathbb{P}(\xi \in A_\infty).$$

□

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