Domain-sensitivity analysis for Dirichlet eigenvalues of the Witten Laplacian in the semiclassical limit.

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Contents

1 Introduction **1**

2 Setting and notations **1**
2.1 Geometric assumptions on the domains Ω_β. 3

3 Limiting behavior of the low-lying spectrum **5**
3.1 Definition of the harmonic approximation 6
3.2 Local harmonic models. 6
3.3 Harmonic eigenmodes. 7
3.4 Critical oscillators. 7
3.5 Global harmonic approximation. 10
3.6 Harmonic quasimodes. 12
3.7 Proof of Theorem 1 15

4 An Eyring–Kramers formula for $\lambda_{1,\beta}$. **20**
4.1 Geometric assumptions 20
4.2 Construction of a precise quasimode 20
4.3 21

5 Application to domain optimization **23**

6 Tools **24**

1 Introduction

2 Setting and notations

In this paragraph, we introduce various notations which will be used throughout this work; We consider a potential function, $V : \mathbb{R}^d \to \mathbb{R}$, which we assume to be smooth and Morse.

A metastable diffusion process. 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. This process is known, under tame assumptions on V, to be 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:

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

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

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

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

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 $-\mathcal{L}^D_\beta$, 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 $-\mathcal{L}^D_\beta$ 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 $+\infty$.

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

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 $\dim\ker(\mathcal{L}_\beta + \lambda_{1,\beta}) = 1$.

In fact, it will sometimes be more convenient to study the spectrum of the Dirichlet realization of an equivalent Schrödinger-like operator:

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

with domains $D(H_\beta) = H^1_0 \cap H^2(\Omega_\beta) \subset L^2(\Omega_\beta)$. A straightforward computation shows that $\frac{1}{\beta}H_\beta$ is the conjugate of $-\mathcal{L}_\beta$ under the unitary transformation $u \mapsto \mathrm{e}^{-\frac{\beta V}{2}}u$ from $L^2_\mu(\Omega_\beta)$ to $L^2(\Omega_\beta)$, so that H_β also has pure point spectrum, and the k-th eigenvalue of H_β, counted with multiplicity, is given by $\beta\lambda_{k,\beta}$.

Moreover, we note that H_β may be written as

$$H_\beta = d^\dagger_{\beta,V} d_{\beta,V}, \tag{5}$$

where $d_{\beta,V}$ is the so-called twisted differential, given, for $u \in \mathcal{C}^\infty_c(\Omega_\beta)$, by the 1-form:

$$d_{\beta,V} u = \mathrm{e}^{-\frac{\beta V}{2}} \nabla\left[\mathrm{e}^{\frac{\beta V}{2}} u\right] = \nabla u + \frac{\beta}{2}\nabla V u, \tag{6}$$

and whose formal adjoint is given by:

$$d^\dagger_{\beta,V}\Theta = -\operatorname{div}\Theta + \frac{\beta}{2}\nabla V \cdot \Theta. \tag{7}$$

It will be convenient to use the quadratic form associated with H_β:

$$Q_\beta(u) = \langle U_\beta u, u\rangle + \|\nabla u\|^2, \tag{8}$$

with form domains $H_0^1(\Omega_\beta)$.

We use the following notation for the spectrum of $\nabla^2 V$ at each critical point z_i:

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

denote the eigenvalues of $\mathrm{Hess}\, V$ at z_i, with associated orthonormal eigenbasis:

$$U^{(i)} = \begin{pmatrix} v_1^{(i)} & \cdots & v_d^{(i)} \end{pmatrix},$$

which induce unitary transformations in L^2, via:

$$\mathcal{U}^{(i)} f(x) = f\left(U^{(i)\intercal} x\right), \quad \mathcal{U}^{(i)*} f(x) = f\left(U^{(i)} x\right). \tag{9}$$

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

For convenience, we will define the following half-spaces associated with each critical point:

$$E^{(i)}(\alpha) = U^{(i)}\left[(-\infty, \alpha) \times \mathbb{R}^{d-1}\right] \tag{10}$$

and, for $r > 0$, B_r will denote the Euclidean ball centered on the origin with radius r.

2.1 Geometric assumptions on 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

$$\dot{X} = -\nabla V(X). \tag{11}$$

We formalize the setting using the following assumptions:

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

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

$$\mathbf{B} = \left\{x \in \mathbb{R}^d : \lim_{t\to\infty} \phi_t(x) = z_0\right\}, \tag{12}$$

where $(\phi_t)_{t\geq 0}$ is the flow associated with the steepest descent dynamics (11), 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:

$$\forall\, \beta > 0,\, \forall\, x \in \partial\Omega_\beta, \mathrm{n}_\beta \cdot \nabla V(x) \leq 0. \tag{13}$$

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 all the order-one saddle points. By assumption i) all these critical points are isolated are non-degenerate, implying that the eigenvalues:

$$\sigma(\operatorname{Hess} V(z_i)) = \left(\nu_1^{(i)} \leq \nu_2^{(i)} \leq \cdots \nu_d^{(i)}\right) \tag{14}$$

are bounded away from zero, uniformly in i). We denote

$$U^{(i)} = \begin{pmatrix} v_1^{(i)} & \cdots & v_d^{(i)} \end{pmatrix}, \quad \operatorname{diag}(\nu_1^{(i)}, \cdots, \nu_d^{(i)}) = U^{(i)\intercal} \operatorname{Hess}(V(z_i)) U^{(i)}. \tag{15}$$

the associated orthonormal eigenbasis.

For $i = 0, \cdots, m+r$, we denote:

$$\varepsilon^{(i)}(\beta) = \sigma_{\Omega_\beta}(z_i), \tag{16}$$

where σ_{Ω_β} is the signed distance function to the boundary:

$$\sigma_{\Omega_\beta}(x) = \begin{cases} d(x, \partial\Omega_\beta) & x \in \Omega_\beta, \\ -d(x, \partial\Omega_\beta) & x \notin \Omega_\beta. \end{cases} \tag{17}$$

Since the Ω_β are assumed to be non-increasing, $\varepsilon^{(i)}$ is also a non-increasing function of β.

When considering a Gaussian approximation of the Boltzmann–Gibbs measure around the minimum z_0, that is, one finds that the covariance scales as β^{-1} when $\beta \to +\infty$. This suggest that the relevant scale on which to analyze concentration phenomena is $\beta^{-\frac{1}{2}}$ in the small temperature regime. This intuition is indeed borne out by analysis, and motivates the following assumption.

Assumption 1. *The following limit is well defined in $\mathbb{R} \cup \{+\infty\}$.*

$$\alpha^{(i)} = \lim_{\beta \to \infty} \sqrt{\beta} \varepsilon^{(i)}(\beta) \in (-\infty, +\infty]. \tag{H0}$$

We will distinguish two regimes depending on the nature of $\alpha^{(i)}$.

- If $\alpha^{(i)} = +\infty$, we say that z_i is **far** from the boundary.
- If $\alpha^{(i)}$ is finite, we say that z_i is **close** to the boundary.
- Finally, we will distinguish points which are **inside** the boundary as those for which $\alpha^{(i)} \geq 0$, and those **outside**, for which $\alpha^{(i)} < 0$. Note that we proclude the case of critical points which are far outside the boundary.

Note that if z_i is far from the boundary, Ω_β contains a ball of radius much larger than $\beta^{-\frac{1}{2}}$, say $\frac{\varepsilon^{(i)}(\beta)}{2}$, centered around z_i. In the case where z_i is close to the boundary, our main hypothesis will be the following assumption on the local geometry of $\partial\Omega_\beta$ around z_i.

Assumption 2. *There exist functions $\delta^{(i)}, \gamma^{(i)} : \mathbb{R}_+^* \to \mathbb{R}_+$ such that the following holds for β large enough:*

$$\begin{cases} \sqrt{\beta}\delta^{(i)}(\beta) \overset{\beta\to\infty}{\longrightarrow} +\infty, \\ \sqrt{\beta}\gamma^{(i)}(\beta) \overset{\beta\to\infty}{\longrightarrow} 0, \\ \mathcal{O}_i^-(\beta) \subseteq B(z_i, \delta^{(i)}(\beta)) \cap \Omega_\beta \subseteq \mathcal{O}_i^+(\beta), \end{cases} \tag{\textbf{H1}}$$

where we denote

$$\mathcal{O}_i^\pm(\beta) = z_i + B_{\delta^{(i)}(\beta)} \cap E^{(i)}\left(\frac{\alpha^{(i)}}{\sqrt{\beta}} \pm \gamma^{(i)}(\beta)\right), \tag{18}$$

recalling the definition of the half-space (10)*.*

Geometrically, the sets (18) correspond to hyperspherical caps centered around z_i and cut in the direction $v_1^{(i)}$. Thus, this condition fixes the orientation convention for $v_i^{(1)}$ in the case z_i is close to the boundary, namely, $v_1^{(i)}$ always points outwards from $\partial\Omega_\beta$ (including when z_i is outside the domain). The content of Assumption (**H1**) is that, up to negligible perturbations relative to $\beta^{-\frac{1}{2}}$, the boundary is shaped like a hyperplane which is normal to the first eigenvector of the Hessian, $v_1^{(i)}$, in a local neighborhood of size $\delta^{(i)}(\beta)$ around z_i. Thus, we also write: we also write

$$\mathcal{O}_i^\pm(\beta) = B(z_i, \delta^{(i)}(\beta)) \setminus C_i^\pm(\beta), \tag{19}$$

where the $C_i^\pm(\beta)$ are the hyperspherical caps:

$$C_i^\pm(\beta) = z_i + B_{\delta^{(i)}(\beta)} \cap \overline{E^{(i)}}\left(\frac{\alpha^{(i)}}{\sqrt{\beta}} \pm \gamma^{(i)}\right), \tag{20}$$

and $\overline{E^{(i)}}$ denotes the closure of $E^{(i)}$.

commenter dans le cas des points selles d'ordre un qu'il s'agit de perturbations d'ordre $1/\sqrt{\beta}$ du bassin d'attraction

In Figure **??**, we represent schematically the local geometry of $\partial\Omega_\beta$, in a case where z_i is close to and inside the boundary.

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We make the following further assumption concerning the scaling of $\varepsilon^{(i)}$ and $\delta^{(i)}$. In fact, assuming (**H1**), it comes at no cost to generality, as will be discussed below.

Assumption 3. *There exists $0 < t < \frac{1}{6}$ such that, for all $0 \le i \le m + r$:*

- *if z_i is close to the boundary:*

$$\varepsilon^{(i)}(\beta) < \delta^{(i)}(\beta) < \beta^{t-\frac{1}{2}}, \tag{\textbf{H2}}$$

- *if z_i is far from the boundary:*

$$\delta^{(i)} < \varepsilon^{(i)}(\beta) \wedge \beta^{t-\frac{1}{2}}. \tag{\textbf{H2'}}$$

This assumption comes at no cost of generality if we assume (**H1**). Indeed, we are always free to consider instead $\delta^{(i)}(\beta) \wedge \beta^{t-\frac{1}{2}}$ in the case where z_i is close to the boundary, and $\delta^{(i)} = (1-\rho)\varepsilon^{(i)}(\beta) \wedge \beta^{t-\frac{1}{2}}$ for some $0 < \rho < 1$ in the case where z_i is far from the boundary. We note that both these choices still satisfy the first condition of (**H1**), and thus also the third for β large enough. The motivation for choosing this range for the exponent t will be made clear in the proof of Lemma 3.

Finally, we will need the following technical assumption on the growth of $\delta^{(i)}(\beta)$.

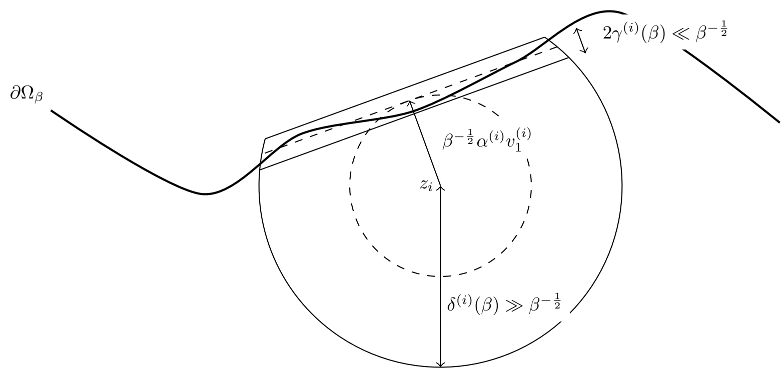

Figure 1: The local geometry of Ω_β in the neighborhood of a critical point z_i which is close to the boundary.

Assumption 4. *The following holds for all* $0 \le i \le m + r$*:*

$$\lim_{\beta\to\infty} \delta^{(i)}(\beta)\sqrt{\frac{\beta}{\log\beta}} = +\infty. \tag{\textbf{H3}}$$

We stress that (**H3**), together with the hypothesis (**H2'**), forces critical points which are far from $\partial\Omega_\beta$ to be sufficiently far relatively to $\sqrt{\beta}$, namely further than $\sqrt{\log\beta}$ in this scaling. Slower rates of divergence lie outside the scope of our analysis.

3 Limiting behavior of the low-lying spectrum

We first aim to generalize the harmonic approximation of [6] to the case of a temperature-dependent Dirichlet boundary condition, treating in particular the case in which the distance to the boundary scales critically with the temperature. We will show the following theorem:

Theorem 1 (Harmonic approximation)**.** *Assume that ,* (**H0**)*,* (**H1**) *and* (**H3**) *hold, and let* $k \ge 1$*. Then the following holds:*

$$\lim_{\beta\to\infty} \lambda_{k,\beta} = \lambda^{\mathrm{H}}_{k,\alpha}, \tag{21}$$

where α *is given by* (41)*, and* $\lambda_{k,\beta}$ *is the* k*-th Dirichlet eigenvalue of the operator* (3) *in* Ω_β*.*

In the above, $\lambda^{\mathrm{H}}_{k,\alpha}$ denotes the k-th eigenvalue of some temperature-independent operator defined in Equation (44), the harmonic approximation to the Witten Laplacian. The vector $\alpha \in (-\infty, +\infty]^{1+m+r}$ encodes the asymptotic distance to the boundary of each critical points in the semiclassical scaling, and its i-th component is given by the limit $\alpha^{(i)}$. The proof of Theorem 1 relies on the construction of approximate eigenvectors for the Witten Laplacian, which are composed

3.1 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 value of the limit $\alpha^{(i)} \in [0, \infty]$.

3.2 Local harmonic models.

The potential part of $H_\beta = U_\beta - \Delta$, given by $U_\beta = \frac{1}{2}\left(\beta^2\frac{|\nabla V|^2}{2} - \beta\Delta V\right)$ is, at dominant order in β, comprised of sharp wells centered around the critical points of V. The purpose of the harmonic approximation is to approximate H_β using independent local models consisting of shifted harmonic oscillators centered around each one of these wells, with frequencies prescribed by the eigenvalues of the $\nabla^2 V$ at z_i. Although very simple, this approximation is sufficient to capture the first-order behaviour of the bottom of the spectrum of $-\mathcal{L}_\beta$.

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

and let

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

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

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

the associated orthonormal eigenbasis, which induces unitary transformation on flast L^2 spaces, 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 $1 \le j \le d$, $0 \le i \le m+r$, and $\nu_1^i < 0$ if and only if $i \ge 1$.

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 direct computation shows that the Dirichlet realization of $H_\beta^{(i)}$ on $L^2(\Omega_\beta)$ is unitarily equivalent to that of $\beta K^{(i)}$ on $L^2(\sqrt{\beta}U^{(i)\intercal}(\Omega_\beta - z_i))$:

$$H_\beta^{(i)} = D_{\sqrt{\beta}}T_{\sqrt{\beta}z_i}\mathcal{U}^{(i)}\left(\beta K^{(i)}\right)\mathcal{U}^{(i)*}T_{-\sqrt{\beta}z_i}D_{1/\sqrt{\beta}}. \tag{22}$$

3.3 Harmonic eigenmodes.

In this section we define a family of self-adjoint realizations of the harmonic oscillators $K^{(i)}$, corresponding to various Dirichlet boundary conditions. These operators in turn will serve as local approximations of H_β around each critical point, allowing the construction of approximate eigenfunctions for H_β in the limit $\beta \to \infty$.

First, we recall classical results (see []) about the one-dimensional harmonic oscillator, and introduce some notation. The differential operator $-\frac{1}{2}\left(\partial_x^2 - x^2\right)$ is essentially self-adjoint on $\mathcal{C}_c^\infty(\mathbb{R})$, and its closure, which we denote by $\mathfrak{H}_\infty$, has compact resolvent. We use the following notation for the eigendecomposition of $\mathfrak{H}_\infty$: for $k \in \mathbb{N}$, we denote:

$$w_{k,\infty}(x) = \frac{1}{\sqrt{2^k k!\sqrt{\pi}}}\mathrm{e}^{-\frac{x^2}{2}}H_k(x), \tag{23}$$

where H_k is the k-th Hermite polynomial. The function $w_{k,\infty}$ is the k-th eigenstate of $\mathfrak{H}_\infty$, with

$$\mathfrak{H}_\infty w_{k,\infty} = \mu_{k,\infty}w_{k,\infty}, \quad \mu_{k,\infty} = k + \frac{1}{2}. \tag{24}$$

The full harmonic oscillator will serve (after an appropriate change of scale), as a local approximation of H_β around critical points z_i which are far from the boundary, or to model the behaviour in the directions $v_j^{(i)}$, $2 \leq j \leq d$ in the case where z_i is (super)critically close to the boundary. To construct a harmonic model for H_β around z_i critically close to the boundary in the direction $v_1^{(i)}$, we must consider Dirichlet realizations of the harmonic oscillator, whose study is the object of the next paragraph.

3.4 Critical oscillators.

In this paragraph, we introduce Dirichlet realizations for the harmonic oscillator which will serve as the basis for the construction of local models for H_β around critical points which are (super)critically close to the boundary.

We consider the following dense subspace of $L^2([a,b))$ for $a < b \leq +\infty$:

$$\mathcal{C}^\infty_{c,0}([a,b)) = \{f \in \mathcal{C}^\infty_c([a,b)) | f(a) = 0\}.$$

First we recall a few properties of the harmonic half-oscillator (see for instance the proof of [1, Proposition S1.2.10]): the symmetric operator

$$\widetilde{\mathfrak{H}}_0 = -\frac{1}{2}(\partial_x^2 - x^2), \quad \mathcal{D}(\widetilde{\mathfrak{H}}_0) = \mathcal{C}^\infty_{c,0}([0,+\infty)),$$

is essentially self-adjoint. Its unique self-adjoint extension, denoted $\mathfrak{H}_0$, has the following spectral decomposition:

$$\mathfrak{H}_0 w_{2k+1,\infty} = \left(2k + \frac{3}{2}\right) w_{2k+1,\infty}, \qquad k \in \mathbb{N}, \tag{25}$$

where the family $(\sqrt{2} w_{2k+1,\infty})_{k \geq 0}$ is an orthonormal eigenbasis for $\mathfrak{H}_0$ (the $\sqrt{2}$ factor accounts for normalization in L^2). Furthermore, $\mathfrak{H}_0$ has compact resolvent, and the following inclusion holds: $\mathcal{D}(\mathfrak{H}_0) \subset H^1_0([0,+\infty))$. We aim to study, for $\alpha \in \mathbb{R}$, the spectrum of a self-adjoint realization of the canonical oscillator $-\frac{1}{2}(\partial_x^2 - \frac{x^2}{2})$ with Dirichlet boundary conditions on $[\alpha, +\infty)$, and in particular show that its spectrum is (essentially) composed of isolated eigenvalues of finite multiplicity which moreover depend analytically on α. To this end, we use a perturbative approach. Changing domains by translating positions with $y = x - \alpha$, we see that the spectral properties of the operator:

$$\widetilde{\mathfrak{H}}_\alpha = -\frac{1}{2}(\partial_x^2 - x^2), \quad \mathcal{D}(\widetilde{\mathfrak{H}}_\alpha) = \mathcal{C}^\infty_{c,0}([-\alpha,+\infty))$$

can be deduced by those of the following operator:

$$-\frac{1}{2}(\partial_y^2 - y^2) + \alpha y + \frac{\alpha^2}{2} = \widetilde{\mathfrak{H}}_0 + V_\alpha + \frac{\alpha^2}{2}, \mathcal{D}(V_\alpha) = C^\infty_{c,0}([0,+\infty)).$$

Since the constant $\frac{\alpha^2}{2}$ only shifts the spectrum by a quantity which is analytic in α, it is enough to consider the operator:

$$\widetilde{\mathfrak{G}}_\alpha = \widetilde{\mathfrak{H}}_0 + \alpha y.$$

We first show that $\widetilde{\mathfrak{G}}_\alpha$ is essentially self-adjoint. To show this, we first show that αy is $\widetilde{\mathfrak{H}}_0$-

bounded with relative norm 0, computing, for $\varphi \in \mathcal{C}_c^\infty([0,+\infty))$ and any $M > 0$:

$$
\begin{aligned}
\|\alpha y \varphi\|^2 &= \alpha^2 \int_0^\infty y^2 \varphi^2(y)\,\mathrm{d}y \\
&\leq \alpha^2 M^2 \int_0^M \varphi^2(y)\,\mathrm{d}y + \frac{\alpha^2}{M^2}\int_M^\infty y^4 \varphi(y)^2\,\mathrm{d}y \\
&\leq \alpha^2 M^2 \|\varphi\|^2 + \frac{\alpha^2}{M^2}\|y^2\varphi\|^2 \\
&= \alpha^2 M^2 \|\varphi\|^2 + \frac{\alpha^2}{M^2}\left(4\|\widetilde{\mathfrak{H}}_0\varphi\|^2 + \int_0^\infty \left[2y^2\varphi(y)\varphi''(y) - \varphi''(y)^2\right]\,\mathrm{d}y\right) \\
&\leq \alpha^2 M^2 \|\varphi\|^2 + \frac{4\alpha^2}{M^2}\|\widetilde{\mathfrak{H}}_0\varphi\|^2 + \frac{2\alpha^2}{M^2}\int_0^\infty y^2\varphi(y)\varphi''(y)\,dy
\end{aligned}
\tag{26}
$$

We may treat the remaining integral using two successive integration by parts, observing that at each step, the boundary term at zero vanishes since $\varphi(0) = 0$ is a factor:

$$
\begin{aligned}
\int_0^\infty y^2\varphi(y)\varphi''(y)\,\mathrm{d}y &= -\int_0^\infty (2y\varphi(y) + y^2\varphi'(y))\varphi'(y)\,\mathrm{d}y \\
&\leq -\int_0^\infty 2y\varphi(y)\varphi'(y)\,\mathrm{d}y \\
&= \|\varphi\|^2.
\end{aligned}
\tag{27}
$$

It follows that

$$
\|\alpha y\varphi\| \leq |\alpha|\sqrt{M^2 + \frac{2}{M^2}}\|\varphi\| + \frac{2|\alpha|}{M}\|\widetilde{\mathfrak{H}}_0\varphi\|,
\tag{28}
$$

and the claim follows by taking $M \to \infty$.

Since αy is $\widetilde{\mathfrak{H}}_0$-bounded with relative norm 0, by the Kato–Rellich theorem [7, Theorem 6.4], $\widetilde{\mathfrak{G}}_\alpha = \widetilde{\mathfrak{H}}_0 + \alpha y$ is essentially self-adjoint on $\mathcal{D}(\widetilde{\mathfrak{H}}_0)$, and its unique self-adjoint extension has domain

$$
\mathcal{D}(\mathfrak{G}_\alpha) = \mathcal{D}(\mathfrak{H}_0),
$$

which is independent of α. We denote by $\mathfrak{G}_\alpha$ the closure of $\widetilde{\mathfrak{G}}_\alpha$, and $\mathfrak{H}_\alpha$ the corresponding self-adjoint operator on $L^2([\alpha,+\infty))$ obtained by translating back to $x = y + \alpha$ coordinates and appropriately shifting the spectrum by $\alpha^2/2$. Let us denote, for $\lambda \notin \sigma(\mathfrak{G}_\alpha)$, the resolvent:

$$
R_\alpha(\lambda) = (\mathfrak{G}_\alpha - \lambda)^{-1}.
$$

A straightforward consequence of the relative bound (28) (which extends to the closures of the operators at play) is that, for fixed $\alpha \in \mathbb{R}$ and $|\operatorname{Im}\lambda|$ sufficiently large, R_α may be expanded into a normally convergent Dyson series:

$$
R_\alpha(\lambda) = R_0(\lambda)\sum_{k=0}^\infty \alpha^k \left(yR_0(\lambda)\right)^k,
\tag{29}
$$

which thus defines an analytic function of α. Furthermore, it is manifest from the expansion (29), since $\mathfrak{H}_0$ has compact resolvent, that $R_\alpha(\lambda)$ is compact, and hence $\mathfrak{G}_\alpha$, $\mathfrak{H}_\alpha$ also have compact resolvent. Since they are manifestly bounded below (by $-\alpha^2/2$ and 0 respectively), their spectra are comprised of isolated eigenvalues of finite multiplicity tending to $+\infty$. Standard results of perturbation theory (see [3, Chapter VII]) apply. In particular, we get from (28) and [3, Theorem VII.2.6,Theorem VII.3.9] that $\mathfrak{G}_\alpha$ and thus $\mathfrak{H}_\alpha$ define self-adjoint holomorphic families of type (A) for $\alpha \in \mathbb{R}$, and that there exists, for every $k \in \mathbb{N}$, holomorphic functions $\mu_{k,\alpha}$, $w_{k,\alpha}$ satisfying the eigenrelation

$$
\mathfrak{H}_\alpha w_{k,\alpha} = \mu_{k,\alpha} w_{k,\alpha},
\tag{30}
$$

such that $(v_{k,\alpha})_{k\in\mathbb{N}}$ is a dense orthonormal family in $L^2([\alpha,+\infty))$. Moreover, the enumeration of these eigenpairs is fixed by the convention chosen for the harmonic half-oscillator, namely:

$$v_{k,0} = \sqrt{2}v_{2k+1}, \qquad \omega_{k,0} = 2k + \frac{3}{2}.$$

We highlight that we slightly abuse terminology when speaking of the holomorphic function $\alpha \mapsto w_{k,\alpha}$, since these functions are, strictly speaking, elements of different Hilbert spaces. We will, here and thereafter, abuse notation and settle this issue by embedding them in $L^2(\mathbb{R})$ by extending them trivially by zero:

$$w_{k,\alpha}(x) = \mathbb{1}_{\alpha\le x} w_{k,\alpha}(x), \quad x \in \mathbb{R}. \tag{31}$$

The case $d = 1$.

Using the change of variables $z = \sqrt{\frac{|\nu_1^{(i)}|}{2}}x$, which gives $\frac{\nu_1^{(i)2}}{4}x^2 - \partial_x^2 = |\nu_1^{(i)}|\frac{1}{2}\left(z^2 - \partial_z^2\right)$, we denote, for $k \ge 0$ and $\alpha \in [0,\infty]$:

$$w_{k,\alpha}^{(i)}(x) = \left(\frac{|\nu_1^{(i)}|}{2}\right)^{\frac{1}{4}} v_{k,-\alpha(|\nu_1^{(i)}|/2)^{\frac{1}{2}}}\left(-\sqrt{\frac{|\nu_1^{(i)}|}{2}}x\right), \qquad \omega_{k,\alpha}^{(i)} = |\nu_1^{(i)}|\mu_{k,-\alpha(|\nu_1^{(i)}|/2)^{\frac{1}{2}}} - \frac{\nu_1^{(i)}}{2}. \tag{32}$$

Note that that the sign of the variable has been flipped to conform with the orientation convention chosen for $v_1^{(i)}$. It is immediate, from the construction performed above, that $(w_{k,\alpha}^{(i)})_k$ forms a complete orthonormal eigenbasis for the Dirichlet realization of the oscillator $K_\alpha^{(i)}$ on $L^2((-\infty,\alpha))$, and hence $K_\alpha^{(i)}$ is self-adjoint with domain:

$$D(K_\alpha^{(i)}) = \left\{u \in L^2(\mathbb{R}) : \sum_{k=0}^{\infty}\left(\omega_{k,\alpha}^{(i)}\right)^2 \left|\left\langle u, w_{k,\alpha}^{(i)}\right\rangle\right|^2 < +\infty\right\} \subset H_0^1(-\infty,\alpha). \tag{33}$$

The higher dimensional case is simply obtained by tensorizing one-dimensional eigenmodes.

The case $d \ge 2$.

We derive the general case by taking tensor products of the one-dimensional oscillators. Namely, we define, for $n \in \mathbb{N}^d$:

$$\lambda_{n,\alpha}^{(i)} = \omega_{n_1,\alpha}^{(i)} + \sum_{j=2}^{d}\left[|\nu_j^{(i)}|\mu_{n_j,\infty} - \frac{\nu_j^{(i)}}{2}\right], \qquad \psi_{n,\alpha}^{(i)}(x) = w_{n_1,\alpha}^{(i)}(x_1)\prod_{j=2}^{d}\left[\left(\frac{|\nu_j^{(i)}|}{2}\right)^{\frac{1}{4}} w_{n_j,\infty}\left(\sqrt{\frac{|\nu_j^{(i)}|}{2}}x_j\right)\right], \tag{34}$$

$$D(K_\alpha^{(i)}) = \left\{u \in L^2\left[(-\infty,\alpha)\times\mathbb{R}^{d-1}\right], \quad \sum_{n\in\mathbb{N}^d}^{\infty}\left(\lambda_{n,\alpha}^{(i)}\right)^2\left|\left\langle u, \psi_{n,\alpha}^{(i)}\right\rangle\right|^2 < +\infty\right\} \subset H_0^1\left[(-\infty,\alpha)\times\mathbb{R}^{d-1}\right], \tag{35}$$

$$K_\alpha^{(i)}u = \sum_{n\in\mathbb{N}^d}^{\infty}\lambda_{n,\alpha}^{(i)}\left\langle u, \psi_{n,\alpha}^{(i)}\right\rangle\psi_{n,\alpha}^{(i)}, \qquad \forall\, u \in D(K_\alpha^{(i)}). \tag{36}$$

It is immediate from the construction performed above that $K_\alpha^{(i)}$ is a self-adjoint on $L^2((-\infty,\alpha)\times\mathbb{R}^{d-1})$, with compact resolvent, and a spectrum consisting of isolated eigenvalues of finite multiplicity tending to $+\infty$. As before, we allow ourselves to consider each $\psi_{n,\alpha}^{(i)}$ as an element of $L^2(\mathbb{R}^d)$ by extending it by zero outside of $(-\infty,\alpha)\times\mathbb{R}^{d-1}$.

Furthermore, we have the following pointwise decay estimate for eigenmodes.

Lemma 1. *For any $n \in \mathbb{N}^d$ and $\alpha \in (-\infty, \infty]$, there exists a constant $C_{i,n,\alpha} > 0$ such that the following inequality holds for almost every x in $\mathbb{R}^d$:*

$$|\psi^{(i)}_{n,\alpha}(x)| \leq C_{i,n,\alpha}\,\mathrm{e}^{-\frac{|x|^2}{C_{i,n,\alpha}}}. \tag{37}$$

Proof. The proof relies on a probabilistic estimate obtained in [2], and a reflection argument. We consider the following anti-symmetrization of the eigenmode $\psi^{(i)}_{n,\alpha}$:

$$\widetilde{\psi}^{(i)}_{n,\alpha}(x) = \psi^{(i)}_{n,\alpha}(x)\mathbb{1}_{x\leq\alpha} - \psi^{(i)}_{n,\alpha}(\iota_\alpha x)\mathbb{1}_{x>\alpha}, \tag{38}$$

where $\iota_\alpha(x) = (2\alpha - x, \dots, x_d)$ denotes the reflection with respect to the $\{x_1 = \alpha\}$ hyperplane. Then, it is easy to check that $\widetilde{\psi}^{(i)}_{n,\alpha}$ is also an eigenmode (for the same eigenvalue $\lambda^{(i)}_{n,\alpha}$) of the Schrödinger operator associated with the symmetrized potential:

$$\widetilde{K}^{(i)}_\alpha = \widetilde{W}^{(i)} - \Delta, \quad \widetilde{W}^{(i)}(x) = W^{(i)}(x)\mathbb{1}_{x\leq\alpha} + W^{(i)}(\iota_\alpha x)\mathbb{1}_{x>\alpha}, \tag{39}$$

We note that there exists a compact set $B_i \subset \mathbb{R}^d$, depending only on i, and $\varepsilon > 0$ such that

$$\widetilde{W}^{(i)} \geq \varepsilon|x|^2, \quad \forall\, x \in \mathbb{R}^d \setminus B_i, \tag{40}$$

owing to the strict positivity of $\Lambda^{(i)}$ (recalling that z_i is a non-degenerate critical point). We consider $\widetilde{K}^{(i)}$ to be the self-adjoint extension of a formal operator defined as a Friedrichs extension of the lower-bounded quadratic form associated with $K^{(i)}$. Then, it immediately follows from [2, Proposition 3.1] and the lower bound (40) that the pointwise estimate (37) holds for $\widetilde{\psi}^{(i)}_{n,\alpha}$ and some constant $C_{i,n,\alpha}$. The proof is concluded, since $|\psi^{(i)}_{n,,\alpha}(x)| \leq |\widetilde{\psi}^{(i)}_{n,\alpha}(x)|$ for all x. □

3.5 Global harmonic approximation.

We now define the global harmonic approximation to H_β, associated with a vector of extended real numbers $\alpha' = (\alpha'_0, \dots, \alpha'_{m+r}) \in (-\infty, \infty]^{1+m+r}$ encoding the Dirichlet boundary conditions. Recall, that for each $i = 0, \cdots, m + r$, the extended real number α_i is defined as the limit $\lim\limits_{\beta\to\infty} \sqrt{\beta}\varepsilon^{(i)}(\beta)$, and so we also denote for convenience:

$$\alpha = (\alpha_i)_{i=0,\dots,m+r}\,. \tag{41}$$

We define, for general α', local oscillators $H^{(i)}_{\beta,\alpha'_i}$ from the definition $K^{(i)}_{\alpha'_i}$ using the unitary equivalence (22). In particular, the domain of $H^{(i)}_{\beta,\alpha'_i}$ is given by

$$D(H^{(i)}_{\beta,\alpha'_i}) = \left\{ u \in L^2\left[z_i + E^{(i)}\left(\frac{\alpha'_i}{\sqrt{\beta}}\right)\right], \quad \mathcal{U}^{(i)*}T_{-\sqrt{\beta}z_i}D_{1/\sqrt{\beta}}u \in D(K^{(i)}_{\alpha'_i})\right\}. \tag{42}$$

We denote by

$$\psi^{(i)}_{\beta,k,\alpha'_i}(x) = \beta^{\frac{1}{4}}\psi^{(i)}_{k,\alpha'_i}(\sqrt{\beta}U^{(i)\intercal}(x - z_i)), \tag{43}$$

the eigenmode of $H^{(i)}_{\beta,\alpha'_i}$ with eigenvalue $\beta\lambda^{(i)}_{,k,\alpha'_i}$ associated with $\psi^{(i)}_{k,\alpha'_i}$ under this correspondence. Note the $\beta^{\frac{1}{4}}$ factor, which accounts for L^2 normalization.

The global approximation is formed by a direct sum of these local oscillators:

$$H^{\mathrm{H}}_{\beta,\alpha'} = \bigoplus_{i=0}^{m+r} H^{(i)}_{\beta,\alpha'_i}, \qquad D(H^{\mathrm{H}}_{\beta,\alpha'}) = \prod_{i=0}^{m+r} D(H^{(i)}_{\beta,\alpha'_i}), \tag{44}$$

whence the harmonic spectrum is given by

$$\sigma(H^{\mathrm{H}}_{\beta,\alpha'}) = \left(\beta\lambda^{(i)}_{n,\alpha'_i}\right)_{\substack{0\leq i\leq m+r\\ n\in\mathbb{N}^d}}. \tag{45}$$

For convenience, we specify the conventions we use to enumerate the various spectra at play. First, we enumerate the spectrum of $K^{(i)}_{\alpha'_i}$ in non-decreasing order, defering to the lexicographic ordering on $\mathbb{N}^d$ to resolve ambiguities from degenerate eigenvalues. Thus we have a non-decreasing family $(\lambda^{(i)}_{n,\alpha})_{n\in\mathbb{N}}$, and corresponding eigenmodes $(\psi^{(i)}_{n,\alpha})_{n\in\mathbb{N}}$. We then enumerate the full harmonic spectrum in non-decreasing order, by defining two integer-valued sequences

$$(k_j)_{j\geq 1} \in \mathbb{N}^{\mathbb{N}^*}, \quad (i_j)_{k\geq 1} \in \{0,\dots,m+r\}^{\mathbb{N}^*}, \tag{46}$$

defined by the condition that the k-th largest eigenvalue of H^{H}_β, counted with multiplicity, is given by:

$$\beta\lambda^{\mathrm{H}}_{k,\alpha'} = \beta\lambda^{(i_k)}_{n_k,\alpha'_{i_k}}, \tag{47}$$

where we first defer to the ordering on $\{0,\dots,m+r\}$ and then to the ordering on each $\sigma(K^{(i)}_{\alpha'_i})$ to resolve ambiguities from degenerate eigenvalues.

For convenience, we also define, for each $0\leq i\leq m+r$, the function which gives, for a given $k\geq 1$, the number of eigenmodes corresponding to energy levels below $\lambda^{\mathrm{H}}_{\alpha'}$ localized around z_i:

$$N_i(k) = \#\{1\leq j\leq k : i_j = i\}. \tag{48}$$

For simplicity, we have omitted to notate the dependence of N_i, i_k and n_k in α', which will be clear from the context. We also note the following obvious relations, valid for any $k\geq 0$:

$$\max_{0\leq i\leq m+r} \lambda^{(i)}_{N_i(k),\alpha'_i} = \lambda^{\mathrm{H}}_{k,\alpha'}, \qquad \min_{0\leq i\leq m+r} \lambda^{(i)}_{N_i(k)+1,\alpha'_i} = \lambda^{\mathrm{H}}_{k+1,\alpha'}, \qquad \sum_{i=0}^{m+r} N_i(k) = k. \tag{49}$$

We highlight that the analyticity of the map $\alpha\mapsto\mu_{k,\alpha}$ for all $k\in\mathbb{N}$ implies that the map:

$$\alpha'\mapsto\lambda^{\mathrm{H}}_{k,\alpha'} \tag{50}$$

is continuous.

3.6 Harmonic quasimodes.

Approximate eigenmodes of H_β may be obtained by localizing the eigenmodes of the harmonic approximation around the corresponding critical point, in such a way that the Dirichlet boundary conditions in Ω_β are met. We will consider so-called quasimodes of the form

$$\widetilde{\psi}^{(i)}_{\beta,k,\alpha} = \frac{\chi^{(i)}_\beta \psi^{(i)}_{\beta,k,\alpha}}{\|\chi^{(i)}_\beta \psi^{(i)}_{\beta,k,\alpha}\|_{L^2(\Omega_\beta)}}, \tag{51}$$

where $\psi^{(i)}_{\beta,k,\alpha}$ is a harmonic mode of $H^{(i),\alpha}_\beta$, multiplied by the cutoff function $\chi^{(i)}_\beta$, and normalized in $L^2(\Omega_\beta)$. The role of $\chi^{(i)}_\beta$ is to localize the quasimode in the vicinity of z_i, and ensure that the boundary conditions are met. To this effect, we fix a reference $\mathcal{C}^\infty_c$ cutoff function χ such that

$$\chi|_{B\left(0,\frac{1}{2}\right)} \equiv 1, \quad \chi|_{\mathbb{R}^d\setminus B(0,1)} \equiv 0.$$

We will furthermore require the following technical condition:

$$\|\nabla\sqrt{1-\chi^2}\|_\infty < +\infty, \tag{52}$$

which may be easily enforced by choosing χ such that $\chi \overset{a^+}{\sim} \exp\left(-\frac{1}{x-a}\right)$, $\chi \overset{b^-}{\sim} \exp\left(-\frac{1}{b-x}\right)$, say for $\operatorname{supp}\chi = [a,b]$. Let us next define the localized cutoff function:

$$\chi^{(i)}_\beta(x) = \chi(\delta^{(i)}(\beta)^{-1}|x-z_i|). \tag{53}$$

Recalling that $\sqrt{\beta}\delta^{(i)}(\beta) \overset{\beta\to\infty}{\longrightarrow} +\infty$, we have that $\mathrm{supp}\chi_\beta^{(i)}$ is contained in a small ball around z_i, but which is large with respect to $\frac{1}{\sqrt{\beta}}$, and $\mathrm{supp}\,\nabla\chi_\beta^{(i)}$ is contained in a hyperspherical shell around z_i:

$$\mathrm{supp}\,\chi_\beta^{(i)} \subset B(z_i, \delta^{(i)}(\beta)), \quad \mathrm{supp}\,\nabla\chi_\beta^{(i)} \subset B(z_i, \delta^{(i)}(\beta)) \setminus B\left(z_i, \frac{1}{2}\delta^{(i)}(\beta)\right). \tag{54}$$

In particular we have

$$\|\partial^\alpha \chi_\beta^{(i)}\|_\infty = \|\partial^\alpha\chi\|_\infty \delta^{(i)}(\beta)^{|\alpha|}, \tag{55}$$

for any multi-index α, hence $\|\partial^\alpha\chi_\beta^{(i)}\|_\infty = \mathrm{o}(\beta^{\frac{|\alpha|}{2}})$ for $|\alpha| \le 2$.

We stress that, although $\chi_\beta^{(i)}$ does not itself vanish on $\partial\Omega_\beta$ in general in the case where z_i is (super)critically close to the boundary, we still have $\widetilde{\psi}_{\beta,k,\alpha}^{(i)} \in H_0^1 \cap H^2(\Omega_\beta)$ provided the harmonic eigenmode $\psi_{\beta,k,\alpha}^{(i)}$ vanishes on $C_i(\beta)$, where we recall the definition (20) of the spherical cap associated with z_i.

In the following lemma, we record some localization estimates.

Lemma 2 (Localization estimates)**.** *We consider normalized eigenvectors $\psi_{\beta,n,\alpha}^{(i)}$ and $\psi_{\beta,m,\alpha}^{(i)}$ of $H_{\beta,\alpha}^{(i)}$ in $L^2\left(E^{(i)}(\frac{\alpha}{\sqrt{\beta}})\right)$, and we define the associated quasimodes $\widetilde{\psi}_{\beta,n,\alpha}^{(i)}$ and $\widetilde{\psi}_{\beta,m,\alpha}^{(i)}$ according to the formula (51). Then, there exists $\beta_0 > 0$ and constants $C_{n,i,\alpha}, C_{m,i,\alpha}, C_{n,m,i,\alpha} > 0$, independent of β such that the following estimates hold for any $\beta > \beta_0$.*

$$\|(1-\chi_\beta^{(i)})\psi_{\beta,n}^{(i)}\|_{L^2(\mathbb{R}^d)} \le \frac{C_{n,i,\alpha}}{\beta^{\frac14}\delta^{(i)}(\beta)^{\frac12}} \mathrm{e}^{-\frac{\beta\delta^{(i)}(\beta)^2}{C_{n,i,\alpha}}}, \tag{56}$$

$$\left|\langle \widetilde{\psi}_{\beta,n}^{(i)}, \widetilde{\psi}_{\beta,m}^{(i)}\rangle - \delta_{nm}\right| \le \frac{C_{n,m,i,\alpha}}{\beta^{\frac14}\delta^{(i)}(\beta)^{\frac12}} \mathrm{e}^{-\frac{\beta\delta^{(i)}(\beta)^2}{C_{n,m,i,\alpha}}}, \tag{57}$$

$$\left|\left\langle H_\beta^{(i)}(1-\chi_\beta^{(i)})\psi_{\beta,n}^{(i)}, (1-\chi_\beta^{(i)})\psi_{\beta,m}^{(i)}\right\rangle_{L^2(\mathbb{R}^d)}\right| \le \frac{C_{n,m,i,\alpha}}{\beta^{\frac12}\delta^{(i)}(\beta)^3} \mathrm{e}^{-\frac{\beta\delta^{(i)}(\beta)^2}{C_{n,m,i,\alpha}}}. \tag{58}$$

Furthermore, assuming (**H3**)*, these bounds decay faster than any polynomial growth in β.*

Proof. We begin by proving (56). Changing coordinates with $y = \sqrt{\beta}U^{(i)\mathsf{T}}(x - z_i)$, we get:

$$\begin{aligned}
\|(1-\chi_\beta^{(i)})\psi_{\beta,n,\alpha}^{(i)}\|_{L^2(\mathbb{R}^d)}^2 &= \int_{\mathbb{R}^d} (1-\chi)\left(\frac{1}{\sqrt{\beta}\delta^{(i)}(\beta)}U^{(i)}y\right)\psi_{n,\alpha}^{(i)}(y)^2\,\mathrm{d}y \\
&\le \int_{\mathbb{R}^d\setminus B(0,\frac12\sqrt{\beta}\delta^{(i)}(\beta))} \psi_{n,\alpha}^{(i)}(y)^2\,\mathrm{d}y \\
&\le |\mathbb{S}^{d-1}|C_{n,i,\alpha}\int_{\frac12\sqrt{\beta}\delta^{(i)}(\beta)}^{\infty} s^{d-1}\mathrm{e}^{-\frac{s^2}{C_{n,i,\alpha}}}\,\mathrm{d}s, \\
&\le C'_{n,i,\alpha}\int_{\frac12\sqrt{\beta}\delta^{(i)}(\beta)}^{\infty} \mathrm{e}^{-\frac{s^2}{C'_{n,i,\alpha}}}\,\mathrm{d}s,
\end{aligned} \tag{59}$$

where we used respectively the condition (54) and the pointwise exponential decay estimate (37) to obtain the first and second inequalities. Applying the standard Gaussian tail bound $\int_t^\infty \mathrm{e}^{-s^2/2}\,\mathrm{d}s \le t^{-1}\mathrm{e}^{-t^2/2}$ yields the desired bound (56) upon taking $C'_{n,i,\alpha}$ as large as necessary.

To show (57), we first note that, since $\|\psi_{\beta,n,\alpha}^{(i)}\| = 1$, and $0 \le \chi_\beta^{(i)} \le 1$, we obtain, by a simple triangle inequality:

$$0 \le 1 - \|\chi_\beta^{(i)}\psi_{\beta,n,\alpha}^{(i)}\| \le \|(1-\chi_\beta^{(i)})\psi_{\beta,n,\alpha}^{(i)}\|,$$

and thus

$$1 \leq \frac{1}{\|\chi_\beta^{(i)} \psi_{\beta,n,\alpha}^{(i)}\|} \leq 1 + 2\|(1-\chi_\beta^{(i)})\psi_{\beta,n,\alpha}^{(i)}\| \tag{60}$$

for β sufficiently large. A similar estimate holds for $\psi_{\beta,m,i}^{(i)}$.

For convenience, we denote $\psi_{\beta,n,\alpha}^{(i)} = \psi_n$, $\psi_{\beta,m,\alpha}^{(i)} = \psi_m$ and $\chi_\beta^{(i)} = \chi$. Then:

$$\langle \chi\psi_n, \chi\psi_m \rangle = \langle \psi_n, \psi_m \rangle - 2\langle \psi_n, (1-\chi)\psi_m \rangle + \langle \psi_n, (1-\chi)^2\psi_m \rangle.$$

Thus, by Cauchy–Schwarz inequalities, and using the orthogonality of ψ_n and ψ_m, we obtain:

$$|\langle \chi\psi_n, \chi\psi_m \rangle - \delta_{n,m}| \leq 2\|\psi_n\|\|(1-\chi)\psi_m\| + \|\psi_n\|\|(1-\chi)^2\psi_m\| \leq 3\|(1-\chi)\psi_m\|,$$

since $(1-\chi)^2 \leq (1-\chi)$.

Denoting $\widetilde{\psi}_n = \chi\psi_n\|\chi\psi_n\|^{-1}, \widetilde{\psi}_m = \chi\psi_m\|\chi\psi_m\|^{-1}$, we deduce from (60) that there exists constants $C, \beta_0 > 0$ such that

$$\left|\langle \widetilde{\psi}_n, \widetilde{\psi}_m \rangle - \delta_{nm}\right| \leq \left|1 - \frac{1}{\|\chi\psi_n\|\|\chi\psi_m\|}\right| \|\chi\psi_n\|\|\chi\psi_m\| \leq C(\|(1-\chi)\psi_m\| + \|(1-\chi)\psi_n\|)$$

for all $\beta > \beta_0$. Using the estimate (56) then yields (57).

For (58), we start with a small computation for a Schrödinger operator $H = V - \Delta$ with domain $D(H) \subset H^1(\mathbb{R}^d)$, two eigenstates u, v with respective eigenvalues λ_u, λ_v, and $\eta \in \mathcal{C}_c^\infty(\mathbb{R}^d)$. Using the relation

$$H(\eta u) = \eta Hu - 2\nabla\eta \cdot \nabla u - u\Delta\eta = \lambda_u \eta u - 2\nabla\eta \cdot \nabla u - u\Delta\eta,$$

we get by integrating against ηv:

$$\langle H\eta u, \eta v \rangle = \lambda_u \langle u, \eta v\eta \rangle - \langle uv, \eta\Delta\eta \rangle - 2\langle v\nabla u, \eta\nabla\eta \rangle.$$

Thus, by symmetry and an integration by parts, we get

$$\langle H\eta u, \eta v \rangle = \langle uv, \frac{\lambda_u + \lambda_v}{2}\eta^2 - \eta\Delta\eta \rangle - \langle \nabla[uv], \nabla[\eta^2] \rangle = \langle uv, \frac{\lambda_u + \lambda_v}{2}\eta^2 + \eta\Delta\eta + 2|\nabla\eta|^2 \rangle. \tag{61}$$

Applying equation (61) to $H = H_{\beta,\alpha}^{(i)}$ with $\eta = (1 - \chi_\beta^{(i)})$, we get, noting that the test function $\frac{\lambda_u+\lambda_v}{2}\eta^2 + \eta\Delta\eta + 2|\nabla\eta|^2$ is supported in:

$$\mathbb{R}^d \setminus B\left(z_i, \frac{1}{2}\sqrt{\beta}\delta^{(i)}(\beta)\right),$$

$$\left\|\frac{\lambda_n + \lambda_m}{2}(1-\chi_\beta^{(i)})^2 + (1-\chi_\beta^{(i)})\Delta(1-\chi_\beta^{(i)}) + 2|\nabla(1-\chi_\beta^{(i)})|^2\right\|_\infty \leq \frac{C_{n,m}}{\delta^{(i)}(\beta)^2},$$

using the crude estimate (55), whereby, using again the pointwise exponential decay of both φ and ψ, and the same Gaussian tail estimate as for (56), we get, for some $C > 0$,

$$\left|\left\langle H_\beta^{(i)}(1-\chi_\beta^{(i)})\varphi_\beta^{(i)}, (1-\chi_\beta^{(i)})\varphi_\beta^{(i)}\right\rangle\right| \leq \frac{C}{\delta^{(i)}(\beta)^2}\int_{\frac{1}{2}\sqrt{\beta}\delta^{(i)}(\beta)}^{+\infty} \mathrm{e}^{-\frac{2s^2}{C}}\,\mathrm{d}s \leq C\frac{\mathrm{e}^{-\frac{\beta\delta^{(i)}(\beta)^2}{C}}}{\beta^{\frac{1}{2}}\delta^{(i)}(\beta)^3}. \tag{62}$$

Finally, each of the bounds may be written in the form $\frac{P(\beta)}{Q(T(\beta))}\mathrm{e}^{-cT(\beta)^2}$, where $T(\beta) = \sqrt{\beta}\delta^{(i)}(\beta)$ and P, Q are polynomials. Since, under Assumption (**H3**), $T(\beta)$ goes to $+\infty$ faster than $\sqrt{\log\beta}$, we also have $\frac{R(\beta)P(\beta)}{Q(T(\beta))}\mathrm{e}^{-cT(\beta)^2} \to 0$ for any polynomial R. □

The following lemma justifies the local approximation of H_β by $H_\beta^{(i)}$ around z_i.

Lemma 3 (Taylor estimate). *Fix $0 \le i \le m+r$ and $u \in L^2(\Omega_\beta)$, and assume* (**H2**), (**H2'**) *hold. There exists $C > 0$ and $\beta_0 > 0$ such that, for all $\beta > \beta_0$, the following estimate holds:*

$$\|(H_\beta - H_\beta^{(i)})\chi_\beta^{(i)} u\| \le C\beta^{3t+\frac{1}{2}}\|\chi_\beta^{(i)} u\| = \mathrm{o}(\beta)\|\chi_\beta^{(i)} u\|. \tag{63}$$

Proof. Since $H_\beta - H_\beta^{(i)}$ is a multiplication operator by a smooth function, it is bounded in $L^2(\Omega_\beta)$, and thus we only need to control the L^∞-norm of the difference in the potential parts:

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

on $\Omega_\beta \cap \operatorname{supp}\chi_\beta^{(i)} \subset B(z_i, \beta^{t-\frac{1}{2}})$. In turn, this is given by the sum of two contributions:

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

Thus, using a second-order Taylor expansion around z_i, there exists $\beta_0 > 0, C > 0$ depending only on V and i such that for all $\beta > \beta_0$ and every $x \in \operatorname{supp}\chi_\beta^{(i)}$,

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

For the Laplacian term, since V is C^∞ and ΔV is thus locally Lipschitz, we have, for β large enough,

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

In turn, we get that

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

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

3.7 Proof of Theorem 1

We conclude this section by giving the proof of the so-called harmonic approximation in the case of a moving boundary, which posits that the first-order asymptotics of any given eigenvalue at the bottom of the spectrum of H_β is given by the corresponding eigenvalue of H_β^{H} in the limit $\beta \to \infty$. The main novelty is the accomodation of moving Dirichlet boundary conditions, and in particular allowing the computation of asymptotic energies for eigenstates localized around critical points which are (super)critically close to the boundary.

Proof of Theorem 1. Without loss of generality, we assume (**H2**) and (**H2'**). To show (21), we study eigenvalues of the Witten Laplacian (4), since these are related to those of $-\mathcal{L}_\beta$ via a simple multiplication by β. As in [6], the strategy is to construct approximate eigenvectors for H_β, which (roughly speaking) consist of eigenvectors of each of the local oscillators $H_{\beta,\alpha_i}^{(i)}$, localized around the critical points z_i by appropriate cutoff functions. The main technical novelty compared to previous constructions, besides the construction of critical harmonic models performed in Section 3.4, is the special care which must be taken to ensure that the quasimodes remain in the appropriate form domains. Once one has constructed valid quasimodes, we will be able to make estimates on the bottom of the spectrum using the Courant–Fischer variational principles.

Step 1: Upper bound. The proof of the upper bound proceeds in two steps. In the first step, we define an appropriate realization of the harmonic approximation (44) so that the associated quasimodes are in the form domain $H_0^1(\Omega_\beta)$. The second step is very similar, once the construction of the harmonic approximation has been performed and the various localization estimates have been verified, to the techniques of [6, 4]. We choose to include it for the sake of completeness.

Step 1a: Perturbation of the local oscillators.
We fix $k \geq 1$. We construct families of quasimodes $\{\varphi_1, \cdots, \varphi_k\}$ associated to the first k harmonic eigenvalues $\lambda^{\mathrm{H}}_{1,\alpha}, \cdots, \lambda^{\mathrm{H}}_{k,\alpha}$. The φ_j will be in the general form (51), however, we must be careful with the chosen realization of $H^{(i_j)}_\beta$ to ensure that the quasimodes are in the form domain of H_β. In fact we need, for each $0 \leq i \leq m+r$, to distinguish two cases:

a) If z_i is far from the boundary, then by Assumption (**H2'**), $\chi^{(i)}_\beta$ is supported inside Ω_β, and thus the associated quasimodes are indeed in $H^1_0(\Omega_\beta)$, the form domain of H_β.

b) If z_i is close to the boundary, then by the third condition in Assumption (**H1**), $\mathcal{O}^-_i(\beta) \subseteq B(z_i, \delta^{(i)}(\beta)) \cap \Omega_\beta$ for β large enough.

Let us fix $\rho > 0$ such that $\rho < \alpha_i$ for $i = 0, \dots, m+r$, and fix i such that z_i is close to the boundary, i.e. $\alpha^{(i)} < +\infty$. Then, Assumption (**H1**), straightforwardly implies that there exists $\beta_0 > 0$ such that, for all $\beta > \beta_0$, we have the inclusion:

$$B(z_i, \delta^{(i)}) \cap \left[z_i + E^{(i)}\left(\frac{\alpha^{(i)} - \rho}{\sqrt{\beta}} \right) \right] \subseteq \mathcal{O}^-_i(\beta) \subseteq \Omega_\beta,$$

recalling the notations (10), (18). Defining the vector,

$$\alpha^\rho = (\alpha_i - \rho \mathbb{1}_{\alpha^{(i)} < +\infty})_{0 \leq j \leq m+r},$$

we consider the perturbed harmonic approximation corresponding to the operator $H^{\mathrm{H}}_{\beta,\alpha^\rho}$, as defined in (44). By construction, for all $\beta > \beta_0$, eigenmodes $\psi^{(i_j)}_{\beta,k_j,\alpha^\rho_{i_j}}$ of $H^{(i_j)}_{\beta,\alpha^\rho_{i_j}}$, are supported in $z_i + E^{(i)}\left(\frac{\alpha^{(i)}-\rho}{\sqrt{\beta}}\right)$, as noted in Equation (42), and it follows the associated quasimode $\widetilde{\psi}^{(i_j)}_{\beta,k_j,\alpha^\rho_{i_j}}$, as defined by (51), belongs to $H^1_0(\Omega_\beta)$.

Step 1b: Energy upper bound.
We set:

$$\varphi_j = \widetilde{\psi}^{(i_j)}_{\beta,k_j,\alpha^\rho_{i_j}}, \quad 1 \leq j \leq k.$$

Note that the $(\varphi_j)_{1 \leq j \leq k}$ span a k-dimensional subspace of $H^1_0(\Omega_\beta)$, since the Gram matrix

$$\big(\langle \varphi_j, \varphi_{j'} \rangle_{L^2(\Omega_\beta)}\big)_{1 \leq j,j' \leq k}$$

is quasi-unitary, i.e. can be written in the form $I + \mathrm{o}(1)$ as $\beta \to \infty$. Indeed, we only need to check that the off-diagonal entries converge to zero in this limit. Fixing $1 \leq j, j' \leq k$, this is clear for $i_j \neq i_{j'}$, since the corresponding test functions $\chi^{(i_j)}_\beta$, $\chi^{(i_{j'})}_\beta$ have disjoint support. If $i_j = i_{j'}$, the statement is an immediate consequence of the quasi-orthogonality estimate (57). By the Min-Max Courant–Fischer principle, it then suffices to show that, for all $u \in \mathrm{Span}(\varphi_j,\, 1 \leq j \leq k)$,

$$Q_\beta(u) \leq (\beta \lambda^{\mathrm{H}}_{k,\alpha^\rho} + \mathrm{o}(\beta)) \|u\|^2, \tag{64}$$

to conclude

$$\overline{\lim_{\beta \to \infty}}\, \beta^{-1} \lambda_{\beta,k} \leq \lambda^{\mathrm{H}}_{k,\alpha^\rho}.$$

We will conclude, observing that the map $\rho \mapsto \lambda^{\mathrm{H}}_{k,\alpha^\rho}$ is continuous and $\alpha^\rho \overset{\rho\to 0}{\longrightarrow} \alpha$, that $\lambda^{\mathrm{H}}_{k,\alpha^\rho} \overset{\rho\to 0}{\longrightarrow} \lambda^{\mathrm{H}}_{k,\alpha}$, yielding the desired upper bound. We first consider $u = \chi^{(i_j)}_\beta \psi^{(i_j)}_{\beta,k_j,\alpha^\rho}$, which for convenience we write $u = \chi\psi$, with $H^{(i_j)}_{\beta,\alpha^\rho_{i_j}} \psi = \beta\lambda\psi$, and denote $H^{(i_j)}_{\beta,\alpha^\rho_{i_j}} = H$. By our choice of $(\varphi_j)_{1 \leq j \leq k}$, we have $\lambda \in (\lambda^{\mathrm{H}}_{j,\alpha^\rho})_{1 \leq j \leq k}$, and so $\lambda \leq \lambda^{\mathrm{H}}_{k,\alpha^\rho}$. We then write:

$$\langle H_\beta u, u \rangle = \langle Hu, u \rangle + \langle (H_\beta - H)u, u \rangle\,.$$

Since $\langle (H_\beta - H)u, u\rangle \leq C_{j,\alpha,\rho}\beta^{3t+\frac{1}{2}}\|u\|^2 = \mathrm{o}\beta)\|u\|^2$ for some constant $C_{j,\alpha,\rho} > 0$, by Lemma 3, we only need to estimate the first term. But, recalling $\|\psi\| = 1$, we have:

$$\begin{aligned}\langle H\chi\psi, \chi\psi\rangle &= \langle H\psi, \psi\rangle - 2\,\langle H\psi, (1-\chi)\psi\rangle + \langle H(1-\chi)\psi, (1-\chi)\psi\rangle \\ &= \beta\lambda\|\psi\|^2 - 2\,\langle H\psi, (1-\chi)\psi\rangle + \langle H(1-\chi)\psi, (1-\chi)\psi\rangle \\ &\leq \beta\lambda\|u\|^2 + 2\beta\lambda\|(1-\chi)\psi\| + \langle H(1-\chi)\psi, (1-\chi)\psi\rangle\end{aligned}$$

where we used a Cauchy–Schwarz inequality to obtain the final inequality. We next use the localization estimates given in Lemma 2 to two rightmost terms. Here, we make crucial use of the hypothesis (**H3**), which , together with (56) implies that $\beta\|(1-\chi)\psi\| = \mathrm{o}(\beta)$, and similarly that $\langle H(1-\chi)\psi, (1-\chi)\psi\rangle = \mathrm{o}(\beta)$. Finally, (58) implies that $\|u\|^2 = 1 + \mathrm{o}(\beta)$, so that we may write $Q(u) \leq \|u\|^2(\beta\lambda + \mathrm{o}(\beta))$. Since $\lambda \leq \lambda^{\mathrm{H}}_{k,\alpha^\rho}$, this implies the upper bound (64) for this particular choice of u. For a general $u = \sum_j g_j\varphi_j$ in the linear span of the quasimodes, in view of the previous estimation, it is enough to show that the cross terms

$$g_j g_{j'}\left\langle H^{(i_j)}_{\beta,\alpha^\rho_{i_j}}\varphi_j, \varphi_{j'}\right\rangle$$

are small whenever $i_j = i_{j'}$. Indeed, the terms for which $i_j \neq i_{j'}$ vanish for β large enough, since the corresponding cutoff functions become disjointly supported. We write, for convenience, $\chi = \chi^{(i_j)}_\beta$, and $\psi = \psi^{(i_j)}_{\beta,k_j,\alpha^\rho}$, $\psi' = \psi^{(i_{j'})}_{\beta,k_{j'},\alpha^\rho}$, so that $\varphi_j = \chi\psi/Z$, $\varphi_{j'} = \chi\psi'/Z'$, where Z, Z' are normalizing constants ensuring that the quasimodes have unit $L^2(\Omega_\beta)$-norm, and again $H^{(i_j)}_{\beta,\alpha^\rho_{i_j}} = H$, so that we may write:

$$\begin{aligned}\langle H\chi\varphi, \chi\varphi'\rangle &= \langle H\psi, \psi'\rangle - \langle H\psi, (1-\chi)\psi'\rangle - \langle H(1-\chi)\psi, \psi'\rangle + \langle H(1-\chi)\psi, (1-\chi)\psi'\rangle \\ &= 0 + \mathrm{o}(\beta)\|\psi\|\|\psi'\|,\end{aligned}$$

using again Cauchy–Schwarz inequalities and the estimates (56), (58), as well as the orthogonality $\langle\psi, \psi'\rangle = 0$. It follows, noting in view of (57) that $Z, Z' = 1 + \mathrm{o}(\beta)$:

$$\langle H_\beta u, u\rangle \leq (\beta\lambda^{\mathrm{H}}_{k,\alpha^\rho} + \mathrm{o}(\beta))\|u\|^2, \quad \forall\, u \in \mathrm{Span}\{\varphi_j\}_{1\leq j\leq k},$$

which concludes the upper bound.

Step 2: Lower bound. We show the lower bound in (21). As in the proof of the upper bound, we proceed in two steps. The first step is to construct an appropriate extension of the domain Ω_β, which will be defined using a local positive perturbation of the signed distance function σ_{Ω_β} around critical points which are close to the boundary. The second is similar (once the previous constructions have been performed) to the proofs of [6, 4] in the boundaryless case, and we include it for completeness.

Step 2a: Perturbation of the domain.
Our analysis requires to consider, in addition to perturbed harmonic eigenvalues, a perturbed domain Ω^ρ_β which contains Ω_β, parametrized by some small $\rho > 0$. We will construct Ω^ρ_β to be smooth and bounded, so that H_β, defined as the Friedrichs extension of the semi-bounded quadratic form Q_β on the domain $\mathcal{C}^\infty_c(\Omega^\rho_\beta)$, is self-adjoint with compact resolvent, with form domain $H^1_0(\Omega^\rho_\beta)$. Thus, we denote $\widetilde{\lambda}^\rho_{\beta,k}$ its k-th eigenvalue which is positive with finite multiplicity. By the Courant–Fischer principle, the inclusion of form domains $H^1_0(\Omega_\beta) \subset H^1_0(\Omega^\rho_\beta)$ implies, for all $k \geq 1$, the inequality $\lambda_{\beta,k} \geq \widetilde{\lambda}^\rho_{\beta,k}$, which we will exploit for a usable lower bound. The key requirement we aim to satisfy in constructing Ω^ρ_β is that the following property holds for each $i = 0, \ldots, m+r$:

$$B\left(z_i, \frac{1}{2}\delta^{(i)}(\beta)\right) \cap \Omega^\rho_\beta = B\left(z_i, \frac{1}{2}\delta^{(i)}(\beta)\right) \cap \left[z_i + E^{(i)}\left(\frac{\alpha^{(i)} + \rho}{\sqrt{\beta}}\right)\right]. \tag{65}$$

Note that this condition is void in the case where z_i is far from the boundary, in the sense that Ω_β trivially satisfies it, and in the case where z_i is close to the boundary, corresponds to the requirement that, locally around z_i, Ω_β^ρ coincides exactly with a hyperspherical cap.

Since Ω_β may be viewed as the positive superlevel set of the signed distance function:

$$\Omega_\beta = \sigma_{\Omega_\beta}^{-1}(0,+\infty),$$

our aim is realize the perturbed domain Ω_β^ρ as the positive superlevel set of a local perturbation of σ_{Ω_β} around each z_i close to the boundary. To this effect, we define, for $x \in \mathbb{R}^d$, and i such that z_i is close to the boundary:

$$h_\beta^{(i),\rho}(x) = \frac{\alpha^{(i)}+\rho}{\sqrt{\beta}} - (x-z_i)^\intercal v_1^{(i)},$$

the signed distance of x to the boundary hyperplane of $E^{(i)}\left(\frac{\alpha^{(i)}+\rho}{\sqrt{\beta}}\right)$, and take:

$$f_\beta^\rho(x) = \sigma_{\Omega_\beta}(x) + \sum_{\substack{i=0,\dots,m+r\\ \alpha_i<+\infty}} \chi_\beta^{(i)}(x)\left(h_\beta^{(i),\rho}(x) - \sigma_{\Omega_\beta}(x)\right), \tag{66}$$

recalling the definition (53). Thus, f_β^ρ is constructed to coincide precisely with $h_\beta^{(i),\rho}$ in the neighborhood of each z_i.

By construction, f_β^ρ

We then define the perturbed domain as the superlevel set:

$$\Omega_\beta^\rho = \{x \in \mathbb{R}^d : f_\beta^\rho(x) > 0\}.$$

By Assumption (**H1**), there exists $\beta_0 > 0$ such that for all $\beta > \beta_0$,

$$B(z_i,\delta^{(i)}) \cap \Omega_\beta \subseteq \mathcal{O}_i^+(\beta) \subseteq B\left(z_i,\delta^{(i)}(\beta)\right) \cap \left[z_i + E^{(i)}\left(\frac{\alpha^{(i)}+\rho}{\sqrt{\beta}}\right)\right].$$

It follows that for all x in $B(z_i,\delta^{(i)}(\beta)) \cap \Omega_\beta$, $\sigma_{\Omega_\beta}(x) < h_\beta^{(i),\rho}$, and since $\chi_\beta^{(i)}$ is supported in $B(z_i,\delta^{(i)})$, $f_\beta^\rho \geq \sigma_{\Omega_\beta}$, thus $\Omega_\beta \subseteq \Omega_\beta^\rho$. Furthermore, since the $\chi_\beta^{(i)}$ have disjoint support for β large enough, and $\chi_\beta^{(i)} \equiv 1$ on $B\left(z_i, \frac{1}{2}\delta^{(i)}(\beta)\right)$, it follows that Ω_β^ρ coincides locally with the superlevel set of $h_\beta^{(i),\rho}$, that is, Equation (65) holds.

Pour pouvoir faire Courant-Fischer ad infinitum, on veut compacité de la resolvante, donc Ω_β^ρ de bord Lipschitzien -¿ argument avec Sard

Dessin!

Step 2b: Energy lower bound.

Throughout the remainder of this proof, α^ρ will denote the vector $(\alpha_i + \rho\mathbb{1}_{\alpha_i<+\infty})_{0\leq i\leq m+r}$, and $\varphi_j, 1 \leq j \leq k-1$ will denote $k-1$ harmonic quasimodes, associated with the Dirichlet harmonic approximation $H_{\beta,\alpha^\rho}^{\mathrm{H}}$. However, due to the construction performed in the previous step, one must slightly adjust the definition (51). We set:

$$\varphi_j = \frac{\eta_\beta^{(i)}\psi_{\beta,k_j,\alpha_{i_j}^\rho}^{(i_j)}}{\|\eta_\beta^{(i)}\psi_{\beta,k_j,\alpha_{i_j}^\rho}^{(i_j)}\|}\, 1 \leq j \leq k-1,$$

where $\eta_\beta^{(i)}(x) = \chi_\beta^{(i)}(2x)$. By construction, each φ_j is supported in $B(z_i, \frac{1}{2}\delta^{(i)}(\beta))$, and thus belongs to $H_0^1(\Omega_\beta^\rho)$, by the inclusion (65). We note that this choice of quasimodes amount to rescaling $\delta^{(i)}$ for each i by a factor $\frac{1}{2}$, and in particular has no bearing on any of the estimates in Lemmas 2 and 3, which we will use freely throughout the remainder of the proof upon replacing $\chi_\beta^{(i)}$ by $\eta_\beta^{(i)}$.

As before, the φ_j span a $(k-1)$-dimensional subspace of $L^2(\Omega_\beta^\rho)$, the proof is identical to the one given in step 1b. Once again, we rely on the Courant–Fischer principle, in its Max-Min form: it suffices to show that, for any $u \in H_0^1(\Omega_\beta^\rho) \cap \mathrm{Span}(\varphi_j, 1 \leq j \leq k-1)^\perp$, the following inequality holds:

$$Q_\beta(u) \geq (\beta \lambda_{k,\alpha^\rho}^{\mathrm{H}} + \mathrm{o}(\beta))\|u\|^2.$$

Since the φ_j are linearly independent for β large enough, as shown above, this implies:

$$\varliminf_{\beta\to\infty} \beta^{-1}\lambda_{\beta,k} \geq \varliminf_{\beta\to\infty} \beta^{-1}\lambda_{\beta,k}^\rho \geq \lambda_{k,\alpha^\rho}^{\mathrm{H}},$$

and the desired lower bound will follow by taking the limit $\rho \to 0$. Hence, let $u \in H_0^1(\Omega_\beta^\rho)$ be orthogonal to φ_j for every $1 \leq j \leq k-1$. The IMS formula gives:

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

where we denote $\eta_\beta^{(m+r+1)} = \sqrt{\mathbb{1}_{\Omega_\beta^\rho} - \sum_{i=0}^{m+r} \eta_\beta^{(i)2}}$. We first estimate, for $0 \leq i \leq m+r$, the terms

$$Q_\beta(\eta_\beta^{(i)} u) - \langle H_\beta^{(i)} \eta_\beta^{(i)} u, \eta_\beta^{(i)} \rangle = \langle (H_\beta - H_\beta^{(i)}) \eta_\beta^{(i)} u, \eta_\beta^{(i)} u \rangle = \mathrm{o}(\beta)\|u\|^2, \tag{67}$$

using Lemma 3. On the other hand, the assumption that u is $L^2(\Omega_\beta^\rho)$-orthogonal to the φ_j for $1 \leq j \leq k-1$ implies, for all $0 \leq i \leq m+r$ and all $j \in \{1 \leq l \leq k-1 : i_l = i\}$, that $\eta_\beta^{(i)} u$ is $L^2\left[z_i + E^{(i)}\left(\frac{\alpha^{(i)}+\rho}{\sqrt{\beta}}\right)\right]$-orthogonal to $\psi_{\beta,k_j,\alpha_i^\rho}^{(i)}$. Furthermore, $\eta_\beta^{(i)} u$ is by construction in the form domain of the self-adjoint operator $H_{\beta,\alpha_i^\rho}^{(i)}$, and thus the Courant–Fischer principle implies:

$$\left\langle H_{\beta,\alpha_i^\rho}^{(i)} \eta_\beta^{(i)} u, \eta_\beta^{(i)} u \right\rangle \geq \beta \lambda_{N_i(k-1)+1,\alpha_i^\rho}^{(i)} \|\eta_\beta^{(i)} u\|^2 \geq \beta \lambda_{k,\alpha^\rho}^{\mathrm{H}} \|\eta_\beta^{(i)} u\|^2, \tag{68}$$

where we use the identity (49).

Furthermore, the L^∞ bound (55) implies that $\||\nabla \eta_\beta^{(i)}| u\|^2 = \mathrm{o}(\beta)\|u\|^2$.

We are left with the terms

$$\left\langle H_\beta \eta_\beta^{(m+1)} u, \eta_\beta^{(m+1)} u \right\rangle - \||\nabla \eta_\beta^{(m+1)}| u\|^2.$$

Note that, since

$$A_\beta = \mathrm{supp}\, \eta_\beta^{(m+1)} \subset \mathbb{R}^d \setminus \bigcup_{i=0}^m B\left(z_i, \frac{1}{2}\delta^{(i)}(\beta)\right),$$

and because V is a C^∞ Morse function in Ω_β^ρ, there exists $c, d, \beta_0 > 0$ such that, for all $\beta > \beta_0$,

$$|\nabla V|^2|_{A_\beta} \geq c\delta^{(i)}(\beta)^2, \quad |\Delta V||_{A_\beta} \leq d,$$

whence:

$$U_\beta = \frac{\beta^2}{4}|\nabla V|^2 - \frac{\beta}{2}\Delta V \geq \frac{c\beta^2\delta^{(i)}(\beta)^2}{4} - \beta d.$$

Using a simple ground state estimate shows that, for $\beta > \beta_0$ and any v in the form domain of H_β on A_β:

$$\langle H_\beta v, v \rangle_{L^2(A_\beta)} \geq \langle U_\beta v, v \rangle \geq \beta\left(\frac{c\beta\delta^{(i)}(\beta)^2}{4} - d\right)\|v\|^2.$$

Since $\sqrt{\beta}\delta^{(i)}(\beta) \overset{\beta\to\infty}{\longrightarrow} +\infty$, we conclude that for β large enough, and since $\eta_\beta^{(m+1)} u$ is in $H_0^1(A_\beta)$ with compact support, we have:

$$\langle H_\beta \eta_\beta^{(m+1)} u, \eta_\beta^{(m+1)} u \rangle \geq \beta \lambda_{k,\alpha^\rho}^{\mathrm{H}} \|\eta_\beta^{(m+1)} u\|^2.$$

Finally, we note that, owing to the condition (52), and the fact that the $\eta_\beta^{(i)}$ have disjoint support for $i = 0, \cdots, m+r$, it also holds:

$$\||\nabla \eta_\beta^{(m+r+1)} u\|^2 = \mathrm{o}(\beta)\|u\|^2,$$

and so we have shown:

$$\langle H_\beta u, u\rangle \geq \beta \lambda^{\mathrm{H}}_{k,\alpha^\rho} \sum_{i=0}^{m+r+1} \|\eta_\beta^{(i)} u\|^2 + \mathrm{o}(\beta)\|u\|^2. \tag{69}$$

The lower bound follows easily since the $\eta_\beta^{(i)}$ for a quadratic partition of unity:

$$\|u\|^2 = \sum_{i=0}^{m+r+1} \|\eta_\beta^{(i)} u\|^2,$$

which implies

$$\varliminf_{\beta\to\infty} \beta^{-1}\lambda_{\beta,k} \geq \lambda^{\mathrm{H}}_{k,\alpha^\rho},$$

and the proof of Theorem 1 is completed upon taking the limit $\rho \to 0$.

□

Remark 1.

Remark 2.

4 An Eyring–Kramers formula for $\lambda_{1,\beta}$.

We dedicate this section to the derivation of finer asymptotics for the first Dirichlet eigenvalue of $-\mathcal{L}_\beta$, $\lambda_{\beta,1}$ in the regime $\beta \to \infty$. More precisely, we aim to show the following Eyring–Kramers type formula for $\lambda_{1,\beta}$, which generalizes well-known formulæ in the presence of saddle points which are close to the boundary:

Theorem 2. *Assume [Single well assumption + scaling constraints ...].*
Then the following asymptotic equivalent holds:

$$\lambda_{1,\beta} \overset{\beta\to+\infty}{\sim} \frac{1}{2\pi} \sum_{i\in I_{\min}} \frac{|\nu_1^{(i)}|}{\Phi\left(|\nu_1^{(i)}|^{\frac{1}{2}}\alpha^{(i)}\right)} \sqrt{\frac{\det\,\nabla^2 V(z_0)}{|\det\,\nabla^2 V(z_i)|}} \mathrm{e}^{-\beta(V(z_i)-V(z_0))}, \tag{70}$$

where Φ denotes the standard normal cumulative distribution function, and

$$I_{\min} = \operatorname*{Argmin}_{i=1,\dots,m} V(z_i) \tag{71}$$

is the set of indices correspondint to the order-one saddle points of lowest energy.

The proof of (70) on the construction of an accurate approximation of the first Dirichlet eigenvector for $-\mathcal{L}_\beta$, which is closely related to the one performed in [5], in the special case of saddle points lying on the boundary of a static domain. More precisely a local ansatz is defined in the neighborhood of each of the low-energy saddle points of V, and it is then extended to an element of $H^1_{0,\mu}(\Omega_\beta)$, the form domain of $-\mathcal{L}_\beta$.

4.1 Geometric assumptions

4.2 Construction of a precise quasimode

Let us fix a parameter $\rho > 0$, and let $i \in \{1, \dots, m\}$. It is convenient to introduce the following neihborhoods, which are similarly defined similarly to the capped balls (18) described in Section 2.1, but in some other norm whose balls are rotated cuboids:

$$\mathcal{R}_i(\beta) = z_i + U^{(i)} \left[\left(-\infty, \frac{\alpha^{(i)}}{\sqrt{\beta}} - \gamma^{(i)}(\beta) \right) \cap \left(-C_d \delta^{(i)}(\beta), C_d \delta^{(i)}(\beta) \right)^d \right] \tag{72}$$

where $C_d > 0$ is a constant depending only on the dimension ensuring that $\mathcal{R}_i(\beta) \subseteq \mathcal{O}_i^-(\beta)$ whenever **H1** is satisfied.

We then define the following function:

$$\varphi_\beta^{(i)}(x) = \frac{\displaystyle\int_{(x-z_i)^\intercal v_1^{(i)}}^{+\infty} \mathrm{e}^{-\beta \frac{|\nu_1^{(i)}|}{2} t^2} \xi_\beta^{(i)}(t)\, \mathrm{d}t}{\displaystyle\int_{-\infty}^{+\infty} \mathrm{e}^{-\beta \frac{|\nu_1^{(i)}|}{2} t^2} \xi_\beta^{(i)}(t)\, \mathrm{d}t}, \tag{73}$$

Motivation:, avec un potentiel en selle de cheval: $\frac{1}{2}(x_2^2 - x_1^2)$, $-\mathcal{L}_\beta \varphi_\beta = 0$ (localement au voisinage de 0)

where $\xi_\beta^{(i)} : \mathbb{R} \to \mathbb{R}$ is a $\mathcal{C}_c^\infty$ cutoff function chosen such that:

$$\operatorname{supp} \xi_\beta^{(i)} \subset \left(-\infty, \frac{\alpha^{(i)}}{\sqrt{\beta}} - \gamma^{(i)}(\beta) \right) \cap \left(-C_d \delta^{(i)}(\beta), C_d \delta^{(i)}(\beta) \right), \tag{74}$$

$$\xi_\beta^{(i)} \equiv 1 \text{ in } \left(-\infty, \frac{\alpha^{(i)}}{\sqrt{\beta}} - 2\gamma^{(i)}(\beta) \right) \cap \left(\frac{-C_d}{2} \delta^{(i)}(\beta), \frac{C_d}{2} \delta^{(i)}(\beta) \right). \tag{75}$$

$$\psi_\beta = \frac{1}{Z_\beta} \left[\eta_\beta + \sum_{i \in I_{\min}} \varphi_\beta^{(i)} \chi_\beta^{(i)} \right], \tag{76}$$

where Z_β is a normalizing constant imposing $\|\psi_\beta\|_{L^2_\mu(\Omega_\beta)} = 1$.

4.3

Proposition 1 (Critical Laplace asymptotics)**.** *For $i = 1, \dots, m$, the following hold:*

$$Z_\beta = \mathrm{e}^{-\frac{\beta}{2} V(z_0)} \left(\frac{2\pi}{\beta} \right)^{\frac{d}{4}} |\det \nabla^2 V(z_0)|^{-\frac{1}{4}} \left(1 + \mathcal{O}()\right). \tag{77}$$

$$\||\nabla \psi_\beta|\|^2_{L^2_\mu(\mathcal{R}_i(\beta))} = \frac{|\nu_1^{(i)}|}{2\pi \Phi\left(|\nu_1^{(i)}|^{\frac{1}{2}} \alpha^{(i)} \right)} \sqrt{\frac{\det \nabla^2 V(z_0)}{|\det \nabla^2 V(z_i)|}} \mathrm{e}^{-\beta(V(z_i) - V(z_0))} \left(1 + \mathcal{O}()\right), \tag{78}$$

$$\|\mathcal{L}_\beta \psi_\beta\|^2_{L^2_\mu(\mathcal{R}_i(\beta))} = \mathcal{O}() \, \||\nabla \psi_\beta|\|^2_{L^2_\mu(\mathcal{R}_i(\beta))} \tag{79}$$

There exists $c > 0$ and β_0 such that for all $\beta > \beta_0$:

$$\||\nabla \psi_\beta|\|^2_{L^2_\mu(\Omega_\beta \setminus \bigcup_{i \in I_{\min}} \mathcal{R}_i(\beta))} = \mathcal{O}\left(\frac{1}{\delta^{(i)}(\beta)^2} \mathrm{e}^{-\beta(V(z_i) - V(z_0) + c\delta^{(i)}(\beta)^2)} \right) \tag{80}$$

Proof. The usual Laplace method yields (77).

à préciser

Let us fix $i = 1, \dots, m$, and for convenience, we use a set of coordinates adapted to the Hessian of V at z_i:

$$y = U^{(i)\intercal}(x - z_i),$$

which ensures, that, on $B(z_i, \delta^{(i)}(\beta))$, we have, in the y coordinates:

$$V(y) = \left[\frac{1}{2}\sum_{j=1}^{d} \nu_j^{(i)} y_j^2\right] \left(1 + \mathcal{O}(\delta^{(i)}(\beta))\right). \tag{81}$$

Besides, since:

$$\int_{-\infty}^{\frac{\alpha^{(i)}}{\sqrt{\beta}} - 2\gamma^{(i)}(\beta)} \mathrm{e}^{-\beta\frac{|\nu_1^{(i)}|}{2}t^2}\,\mathrm{d}t \le \int_{-\infty}^{\infty} \mathrm{e}^{-\beta\frac{|\nu_1^{(i)}|}{2}t^2}\xi_\beta^{(i)}(t)\,\mathrm{d}t \le \int_{-\infty}^{\frac{\alpha^{(i)}}{\sqrt{\beta}} - \gamma^{(i)}(\beta)} \mathrm{e}^{-\beta\frac{|\nu_1^{(i)}|}{2}t^2}\,\mathrm{d}t, \tag{82}$$

we get, using the one-dimensional case of Lemma 8 and Assumption (**H3**), that:

$$C_\beta = \int_{-\infty}^{\infty} \mathrm{e}^{-\beta\frac{|\nu_1^{(i)}|}{2}t^2}\xi_\beta^{(i)}(t)\,\mathrm{d}t = \sqrt{\frac{2\pi}{\beta|\nu_1^{(i)}|}}\Phi(|\nu_1^{(i)}|\alpha^{(i)})\left(1 + \mathcal{O}()\right). \tag{83}$$

Furthermore, we may write in the y-coordinates:

$$\nabla\varphi_\beta^{(i)}(y) = -C_\beta^{-1}\mathrm{e}^{-\frac{\beta}{2}|\nu_1^{(i)}|y_1^2}\xi_\beta^{(i)}(y_1)v_1^{(i)},$$

whence

$$|\nabla\varphi_\beta^{(i)}|^2\mathrm{e}^{-\beta V}(y) = C_\beta^{-2}\mathrm{e}^{-\beta\left(|\nu_1^{(i)}|y_1^2 + V(y)\right)}\xi_\beta^{(i)}(y_1)^2.$$

The estimation (81) implies that $W(y) = |\nu_1^{(i)}|y_1^2 + V(y)$ has a strict minimum at $y = 0$, with $\nabla_y^2 W(0) = \mathrm{diag}\left(|\nu_1^{(i)}|, \dots, \nu_d^{(i)}\right)$, and this minimum is unique in $\mathcal{R}_i(\beta)$.

Hence, using identical bounds on $\xi_\beta^{(i)\,2}$ as the ones leading to (82), we get, by the d-dimensional case of Lemma 8 and the convergence of $\sqrt{\beta}\mathcal{R}_i(\beta)$ to the half-space $E^{(i)}(\alpha^{(i)})$ under Assumption (**H3**), by going back to x coordinates:

$$\||\nabla\psi_\beta|\|^2_{L^2_\mu(\mathcal{R}_i(\beta))} = Z_\beta^{-2}C_\beta^{-2}\mathrm{e}^{-\beta V(z_i)}\left(\frac{2\pi}{\beta}\right)^{\frac{d}{2}}|\det\nabla^2 W(z_i)|^{-\frac{1}{2}}\mathbb{P}(\xi \in E^{(i)}(\alpha^{(i)}))(1 + \mathcal{O}()),$$

where $\xi \sim \mathcal{N}(0, \nabla^2 W(z_i)^{-1})$. We then note:

$$\mathbb{P}(\xi \in E^{(i)}(\alpha^{(i)})) = \Phi(|\nu_1^{(i)}|\alpha^{(i)}),$$

$$|\det\nabla^2 W(z_i)| = |\det\nabla^2 V(z_i)|,$$

and combine the asymptotic equivalents (77), (83) to obtain (78).

To show (79), we write, for all $x \in \mathcal{R}_i$, in the y-coordinates:

$$\begin{aligned}
\mathcal{L}_\beta\psi_\beta(y) &= \frac{1}{C_\beta Z_\beta}\left(-\nabla V\cdot\nabla\varphi_\beta^{(i)} + \frac{1}{\beta}\Delta\varphi_\beta^{(i)}\right)(y) \\
&= \frac{1}{Z_\beta C_\beta}\left(\frac{\partial V}{\partial y_1}(y)\xi_\beta^{(i)}(y_1) + \left[\frac{\xi_\beta^{(i)\prime}(y_1)}{\beta} - |\nu_1^{(i)}|y_1\xi_\beta^{(i)}(y_1)\right]\right)\mathrm{e}^{-\beta\frac{|\nu_1^{(i)}|}{2}y_1^2} \\
&= \frac{1}{Z_\beta C_\beta}\left(\mathcal{O}(|y|) + \mathcal{O}\left(\beta^{-1}\|\xi_\beta^{(i)\prime}\|_\infty\right)\right)\mathrm{e}^{-\beta\frac{|\nu_1^{(i)}|}{2}y_1^2},
\end{aligned}$$

using a first-order Taylor expansion of $\frac{\partial V}{\partial y_1}$ around $y = 0$ in the last line. Now, estimating the $L^2_\mu(\mathcal{R}_i(\beta))$-norm yields, using $|y| = \mathcal{O}\left(\delta^{(i)}(\beta)\right)$ in $\mathcal{R}_i$, $\|\xi_\beta^{(i)\prime}\|_\infty = \mathcal{O}(1/\gamma^{(i)}(\beta))$:

$$\begin{aligned}\|\mathcal{L}_\beta\psi_\beta\|^2_{L^2_\mu(\mathcal{R}_i(\beta))} &= \frac{1}{Z_\beta C_\beta}\mathcal{O}\left(\delta^{(i)}(\beta)^2 \vee \beta^{-2}\gamma^{(i)}(\beta)^{-2}\right)\int_{y^{-1}(\mathcal{R}_i(\beta))} \mathrm{e}^{-\beta|\nu_1^{(i)}|y_1^2}\mathrm{e}^{-\beta V(y)}\,\mathrm{d}y \\ &= \mathcal{O}\left(\delta^{(i)}(\beta)^2 \vee \beta^{-2}\gamma^{(i)}(\beta)^{-2}\right)\||\nabla\psi_\beta|\|^2_{L^2_\mu(\mathcal{R}_i(\beta))}\end{aligned}$$

Construire η_β tq le support de $\nabla\eta_\beta$ se concentre sur une zone de haute énergie (hypothèse nécessaire sur le domaine)

$\square$

Lemma 4 (Resolvent estimate)**.** *Let $u \in H^1_{0,\mu}(\Omega_\beta) \cap H^2_\mu(\Omega_\beta) = \mathcal{D}(\mathcal{L}_\beta)$. Then the following holds:*

$$\|(1-\pi_{\lambda_{1,\beta}})u\|_{L^2_\mu(\Omega_\beta)} = \mathcal{O}(\|\mathcal{L}_\beta u\|_{L^2_\mu(\Omega_\beta)}). \tag{84}$$

$$\left\||\nabla\pi_{\lambda_{1,\beta}}u|\right\|^2_{L^2_\mu(\Omega_\beta)} = \||\nabla u|\|^2_{L^2_\mu(\Omega_\beta)} + \mathcal{O}\left(\|\mathcal{L}_\beta u\|^2_{L^2_\mu(\Omega_\beta)}\right). \tag{85}$$

Proof. The estimates (84) and (85) are standard in the semiclassical analysis of the Witten Laplacian, see for instance [5, Proposition 27]. We include its proof (in the equivalent weighted L^2 setting) for the sake of completeness. Since $\lambda_2^{\mathrm{H}} > 0$ by Assumption (one-well, minimum far from boundary), Theorem 1 implies that there exists $r, \beta_0 > 0$ such that for all $\beta > \beta_0$:

$$|\lambda_{1,\beta}| < r, \quad \lambda_{2,\beta} > 3r,$$

so that the circular contour $\Gamma_{2r} = \{2r\mathrm{e}^{2i\pi t}, 0 \le t \le 1\}$ is at distance at least r from $\sigma(-\mathcal{L}_\beta)$. A standard corollary of the spectral theorem yields the following uniform resolvent estimate:

$$\|(-\mathcal{L}_\beta - z)^{-1}\|_{L^\infty\left(\Gamma_{2r};\mathcal{B}(L^2_\mu(\Omega_\beta))\right)} \le \frac{1}{r}.$$

Furthermore, the spectral projector $\pi_{\lambda_{1,\beta}}$ onto $\ker(-\mathcal{L}_\beta - \lambda_{1,\beta})$ may be expressed using the following contour integral:

$$\frac{1}{2i\pi}\oint_{\Gamma_{2r}} (\mathcal{L}_\beta + z)^{-1}\,\mathrm{d}z, \tag{86}$$

whereby, using the residue theorem once again:

$$\begin{aligned}(1-\pi_{\lambda_{1,\beta}})u &= \frac{1}{2i\pi}\oint_{\Gamma_{2r}}\left[z^{-1} - (\mathcal{L}_\beta + z)^{-1}\right]u\,\mathrm{d}z \\ &= \left(\frac{1}{2i\pi}\oint_{\Gamma_{2r}} z^{-1}(\mathcal{L}_\beta + z)^{-1}\,\mathrm{d}z\right)\mathcal{L}_\beta u.\end{aligned}$$

Estimating the L^2_μ norm then yields (84):

$$\|(1-\pi_{\lambda_{1,\beta}})u\|_{L^2_\mu(\Omega_\beta)} \le \frac{1}{r}\|\mathcal{L}_\beta u\|_{L^2_\mu(\Omega_\beta)}.$$

For (85), we use the commutativity $\pi_{\lambda_{1,\beta}}\mathcal{L}_\beta\pi_{\lambda_{1,\beta}} = \pi_{\lambda_{1,\beta}}\mathcal{L}_\beta$ to write:

$$\begin{aligned}\left\||\nabla\pi_{\lambda_{\beta,1}}u|\right\|^2_{L^2_\mu(\Omega_\beta)} &= \left\langle \pi_{\lambda_{\beta,1}}u, \mathcal{L}_\beta\pi_{\lambda_{\beta,1}}u\right\rangle_{L^2_\mu(\Omega_\beta)} \\ &= \left\langle \pi_{\lambda_{\beta,1}}u, \mathcal{L}_\beta u\right\rangle_{L^2_\mu(\Omega_\beta)} \\ &= \langle u, \mathcal{L}_\beta u\rangle_{L^2_\mu(\Omega_\beta)} + \left\langle(\pi_{\lambda_{\beta,1}} - 1)u, \mathcal{L}_\beta u\right\rangle_{L^2_\mu(\Omega_\beta)} \\ &= \||\nabla u|\|^2_{L^2_\mu(\Omega_\beta)} + \mathcal{O}(\|\mathcal{L}_\beta u\|^2_{L^2_\mu(\Omega_\beta)}),\end{aligned}$$

where we used a Cauchy–Schwarz inequality and (84) to obtain the last equality. $\square$

We are now in a position to prove the critical Eyring–Kramers formula.

Proof of Theorem 2. We write, using (85):

$$
\begin{aligned}
\lambda_{1,\beta} &= \frac{\big\||\nabla \pi_{\lambda_{1,\beta}}\psi_\beta|\big\|^2_{L^2_\mu(\Omega_\beta)}}{\|\pi_{\lambda_{1,\beta}}\psi_\beta\|^2_{L^2_\mu(\Omega_\beta)}} \\
&= \frac{\||\nabla\psi_\beta|\|^2_{L^2_\mu(\Omega_\beta)} + \mathcal{O}(\|\mathcal{L}_\beta\psi_\beta\|^2_{L^2_\mu(\Omega_\beta)})}{\|\psi_\beta - (1-\pi_{\lambda_{1,\beta}})\psi_\beta\|^2_{L^2_\mu(\Omega_\beta)}} \\
&= \frac{\||\nabla\psi_\beta|\|^2_{L^2_\mu(\Omega_\beta)} + \mathcal{O}(\|\mathcal{L}_\beta\psi_\beta\|^2_{L^2_\mu(\Omega_\beta)})}{1 + \|(1-\pi_{\lambda_{\beta,1}})\psi_\beta\|^2_{L^2_\mu(\Omega_\beta)} - 2\left\langle (1-\pi_{\lambda_{\beta,1}})\psi_\beta, \psi_\beta\right\rangle_{L^2_\mu(\Omega_\beta)}} \\
&= \frac{\||\nabla\psi_\beta|\|^2_{L^2_\mu(\Omega_\beta)} + \mathcal{O}(\|\mathcal{L}_\beta\psi_\beta\|^2_{L^2_\mu(\Omega_\beta)})}{1 + \mathcal{O}(\|\mathcal{L}_\beta\psi_\beta\|_{L^2_\mu(\Omega)})}
\end{aligned}
$$

We estimate the denominator, using a Cauchy–Schwarz inequality and $\|\psi_\beta\|_{L^2_\mu(\Omega_\beta)} = 1$:

$$
\begin{aligned}
\|\psi_\beta - (1-\pi_{\lambda_{1,\beta}})\psi_\beta\|^2_{L^2_\mu(\Omega_\beta)} &= 1 + \mathcal{O}(\|(1-\pi_{\lambda_{1,\beta}})\psi_\beta\|^2_{L^2_\mu(\Omega_\beta)}) + \mathcal{O}(\|(1-\pi_{\lambda_{1,\beta}})\psi_\beta\|_{L^2_\mu(\Omega_\beta)}) \\
&= 1 + \mathcal{O}(\|(1-\pi_{\lambda_{1,\beta}})\psi_\beta\|_{L^2_\mu(\Omega_\beta)}) \\
&= 1 + \mathcal{O}(\|\mathcal{L}_\beta\psi_\beta\|_{L^2_\mu(\Omega_\beta)}) \\
&= 1 + \mathcal{O}()\|\|
\end{aligned}
$$

□

5 Application to domain optimization

In this Section, we describe how to use the analysis performed in Sections 3 and 4

6 Tools

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 $0 \le \lambda_1(D_i) \le \lambda_2(D_i) \le \dots$ the sequence of ordered eigenvalues (counted with multiplicity) below the essential spectrum for the realization of A on D_i.*

Then, $\lambda_k(D_1) \ge \lambda_k(D_2)$ 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 $H_0^1 \cap H^2(\Omega) \subset L^2(\Omega)$. Then the following identity holds:

$$H = \sum_{i=1}^{m} \chi_i H \chi_i - \sum_{i=1}^{m} |\nabla \chi_i|^2. \tag{87}$$

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

$$Q(u) = \sum_{i=1}^{m} Q(\chi_i u) - \||\nabla \chi_i| u\|^2. \tag{88}$$

Proof. We compute the following commutator in two ways:

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

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 $\varphi \in \mathcal{C}_c^\infty(\Omega)$,

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

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

$$\|(z - P)^{-1}\|_{\mathcal{B}(\mathcal{H})} = \mathrm{d}(z, \sigma(P))^{-1} \tag{89}$$

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

$$\|(P - \mu)u\| \le \varepsilon \implies \exists \lambda \in \sigma(P),\ |\mu - \lambda| \le \varepsilon. \tag{90}$$

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

$$\|u-\pi_\lambda u\| \leq \frac{2\varepsilon}{\delta}, \tag{91}$$

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

$$\|\pi_{[b,+\infty)}u\|^2 \leq \frac{Q(u)}{b}. \tag{92}$$

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 $\sigma(P_\lambda)=\sigma(P)\backslash\{\lambda\}$, 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:

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

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:

$$\|\pi_{[b,+\infty)}u\|^2=\mathbb{P}(U\geq b)\leq\frac{\mathbb{E}[U]}{b}=\frac{1}{b}\int_0^\infty\langle\lambda\,\mathrm{d}\pi_\lambda u,u\rangle=\frac{1}{b}\langle Pu,u\rangle=\frac{Q(u)}{b}. \tag{93}$$

□

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:

$$I_\lambda \overset{\lambda \to \infty}{\sim} \mathrm{e}^{-\lambda f(x_0)} g(x_0) \left(\frac{2\pi}{\lambda}\right)^{\frac{d}{2}} \left|\det \nabla^2 f(x_0)\right|^{-\frac{1}{2}} \mathbb{P}\left(\xi \in A_\infty\right), \quad \xi \sim \mathcal{N}\left(0, \nabla^2 f(x_0)^{-1}\right) \tag{94}$$

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 $|x| < \delta$.

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

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,

$$I_\lambda = \int_{A_\lambda \cap B(0,\delta)} \mathrm{e}^{-\lambda f(x)} g(x) \, \mathrm{d}x + \int_{A_\lambda \setminus B(0,\delta)} \mathrm{e}^{-\lambda f(x)} g(x) \, \mathrm{d}x, \tag{95}$$

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:

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

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

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

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

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

whereby an identical argument yields

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

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

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

□

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