HAL
open science

Small eigenvalues of the Witten Laplacian with Dirichlet boundary conditions: the case with critical points on the boundary

Dorian Le Peutrec, Boris Nectoux

To cite this version:

Dorian Le Peutrec, Boris Nectoux. Small eigenvalues of the Witten Laplacian with Dirichlet boundary conditions: the case with critical points on the boundary. Analysis & PDE, 2021, 14 (8), pp.2595-2651. 10.2140/apde.2021.14.2595 . hal-02185083v2

HAL Id: hal-02185083

https://hal.science/hal-02185083v2

Submitted on 10 Aug 2020

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Small eigenvalues of the Witten Laplacian with Dirichlet boundary conditions: the case with critical points on the boundary

Dorian Le Peutrec* and Boris Nectoux †

Abstract

In this work, we give sharp asymptotic equivalents in the limit $h \to 0$ of the small eigenvalues of the Witten Laplacian, that is the operator associated with the quadratic form

$$\psi \in H_0^1(\Omega) \mapsto h^2 \int_\Omega \left|\nabla\left(e^{\frac{1}{h}f}\psi\right)\right|^2 e^{-\frac{2}{h}f},$$

where $\overline{\Omega} = \Omega \cup \partial\Omega$ is an oriented C^∞ compact and connected Riemannian manifold with non empty boundary $\partial\Omega$ and $f : \overline{\Omega} \to \mathbb{R}$ is a C^∞ Morse function. The function f is allowed to admit critical points on $\partial\Omega$, which is the main novelty of this work in comparison with the existing literature.
Keywords: Witten Laplacian, overdamped Langevin dynamics, semiclassical analysis, metastability, spectral theory, Eyring-Kramers formulas.
MSC 2010: 35P15, 35P20, 47F05, 35Q82.

Contents

1 Introduction **2**
1.1 Setting 2
1.2 Spectral approach of metastability in statistical physics 3
1.3 Motivation and results 4
1.4 Strategy and organization of the paper 8

2 On the number of small eigenvalues of $\Delta_{f,h}^D$ **10**
2.1 Preliminary results 11
2.2 Proof of Theorem 1 12

*Laboratoire de Mathématiques d'Orsay, Univ. Paris-Sud, CNRS, Université Paris-Saclay, 91405 Orsay, France. E-mail: dorian.lepeutrec@math.u-psud.fr

†Institut für Analysis und Scientific Computing, TU Wien, Wiedner Hauptstr. 8, 1040 Wien, Austria. E-mail: boris.nectoux@enpc.fr

3 Study of the characteristic wells of the function f **16**
3.1 Principal wells of f in Ω 16
3.2 Separating saddle points 17
3.2.1 Separating saddle points of f in Ω 17
3.2.2 Separating saddle points of f in $\overline{\Omega}$ 18
3.3 Construction of the maps j and C_{j} 25

4 Quasi-modal construction **29**
4.1 Adapted coordinate systems 30
4.2 Quasi-modal construction near the elements of $\cup_{x\in\mathsf{U}_0}\mathsf{j}(x)$ 33
4.3 Construction of m_0 quasi-modes for $\Delta^D_{f,h}$ 35

5 Asymptotic equivalents of the small eigenvalues of $\Delta^D_{f,h}$ **38**
5.1 First quasi-modal estimates 38
5.2 Linear independence of the quasi-modes 45
5.3 An accurate interaction matrix 50
5.4 Asymptotic behaviour of the small eigenvalues of $\Delta^D_{f,h}$ 53

1 Introduction

1.1 Setting

Let $(\overline{\Omega}, g)$ be an oriented C^∞ compact and connected Riemannian manifold of dimension d with interior Ω and non empty boundary $\partial\Omega$, and let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ function. Let us moreover denote by d the exterior derivative acting on functions on $\overline{\Omega}$ and by d^* its formal adjoint (called the co-differential) acting on 1-forms (which are naturally identified with vector fields). For any $h > 0$, the semiclassical Witten Laplacian acting on functions on $\overline{\Omega}$ is then the Schrödinger operator defined by

$$\Delta_{f,h} \;:=\; d^*_{f,h} d_{f,h} \;=\; h^2\Delta_H + |\nabla f|^2 + h\Delta_H f\,,$$

where $\Delta_H = d^*d$ is the Hodge Laplacian acting on functions, that is the negative of the Laplace–Beltrami operator, and

$$d_{f,h} \;:=\; h\, e^{-\frac{f}{h}} d\, e^{\frac{f}{h}} \quad \text{and} \quad d^*_{f,h} = h\, e^{\frac{f}{h}} d^*\, e^{-\frac{f}{h}}$$

are respectively the distorted exterior derivative and co-differential. This operator was originally introduced by Witten in [42] and acts more generally on the algebra of differential forms. Note also the relation

$$\Delta_{f,h} \;=\; h\, e^{-\frac{V}{2h}} \left(h\Delta_H + \nabla V\cdot\nabla\right) e^{\frac{V}{2h}} \quad \text{where} \quad V = 2f, \tag{1}$$

where the notation $\nabla V\cdot\nabla$ stands for $g(\nabla V, \nabla\cdot)$. It is then equivalent to study the Witten Laplacian $\Delta_{f,h}$ acting in the flat space $L^2(\Omega) = L^2(\Omega, d\mathrm{Vol}_\Omega)$ or the weighted Laplacian

$$L_{V,h} := h\Delta_H + \nabla V\cdot\nabla = d^*_{V,h}\, d$$

acting in the weighted space $L^2(\Omega, e^{-\frac{V}{h}} d\mathrm{Vol}_\Omega)$.

Let us now consider the usual self-adjoint Dirichlet realization $\Delta^D_{f,h}$ of the Witten Laplacian $\Delta_{f,h}$ on the Hilbert space $L^2(\Omega)$. Its domain is given by

$$D\big(\Delta^D_{f,h}\big) = H^2(\Omega) \cap H^1_0(\Omega),$$

where, for $p \in \mathbb{N}^*$, we denote by $H^p(\Omega)$ the usual Sobolev space with order p and by $H^1_0(\Omega)$ the set made of the functions in $H^1(\Omega)$ with vanishing trace on $\partial\Omega$. We refer for instance to [35] for more material about Sobolev spaces on manifolds with boundary. The operator $\Delta^D_{f,h}$ has a compact resolvent, and thus its spectrum $\sigma(\Delta^D_{f,h})$ is discrete. This operator is moreover nonnegative since it satisfies:

$$\forall \psi \in D\big(\Delta^D_{f,h}\big)\,, \quad \langle \Delta^D_{f,h}\psi, \psi\rangle_{L^2(\Omega)} \;=\; \|d_{f,h}\psi\|^2_{\Lambda^1 L^2(\Omega)} \;=\; h^2 \int_\Omega |d(e^{\frac{f}{h}}\psi)|^2 e^{-\frac{2f}{h}}\,, \quad (2)$$

where $\Lambda^1 L^2(\Omega)$ denotes the space of 1-forms in $L^2(\Omega)$ and $\|d_{f,h}\psi\|^2_{\Lambda^1 L^2(\Omega)} = \int_\Omega |d_{f,h}\psi|^2$. Let us also mention here that the (closed) quadratic form $Q_{f,h}$ associated with $\Delta^D_{f,h}$ has domain $H^1_0(\Omega)$ and satisfies, for every $\psi \in H^1_0(\Omega)$,

$$Q_{f,h}(\psi) := Q_{f,h}(\psi,\psi) = \|d_{f,h}\psi\|^2_{\Lambda^1 L^2(\Omega)} = h^2 \int_\Omega |d\psi|^2 + \int_\Omega \big(|\nabla f|^2 + h\Delta_H f\big)\,|\psi|^2\,. \quad (3)$$

Remark 1. *From standard results on elliptic operators, the principal eigenvalue of $\Delta^D_{f,h}$, which is positive since $e^{-\frac{f}{h}} \notin H^1_0(\Omega)$ (see (2)), is moreover non degenerate and any associated eigenfunction has a sign on Ω (see for example [12, 15]).*

1.2 Spectral approach of metastability in statistical physics

The operator $L_{V,h} = \frac{1}{h} e^{\frac{f}{h}}\, \Delta_{f,h} e^{-\frac{f}{h}}$, where we recall that $V = 2f$ (see (1)), is the infinitesimal generator of the overdamped Langevin process

$$dX_t = -\nabla V(X_t)dt + \sqrt{2h}\, dB_t \quad (4)$$

which is for instance used to describe the motion of the atoms of a molecule or the diffusion of impurities in a crystal. When the temperature of the system is small, i.e. when $h \ll 1$, the process (4) is typically metastable: it is trapped during a long period of time in a neighborhood of a local minimum of V, called a metastable region, before reaching another metastable region.

When one looks at the process (4) on a metastable region Ω with absorbing boundary conditions, the evolution of observables is in particular given by the semigroup $e^{-tL^D_{V,h}}$, where $L^D_{V,h} := \frac{1}{h} e^{-\frac{f}{h}}\, \Delta^D_{f,h} e^{-\frac{f}{h}}$ is the Dirichlet realization of the weighted Laplacian $L_{V,h}$ in the weighted space $L^2(\Omega, e^{-\frac{V}{h}} d\mathrm{Vol}_\Omega)$, see (1). A first description of the metastability of the process (4) with absorbing boundary conditions is then given by the behaviour of the low-lying spectrum of the Dirichlet realization $\Delta^D_{f,h}$ of the Witten Laplacian in the limit $h \to 0$. The metastable behaviour of the dynamics is more precisely characterized by the fact that the low-lying spectrum of $\Delta^D_{f,h}$ contains

exponentially small eigenvalues, i.e. eigenvalues of order $O(e^{-\frac{c}{h}})$ where $C > 0$. The first mathematical results in this direction probably go back to the works of Freidlin-Wentzell in the framework of their large deviation theory developed in the 70's and we refer in particular to their book [14] for an overview on this topic. In this context, when λ_h is some exponentially small eigenvalue of $\Delta^D_{f,h}$, the limit of $h \ln \lambda_h$ has been investigated assuming that (see [14, Section 6.7])

$$|\nabla f| \neq 0 \text{ on } \partial\Omega. \tag{5}$$

The results of [14] imply in particular that, when $\partial_n f > 0$ on $\partial\Omega$ and Ω contains a unique critical point of f which is non degenerate and is hence the global minimum of f in $\overline{\Omega}$, the principal eigenvalue $\lambda_{1,h}$ of $\Delta^D_{f,h}$ satisfies

$$\lim_{h\to 0} h \ln \lambda_{1,h} \;=\; -2\,(\min_{\partial\Omega} f - \min_{\overline{\Omega}} f)\,.$$

The asymptotic logarithmic behaviour of the low-lying spectrum of $\Delta^D_{f,h}$ has also been studied in [28] dropping the assumption (5). When f and $f|_{\partial\Omega}$ are smooth Morse functions and (5) holds, precise asymptotic formulas in the limit $h \to 0$ have been given by Helffer-Nier in [17] where they prove in particular that under additional generic hypotheses on the function f, any exponentially small eigenvalue λ_h of $\Delta^D_{f,h}$ satisfies the following Eyring-Kramers type formula when $h \to 0$:

$$\lambda_h \;=\; A\, h^{\gamma}\, e^{-\frac{2}{h}E}\,\big(1 + \varepsilon(h)\big), \tag{6}$$

where $A > 0$, $E > 0$, and $\gamma \in \{\frac{1}{2}, 1\}$ are explicit, and the error term $\varepsilon(h)$ is of the order $O(h)$ and admits a full asymptotic expansion in h. The constants E's involved in (6) are the depths of some characteristic wells of the potential f in Ω. The results of [17], obtained by a semiclassical approach, were following similar results obtained in the case without boundary in [5,6,20,30] by a probabilistic approach and in [16] by a semiclassical approach. We also refer to [19, 29] for a generalization of the results obtained in [16] in the case without boundary (see also [2, 3, 22] for related results), to [11][1] for a generalization of the results obtained in [17] in the case of Dirichlet boundary conditions (see also [4, 26, 27, 32] for related results), and to [24, 28] in the case of Neumann boundary conditions. Finally, we refer to [1,25] for a comprehensive review on this topic.

1.3 Motivation and results

Motivation. These past few years, several efficient algorithms have been designed to accelerate the sampling of the exit event from a metastable region Ω, such as for instance the Monte Carlo methods [7, 13, 33, 34, 40, 41] or the *accelerated dynamics* algorithms [37–39]. These algorithms rely on a very precise asymptotic understanding of the metastable behaviour of the process $(X_t)_{t\geq 0}$ in a metastable region Ω when $h \to 0$, and in particular on the validity of Eyring-Kramers type formulas of the

[1] This work corresponds to the first part of the preprint [10].

type (6) in the limit $h \to 0$. Moreover, though the hypothesis (5) considered in [11,17] is generic, in most applications of the accelerated algorithms mentioned above, the domain Ω is the basin of attraction of some local minimum of f for the dynamics $\dot{X} = -\nabla f(X)$ so that the function f admits critical points on the boundary of Ω.

In this work, we precisely aim at giving a precise description of the low-lying spectrum of $\Delta^D_{f,h}$ in the limit $h \to 0$ of the type (6) in a rather general geometric setting covering the latter case (though we assume Ω to have a smooth boundary). This establishes the first step to precisely describe the metastable behaviour of the overdamped Langevin process (4) with absorbing boundary conditions in Ω when $\partial\Omega$ contains critical points of f. Let us also point out that, though the spectrum of $\Delta^D_{f,h}$ (or equivalently of $L^D_{V,h}$) has been widely studied these past few decades, up to our knowledge, this setting has not been treated in the mathematical literature. Our techniques come from semiclassical analysis and, in Section 1.4 below, we detail various difficulties arising when considering critical points of f on $\partial\Omega$ with such techniques.

Results. We recall that we assume that $\overline{\Omega}$ is a C^∞ oriented compact and connected Riemannian manifold of dimension d with interior Ω and boundary $\partial\Omega \neq \emptyset$, and that $f : \overline{\Omega} \to \mathbb{R}$ is a C^∞ Morse function. For $\mu \in \mathbb{R}$, we will use the notation

$$\{f \leq \mu\} = \{x \in \overline{\Omega},\ f(x) \leq \mu\}, \quad \{f < \mu\} = \{x \in \overline{\Omega},\ f(x) < \mu\},$$

and

$$\{f = \mu\} = \{x \in \overline{\Omega},\ f(x) = \mu\}.$$

Moreover, for all $z \in \partial\Omega$, $\mathsf{n}_\Omega(z)$ will denote the unit outward vector to Ω at z. Finally, for $r > 0$ and $y \in \overline{\Omega}$, $B(y,r)$ will denote the open ball of radius r centered at y in $\overline{\Omega}$:

$$B(y,r) := \{z \in \overline{\Omega},\ |y - z| < r\},$$

where, for $y \in \overline{\Omega}$, $|y - z|$ is the geodesic distance between y and z in $\overline{\Omega}$.

Since stating our main results, which are Theorems 2 and 3 (see Section 5.4), requires substantial additional material, we just give here simplified (and weaker) versions of these results. We first give a preliminary result stating that, when $f : \overline{\Omega} \to \mathbb{R}$ is a Morse function, the number of small eigenvalues of $\Delta^D_{f,h}$ is the number of local minima of f in Ω. This requires the following definition.

Definition 2. *Let us assume that $f : \overline{\Omega} \to \mathbb{R}$ is a C^∞ Morse function. The set of local minima of f in Ω is then denoted by U_0 and one defines*

$$\mathsf{m}_0 := \mathrm{Card}\big(\mathsf{U}_0\big) \ \in\ \mathbb{N}.$$

Theorem 1. *Let us assume that $f : \overline{\Omega} \to \mathbb{R}$ is a C^∞ Morse function. Then, there exist $c_0 > 0$ and $h_0 > 0$ such that for all $h \in (0, h_0)$:*

$$\dim \mathrm{Ran}\, \pi_{[0,c_0 h]}\big(\Delta^D_{f,h}\big) \ = \ \dim \mathrm{Ran}\, \pi_{\left(0, e^{-\frac{c_0}{h}}\right)}\big(\Delta^D_{f,h}\big) \ = \ \mathsf{m}_0\,,$$

where, for a Borel set $E \subset \mathbb{R}$, $\pi_E(\Delta^D_{f,h})$ denotes the spectral projector associated with $\Delta^D_{f,h}$ and E, and the nonnegative integer m_0 is defined in Definition 2.

Let us emphasize that the local minima of f included in $\partial\Omega$ are not listed in U_0. This preliminary result is expected from works such as [17,18] but we did not find any such statement in the literature in our setting when the boundary admits critical points of f. Theorem 1 will be proven in Section 2.

In the sequel, when $\mathsf{m}_0 > 0$, we will denote by

$$0 \;<\; \lambda_{1,h} \;<\; \lambda_{2,h} \;\leq\; \cdots \;\leq\; \lambda_{\mathsf{m}_0,h}$$

the m_0 exponentially small eigenvalues of $\Delta^D_{f,h}$ in the limit $h \to 0$ (see Theorem 1). The first main result of this paper is Theorem 2, which is stated and proven in Section 5.4. Here is a simplified version of this result, in a less general setting. The notation $\mathrm{Hess}\, f(z)$ at a critical point z of f below stands for the endomorphism of the tangent space $T_z\overline{\Omega}$ canonically associated with the usual symmetric bilinear form $\mathrm{Hess}\, f(z)$ on $T_z\overline{\Omega} \times T_z\overline{\Omega}$ via the metric g.

Theorem 2'. *Let us assume that the number of local minima m_0 of the Morse function f is positive, that $f|_{\partial\Omega}$ has only non degenerate local minima, and that at any saddle point (i.e. critical point of index 1) z of f which belongs to $\partial\Omega$, $\mathsf{n}_\Omega(z)$ is an eigenvector of $\mathrm{Hess}\, f(z)$ associated with its unique negative eigenvalue. Then, there exists $C > 0$ such that one has in the limit $h \to 0$:*

$$\forall j \in \{1, \ldots, \mathsf{m}_0\}\,, \quad \frac{1}{C}\, h^{\gamma_j}\, e^{-\frac{2}{h}E_j} \;\leq\; \lambda_{j,h} \;\leq\; C\, h^{\gamma_j}\, e^{-\frac{2}{h}E_j}\,, \tag{7}$$

where, for $j \in \{1, \ldots, \mathsf{m}_0\}$, $E_j > 0$, and γ_j are explicit with moreover $\gamma_j \in \{\frac{1}{2}, 1\}$.

The above constants E_j's are the depths of some characteristic wells of the potential f in Ω which are defined through the map

$$\mathbf{j} : \mathsf{U}_0 \to \mathcal{P}(\mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega})) \tag{8}$$

constructed in Section 3.3 (see (43) there). Here $\mathcal{P}(\mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega}))$ denotes the power set of $\mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega})$, the set of relevant *generalized* saddle points (or critical points of index 1) of f in $\overline{\Omega}$ (see Definition 17 at the end of Section 3.2). To be a little more precise here, we have the inclusion

$$\begin{aligned}\mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega}) \;&\subset \{\text{critical points of } f \text{ in } \overline{\Omega} \text{ of index } 1\}\\ &\quad\cup \{\text{local minima } z \text{ of } f|_{\partial\Omega} \text{ in } \partial\Omega \text{ such that } \partial_{\mathsf{n}_\Omega} f(z) > 0\},\end{aligned}$$

where $\partial_{\mathsf{n}_\Omega} f(z) = \mathsf{n}_\Omega(z) \cdot \nabla f(z)$ denotes the normal derivative of f at z. Moreover, f is constant on each $\mathbf{j}(x)$, $x \in \mathsf{U}_0$, and the E_j's are precisely the $f(\mathbf{j}(x)) - f(x)$'s, where, with a slight abuse of notation, we have identified $f(\mathbf{j}(x))$ with its unique element, see Section 3 for precise statements. Note that the E_j's give the logarithmic equivalents of the small eigenvalues of $\Delta^D_{f,h}$ since the relation (7) obviously implies:

$$\forall j \in \{1, \ldots, \mathsf{m}_0\}\,, \quad \lim_{h \to 0} h \ln \lambda_{j,h} \;=\; -2E_j\,.$$

Note also that when Ω is the basin of attraction of some local minimum (or of some family of local minima) of some Morse function f for the flow of $\dot{X} = -\nabla f(X)$ and z is

a saddle point of f which belongs to $\partial\Omega$, the following holds: $\partial\Omega$ is a smooth manifold of dimension $d-1$ near z and $\mathsf{n}_\Omega(z)$ is an eigenvector of Hess $f(z)$ associated with its unique negative eigenvalue. More precisely, $\partial\Omega$ coincides with the stable manifold of z for the dynamics $\dot{X} = -\nabla f(X)$ near the saddle point z (see (12) in Section 2). In Theorem 2, the corresponding assumption is more general since we just assume that the boundary $\partial\Omega$ of Ω is, at the saddle points $z \in \mathbf{j}(\mathsf{U}_0) \cap \partial\Omega$, tangent to the stable manifold of z.

Finally, the second main result of this work is Theorem 3, which is stated and proven in Section 5.4. It states that, under the hypotheses of Theorem 2, which, we recall, are a little more general than the ones of Theorem 2', plus additional very general generic hypotheses on the separation of the characteristic wells of f defined through the map $\mathbf{j} : \mathsf{U}_0 \to \mathcal{P}(\mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega}))$ (see (8) and the lines below), one has in the limit $h \to 0$ sharp asymptotic estimates of the type (6) on all or part of the smallest eigenvalues of $\Delta_{f,h}^D$. We state below a simplified version of Theorem 3, in a less general setting, where we do not make explicit the pre-exponential factors (see Theorem 3 for explicit formulas).

Theorem 3'. *Let us assume the hypotheses of Theorem 2'. Then, under generic hypotheses on the characteristic wells of f defined through the map $\mathbf{j} : \mathsf{U}_0 \to \mathcal{P}(\mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega}))$ defined in 43, one has in the limit $h \to 0$:*

$$\forall j \in \{1, \dots, \mathsf{m}_0\}, \quad \lambda_{j,h} \;=\; A_j\, h^{\gamma_j}\, e^{-\frac{2}{h}E_j} \left(1 + O(\sqrt{h})\right), \tag{9}$$

where, for $j \in \{1, \dots, \mathsf{m}_0\}$, $A_j > 0$, $E_j > 0$, and γ_j are explicit with moreover $\gamma_j \in \{\frac{1}{2}, 1\}$, and the remainder term $O(\sqrt{h})$ is actually of the order $O(h)$ when the boundary of the associated characteristic well does not meet both $(|\nabla f|)^{-1}(\{0\})$ and $\partial\Omega$.
In addition, when $\mathsf{m}_0 \geq 2$ and $E_{\mathsf{m}^*} > E_{\mathsf{m}^*+1}$ for some $\mathsf{m}^* \in \{1, \dots, \mathsf{m}_0 - 1\}$, the previous estimates remain valid for $\lambda_{1,h}, \dots, \lambda_{\mathsf{m}^*,h}$ under more general hypotheses:

$$\forall j \in \{1, \dots, \mathsf{m}^*\}, \quad \lambda_{j,h} \;=\; A_j\, h^{\gamma_j}\, e^{-\frac{2}{h}E_j} \left(1 + O(\sqrt{h})\right), \tag{10}$$

where, for $j \in \{1, \dots, \mathsf{m}_0\}$, $A_j > 0$, $E_j > 0$, and γ_j are explicit with moreover $\gamma_j \in \{\frac{1}{2}, 1\}$, and the remainder term $O(\sqrt{h})$ is actually of the order $O(h)$ when the boundary of the associated characteristic well does not meet both $(|\nabla f|)^{-1}(\{0\})$ and $\partial\Omega$.

Let us now comment about this result.

First, the above error terms $O(\sqrt{h})$ or $O(h)$ are in general optimal, see indeed Remark 39 below.

Moreover, even when $\mathsf{m}^* = \mathsf{m}_0$ in Theorem 3', the geometric assumptions on the characteristic wells of f are still more general than the generic hypotheses made e.g. in [6, 16] in the case without boundary or in [17] in the case with boundary, see indeed [17, Assumption 5.3.1]. For instance, our hypotheses neither imply that the E_j's are distinct, nor that the $\mathbf{j}(x)$, $x \in \mathsf{U}_0$, are singletons, as assumed in [17]. More precisely, the main result of [17] is a particular case of Theorem 3' when $|\nabla f| \neq 0$

on $\partial\Omega$, except that we do not prove in this work the possible existence of a full asymptotic expansion of the low-lying spectrum of $\Delta^D_{f,h}$.

Furthermore, our results have the advantage to give assumptions on f leading to sharp asymptotic estimates on the sole m^* smallest eigenvalues $\lambda_{1,h}, \dots, \lambda_{\mathsf{m}^*,h}$ of $\Delta^D_{f,h}$ when $\mathsf{m}^* < \mathsf{m}_0$, and the more m^* is small, the less restrictive are these assumptions. This was not allowed in [17]. In particular, in the case when $\mathsf{m}^* = 1$ is given a sharp equivalent of the sole principal eigenvalue $\lambda_{1,h}$. This is appreciable since it gives the leading term of the semigroup $(e^{-t\Delta^D_{f,h}})_{t\geq 0}$ under very general assumptions. On this point, Theorem 3 also generalizes [11, Theorem 3] when f admits critical points on $\partial\Omega$. To be a little more precise here, we have for example the following corollary of Theorem 3 (see also Remark 40 in this connection).

Corollary 3. *Let us assume that f is a Morse function, that $\{f < \min_{\partial\Omega} f\}$ is non empty, connected, contains all the local minima of f in Ω, and that*

$$\overline{\{f < \min_{\partial\Omega} f\}} \cap \partial\Omega \;=\; \{z_1, \dots, z_N\}\,,$$

where $N \in \mathbb{N}^*$ and, for $k \in \{1, \dots, N\}$, z_k is a saddle point of f such that $\mathsf{n}_\Omega(z_k)$ is an eigenvector of $\operatorname{Hess} f(z_k)$ associated with its unique negative eigenvalue $\lambda(z_k)$. The principal eigenvalue of $\Delta^D_{f,h}$ then satisfies the following Eyring-Kramers formula in the limit $h \to 0$:

$$\lambda_{1,h} \;=\; \frac{2}{\pi}\,\frac{\sum_{k=1}^N |\lambda(z_k)|\,|\det \operatorname{Hess} f(z_k)|^{-\frac{1}{2}}}{\sum\limits_{y\in \arg\min_\Omega f} \big(\det \operatorname{Hess} f(y)\big)^{-\frac{1}{2}}}\, h\, e^{-\frac{2}{h}(\min_{\partial\Omega} f - \min_\Omega f)} \big(1 + O(\sqrt{h})\big)\,. \quad (11)$$

Let us also mention the work [29], where the author treats the case of general Morse functions in the case without boundary. We believe that the analysis done in [29] can be adapted to our setting, which would lead to the existence of an Eyring-Kramers type formula for each small eigenvalue of $\Delta^D_{f,h}$ under the sole assumptions of Theorem 2'. Nevertheless, we made the choice to not follow this way here since these precise formulas are in general very complicated to make explicit. Indeed, the pre-exponential factors are not computed in general in [29], but are shown to be computable by following an arbitrary long algorithm. This follows from the fact that in the general case, some tunneling effect between the characteristic wells of f mixes their corresponding pre-exponential factors, see [29] for more details. Our hypotheses remain however very general and lead to explicit Eyring-Kramers type formulas in Theorem 3.

1.4 Strategy and organization of the paper

In works such as [11, 16, 17, 19, 24, 29], a part of the analysis relies on the construction of 0-forms (i.e. functions) quasi-modes supported in some characteristic wells of the potential f and of 1-forms quasi-modes supported near the saddle points of f, and, in [11, 17, 24], near its so-called generalized saddle points on the boundary. Very

accurate WKB approximations of these local 1-forms quasi-modes then finally lead to the asymptotic expansions of the low-lying spectrum of the Witten Laplacian acting on functions. This approach is based on the supersymmetric structure of the latter operator, once restricted to the interplay between 0- and 1-forms.

Near the generalized saddle points on the boundary as considered in [17,24], where one recalls that $|\nabla f| \neq 0$ there and actually where the normal derivative $\partial_{\mathsf{n}_\Omega} f$ does not vanish, this construction means solving non characteristic transport equations with prescribed initial boundary conditions, see in particular [17,23,24]. Near a usual saddle point z in Ω (i.e. a critical point z with index 1), this construction follows from the work [18] of Helffer-Sjöstrand and means solving transport equations which are degenerate at z (see in particular Section 2 there). In this case, the problem is well-posed only for prescribed initial condition at the single point z. In particular, when one drops the assumption (5) and z is a usual saddle point which belongs to $\partial\Omega$, the corresponding transport equations, which are the same as for interior saddle points, are uniquely solved as in [18], but the resulting WKB ansatz does not in general satisfy the required boundary conditions, except its leading term when the boundary $\partial\Omega$ has a specific shape near z. To be more precise, and to make the connection with the hypotheses of Theorems 2' and 3' (and Theorems 2 and 3), the leading term of this WKB ansatz satisfies the required boundary conditions if and only if $\partial\Omega$ coincides near z with the stable manifold of z for the dynamics $\dot{X} = -\nabla f(X)$ (see (12) in Section 2). This compatibility condition imposes in particular that $\mathsf{n}_\Omega(z)$ spans the negative direction of $\mathrm{Hess}\, f(z)$. The fact that the remaining part of the WKB ansatz does in general not satisfy the required boundary conditions for a compatible boundary $\partial\Omega$ arises from the curvature of this boundary.

The above considerations show that, when $z \in \partial\Omega$ is a saddle point of f and $\mathsf{n}_\Omega(z)$ does not span the negative direction of $\mathrm{Hess}\, f(z)$, the classical WKB ansatz constructed near z will not be an accurate approximation of the local 1-form quasi-mode associated with z. They also imply that the potential existence of full asymptotic expansions of the small eigenvalues of $\Delta^D_{f,h}$ will in general not follow from the existence of these WKB ansätze when f admits saddle points on the boundary. Moreover, we expect that sharp asymptotic equivalents such as (11) are not valid in general when $\mathsf{n}_\Omega(z)$ does not span the negative direction of $\mathrm{Hess}\, f(z)$ at the relevant saddle points $z \in \partial\Omega$. In the latter case, we expect that the corresponding possible sharp asymptotic equivalents should also rely on the angle between $\mathsf{n}_\Omega(z)$ and the negative direction of $\mathrm{Hess}\, f(z)$.

In this work, we follow a different strategy based on the constructions of very accurate quasi-modes for $\Delta^D_{f,h}$. This approach, which is partly inspired by the quasi-modal construction made in [9] (see also [5, 22, 32]), requires a careful construction of these functions quasi-modes around the relevant (possibly generalized) saddle points z of f, whereas these points were not in the supports of the corresponding quasi-modes constructed in [11,16,17,19,24,29]. One advantage of this method is to avoid a careful study of the Witten Laplacian acting on 1-forms near the boundary $\partial\Omega$, which would

finally lead to more stringent hypotheses on f and on $f|_{\partial\Omega}$, that is precisely to the hypotheses made in the statement of Theorem 2'[2]

The rest of the paper is organized as follows. In Section 2, we prove Theorem 1 about the number of small eigenvalues of $\Delta^D_{f,h}$. This is done using spectral and localization arguments. Then, in Section 3, we construct the map $\mathbf{j}$ characterizing the relevant wells of the potential function f. This permits to construct very accurate quasi-modes in Section 4 and then to state and prove our main results, namely Theorems 2 and 3, in Section 5. As in [11, 16, 17, 19, 24, 29], the analysis of the precise asymptotic behaviour of the low-lying spectrum of $\Delta^D_{f,h} = d^{D,*}_{f,h} d^D_{f,h}$ is finally reduced to the computation of the small singular values of $d^D_{f,h}$.

2 On the number of small eigenvalues of $\Delta^D_{f,h}$

This section is dedicated to the proof of Theorem 1. Before going into its proof, we briefly recall basic facts about smooth Morse functions on a C^∞ compact Riemannian manifold with boundary $\overline{\Omega} = \Omega \cup \partial\Omega$ of dimension d.

Let $z \in \partial\Omega$. Let us consider a neighborhood V_z of z in $\overline{\Omega}$ and a coordinate system $p \in \mathsf{V}_z \mapsto x = (x', x_d) \in \mathbb{R}^d_- = \mathbb{R}^{d-1} \times \mathbb{R}_-$ such that: $x(z) = 0$, $\{p \in \mathsf{V}_z,\, x_d(p) < 0\} = \Omega \cap \mathsf{V}_z$ and $\{p \in \mathsf{V}_z,\, x_d(p) = 0\} = \partial\Omega \cap \mathsf{V}_z$. By definition, the function f is C^∞ on V_z if, in the x-coordinates, the function $f : x(\mathsf{V}_z) \to \mathbb{R}$ is the restriction of a C^∞ function defined on an open subset O of $\mathbb{R}^d$ containing $x(\mathsf{V}_z)$. Moreover, $z \in \partial\Omega$ is a non degenerate critical point of $f : \overline{\Omega} \to \mathbb{R}$ of index $p \in \{0, \dots, d\}$ if it is a non degenerate critical point of index p for this extension. Notice that this definition is independent of the choice of the extension. A C^∞ function $f : \overline{\Omega} \to \mathbb{R}$ is then said to be a Morse function if all its critical points in $\overline{\Omega}$ are non degenerate. In the following, we will also say that $z \in \overline{\Omega}$ is a saddle point of the Morse function f if it is a critical point of f with index 1.

Let now $f : \overline{\Omega} \to \mathbb{R}$ be a Morse fonction. By the above, there exist a C^∞ Riemannian manifold $\widetilde{\Omega}$ (without boundary) of dimension d and a C^∞ Morse function $\tilde{f} : \widetilde{\Omega} \to \mathbb{R}$ such that

$$\tilde{f}|_{\overline{\Omega}} = f \quad \text{and} \quad \overline{\Omega} \subset \widetilde{\Omega}\,.$$

For a critical point $z \in \overline{\Omega}$ of $\tilde{f}$, the sets $\mathsf{W}^+(z)$ and $\mathsf{W}^-(z)$ will respectively denote the so-called stable and unstable manifolds of z for the dynamics $\dot{X} = -\nabla\tilde{f}(X)$ in $\widetilde{\Omega}$. In other words, denoting by $X_y(t)$ the solution to $\frac{d}{dt}X_y(t) = -\nabla\tilde{f}(X_y(t))$ with initial condition $X_y(0) = y \in \widetilde{\Omega}$, one has (see for example [21, Definition 7.3.2]):

$$\mathsf{W}^\pm(z) \;=\; \{y \in \widetilde{\Omega} \;\text{ s.t. }\; X_y(t) \in \widetilde{\Omega} \text{ for every } \pm t \geq 0 \;\text{ and }\; \lim_{t\to\pm\infty} X_y(t) = z\}. \tag{12}$$

We recall that when z has index $p \in \{0, \dots, d\}$, the sets $\mathsf{W}^+(z)$ and $\mathsf{W}^-(z)$ are indeed smooth submanifolds of $\widetilde{\Omega}$; they moreover intersect orthogonally at z and

[2] For example, in the statement of Corollary 3, the "1-form approach" would require that *all* the local minima of $f|_{\partial\Omega}$ are non degenerate and that $\mathsf{n}_\Omega(z)$ spans the negative direction of Hess $f(z)$ at *any* saddle point $z \in \partial\Omega$.

have respective dimensions $d-p$ and p (see for example [21, Theorem 7.3.1 and Corollary 7.4.1]). Note lastly that the part of $\mathsf{W}^{\pm}(z)$ leaving outside $\overline{\Omega}$ of course depends on the choice of the extension $\tilde{f}$.

2.1 Preliminary results

In order to prove Theorem 1, one will make use of the following proposition which results from [18, Théorème 1.4].

Proposition 4. *Let $\overline{\mathsf{O}}$ be an oriented C^∞ compact and connected Riemannian manifold of dimension d with interior O and non empty boundary $\partial\mathsf{O}$, let $\phi : \overline{\mathsf{O}} \to \mathbb{R}$ be a C^∞ Morse function, and let x_0 be a critical point of ϕ in O with index $\ell \in \{0,\dots,d\}$ such that x_0 is the only critical point of ϕ in $\overline{\mathsf{O}}$. Then, the Dirichlet realization $\Delta^D_{\phi,h}(\mathsf{O})$ of the Witten Laplacian acting on functions on O satisfies the following estimate: there exist $\eta_0 > 0$ and $h_0 > 0$ such that for all $h \in (0,h_0)$,*

$$\dim \operatorname{Ran} \pi_{[0,\eta_0 h]}\big(\Delta^D_{\phi,h}(\mathsf{O})\big) = \delta_{\ell,0}.$$

The following result is a direct consequence of Proposition 4.

Corollary 5. *Let $\overline{\mathsf{O}}$, ϕ, x_0, and $\ell \in \{0,\dots,d\}$ be as in Proposition 4. Let us assume that $\ell = 0$, i.e. that x_0 is a local minimum of ϕ in O, and that ϕ only attains its minimal value on $\overline{\mathsf{O}}$ at x_0. Let moreover, for every h small enough, $\Psi \geq 0$ be the $L^2(\mathsf{O})$-normalized eigenfunction of $\Delta^D_{\phi,h}(\mathsf{O})$ associated with its unique eigenvalue λ_h in $(0,\eta_0 h]$ (see Proposition 4 and Remark 1). Lastly, let $\xi \in C^\infty_c(\mathsf{O},[0,1])$ be a cut-off function such that $\xi = 1$ in a neighborhood of x_0 in O. Then, defining $\chi := \frac{\xi\, e^{-\frac{1}{h}\phi}}{\left\|\xi\, e^{-\frac{1}{h}\phi}\right\|_{L^2(\mathsf{O})}}$, there exists $c > 0$ such that for every h small enough:*

$$\Psi = \chi + O\big(e^{-\frac{c}{h}}\big) \quad \text{in} \quad L^2(\mathsf{O}) \quad \text{and} \quad 0 < \lambda_h \leq \left\|d_{\phi,h}\chi\right\|^2_{\Lambda^1 L^2(\mathsf{O})} \leq e^{-\frac{c}{h}}\,. \tag{13}$$

Proof. The proof of (13) is standard but we give it for the sake of completeness. As in the statement of Corollary 5, let us define

$$\chi := \frac{\xi\, e^{-\frac{1}{h}\phi}}{\left\|\xi\, e^{-\frac{1}{h}\phi}\right\|_{L^2(\mathsf{O})}}\,.$$

From the definition of ξ and the Laplace method together with the fact that ϕ only attains its minimal value on $\overline{\mathsf{O}}$ at x_0, it holds

$$\left\|\xi\, e^{-\frac{1}{h}\phi}\right\|^2_{L^2(\mathsf{O})} = \frac{(\pi h)^{\frac{d}{2}}}{\sqrt{\det \operatorname{Hess}\phi(x_0)}} e^{-\frac{2}{h}\phi(x_0)}\big(1+O(h)\big).$$

According to Proposition 4, there exist $\eta_0 > 0$ and $h_0 > 0$ such that for all $h \in (0,h_0)$, $\pi_{[0,\eta_0 h]}\big(\Delta^D_{f,h}(\mathsf{O})\big)$ is the orthogonal projector on $\operatorname{Span}\{\Psi\}$. Moreover, using the following spectral estimate, valid for any nonnegative self-adjoint operator $(T, D(T))$ on a Hilbert space $(\mathcal{H}, \|\cdot\|)$ with associated quadratic form $(q_T, Q(T))$,

$$\forall b > 0\,,\ \forall u \in Q\,(T)\ ,\ \left\|\pi_{[b,+\infty)}(T)\, u\right\|^2 \leq \frac{q_T(u)}{b}, \tag{14}$$

it holds (see (2) and (3))

$$\left\|\chi - \pi_{[0,\eta_0 h]}\big(\Delta^D_{\phi,h}(\mathsf{O})\big)\chi\right\|^2_{L^2(\mathsf{O})} \leq \frac{\left\|d_{\phi,h}\chi\right\|^2_{\Lambda^1 L^2(\mathsf{O})}}{\eta_0 h} = \frac{h}{\eta_0}\frac{\int_{\mathsf{O}}|d\xi|^2 e^{-\frac{2}{h}\phi}}{\left\|\xi\, e^{-\frac{1}{h}\phi}\right\|^2_{L^2(\mathsf{O})}}.$$

Hence, since $\xi = 1$ in a neighborhood of x_0 and thus, for some $c > 0$, $\phi(y) \geq \phi(x_0) + c$ for every $y \in \operatorname{supp} d\xi$, one has for every $h > 0$ small enough,

$$\left\|d_{\phi,h}\chi\right\|^2_{\Lambda^1 L^2(\mathsf{O})} \leq e^{-\frac{c}{h}} \quad \text{and} \quad \left\|\chi - \pi_{[0,\eta_0 h]}\big(\Delta^D_{\phi,h}(\mathsf{O})\big)\chi\right\|^2_{L^2(\mathsf{O})} \leq e^{-\frac{c}{h}}, \tag{15}$$

where $c > 0$ is independent of h. Since $\|\chi\|_{L^2(\mathsf{O})} = 1$, the first relation in (15) together with the Min-Max principle leads to (see (2))

$$\lambda_h \;\leq\; \langle \Delta^D_{\phi,h}(\mathsf{O})\chi, \chi\rangle_{L^2(\mathsf{O})} \;=\; \left\|d_{\phi,h}\chi\right\|^2_{\Lambda^1 L^2(\mathsf{O})} \;\leq\; e^{-\frac{c}{h}}\,.$$

Moreover, using the second relation in (15) and the Pythagorean theorem, one obtains for every $h > 0$ small enough:

$$\left\|\pi_{[0,\eta_0 h]}\big(\Delta^D_{\phi,h}(\mathsf{O})\big)\chi\right\|_{L^2(\mathsf{O})} = 1 + O(e^{-\frac{c}{h}}). \tag{16}$$

In conclusion, from (15), (16), and since χ and Ψ are nonnegative, it holds, in $L^2(\mathsf{O})$, for some $c > 0$ and every $h > 0$ small enough:

$$\Psi = \frac{\pi_{[0,\eta_0 h]}\big(\Delta^D_{\phi,h}(\mathsf{O})\big)\chi}{\left\|\pi_{[0,\eta_0 h]}\big(\Delta^D_{\phi,h}(\mathsf{O})\big)\chi\right\|_{L^2(\mathsf{O})}} = \chi + O\big(e^{-\frac{c}{h}}\big).$$

This concludes the proof of (13) and then the proof of Corollary 5. ∎

We are now in position to prove Theorem 1.

2.2 Proof of Theorem 1

Let $\{x_1, \ldots, x_n\}$ be the set of the critical points of f in $\overline{\Omega}$, i.e.

$$\big\{x_1, \ldots, x_n\big\} \;=\; \big\{x \in \overline{\Omega},\ |\nabla f(x)| = 0\big\}\,.$$

From the preliminary discussion in the beginning of Section 2, there exist an oriented C^∞ compact and connected Riemannian manifold $\overline{\widetilde{\Omega}}$ of dimension d with interior $\widetilde{\Omega}$ and boundary $\partial\widetilde{\Omega}$, and a C^∞ Morse function $\tilde{f} : \overline{\widetilde{\Omega}} \to \mathbb{R}$ such that

$$\tilde{f}|_{\overline{\Omega}} = f\,,\ \ \overline{\Omega} \;\subset\; \overline{\widetilde{\Omega}} \quad \text{and} \quad \big\{x_1, \ldots, x_n\big\} \;\subset\; \widetilde{\Omega}\,.$$

We recall that m_0 denotes the number of local minima of f in Ω (see Definition 2), and thus that $0 \leq \mathsf{m}_0 \leq n$. When $\mathsf{m}_0 > 0$, the elements $x_1, \ldots, x_n$ are moreover ordered such that

$$\big\{x_1, \ldots, x_{\mathsf{m}_0}\big\} \;=\; \mathsf{U}_0.$$

In addition, one introduces for every $j \in \{1, \dots, \mathsf{m}_0\}$ a smooth open neighborhood O_j of x_j such that $\overline{\mathsf{O}_j} \subset \Omega$ and such that x_j is the only critical point of f in $\overline{\mathsf{O}_j}$ as well as the only point where f attains its minimal value in $\overline{\mathsf{O}_j}$. Similarly, when $x_j \in \Omega$ is not a local minimum of f, one introduces a smooth open neighborhood O_j of x_j such that $\overline{\mathsf{O}_j} \subset \Omega$ and such that x_j is the only critical point of f in $\overline{\mathsf{O}_j}$. Lastly, when $x_j \in \partial\Omega$, one now introduces a smooth open neighborhood O_j of x_j in $\overline{\widetilde{\Omega}}$ such that $\overline{\mathsf{O}_j} \subset \widetilde{\Omega}$ and such that x_j is the only critical point of $\tilde{f}$ in $\overline{\mathsf{O}_j}$. When such a x_j is a local minimum of f, the set O_j is moreover chosen small enough such that the minimal value of $\tilde{f}$ in $\overline{\mathsf{O}_j}$ is only attained at x_j. Let us also introduce a quadratic partition of unity $(\chi_j)_{j\in\{1,\dots,n+1\}}$ such that:

1. For all $j \in \{1, \dots, n+1\}$, $\chi_j \in C^\infty(\overline{\widetilde{\Omega}}, [0,1])$ and $\sum_{j=1}^{n+1} \chi_j^2 = 1$ on $\overline{\widetilde{\Omega}}$.
2. For all $j \in \{1, \dots, n\}$, $\chi_j = 1$ near x_j and $\operatorname{supp} \chi_j \subset \mathsf{O}_j$. In particular, $\operatorname{supp} \chi_j \subset \Omega$ when $x_j \in \Omega$.
3. For all $(i,j) \in \{1, \dots, n\}^2$, $i \neq j$ implies $\operatorname{supp} \chi_i \cap \operatorname{supp} \chi_j = \emptyset$.

In the following, we will also use the so-called IMS localization formula (see for example [8]): for all $\psi \in H_0^1(\Omega)$, it holds

$$Q_{f,h}(\psi) = \sum_{j=1}^{n+1} Q_{f,h}(\chi_j\, \psi) - \sum_{j=1}^{n+1} h^2 \left\| |\nabla \chi_j|\, \psi \right\|^2_{L^2(\Omega)}, \tag{17}$$

where $Q_{f,h}$ is the quadratic form defined in (3).

Step 1. Let us first show that there exists $c_0 > 0$ such that for every h small enough, it holds

$$\dim \operatorname{Ran} \pi_{(0, e^{-\frac{c_0}{h}})}\big(\Delta^D_{f,h}\big) \;\geq\; \mathsf{m}_0\,. \tag{18}$$

This relation is obvious when $\mathsf{m}_0 = 0$. When $\mathsf{m}_0 > 0$, the family $(\overline{\mathsf{O}_j}, f|_{\overline{\mathsf{O}_j}}, x_j)$ satisfies, for every $j \in \{1, \dots, \mathsf{m}_0\}$, the hypotheses of Corollary 5. Then, according to (13), the function

$$\psi_j := \frac{\chi_j e^{-\frac{f}{h}}}{\|\chi_j e^{-\frac{f}{h}}\|_{L^2(\mathsf{O}_j)}}$$

satisfies, for some $c_j > 0$ and every $h > 0$ small enough (see (3)),

$$Q_{f,h}(\psi_j) \leq e^{-\frac{c_j}{h}}\,.$$

Since the ψ_j's, $j \in \{1, \dots, \mathsf{m}_0\}$, are unitary in $L^2(\Omega)$ and have disjoint supports, it follows from the Min-Max principle that $\Delta^D_{f,h}$ admits at least m_0 exponentially small eigenvalues when $h \to 0$, which proves (18).

Step 2. Let us now show that there exists $c_0' > 0$ such that for every h small enough, it holds

$$\dim \operatorname{Ran} \pi_{[0, c_0' h]}\big(\Delta^D_{f,h}\big) \;\leq\; \mathsf{m}_0\,. \tag{19}$$

According to the Min-Max principle, it is sufficient to show that there exist $h_0 > 0$ and $C > 0$ such that for every $h \in (0, h_0]$, there exist $u_1, \dots, u_{\mathsf{m}_0}$ in $L^2(\Omega)$ such that for any $\psi \in D(Q_{f,h}) = H_0^1(\Omega)$, it holds

$$Q_{f,h}(\psi) \;\geq\; Ch\,\|\psi\|^2_{L^2(\Omega)} - \sum_{i=1}^{\mathsf{m}_0} \langle \psi, u_i\rangle^2_{L^2(\Omega)}\,. \tag{20}$$

Analysis on $\operatorname{supp}\chi_{n+1}$**.**

Since $\operatorname{supp}\chi_{n+1} \cap \overline{\Omega}$ does not meet $\{x_1, \dots, x_n\}$, there exists $C > 0$ such that $|\nabla f| \geq 3C$ on $\operatorname{supp}\chi_{n+1} \cap \overline{\Omega}$. It then follows from (3) that there exists $C > 0$ such that for every h small enough and for every $\psi \in H_0^1(\Omega)$, it holds

$$\begin{aligned} Q_{f,h}(\chi_{n+1}\psi) \;&\geq\; \big\langle \chi_{n+1}\psi, \big(|\nabla f|^2 + h\Delta_H f\big)\chi_{n+1}\psi\big\rangle_{L^2(\Omega)} \\ &\geq\; 2C\,\|\chi_{n+1}\psi\|^2_{L^2(\Omega)}. \end{aligned} \tag{21}$$

Analysis on $\operatorname{supp}\chi_j$**,** $j \in \{1, \dots, \mathsf{m}_0\}$**.**

We assume here that $\mathsf{m}_0 > 0$. We recall that for every $j \in \{1, \dots, \mathsf{m}_0\}$, $(\overline{\mathsf{O}_j}, f|_{\overline{\mathsf{O}_j}}, x_j)$ satisfies the hypotheses of Corollary 5, and we denote, for $h > 0$, by $\Psi_j \geq 0$ the $L^2(\mathsf{O}_j)$-normalized eigenfunction of $\Delta^D_{f,h}(\mathsf{O}_j)$ associated with its principal eigenvalue λ^j_h (which is positive, and exponentially small when $h \to 0$). It then follows from Proposition 4 and Corollary 5 that for some $C > 0$ and every $h > 0$ small enough, it holds, for every $j \in \{1, \dots, \mathsf{m}_0\}$ and for every $\psi \in H_0^1(\Omega)$,

$$\begin{aligned} Q_{f,h}(\chi_j\psi) \;&\geq\; \lambda^j_h \langle \chi_j\psi, \Psi_j\rangle^2_{L^2(\Omega)} + 2Ch\|\chi_j\psi - \langle \chi_j\psi, \Psi_j\rangle\Psi_j\|^2_{L^2(\Omega)} \\ &\geq\; 2Ch\,\|\chi_j\psi\|^2_{L^2(\Omega)} - 2Ch\,\langle \chi_j\psi, \Psi_j\rangle^2_{L^2(\Omega)} \\ &=\; 2Ch\,\|\chi_j\psi\|^2_{L^2(\Omega)} - \langle \psi, u_j\rangle^2_{L^2(\Omega)}\,, \end{aligned} \tag{22}$$

where one has defined $u_j := \sqrt{2Ch}\,\chi_j\Psi_j$.

Analysis on $\operatorname{supp}\chi_j$**, when** $x_j \in \Omega$ **is not a local minimum of** f**.**

In this case, applying Proposition 4 with O_j and $\Delta^D_{f,h}(\mathsf{O}_j)$, it follows that for some $C > 0$ and every $h > 0$ small enough, it holds, for every $\psi \in H_0^1(\Omega)$,

$$Q_{f,h}(\chi_j\psi) \;\geq\; 2Ch\,\|\chi_j\psi\|^2_{L^2(\Omega)}\,. \tag{23}$$

Analysis on $\operatorname{supp}\chi_j$**, when** $x_j \in \partial\Omega$ **is not a local minimum of** f**.**

In this case, applying as previously Proposition 4 with O_j but here with $\Delta^D_{\tilde{f},h}(\mathsf{O}_j)$ and denoting by $Q_{\tilde{f},h,\mathsf{O}_j}$ its associated quadratic form, it follows that for some $C > 0$ and every $h > 0$ small enough, it holds, for every $\psi \in H_0^1(\widetilde{\Omega})$,

$$Q_{\tilde{f},h,\mathsf{O}_j}(\chi_j\psi) \;=\; \big\|d_{\tilde{f},h}\chi_j\psi\big\|^2_{\Lambda^1 L^2(\mathsf{O}_j)} \;\geq\; 2Ch\,\|\chi_j\psi\|^2_{L^2(\widetilde{\Omega})}\,.$$

Let us now consider the application $\psi \in L^2(\Omega) \mapsto \overline{\psi} \in L^2(\widetilde{\Omega})$, where $\overline{\psi}$ extends ψ on $\widetilde{\Omega}$ by $\overline{\psi}|_{\widetilde{\Omega}\setminus\overline{\Omega}} = 0$. Since $\overline{\psi}$ belongs to $H_0^1(\widetilde{\Omega})$ for every $\psi \in H_0^1(\Omega)$ with moreover

$(d\overline{\psi})|_{\widetilde{\Omega}\setminus\overline{\Omega}} = 0$, it holds, for every h small enough and for every $\psi \in H_0^1(\Omega)$,

$$\begin{aligned} Q_{f,h}(\chi_j\psi) \;&=\; \left\|d_{f,h}(\chi_j\psi)\right\|^2_{\Lambda^1 L^2(\Omega)} \;=\; \left\|d_{\tilde{f},h}(\chi_j\overline{\psi})\right\|^2_{\Lambda^1 L^2(\mathsf{O}_j)} \\ &\geq\; 2Ch\,\|\chi_j\overline{\psi}\|^2_{L^2(\widetilde{\Omega})} \;=\; 2Ch\,\|\chi_j\psi\|^2_{L^2(\Omega)}\,. \end{aligned} \tag{24}$$

Analysis on $\operatorname{supp}\chi_j$**, when** $x_j \in \partial\Omega$ **is a local minimum of** f**.**

Let us now consider, as previously, the extension map $\psi \in H_0^1(\Omega) \mapsto \overline{\psi} \in H_0^1(\widetilde{\Omega})$ by 0 outside $\overline{\Omega}$, and let $\Psi_j \geq 0$ be the $L^2(\mathsf{O}_j)$-normalized eigenfunction of $\Delta^D_{\tilde{f},h}(\mathsf{O}_j)$ associated with its principal eigenvalue λ_h^j (see Remark 1). Then, according to Proposition 4, one has for some $C > 0$, for every h small enough, and for every $\psi \in H_0^1(\Omega)$,

$$\begin{aligned} Q_{f,h}(\chi_j\psi) \;&=\; Q_{\tilde{f},h,\mathsf{O}_j}(\chi_j\overline{\psi}) \\ &\geq\; \lambda_h^j\langle\chi_j\overline{\psi},\Psi_j\rangle^2_{L^2(\mathsf{O}_j)} + 6Ch\|\chi_j\overline{\psi} - \langle\chi_j\overline{\psi},\Psi_j\rangle\Psi_j\|^2_{L^2(\mathsf{O}_j)} \\ &\geq\; 6Ch\,\|\chi_j\overline{\psi}\|^2_{L^2(\mathsf{O}_j)} - 6Ch\,\langle\chi_j\overline{\psi},\Psi_j\rangle^2_{L^2(\mathsf{O}_j)} \\ &=\; 6Ch\,\|\chi_j\psi\|^2_{L^2(\Omega)} - 6Ch\,\langle\chi_j\psi,\Psi_j\rangle^2_{L^2(\Omega\cap\mathsf{O}_j)}\,. \end{aligned} \tag{25}$$

Moreover, applying Corollary 5 with $\mathsf{O} = \mathsf{O}_j$, $\phi = \tilde{f}|_{\overline{\mathsf{O}_j}}$, and $\xi = \chi_j$, it follows from (13) that for every h small enough, one has

$$\left\|\Psi_j\right\|^2_{L^2(\Omega\cap\mathsf{O}_j)} = \frac{\left\|\chi_j e^{-\frac{1}{h}\tilde{f}}\right\|^2_{L^2(\Omega\cap\mathsf{O}_j)}}{\left\|\chi_j e^{-\frac{1}{h}\tilde{f}}\right\|^2_{L^2(\mathsf{O}_j)}} + O\big(e^{-\frac{c}{h}}\big).$$

From the Laplace method together with the fact that $\tilde{f}$ only attains its minimal value on $\overline{\mathsf{O}_j}$ at x_j, it then holds in the limit $h \to 0$:

$$\left\|\Psi_j\right\|^2_{L^2(\Omega\cap\mathsf{O}_j)} \;=\; \frac{1}{2} + o(1)\,.$$

According to (25), this implies, using the Cauchy-Schwarz inequality

$$\langle\chi_j\psi,\Psi_j\rangle^2_{L^2(\Omega)} \;\leq\; \left\|\chi_j\psi\right\|^2_{L^2(\Omega)}\left\|\Psi_j\right\|^2_{L^2(\Omega\cap\mathsf{O}_j)}\,,$$

that for some $C > 0$, for every h small enough, and for every $\psi \in H_0^1(\Omega)$, it holds:

$$Q_{f,h}(\chi_j\psi) \;\geq\; 2Ch\,\|\chi_j\psi\|^2_{L^2(\Omega)}\,. \tag{26}$$

Conclusion.

Adding the estimates (21) to (24) and (26), we deduce from the IMS localization formula (17) that there exists $C > 0$ such that for every h small enough and for every $\psi \in H_0^1(\Omega)$, it holds

$$\begin{aligned} Q_{f,h}(\psi) \;&=\; \sum_{j=1}^{n+1} Q_{f,h}(\chi_j\,\psi) - \sum_{j=1}^{n+1} h^2\,\left\||\nabla\chi_j|\,\psi\right\|^2_{L^2(\Omega)} \\ &\geq\; \sum_{j=1}^{n+1} 2Ch\|\chi_j\psi\|^2_{L^2(\Omega)} - \sum_{j=1}^{\mathsf{m}_0}\langle\psi,u_j\rangle^2_{L^2(\Omega)} + O(h^2)\|\psi\|^2_{L^2(\Omega)} \\ &\geq\; Ch\,\|\psi\|^2_{L^2(\Omega)} - \sum_{j=1}^{\mathsf{m}_0}\langle\psi,u_j\rangle^2_{L^2(\Omega)}\,, \end{aligned}$$

where, for $j \in \{1, \dots, \mathsf{m}_0\}$, we recall that $u_j = \sqrt{2Ch}\,\chi_j \Psi_j$. This implies the relation (20) and then (19), which concludes the proof of Theorem 1.

3 Study of the characteristic wells of the function f

In this section, one constructs two maps, $\mathbf{j}$ and $\mathsf{C}_{\mathbf{j}}$. The map $\mathbf{j}$ associates each local minimum of f in Ω with a set of relevant saddle points, here called *separating saddle points*, of f in $\overline{\Omega}$, and the map $\mathsf{C}_{\mathbf{j}}$ associates each local minimum of f in Ω with a characteristic well, here called a *critical component*, of f in Ω (see Definition 17 below). Our construction is strongly inspired by a similar construction made in [19] in the case without boundary, where the notions of separating saddle point and of critical component were defined in this setting. The depths of the wells $\mathsf{C}_{\mathbf{j}}(x)$, $x \in \mathsf{U}_0$, which can be expressed in terms of $\mathbf{j}(x)$, will finally give, up to some multiplicative factor -2, the logarithmic equivalents of the small eigenvalues of $\Delta^D_{f,h}$ (see indeed Theorems 2' and 2). The maps $\mathbf{j}$ and $\mathsf{C}_{\mathbf{j}}$ will also be used in the next section to define accurate quasi-modes for $\Delta^D_{f,h}$.

This section is organized as follows. In Section 3.1, one defines the *principal (characteristic) wells* of the function f in Ω. Then, in Section 3.2, one defines the separating saddle points of f in $\overline{\Omega}$ and the critical components of f. Finally, Section 3.3 is dedicated to the constructions of the maps $\mathbf{j}$ and $\mathsf{C}_{\mathbf{j}}$.

3.1 Principal wells of f in Ω

Definition 6. *Let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ Morse function such that $\mathsf{U}_0 \neq \emptyset$. For all $x \in \mathsf{U}_0$ (see Definition 2) and $\lambda > f(x)$, one defines*

$$\mathsf{C}(\lambda, x) \quad \textit{as the connected component of } \{f < \lambda\} \textit{ in } \overline{\Omega} \textit{ containing } x.$$

Moreover, for every $x \in \mathsf{U}_0$, one defines

$$\lambda(x) := \sup\{\lambda > f(x) \ \textit{ such that } \ \mathsf{C}(\lambda, x) \cap \partial\Omega = \emptyset\} \quad \textit{and} \quad \mathsf{C}(x) := \mathsf{C}(\lambda(x), x).$$

Since for every $x \in \mathsf{U}_0$, x is a non degenerate local minimum of f in Ω, notice that the real value $\lambda(x)$ is well defined and belongs to $(f(x), +\infty)$. The *principal wells* of the function f in Ω are then defined as follows.

Definition 7. *Let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ Morse function such that $\mathsf{U}_0 \neq \emptyset$. The set*

$$\mathcal{C} = \big\{\mathsf{C}(x),\, x \in \mathsf{U}_0\big\}$$

is called the set of principal wells of the function f in Ω. The number of principal wells is denoted by

$$\mathsf{N}_1 := \mathrm{Card}(\mathcal{C}) \in \{1, \dots, \mathsf{m}_0\}.$$

Finally, the principal wells of f in Ω (i.e. the elements of $\mathcal{C}$) are denoted by:

$$\mathcal{C} = \{\mathsf{C}_{1,1}, \dots, \mathsf{C}_{1,\mathsf{N}_1}\}.$$

In Remark 19 below, one explains why the elements of $\mathcal{C}$ are called the principal wells of f in Ω. Notice that they obviously satisfy $\partial\mathsf{C}(x) \subset \{f = \lambda(x)\}$ for every $x \in \mathsf{U}_0$. These wells satisfy moreover the following property.

Proposition 8. *Let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ Morse function such that $\mathsf{U}_0 \neq \emptyset$ and let $\mathcal{C} = \{\mathsf{C}_{1,1}, \dots, \mathsf{C}_{1,\mathsf{N}_1}\}$ be the set of its principal wells defined in Definition 7. Then, for every $k \in \{1, \dots, \mathsf{N}_1\}$, it holds:*

$$\begin{cases} \mathsf{C}_{1,k} \text{ is an open subset of } \Omega, \text{ and} \\ \text{for all } \ell \in \{1, \dots, \mathsf{N}_1\} \text{ with } \ell \neq k,\ \mathsf{C}_{1,k} \cap \mathsf{C}_{1,\ell} = \emptyset. \end{cases} \tag{27}$$

Proof. The proof of (27) is included in the proof of [10, Proposition 20]. Let us mention that in [10, Proposition 20], it is also assumed that $f|_{\partial\Omega}$ is a Morse function, but this assumption is not used in the proof of (27) there. ∎

3.2 Separating saddle points

3.2.1 Separating saddle points of f in Ω

Before giving the definition of the separating saddle points of f in Ω, let us first recall the local structure of the sublevel sets of f near a point $z \in \Omega$.

Lemma 9. *Let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ Morse function, let $z \in \Omega$, and let us recall that, for $r > 0$, $B(z, r) := \{x \in \overline{\Omega} \text{ s.t. } |x - z| < r\}$. For every $r > 0$ small enough, the following holds:*

1. *When $|\nabla f(z)| \neq 0$, the set $\{f < f(z)\} \cap B(z, r)$ is connected.*
2. *When z is a critical point of f with index $p \in \{0, \dots, d\}$, one has:*
   - *(a) if $p = 0$, i.e. if $z \in \mathsf{U}_0$, then $\{f < f(z)\} \cap B(z, r) = \emptyset$,*
   - *(b) if $p = 1$, then $\{f < f(z)\} \cap B(z, r)$ has precisely two connected components,*
   - *(c) if $p \geq 2$, then $\{f < f(z)\} \cap B(z, r)$ is connected.*

The notion of separating saddle point of f in Ω was introduced in [19, Section 4.1] for a Morse function on a manifold without boundary.

Definition 10. *Let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ Morse function. The point $z \in \Omega$ is a separating saddle point of f in Ω if it is a saddle point of f (i.e. a critical point of f of index 1) and if for every $r > 0$ small enough, the two connected components of $\{f < f(z)\} \cap B(z, r)$ are contained in different connected components of $\{f < f(z)\}$. The set of separating saddle points of f in Ω is denoted by $\mathsf{U}_1^{\mathsf{ssp}}(\Omega)$.*

With this definition, one has the following result which will be needed later to construct the maps $\mathbf{j}$ and $\mathsf{C}_{\mathbf{j}}$ in Section 3.3.

Proposition 11. *Let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ Morse function such that $\mathsf{U}_0 \neq \emptyset$. Let us consider $\mathsf{C}_{1,q}$ for $q \in \{1, \dots, \mathsf{N}_1\}$. The set $\mathsf{C}_{1,q}$ and its sublevel sets satisfy the following properties.*

1. *It holds,*

$$\text{if } \partial\mathsf{C}_{1,q} \cap \partial\Omega = \emptyset\,, \text{ i.e. if } \overline{\mathsf{C}_{1,q}} \subset \Omega, \text{ then } \partial\mathsf{C}_{1,q} \cap \mathsf{U}_1^{\mathsf{ssp}}(\Omega) \neq \emptyset. \tag{28}$$

2. *Let λ_q be such that $\mathsf{C}_{1,q}$ is a connected component of $\{f < \lambda_q\}$ (see Definitions 6 and 7). Let $\lambda \in (\min_{\overline{\mathsf{C}_{1,q}}} f, \lambda_q]$ and C be a connected component of $\mathsf{C}_{1,q} \cap \{f < \lambda\}$. Then,*

$$\big(\mathsf{C} \cap \mathsf{U}_1^{\mathsf{ssp}}(\Omega) \neq \emptyset\big) \quad \text{iff} \quad \mathsf{C} \cap \mathsf{U}_0 \text{ contains more than one point.}$$

Moreover, let us define

$$\sigma := \max_{y \in \mathsf{C} \cap \mathsf{U}_1^{\mathsf{ssp}}(\Omega)} f(y)$$

with the convention $\sigma = \min_{\overline{\mathsf{C}}} f$ when $\mathsf{C} \cap \mathsf{U}_1^{\mathsf{ssp}}(\Omega) = \emptyset$. Then, the following assertions hold.

- *For all $\mu \in (\sigma, \lambda]$, the set $\mathsf{C} \cap \{f < \mu\}$ is a connected component of $\{f < \mu\}$.*
- *If $\mathsf{C} \cap \mathsf{U}_1^{\mathsf{ssp}}(\Omega) \neq \emptyset$, one has $\mathsf{C} \cap \mathsf{U}_0 \subset \{f < \sigma\}$ and the boundary of any of the connected components of $\mathsf{C} \cap \{f < \sigma\}$ contains a separating saddle point of f in Ω (i.e. a point in $\mathsf{U}_1^{\mathsf{ssp}}(\Omega)$).*

Proof. The proof of the first item of Proposition 11 is the same as the proof of the last point of [10, Proposition 20] (see Step 5 there), while the proof of the second item of Proposition 11 is the same as the proof of [10, Proposition 22], which follows from the study of the sublevel sets of a Morse function on a manifold without boundary (since the principal wells $\mathsf{C}_{1,k}$'s are included in Ω). Again, the assumption that $f|_{\partial\Omega}$ is a Morse function made in [10] is not used in these proofs. ∎

3.2.2 Separating saddle points of f in $\overline{\Omega}$

In this section, we specify and extend Definition 10 in our setting by taking into account the boundary of Ω and the principal wells $\{\mathsf{C}_1, \ldots, \mathsf{C}_{\mathsf{N}_1}\}$ of f introduced in Definition 7. To this end, we first state the following result which describes the local structure of f near $\bigcup_{k \in \{1,\ldots,\mathsf{N}_1\}} \partial\mathsf{C}_{1,k} \cap \partial\Omega$ and which will be used to state an additional assumption on f, assumption **(H1)** below, ensuring that the critical points of f in $\partial\mathsf{C}_{1,k} \cap \partial\Omega$ are geometrical saddle points of f in $\overline{\Omega}$ (see Remark 15 below).

Proposition 12. *Let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ Morse function such that $\mathsf{U}_0 \neq \emptyset$. Let $k \in \{1, \ldots, \mathsf{N}_1\}$. Then, if $\partial\mathsf{C}_{1,k} \cap \partial\Omega \neq \emptyset$, for $z \in \partial\mathsf{C}_{1,k} \cap \partial\Omega$ (see Definition 7), one has:*

(a) If $|\nabla f(z)| \neq 0$, then z is a local minimum of $f|_{\partial\Omega}$ and $\partial_{\mathsf{n}_\Omega} f(z) > 0$.

(b) If $|\nabla f(z)| = 0$, then z is saddle point of f. In addition, if the unit outward normal vector $\mathsf{n}_\Omega(z)$ to Ω at z is an eigenvector of $\operatorname{Hess} f(z)$ associated with its negative eigenvalue, then z is a non degenerate local minimum of $f|_{\partial\Omega}$ (where $\operatorname{Hess} f(z)$ denotes the endomorphism of $T_z\overline{\Omega}$ canonically associated with the usual symmetric bilinear form $\operatorname{Hess} f(z) : T_z\overline{\Omega} \times T_z\overline{\Omega} \to \mathbb{R}$ via the metric g).

Besides, it holds,

$$\text{for all } \ell \in \{1,\dots,\mathsf{N}_1\} \text{ with } \ell \neq k,\ \overline{\mathsf{C}_{1,\ell}} \cap \overline{\mathsf{C}_{1,k}} = \partial \mathsf{C}_{1,k} \cap \partial \mathsf{C}_{1,\ell} \subset \mathsf{U}_1^{\mathsf{ssp}}(\Omega). \tag{29}$$

Remark 13. *As it will be clear from the proof of Proposition 12, the fact that $f : \overline{\Omega} \to \mathbb{R}$ is a Morse function is not needed in the proof of item (a) in Proposition 12.*

Proof. Let $z \in \partial \mathsf{C}_{1,k} \cap \partial\Omega$. Let V_z be a neighborhood of z in $\overline{\Omega}$ and let

$$p \in \mathsf{V}_z \mapsto x = (x', x_d) \in \mathbb{R}^{d-1} \times \mathbb{R}_- \tag{30}$$

be a coordinate system such that $x(z) = 0$,

$$\{p \in \mathsf{V}_z,\, x_d(p) < 0\} = \Omega \cap \mathsf{V}_z \quad \text{and} \quad \{p \in \mathsf{V}_z,\, x_d(p) = 0\} = \partial\Omega \cap \mathsf{V}_z \tag{31}$$

and

$$\forall i,j \in \{1,\dots,d\}\,,\ g_z\big(\frac{\partial}{\partial x_i}(z), \frac{\partial}{\partial x_j}(z)\big) = \delta_{ij} \quad \text{and} \quad \frac{\partial}{\partial x_d}(z) = \mathsf{n}_\Omega(z)\,. \tag{32}$$

The set $x(\mathsf{V}_z)$ is a neighborhood of 0 in $\mathbb{R}^{d-1} \times \mathbb{R}_-$. With a slight abuse of notation, the function f in the coordinates x is still denoted by f. The set $x(\mathsf{C}_{1,k} \cap \mathsf{V}_z)$ is included in $\{x_d < 0\}$ since $\mathsf{C}_{1,k} \subset \Omega$ (see Proposition 8). For ease of notation, the set $x(\mathsf{C}_{1,k} \cap \mathsf{V}_z)$ will also be denoted by $\mathsf{C}_{1,k}$. Let us now introduce a C^∞ extension of $f : x(\mathsf{V}_z) \subset \{x \in \mathbb{R}^d,\, x_d \leq 0\} \to \mathbb{R}$ to a neighborhood V_0 of 0 in $\mathbb{R}^d$ such that $\mathsf{V}_0 \cap \{x \in \mathbb{R}^d,\, x_d \leq 0\} \subset x(\mathsf{V}_z)$. In the following this extension is still denoted by f. Note that according to (32), the matrix $\operatorname{Hess} f(0)$ is then at the same time the matrix of the symmetric bilinear form $\operatorname{Hess} f(z) : T_z\overline{\Omega} \times T_z\overline{\Omega} \to \mathbb{R}$ and of its canonically associated (via the metric g) endomorphism $\operatorname{Hess} f(z) : T_z\overline{\Omega} \to T_z\overline{\Omega}$, in the basis $\big(\frac{\partial}{\partial x_1}(z), \dots, \frac{\partial}{\partial x_d}(z) = \mathsf{n}_\Omega(z)\big)$ of $T_z\overline{\Omega}$.

Let $r_0 > 0$ be such that $\{x \in \mathbb{R}^d,\, |x| < r_0\} \subset \mathsf{V}_0$ and let $r \in (0, r_0)$. To prove Proposition 12, one will both work with the initial function f and with the above associated function still denoted by f,

$$f :\, x = (x', x_d) \in \mathsf{V}_0 \subset \mathbb{R}^d \mapsto f(x) \in \mathbb{R}. \tag{33}$$

The proof of Proposition 12 is divided into several steps.

Step 1. Proof of item (a) in Proposition 12. Let us assume that $|\nabla f(z)| \neq 0$. According to Lemma 9, for all $r > 0$ small enough, the set $\{x \in \mathbb{R}^d, |x| < r \text{ and } f(x) < f(0)\}$ is connected. Let us also notice that it clearly holds

$$\emptyset \neq \mathsf{C}_{1,k} \cap \{x \in \mathbb{R}^d, |x| < r\} \subset \{x \in \mathbb{R}^d, |x| < r \text{ and } f(x) < f(0)\}.$$

Let us now prove that

$$\{x \in \mathbb{R}^d, |x| < r \text{ and } f(x) < f(0)\} \subset \{x_d < 0\}. \tag{34}$$

If it is not the case, there exists $y_2 \in \{x \in \mathbb{R}^d, |x| < r\}$ such that $x_d(y_2) \geq 0$ and $f(y_2) < f(0)$. The set $\{x \in \mathbb{R}^d, |x| < r \text{ and } f(x) < f(0)\}$ is connected and thus, since

it is locally path-connected, it is path-connected. Then, let $y_1 \in \mathsf{C}_{1,k} \cap \{x \in \mathbb{R}^d, |x| < r\}$ and consider a continuous curve $\gamma : [0,1] \to \{x \in \mathbb{R}^d, |x| < r \text{ and } f(x) < f(0)\}$ such that $\gamma(0) = y_1$ and $\gamma(1) = y_2$. Let us define $t_0 := \inf\{t \geq 0,\, x_d(\gamma(t)) \geq 0\}$. Since $x_d(\gamma(0)) < 0$ and $x_d(\gamma(1)) \geq 0$, it holds $t_0 > 0$. Then, for all $t \in [0, t_0]$, it holds $x_d(\gamma(t)) \leq 0$ (with equality if and only if $t = t_0$), $|\gamma(t)| < r$, and $f(\gamma(t)) < f(0)$. Therefore, since by definition $\mathsf{C}_{1,k}$ is a connected component of $\{q \in \overline{\Omega}, f(q) < f(z)\}$, it holds $\gamma(t_0) \in \mathsf{C}_{1,k} \subset \{x_d < 0\}$. This contradicts $x_d(\gamma(t_0)) = 0$ and proves (34). Hence, since $\mathsf{C}_{1,k}$ is a connected component of $\{f < f(z)\}$ in Ω which intersects the connected set $p(\{x \in \mathbb{R}^d, |x| < r \text{ and } f(x) < f(0)\}) \subset \Omega$, it holds

$$\mathsf{C}_{1,k} \cap \{x \in \mathbb{R}^d, |x| < r\} = \{x \in \mathbb{R}^d, |x| < r \text{ and } f(x) < f(0)\}. \tag{35}$$

Equations (31) and (34) imply that z is a local minimum of $f|_{\partial\Omega}$. Using in addition the fact that $|\nabla f(z)| \neq 0$, it holds $\partial_{\mathsf{n}_\Omega} f(z) \neq 0$ and hence $\partial_{\mathsf{n}_\Omega} f(z) > 0$, since $\partial_{\mathsf{n}_\Omega} f(z) < 0$ would imply that z is a local minimum of f in $\overline{\Omega}$ which would thus not belong to $\overline{\mathsf{C}_{1,k}}$. This proves item (a) in Proposition 12. Let us mention that one can prove in addition that $\partial\Omega$ and $\partial\mathsf{C}_{1,k}$ are tangent at z.

Step 2. Proof of item (b) in Proposition 12. Let us now assume that $|\nabla f(z)| = 0$.

Step 2a. Let us prove that 0 is a saddle point of $f : \mathsf{V}_0 \to \mathbb{R}$. The point 0 is a non degenerate critical point of f. Moreover, because 0 is not a local minimum of f in $\{x_d \leq 0\}$ (since $0 \in \partial\mathsf{C}_{1,k}$), $\operatorname{Hess} f(0)$ has at least one negative eigenvalue. To prove that 0 is a saddle point of f, let us argue by contradiction: assume that $\operatorname{Hess} f(0)$ has at least two negative eigenvalues. Then, according to Lemma 9 (with $p \geq 2$ there), for all $r \in (0, r_0)$ small enough, the set $\{x \in \mathbb{R}^d, f(x) < f(0)\} \cap \{x \in \mathbb{R}^d, |x| < r\}$ is connected. In particular, the same arguments as those used to prove (34) and (35) imply that:

$$\mathsf{C}_{1,k} \cap \{x \in \mathbb{R}^d, |x| < r\} = \{x \in \mathbb{R}^d, |x| < r \text{ and } f(x) < f(0)\} \subset \{x_d < 0\}. \tag{36}$$

To conclude, let us now prove that

$$\{x \in \mathbb{R}^d, |x| < r \ \text{ and } f(x) < f(0)\} \cap \{x \in \mathbb{R}^d, x_d = 0\} \neq \emptyset, \tag{37}$$

which will contradict (36). To this end, let $(\mathsf{e}_1, \mathsf{e}_2, \ldots, \mathsf{e}_d) \subset \mathbb{R}^d$ be an orthonormal basis of eigenvectors of $\operatorname{Hess} f(0)$ associated with its eigenvalues $(\mu_1, \ldots, \mu_d)$ ordered such that $\mu_1 < 0$ and $\mu_2 < 0$. Since $\{x_d = 0\}$ is a $d-1$ dimensional vector space, there exists $\mathsf{v} \in \{x_d = 0\} \cap \operatorname{Span}(\mathsf{e}_1, \mathsf{e}_2) \setminus \{0\}$. An order 2 Taylor expansion then shows that $f(t\,\mathsf{v}) < f(0)$ for every $t > 0$ small enough, which implies (37) since $t\,\mathsf{v} \in \{x_d = 0\}$. Thus, $\operatorname{Hess} f(0)$ has only one negative eigenvalue, i.e. 0 is a saddle point of f.

Step 2b. Let us now end the proof of item (b) in Proposition 12. The point 0 is clearly a critical point of $f|_{\{x_d=0\}}$ since it is a critical point, and more precisely a saddle point by the above analysis, of $f : \mathsf{V}_0 \to \mathbb{R}$. Let us also emphasize here that without any additional assumption, 0 is not necessarily a non degenerate critical point of $f|_{\{x_d=0\}}$, nor a local minimum of $f|_{\{x_d=0\}}$ (see indeed Remark 16 below). Let us now make

the following additional assumption: let us assume that the unit outward normal vector $\mathsf{n}_\Omega(z)$ is an eigenvector of $\operatorname{Hess} f(z)$ associated with its negative eigenvalue. According to (31) and (32), this means that $\mathsf{e}_d = (0, \dots, 0, 1) \in \mathbb{R}^d$ is an eigenvector of $\operatorname{Hess} f(0)$ associated with its unique negative eigenvalue. Since in the Euclidean space $\mathbb{R}^d$, it holds $\{x_d = 0\} = \mathsf{e}_d^\perp$, it follows that $\operatorname{Hess} f|_{\{x_d=0\}}(0)$ is positive definite and hence that 0 is a non degenerate local minimum of $f|_{\{x_d=0\}}$. This concludes the proof of item (b) in Proposition 12.

Step 3. Proof of the relation (29). Let us recall that for every k, the set $\mathsf{C}_{1,k}$ is an open subset of Ω such that for all $\ell \neq k$, it holds $\mathsf{C}_{1,\ell} \cap \mathsf{C}_{1,k} = \emptyset$ (see Proposition 8), and hence $\overline{\mathsf{C}_{1,\ell}} \cap \overline{\mathsf{C}_{1,k}} = \partial \mathsf{C}_{1,\ell} \cap \partial \mathsf{C}_{1,k}$. The proof of (29) is divided into two steps.

Step 3a. Let us prove that for all $\ell \in \{1, \dots, \mathsf{N}_1\}$, $\ell \neq k$, it holds

$$\partial \mathsf{C}_{1,\ell} \cap \partial \mathsf{C}_{1,k} \subset \Omega. \tag{38}$$

To this end, let us consider $z \in \partial \mathsf{C}_{1,k} \cap \partial\Omega$. Let us work again in the x-coordinates satisfying (30) and (31), and with the function

$$f : x = (x', x_d) \in \mathsf{V}_0 \subset \mathbb{R}^d \mapsto f(x) \in \mathbb{R}$$

which was introduced in (33).

Let us first consider the case when $|\nabla f(0)| \neq 0$. Let us recall that according to Lemma 9 and (35), for $r > 0$ small enough, $\{x \in \mathbb{R}^d, |x| < r \text{ and } f(x) < f(0)\}$ is connected and equals $\mathsf{C}_{1,k} \cap \{x \in \mathbb{R}^d, |x| < r\}$. Let $\ell \in \{1, \dots, \mathsf{N}_1\}$, $\ell \neq k$. Since in addition $\mathsf{C}_{1,\ell} \cap \mathsf{C}_{1,k} = \emptyset$, one has $0 \notin \partial \mathsf{C}_{1,\ell}$. This concludes the proof of (38) when $|\nabla f(0)| \neq 0$.

Let us now consider the case when $|\nabla f(0)| = 0$. According to item (b), 0 is a saddle point of f. According to Lemma 9 and since 0 is a non degenerate saddle point of f, for $r > 0$ small enough, $\{x \in \mathbb{R}^d, |x| < r \text{ and } f(x) < f(0)\}$ has two connected components which are denoted by A_1 and A_2. To prove (38), let us argue by contradiction and let us assume that $0 \in \partial \mathsf{C}_{1,\ell} \cap \partial \mathsf{C}_{1,k}$ for some $\ell \in \{1, \dots, \mathsf{N}_1\}$ with $\ell \neq k$. Since both $\mathsf{C}_{1,k}$ and $\mathsf{C}_{1,\ell}$ meet $\mathsf{A}_1 \cup \mathsf{A}_2$, the same arguments as those used to prove (34) and (35) then lead, up to switching A_1 and A_2, to

$$\mathsf{C}_{1,k} \cap \{x \in \mathbb{R}^d, |x| < r\} = \mathsf{A}_1 \quad \text{and} \quad \mathsf{C}_{1,\ell} \cap \{x \in \mathbb{R}^d, |x| < r\} = \mathsf{A}_2$$

and to

$$\{x \in \mathbb{R}^d, |x| < r \text{ and } f(x) < f(0)\} = \mathsf{A}_1 \cup \mathsf{A}_2 \subset \{x_d < 0\}. \tag{39}$$

This imposes that the eigenvector e_d of $\operatorname{Hess} f(0)$ associated with its negative eigenvalue satisfies

$$\mathsf{e}_d \in \{x_d = 0\}.$$

Indeed, if it was not the case, an order 2 Taylor expansion of $t \mapsto f(t\,\mathsf{e}_d)$ at $t = 0$ would imply that $f - f(0)$ admits negative values in $\{x_d > 0\} \cap \{|x| < r\}$ for every $r > 0$, contradicting (39). Thus, $\mathsf{e}_d \in \{x_d = 0\}$. Then, the order 2 Taylor expansion of

$t \mapsto f(t\,\mathsf{e}_d)$ at $t=0$ shows that $f-f(0)$ admits negative values in $\{x_d=0\}\cap\{|x|<r\}$ for every $r>0$, which also contradicts (39). This concludes the proof of (38) when $|\nabla f(0)|=0$.

Step 3b. Proof of (29). According to (38), for all $\ell \neq k$, it holds $\partial\mathsf{C}_{1,k}\cap\partial\mathsf{C}_{1,\ell}\subset\Omega$. Let us now consider $z\in\partial\mathsf{C}_{1,k}\cap\partial\mathsf{C}_{1,\ell}$ when the latter set in non empty, which implies that $\mathsf{C}_{1,k}$ and $\mathsf{C}_{1,\ell}$ are two connected components of $\{f<f(z)\}$. Then, for $r>0$ small enough, $\{f<f(z)\}\cap B(z,r)$ has at least two connected components, respectively included in $\mathsf{C}_{1,k}$ and in $\mathsf{C}_{1,\ell}$. From Lemma 9, z is then a saddle point of f and, according to Definition 10, it thus belongs to $\mathsf{U}_1^{\mathsf{ssp}}(\Omega)$. This concludes the proof of (29) and then the proof of Proposition 12. ∎

We are now in position to state the following assumption which will be used to construct the maps $\mathbf{j}$ and $\mathsf{C}_{\mathbf{j}}$ at the end of this section. Before stating it, let us recall that from item (b) in Proposition 12, any point z belonging to $\partial\mathsf{C}_{1,k}\cap\partial\Omega$ for some $k\in\{1,\dots,\mathsf{N}_1\}$ and such that $|\nabla f(z)|=0$ is a saddle point of f. Using moreover (29), such a z does not belong to $\overline{\mathsf{C}_{1,\ell}}$ when $\ell\in\{1,\dots,\mathsf{N}_1\}\setminus\{k\}$.

Assumption (H1). *The function $f:\overline{\Omega}\to\mathbb{R}$ is a C^∞ Morse function such that $\mathsf{U}_0\neq\emptyset$ and whose principal wells $\mathsf{C}_{1,1},\dots,\mathsf{C}_{1,\mathsf{N}_1}$ defined in Definition 7 satisfy the following property: for every $k\in\{1,\dots,\mathsf{N}_1\}$ and every $z\in\partial\mathsf{C}_{1,k}\cap\partial\Omega$ such that $|\nabla f(z)|=0$, the unit outward normal vector $\mathsf{n}_\Omega(z)$ to Ω at z is an eigenvector of* $\operatorname{Hess} f(z)$ *associated with its negative eigenvalue, where* $\operatorname{Hess} f(z)$ *denotes the endomorphism of $T_z\overline{\Omega}$ canonically associated with the symmetric bilinear form* $\operatorname{Hess} f(z): T_z\overline{\Omega}\times T_z\overline{\Omega}\to\mathbb{R}$ *via the metric g.*

When **(H1)** is satisfied, according to Proposition 12, the sublevel sets $\{f<f(z)\}$ have the following local structure near the points $z\in\bigcup_{k=1}^{\mathsf{N}_1}\partial\mathsf{C}_{1,k}\cap\partial\Omega$.

Corollary 14. *Let $f:\overline{\Omega}\to\mathbb{R}$ be a C^∞ Morse function satisfying* **(H1)**. *Then, for all $k\in\{1,\dots,\mathsf{N}_1\}$ such that $\partial\mathsf{C}_{1,k}\cap\partial\Omega\neq\emptyset$ and for all $z\in\partial\mathsf{C}_{1,k}\cap\partial\Omega$, one has:*

(a) If $|\nabla f(z)|\neq 0$, z is a local minimum of $f|_{\partial\Omega}$ and $\partial_{\mathsf{n}_\Omega} f(z)>0$ (see Figure 1).

(b) If $|\nabla f(z)|=0$, z is a saddle point of f and the unit outward normal vector $\mathsf{n}_\Omega(z)$ to Ω at z is an eigenvector of $\operatorname{Hess} f(z)$ *associated with its negative eigenvalue. Moreover, the point z is a non degenerate local minimum of $f|_{\partial\Omega}$ (see Figure 2).*

Note that when **(H1)** is satisfied, it follows from Corollary 14 that the points $z\in\bigcup_{k=1}^{\mathsf{N}_1}\partial\mathsf{C}_{1,k}\cap\partial\Omega$ such that $|\nabla f(z)|=0$ are isolated in $\bigcup_{k=1}^{\mathsf{N}_1}\partial\mathsf{C}_{1,k}\cap\partial\Omega$. Indeed, they are non degenerate critical points of $f|_{\partial\Omega}$ and $\bigcup_{k=1}^{\mathsf{N}_1}\partial\mathsf{C}_{1,k}\cap\partial\Omega$ is composed of critical points of $f|_{\partial\Omega}$. Note also that this is in general not the case for the points $z\in\bigcup_{k=1}^{\mathsf{N}_1}\partial\mathsf{C}_{1,k}\cap\partial\Omega$ such that $|\nabla f(z)|\neq 0$.

Remark 15. *When* **(H1)** *holds, it follows from items (a) and (b) in Corollary 14 that the elements of $\bigcup_{k=1}^{\mathsf{N}_1}\big(\partial\mathsf{C}_{1,k}\cap\partial\Omega\big)$ play geometrically the role of saddle points of f in $\overline{\Omega}$. Indeed, when f is extended by $-\infty$ outside $\overline{\Omega}$ (this extension is consistent with the*

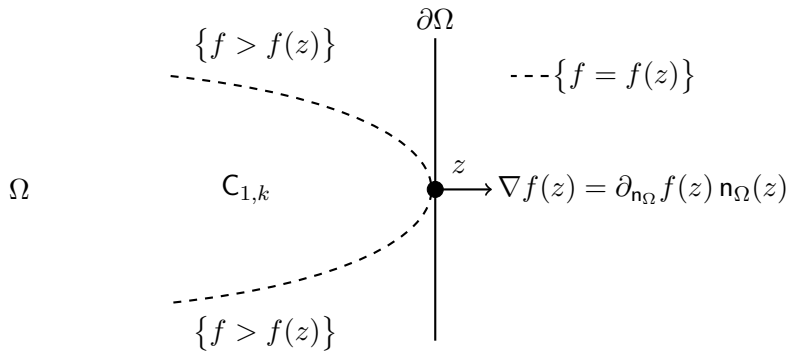

Figure 1: Behaviour of f in a neighborhood of $z \in \partial\mathsf{C}_{1,k} \cap \partial\Omega$ when $|\nabla f(z)| \neq 0$ and z is isolated in $\partial\mathsf{C}_{1,k} \cap \partial\Omega$.

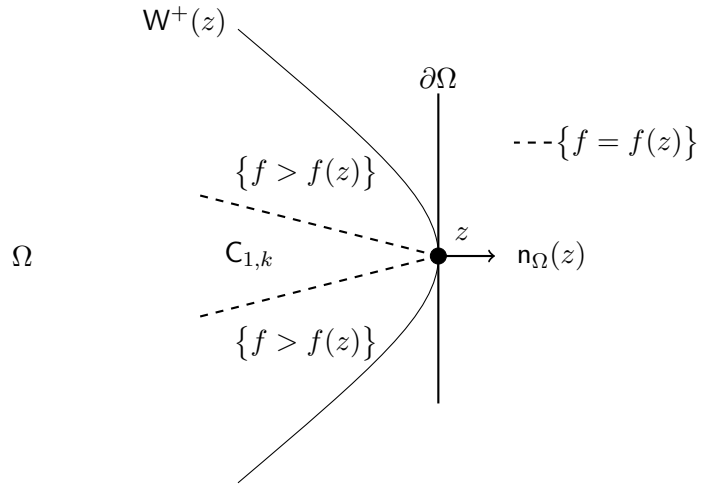

Figure 2: Behaviour of f in a neighborhood of $z \in \partial\mathsf{C}_{1,k} \cap \partial\Omega$ when $|\nabla f(z)| = 0$ and **(H1)** *is satisfied. On this figure, $\mathsf{W}^+(z)$ is the stable manifold of z for the dynamics $\dot{X} = -\nabla f(X)$.*

Dirichlet boundary conditions used to define $\Delta^D_{f,h}$), the points $z \in \bigcup_{k=1}^{\mathsf{N}_1} \partial\mathsf{C}_{1,k} \cap \partial\Omega$ are local minima of $f|_{\partial\Omega}$ and local maxima of $f|_{D_z}$, where D_z is the straight line passing through z and orthogonal to $\partial\Omega$ at z. Note however that when $|\nabla f(z)| \neq 0$, z can be a degenerate local minimum of $f|_{\partial\Omega}$ (which can even be constant around z). This extends the definition of generalized saddle points *of f in $\partial\Omega$ as introduced in [17, Definition 3.2.2] to the case when $f|_{\partial\Omega}$ is not a Morse function and f has critical points on $\partial\Omega$. Moreover, when* **(H1)** *does not hold, the points $z \in \bigcup_{k=1}^{\mathsf{N}_1} \partial\mathsf{C}_{1,k} \cap \partial\Omega$ such that $|\nabla f(z)| = 0$, which are thus saddle points of f according to Proposition 12, do actually not necessarily play the role of saddle points of f in $\overline{\Omega}$ in the above sense, as explained in Remark 16 below.*

Remark 16. *Let $k \in \{1, \ldots, \mathsf{N}_1\}$ and $z \in \partial\mathsf{C}_{1,k} \cap \partial\Omega$ be such that $|\nabla f(z)| = 0$. We recall that, according to Proposition 12, z is a saddle point of f, and that, by*

Corollary 14, when $\mathsf{n}_\Omega(z)$ *is an eigenvector of* $\operatorname{Hess} f(z)$ *associated with its negative eigenvalue,* z *is a local minimum of* $f|_{\partial\Omega}$ *and thus a geometrical saddle point of* f *in* $\overline{\Omega}$ *in the sense of Remark 15. We show below that the latter property fails to be true in general when* $z \in \partial\mathsf{C}_{1,k} \cap \partial\Omega$ *is only assumed to be a critical point, and is hence a saddle point, of* f*. To this end, let us consider, in the canonical basis* $(\mathsf{e}_x, \mathsf{e}_y)$ *of* $\mathbb{R}^2$*, the Morse function*

$$\psi(x, y) = y^2 - x^2\,,$$

whose only critical point in $\mathbb{R}^2$ *is* 0 *and is a saddle point. Let us then introduce the two vectors*

$$\mathsf{u} = \frac{1}{\sqrt{2}}(\mathsf{e}_x - \mathsf{e}_y) \text{ and } \mathsf{v} = \frac{1}{\sqrt{2}}(\mathsf{e}_x + \mathsf{e}_y).$$

In the orthonormal basis (u, v)*, the function* ψ *writes* $\psi(u, v) = -2uv$*. Hence, defining the smooth curve*

$$\Gamma := \{p = (u, u^2) \text{ in the basis } (\mathsf{u}, \mathsf{v}), u \in \mathbb{R}\} \text{ (see Figure 3)},$$

it holds $\psi|_\Gamma : p = (u, u^2) \in \Gamma \mapsto -2u^3$ *and* 0 *is then not a local minimum of* $f|_\Gamma$*. In particular, if, in a neighborhood of* 0 *in* $\mathbb{R}^2$*,* $\partial\Omega$ *coincides with* Γ *and* Ω *is chosen such that* $\mathsf{n}_\Omega(0) = \mathsf{v}$*, and if* $f = \psi$*, then, locally around* 0 *in* $\overline{\Omega}$*,* $\{f < 0\} \cap \{x < 0\}$ *is a connected component of* $\{f < 0\}$ *included in* Ω *such that* $\overline{\{f < 0\} \cap \{x < 0\}} \cap \partial\Omega = \{0\}$ *but* 0 *is not a local minimum of* $f|_{\partial\Omega}$ *(see Figure 3).*

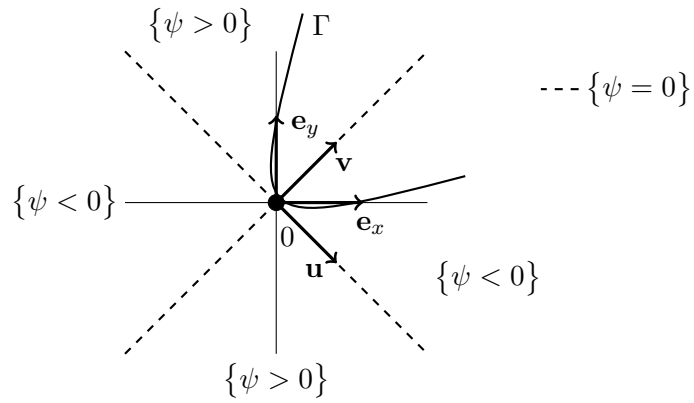

Figure 3: The function ψ *and the curve* Γ *in a neighborhood of* 0 *in* $\mathbb{R}^2$*.*

When **(H1)** holds, one adapts the definition of a separating saddle point of f in Ω given in Definition 10 to our setting by: i) only considering the relevant elements of $\mathsf{U}_1^{\mathsf{ssp}}(\Omega)$ for our study, and ii) taking into account the points in $\bigcup_{i=1}^{\mathsf{N}_1} \partial\mathsf{C}_i \cap \partial\Omega$ which are, according to Remark 15, geometrical saddle points of f in $\overline{\Omega}$. Note in particular that with this definition of $\mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega})$ given below, it does not hold $\mathsf{U}_1^{\mathsf{ssp}}(\Omega) \subset \mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega})$ in general.

Definition 17. *Let* $f : \overline{\Omega} \to \mathbb{R}$ *be a* C^∞ *Morse function satisfying* **(H1)** *and let* $\mathsf{C}_{1,1}, \ldots, \mathsf{C}_{1,\mathsf{N}_1}$ *be its principal wells defined in Definition 7.*

1. *A point $z \in \overline{\Omega}$ is a separating saddle point of f in $\overline{\Omega}$ if*

$$\text{either } z \in \bigcup_{k=1}^{\mathsf{N}_1} \left(\overline{\mathsf{C}_{1,k}} \cap \mathsf{U}_1^{\mathsf{ssp}}(\Omega) \right), \text{ or } z \in \bigcup_{k=1}^{\mathsf{N}_1} \left(\partial \mathsf{C}_{1,k} \cap \partial\Omega \right).$$

Notice that in the first case $z \in \Omega$ whereas in the second case $z \in \partial\Omega$. The set of separating saddle points of f in $\overline{\Omega}$ is denoted by $\mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega})$.

2. *For any $\sigma \in \mathbb{R}$, a connected component C of the sublevel set $\{f < \sigma\}$ in $\overline{\Omega}$ is called a critical connected component of f if $\partial\mathsf{C} \cap \mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega}) \neq \emptyset$. The family of critical connected components is denoted by $\mathcal{C}_{crit}$.*

Equation (28) and item 1 in Definition 17 imply that the principal wells $(\mathsf{C}_{1,\ell})_{\ell \in \{1,\ldots\ldots,\mathsf{N}_1\}}$ are critical connected components, as stated in the next corollary. This will be used in the first step of the construction of the maps $\mathbf{j}$ and $\mathsf{C}_{\mathbf{j}}$.

Corollary 18. *Let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ Morse function satisfying* **(H1)**. *Then, it holds:*

$$\text{for all } \ell \in \{1, \ldots, \mathsf{N}_1\}, \ \ \partial\mathsf{C}_{1,\ell} \cap \mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega}) \neq \emptyset.$$

3.3 Construction of the maps j and $\mathsf{C}_{\mathbf{j}}$

Let us now construct the maps $\mathbf{j}$ and $\mathsf{C}_{\mathbf{j}}$, which respectively associate each local minimum of f in Ω with a set of $\mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega})$ and with an element of $\mathcal{C}_{crit}$ (see Definition 17). We closely follow the presentation of [10, Section 2.4] in the case when f does not have any critical point on the boundary and $f|_{\partial\Omega}$ is a Morse function and which was inspired by [19] in the case without boundary.

Let us assume that $f : \overline{\Omega} \to \mathbb{R}$ is a C^∞ Morse function satisfying **(H1)** (and thus such that $\mathsf{U}_0 \neq \emptyset$.) The maps $\mathbf{j}$ and $\mathsf{C}_{\mathbf{j}}$ are then defined recursively as follows.

1. Initialization ($q = 1$). Let us consider the principal wells $\mathsf{C}_{1,1}, \ldots, \mathsf{C}_{1,\mathsf{N}_1}$ of f in Ω (see Definition 7).

For every $\ell \in \{1, \ldots, \mathsf{N}_1\}$, let us choose

$$x_{1,\ell} \in \arg\min_{\mathsf{C}_{1,\ell}} f.$$

Then, for all $\ell \in \{1, \ldots, \mathsf{N}_1\}$, one defines

$$\kappa_{1,\ell} := \max_{\overline{\mathsf{C}_{1,\ell}}} f, \quad \mathsf{C}_{\mathbf{j}}(x_{1,\ell}) := \mathsf{C}_{1,\ell}, \text{ and } \mathbf{j}(x_{1,\ell}) := \partial\mathsf{C}_{1,\ell} \cap \mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega}). \tag{40}$$

From Definitions 6 and 7, $\partial\mathsf{C}_{\mathbf{j}}(x_{1,\ell}) \subset \{f = \kappa_{1,\ell}\}$ for all $\ell \in \{1, \ldots, \mathsf{N}_1\}$. According moreover to Corollary 18, one has $\mathbf{j}(x_{1,\ell}) \neq \emptyset$ for all $\ell \in \{1, \ldots, \mathsf{N}_1\}$ and thus, $\mathsf{C}_{\mathbf{j}}(x_{1,\ell}) \in \mathcal{C}_{crit}$ (see item 2 in Definition 17). Finally, it holds from (29),

$$\forall \ell \neq q \in \{1, \ldots, \mathsf{N}_1\}^2, \ \partial\mathsf{C}_{1,\ell} \cap \partial\mathsf{C}_{1,q} \subset \mathsf{U}_1^{\mathsf{ssp}}(\Omega).$$

2. First step ($q = 2$).

From item 2 in Proposition 11, for each $\ell \in \{1, \dots, \mathsf{N}_1\}$, $\mathsf{C}_{1,\ell} \cap \mathsf{U}_0 \neq \{x_{1,\ell}\}$ if and only if $\mathsf{U}_1^{\mathsf{ssp}}(\Omega) \cap \mathsf{C}_{1,\ell} \neq \emptyset$. Consequently, one has:

$$\mathsf{U}_1^{\mathsf{ssp}}(\Omega) \bigcap \Big(\cup_{\ell=1}^{\mathsf{N}_1} \mathsf{C}_{1,\ell} \Big) \neq \emptyset \ \text{ iff } \ \{x_{1,1}, \dots, x_{1,\mathsf{N}_1}\} \neq \mathsf{U}_0.$$

If $\mathsf{U}_1^{\mathsf{ssp}}(\Omega) \bigcap \Big(\cup_{\ell=1}^{\mathsf{N}_1} \mathsf{C}_{1,\ell} \Big) = \emptyset$ (or equivalently if $\mathsf{N}_1 = \mathsf{m}_0$), the constructions of the maps $\mathbf{j}$ and $\mathsf{C}_{\mathbf{j}}$ are finished and one goes to item 4 below. If $\mathsf{U}_1^{\mathsf{ssp}}(\Omega) \bigcap \Big(\cup_{\ell=1}^{\mathsf{N}_1} \mathsf{C}_{1,\ell} \Big) \neq \emptyset$, one defines

$$\kappa_2 := \max_{x \in \mathsf{U}_1^{\mathsf{ssp}}(\Omega) \bigcap \left(\cup_{\ell=1}^{\mathsf{N}_1} \mathsf{C}_{1,\ell} \right)} f(x) \ \in \ \Big(\min_{\cup_{\ell=1}^{\mathsf{N}_1} \mathsf{C}_{1,\ell}} f, \max_{\ell \in \{1,\dots,\mathsf{N}_1\}} \kappa_{1,\ell} \Big).$$

The set

$$\bigcup_{\ell=1}^{\mathsf{N}_1} \Big(\mathsf{C}_{1,\ell} \cap \{f < \kappa_2\} \Big)$$

is then the union of finitely many connected components. We denote by $\mathsf{C}_{2,1}, \dots, \mathsf{C}_{2,\mathsf{N}_2}$ (with $\mathsf{N}_2 \geq 1$) the connected components of $\bigcup_{\ell=1}^{\mathsf{N}_1} \big(\mathsf{C}_{1,\ell} \cap \{f < \kappa_2\} \big)$ which do not contain any of the minima $\{x_{1,1}, \dots, x_{1,\mathsf{N}_1}\}$. From item 2 in Proposition 11 (applied for each $\ell \in \{1, \dots, \mathsf{N}_1\}$ with $\mathsf{C} = \mathsf{C}_{1,\ell} \cap \{f < \kappa_2\}$ there) and item 2 in Definition 17,

$$\forall \ell \in \{1, \dots, \mathsf{N}_2\}, \ \mathsf{C}_{2,\ell} \in \mathcal{C}_{crit}.$$

Let us mention that the other connected components (i.e. those containing the points $\{x_{1,1}, \dots, x_{1,\mathsf{N}_1}\}$) may be not critical. For each $1 \leq \ell \leq \mathsf{N}_2$, one then considers an element $x_{2,\ell}$ arbitrarily chosen in $\arg\min_{\overline{\mathsf{C}_{2,\ell}}} f = \arg\min_{\mathsf{C}_{2,\ell}} f$ (the equality follows from $\partial \mathsf{C}_{2,\ell} \subset \{f = \kappa_2\}$) and one defines:

$$\mathsf{C}_{\mathbf{j}}(x_{2,\ell}) := \mathsf{C}_{2,\ell} \ \text{ and } \ \mathbf{j}(x_{2,\ell}) := \partial \mathsf{C}_{2,\ell} \cap \mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega}) \, (\neq \emptyset) \subset \mathsf{U}_1^{\mathsf{ssp}}(\Omega) \cap \{f = \kappa_2\}.$$

3. Recurrence ($q \geq 3$).

If all the local minima of f in Ω have been labeled at the end of the previous step, i.e. if $\cup_{j=1}^{2} \{x_{j,1}, \dots, x_{j,\mathsf{N}_j}\} = \mathsf{U}_0$ (or equivalently if $\mathsf{N}_1 + \mathsf{N}_2 = \mathsf{m}_0$), the constructions of the maps $\mathsf{C}_{\mathbf{j}}$ and $\mathbf{j}$ are finished, all the local minima of f have been labeled and one goes to item 4 below. If it is not the case, from item 2 in Proposition 11, there exists $m \in \mathbb{N}^*$ such that

$$\text{for all } q \in \{2, \dots, m+1\}, \ \mathsf{U}_1^{\mathsf{ssp}}(\Omega) \bigcap \bigcup_{\ell=1}^{\mathsf{N}_1} \Big(\mathsf{C}_{1,\ell} \cap \{f < \kappa_q\} \Big) \neq \emptyset, \tag{41}$$

where the decreasing sequence $(\kappa_q)_{q=3,\dots,m+2}$ is defined recursively by

$$\kappa_q := \max_{x \in \mathsf{U}_1^{\mathsf{ssp}}(\Omega) \bigcap \bigcup_{\ell=1}^{\mathsf{N}_1} \left(\mathsf{C}_{1,\ell} \cap \{f < \kappa_{q-1}\} \right)} f(x) \ \in \ \Big(\min_{\cup_{\ell=1}^{\mathsf{N}_1} \mathsf{C}_{1,\ell}} f, \kappa_{q-1} \Big).$$

Let now $m^* \in \mathbb{N}^*$ be the largest $m \in \mathbb{N}^*$ such that (41) holds. Notice that m^* is well defined since the cardinal of $\mathsf{U}_1^{\mathsf{ssp}}(\Omega)$ is finite. By definition of m^*, one has moreover:

$$\mathsf{U}_1^{\mathsf{ssp}}(\Omega) \bigcap \bigcup_{\ell=1}^{\mathsf{N}_1} \Big(\mathsf{C}_{1,\ell} \cap \{f < \kappa_{m^*+2}\} \Big) = \emptyset. \tag{42}$$

Then, one repeats recursively m^* times the procedure described above defining $\big(\mathsf{C}_{2,\ell}, \mathbf{j}(x_{2,\ell}), \mathsf{C}_{\mathbf{j}}(x_{2,\ell})\big)_{1\le\ell\le\mathsf{N}_2}$: for $q \in \{2,\dots,m^*+1\}$, one defines $(\mathsf{C}_{q+1,\ell})_{\ell\in\{1,\dots,\mathsf{N}_{q+1}\}}$ as the set of the connected components of

$$\bigcup_{\ell=1}^{\mathsf{N}_1}\Big(\mathsf{C}_{1,\ell}\cap\{f<\kappa_{q+1}\}\Big)$$

which do not contain any of the local minima $\cup_{j=1}^{q}\{x_{j,1},\dots,x_{j,\mathsf{N}_j}\}$ of f in Ω which have been previously labeled. From items 1 and 2 in Proposition 11 (applied for each $\ell\in\{1,\dots,\mathsf{N}_1\}$ with $\mathsf{C}=\mathsf{C}_{1,\ell}\cap\{f<\kappa_{q+1}\}$ there),

$$\forall\ell\in\{1,\dots,\mathsf{N}_{q+1}\},\ \mathsf{C}_{q+1,\ell}\in\mathcal{C}_{crit}.$$

For $\ell\in\{1,\dots,\mathsf{N}_{q+1}\}$, we then associate with each $\mathsf{C}_{q+1,\ell}$ one point $x_{q+1,\ell}$ arbitrarily chosen in $\arg\min_{\mathsf{C}_{q+1,\ell}} f$ and we define:

$$\mathsf{C}_{\mathbf{j}}(x_{q+1,\ell}) := \mathsf{C}_{q+1,\ell}\ \text{ and }\ \mathbf{j}(x_{q+1,\ell}) := \partial\mathsf{C}_{q+1,\ell}\cap\mathsf{U}_1^{\mathsf{ssp}}(\Omega)\,(\neq\emptyset)\subset\{f=\kappa_{q+1}\}.$$

From (42) and item 2 in Proposition 11, $\mathsf{U}_0=\cup_{j=1}^{m^*+2}\{x_{j,1},\dots,x_{j,\mathsf{N}_j}\}$. Thus, all the local minima of f in Ω are labeled. This finishes the constructions of the maps $\mathbf{j}$ and $\mathsf{C}_{\mathbf{j}}$. We refer to Figures 8 and 9 in [10] to illustrate these constructions.

4. Properties of the maps j and $\mathsf{C}_{\mathbf{j}}$.

Let us now give important features of the map $\mathbf{j}$ which follow directly from its construction and which will be used in the sequel. Two maps have been defined

$$\mathsf{C}_{\mathbf{j}}\ :\ \mathsf{U}_0\longrightarrow\mathcal{C}_{crit}\quad\text{and}\quad\mathbf{j}\ :\ \mathsf{U}_0\longrightarrow\mathcal{P}(\mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega}))\tag{43}$$

which are clearly injective. For every $x\in\mathsf{U}_0$, the set $\mathbf{j}(x)$ is the set made of the separating saddle points of f in $\overline{\Omega}$ on $\partial\mathsf{C}_{\mathbf{j}}(x)$. Notice that the $\mathbf{j}(x)$, $x\in\mathsf{U}_0$, are not disjoint in general. For all $x\in\mathsf{U}_0$, the set $f(\mathbf{j}(x))$ contains exactly one value, which will be denoted by $f(\mathbf{j}(x))$. Moreover, for all $x\in\mathsf{U}_0$, it holds

$$f(\mathbf{j}(x))-f(x)>0.\tag{44}$$

Since $\cup_{\ell=1}^{\mathsf{N}_1}\mathsf{C}_{1,\ell}\subset\Omega$ (see the first statement in (27)), one has $\mathsf{C}_{\mathbf{j}}(x)\subset\Omega$ for all $x\in\mathsf{U}_0$. Moreover, only the boundaries of the principal wells can contain separating saddle points of f on $\partial\Omega$, i.e.:

$$\forall x\in\mathsf{U}_0\setminus\{x_{1,1},\dots,x_{1,\mathsf{N}_1}\},\ \ \mathbf{j}(x)\subset\mathsf{U}_1^{\mathsf{ssp}}(\Omega)\ \text{(see Definition 10)}.\tag{45}$$

In addition, for all $x,y\in\mathsf{U}_0$ such that $x\neq y$, since by construction $\mathbf{j}(y)\cap\mathbf{j}(x)=\partial\mathsf{C}_{\mathbf{j}}(y)\cap\partial\mathsf{C}_{\mathbf{j}}(x)$ (see (29)), one has two possible cases:

(i) either $\mathbf{j}(x)\cap\mathbf{j}(y)=\emptyset$, in which case either $\overline{\mathsf{C}_{\mathbf{j}}(y)}\cap\overline{\mathsf{C}_{\mathbf{j}}(x)}=\emptyset$ or, up to interchanging x with y, $\overline{\mathsf{C}_{\mathbf{j}}(y)}\subset\mathsf{C}_{\mathbf{j}}(x)$,

(ii) or $\mathbf{j}(x)\cap\mathbf{j}(y)\neq\emptyset$, in which case $f(\mathbf{j}(x))=f(\mathbf{j}(y))$ and the sets $\mathsf{C}_{\mathbf{j}}(x)$ and $\mathsf{C}_{\mathbf{j}}(y)$ are two different connected components of $\{f<f(\mathbf{j}(x))\}$.

Finally, for all $\ell \in \{1, \dots, \mathsf{N}_1\}$ and all $x \in \mathsf{U}_0 \cap \mathsf{C}_{\mathbf{j}}(x_{1,\ell}) \setminus \{x_{1,\ell}\}$, note that

$$f(x) \geq f(x_{1,\ell})\,,\ \ f(\mathbf{j}(x)) < f(\mathbf{j}(x_{1,\ell})) \ \text{ and then } \ f(\mathbf{j}(x)) - f(x) < f(\mathbf{j}(x_{1,\ell})) - f(x_{1,\ell}).$$

Let us also mention that the maps $\mathbf{j}$ and $\mathsf{C}_{\mathbf{j}}$ are not uniquely defined as soon as there exists some $\mathsf{C}_{k,\ell}$, $k \geq 1$, $\ell \in \{1, \dots, \mathsf{N}_k\}$, such that f has more than one global minimum in $\mathsf{C}_{k,\ell}$. However, this non-uniqueness has no influence on the results proven below (in particular Theorems 2 and 3).

Remark 19. *The relevant wells of the potential f for our study are the sets $\mathsf{C}_{\mathbf{j}}(x)$, $x \in \mathsf{U}_0$, and the elements of $\mathcal{C}$ (see Definition 7) are called the principal wells of f in Ω since, for any $x \in \mathsf{U}_0$, $\mathsf{C}_{\mathbf{j}}(x)$ is either an element of $\mathcal{C}$ or a subset of an element of $\mathcal{C}$.*

Let us end this section with the following result which will be used in the proof of Proposition 33 below.

Lemma 20. *Let us assume that $f : \overline{\Omega} \to \mathbb{R}$ is a C^∞ Morse function which satisfies* **(H1)**. *Let $(\mathsf{C}_{\mathbf{j}}(x))_{x \in \mathsf{U}_0}$ be as defined in* (43) *and let $k \geq 1$. Let us consider, for some $m \geq 1$, $\left\{\mathsf{C}^1, \dots, \mathsf{C}^m\right\} \subset \left\{\mathsf{C}_{\mathbf{j}}(x_{k,1}), \dots, \mathsf{C}_{\mathbf{j}}(x_{k,\mathsf{N}_k})\right\}$ such that*

$$\begin{cases} \bigcup_{\ell=1}^m \overline{\mathsf{C}^\ell} \text{ is connected, and} \\ \text{for all } \mathsf{C} \in \left\{\mathsf{C}_{\mathbf{j}}(x_{k,1}), \dots, \mathsf{C}_{\mathbf{j}}(x_{k,\mathsf{N}_k})\right\} \setminus \left\{\mathsf{C}^1, \dots, \mathsf{C}^m\right\}, \ \ \overline{\mathsf{C}} \cap \bigcup_{\ell=1}^m \overline{\mathsf{C}^\ell} = \emptyset. \end{cases}$$

Then, there exist $\ell_0 \in \{1, \dots, m\}$ and $z \in \mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega})$ such that

$$z \in \partial \mathsf{C}^{\ell_0} \setminus \Big(\cup_{\ell=1, \ell \neq \ell_0}^m \partial \mathsf{C}^\ell \Big). \tag{46}$$

Proof. Let $\left\{\mathsf{C}^1, \dots, \mathsf{C}^m\right\}$ be as in Lemma 20.

When $k = 1$, the set $\left\{\mathsf{C}_{\mathbf{j}}(x_{1,1}), \dots, \mathsf{C}_{\mathbf{j}}(x_{1,\mathsf{N}_1})\right\}$ is the set of the principal wells of f, i.e. the set $\mathcal{C}$ of Definition 7, and the proof of Lemma 46 follows exactly the same lines as the proof of [10, Lemma 21].

Let us now consider the case when $k \geq 2$. Let us first notice that according to the construction of the maps $\mathbf{j}$ and $\mathsf{C}_{\mathbf{j}}$, for all $\ell \in \{1, \dots, m\}$, C^ℓ is a connected component of $\{f < \kappa_k\}$ which has been labelled at the k-th iteration. Since $\bigcup_{\ell=1}^m \overline{\mathsf{C}^\ell}$ is connected, there exists $q \in \{1, \dots, \mathsf{N}_1\}$ such that $\bigcup_{\ell=1}^m \overline{\mathsf{C}^\ell} \subset \mathsf{C}_{1,q} = \{f < \kappa_{1,q}\}$, where, since $k \geq 2$, $\kappa_k < \kappa_{1,q}$. Since, from Corollary 18, it holds $\emptyset \neq \partial \mathsf{C}_{1,q} \cap \mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega}) \subset \{f = \kappa_{1,q}\}$, one can define $\kappa^* \in (\kappa_k, \kappa_{1,q}]$ as the minimum of the $\lambda \in (\kappa_k, \kappa_{1,q}]$ such that the connected component of $\{f < \lambda\} \cap \mathsf{C}_{1,q}$ containing $\bigcup_{\ell=1}^m \overline{\mathsf{C}^\ell}$ is critical (see Definition 17). We then define C^* as the connected component of $\{f < \kappa^*\} \cap \mathsf{C}_{1,q}$ containing $\bigcup_{\ell=1}^m \overline{\mathsf{C}^\ell}$. By definition, C^* is critical, and, from the construction of the maps $\mathbf{j}$ and $\mathsf{C}_{\mathbf{j}}$, it thus holds:

$$\mathsf{C}^* \bigcap \cup_{j=1}^{k-1} \{x_{j,1}, \dots, x_{j,\mathsf{N}_j}\} \neq \emptyset. \tag{47}$$

Moreover, since all the C^ℓ's are critical, and thus $\mathsf{C}^* \cap \mathsf{U}_1^{\mathsf{ssp}}(\Omega) \neq \emptyset$, the definitions of κ^* and C^* together with item 2 in Proposition 11 applied to $\mathsf{C} = \mathsf{C}^*$ imply that

$$\kappa_k = \max_{y \in \mathsf{C}^* \cap \mathsf{U}_1^{\mathsf{ssp}}(\Omega)} f(y),$$

where we recall that $\kappa_k < \kappa^*$. Therefore, using again item 2 in Proposition 11 with $\mathsf{C} = \mathsf{C}^*$,

$$\{f \leq \kappa_k\} \cap \mathsf{C}^* \text{ is connected} \quad \text{and} \quad \mathsf{C}^* \cap \mathsf{U}_0 \subset \{f < \kappa_k\}, \tag{48}$$

where the first claim follows from the fact that, for every $\lambda \in (\kappa_k, \kappa^*)$, $\mathsf{C}^* \cap \{f < \lambda\}$ is connected.

To prove (46), one argues by contradiction assuming that (46) is not satisfied. It then follows from the local structure of the sublevel sets of a Morse function given in Lemma 9 that there exists some open set $O \subset \Omega$ such that $O \cap \{f \leq \kappa_k\} = \bigcup_{\ell=1}^m \overline{\mathsf{C}^\ell}$ (see, in [10], the arguments used to prove Equation (50) there for more details). In other words, the connected set $\bigcup_{\ell=1}^m \overline{\mathsf{C}^\ell}$ is open in $\{f \leq \kappa_k\}$ and thus, since it is closed and then closed in $\{f \leq \kappa_k\}$, it is a connected component of $\{f \leq \kappa_k\}$. It thus follows from (48) that $\{f \leq \kappa_k\} \cap \mathsf{C}^* = \bigcup_{\ell=1}^m \overline{\mathsf{C}^\ell}$ contains all the local minima of f in C^*. According to (47), this implies, since $\bigcup_{\ell=1}^m \partial\mathsf{C}^\ell$ does not contain any local minimum of f, that at least one of the C^ℓ's, $\ell \in \{1, \ldots, m\}$, does intersect $\cup_{j=1}^{k-1}\{x_{j,1}, \ldots, x_{j,\mathsf{N}_j}\}$. This leads to a contradiction since the C^ℓ's ($\ell \in \{1, \ldots, m\}$) are labelled at the k-th iteration ($k \geq 2$) and thus, each C^ℓ ($\ell \in \{1, \ldots, m\}$) does not intersect $\cup_{j=1}^{k-1}\{x_{j,1}, \ldots, x_{j,\mathsf{N}_j}\}$. This concludes the proof of Lemma 20. ∎

4 Quasi-modal construction

The aim of this section is to construct, for every $x \in \mathsf{U}_0$, a quasi-mode ψ_x associated with x, or more exactly with $\mathsf{C}_{\mathbf{j}}(x)$, and whose energy in the limit $h \to 0$ will be shown to give the asymptotic behaviour of one of the m_0 first eigenvalues of $\Delta_{f,h}^D$ as exhibited in Theorems 2' and 2.

More precisely, our quasi-modes $(\psi_x)_{x\in\mathsf{U}_0}$ are built as suitable normalisations of auxiliary functions $(\phi_x)_{x\in\mathsf{U}_0}$, which are first explicitly constructed in a neighborhood of the elements of $\mathbf{j}(x) \subset \overline{\Omega}$, and then suitably extended to $\overline{\Omega}$. This construction is partly inspired by the construction made in [9] when $\Omega = \mathbb{R}^d$, see also [5, 22, 32]. We also refer to [11, 16, 17, 19, 24, 27, 29] for related constructions.

This section is organized as follows. In Section 4.1, one introduces adapted coordinate systems in a neighborhood of the elements of $\mathbf{j}(x)$, where $x \in \mathsf{U}_0$, which then permit in Section 4.2 to construct the auxiliary functions ϕ_x in a neighborhood of $\mathbf{j}(x)$. The functions $(\phi_x)_{x\in\mathsf{U}_0}$ and $(\psi_x)_{x\in\mathsf{U}_0}$ are then defined in Section 4.3.

Before, let us introduce the following assumption which will be used throughout the rest of this work.

Assumption (H2). *The function $f : \overline{\Omega} \to \mathbb{R}$ is a C^∞ Morse function such that $\mathsf{U}_0 \neq \emptyset$. Moreover, for all $z \in \bigcup_{k=1}^{\mathsf{N}_1} \partial\mathsf{C}_{1,k} \cap \partial\Omega$ (see Definition 7) such that $|\nabla f(z)| \neq 0$ (we recall that in this case, z is a local minimum of $f|_{\partial\Omega}$ by item (a) in Proposition 12),*

$$z \text{ is a non degenerate local minimum of } f|_{\partial\Omega} \ . \tag{49}$$

When f satisfies the assumptions **(H1)** and **(H2)**, it holds

$$\mathrm{Card}\Big(\bigcup_{k=1}^{\mathsf{N}_1} \partial\mathsf{C}_{1,k} \cap \partial\Omega\Big) < \infty \quad \text{and then} \quad \mathrm{Card}\Big(\bigcup_{x\in\mathsf{U}_0} \mathbf{j}(x)\Big) < \infty. \tag{50}$$

Indeed, $\mathrm{Card}\big(\bigcup_{x\in\mathsf{U}_0} \mathbf{j}(x) \cap \Omega\big) < \infty$ since $\bigcup_{x\in\mathsf{U}_0} \mathbf{j}(x) \cap \Omega$ is composed of non degenerate saddle points of f in Ω (see the construction of the map $\mathbf{j}$ in Section 3.3 and Definition 10) and, according to item (b) in Corollary 14 and to (49), the elements of

$$\bigcup_{x\in\mathsf{U}_0} \mathbf{j}(x) \cap \partial\Omega = \bigcup_{k=1}^{\mathsf{N}_1} \partial\mathsf{C}_{1,k} \cap \partial\Omega \ \text{ are non degenerate local minima of } f|_{\partial\Omega}. \tag{51}$$

In the rest of this section, one assumes that $f : \overline{\Omega} \to \mathbb{R}$ is a C^∞ Morse function which satisfies the assumptions **(H1)** and **(H2)**.

4.1 Adapted coordinate systems

Let us recall that for any $x \in \mathsf{U}_0$, from the construction of the map $\mathbf{j}$ made in Section 3.3 and from **(H1)**–**(H2)**, $\mathbf{j}(x)$ contains saddle points of f in $\overline{\Omega}$ (see Definition 17) which are in finite number and may be of two kinds: the elements $z \in \mathbf{j}(x) \cap \partial\Omega$, such that either $|\nabla f(z)| \neq 0$ or $|\nabla f(z)| = 0$, and the elements $z \in \mathbf{j}(x) \cap \Omega$, such that $|\nabla f(z)| = 0$.

For any $x \in \mathsf{U}_0$ and $z \in \mathbf{j}(x)$, we first construct a coordinate systems in a neighborhood of z as follows.

1.a) The case when $z \in \partial\Omega$ and $|\nabla f(z)| \neq 0$.

Let us recall that, thanks to **(H2)**, z is in this case a non degenerate local minimum of $f|_{\partial\Omega}$ and that $\mu := \partial_{\mathsf{n}_\Omega} f(z) > 0$. Then, according for example to [17, Section 3.4], there exists a neighbourhood V_z of z in $\overline{\Omega}$ and a coordinate system

$$p \in \mathsf{V}_z \mapsto v = (v', v_d) = (v_1, \dots, v_{d-1}, v_d) \in \mathbb{R}^{d-1} \times \mathbb{R}_- \tag{52}$$

such that

$$v(z) = 0\,, \quad \{p \in \mathsf{V}_z,\, v_d(p) < 0\} = \Omega \cap \mathsf{V}_z,\ \{p \in \mathsf{V}_z,\, v_d(p) = 0\} = \partial\Omega \cap \mathsf{V}_z, \tag{53}$$

and

$$\forall i, j \in \{1, \dots, d\}, \quad g_z\big(\frac{\partial}{\partial v_i}(z), \frac{\partial}{\partial v_j}(z)\big) = \delta_{ij} \quad \text{and} \quad \frac{\partial}{\partial v_d}(z) = \mathsf{n}_\Omega(z), \tag{54}$$

with moreover, in the v coordinates,

$$f(v', v_d) = f(0) + \mu v_d + \frac{1}{2}(v')^T \mathrm{Hess}\, f|_{\{v_d=0\}}(0)\, v'. \tag{55}$$

For $\delta_1 > 0$ and $\delta_2 > 0$ small enough, one then defines the following neighborhood of z in $\partial\Omega$,

$$\mathsf{V}^{\delta_2}_{\partial\Omega}(z) := \{p \in \mathsf{V}_z,\, v_d(p) = 0 \text{ and } |v'(p)| \leq \delta_2\} \ \text{ (see (52)-(53))} \tag{56}$$

and the following neighbourhood of z in $\overline{\Omega}$,

$$\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z) = \big\{p \in \mathsf{V}_z, |v'(p)| \leq \delta_2 \text{ and } v_d(p) \in [-2\delta_1, 0]\big\}. \tag{57}$$

1.b) The case when $z \in \partial\Omega$ and $|\nabla f(z)| = 0$.

Let V_z be a neighborhood of z in $\overline{\Omega}$ and let

$$p \in \mathsf{V}_z \mapsto v = (v', v_d) \in \mathbb{R}^{d-1} \times \mathbb{R}_- \tag{58}$$

be a coordinate system such that

$$v(z) = 0\,, \quad \{p \in \mathsf{V}_z,\, v_d(p) < 0\} = \Omega \cap \mathsf{V}_z\,, \quad \{p \in \mathsf{V}_z,\, v_d(p) = 0\} = \partial\Omega \cap \mathsf{V}_z\,, \tag{59}$$

and

$$\forall i, j \in \{1, \ldots, d\}\,,\ g_z\big(\frac{\partial}{\partial v_i}(z), \frac{\partial}{\partial v_j}(z)\big) = \delta_{ij} \quad \text{and} \quad \frac{\partial}{\partial v_d}(z) = \mathsf{n}_\Omega(z)\,. \tag{60}$$

Let us also recall that z is a non degenerate saddle point of f in $\partial\Omega$ such that, according to **(H1)**, $\mathsf{n}_\Omega(z)$ is an eigenvector associated with the negative eigenvalue μ_d of Hess $f(z)$. Thus, denoting by $\mu_1, \ldots, \mu_{d-1}$ the positive eigenvalues of Hess $f(z)$, the coordinates $v' = (v_1, \ldots, v_{d-1})$ can be chosen so that it holds, in the v coordinates,

$$f(v) \;=\; f(0) + \frac{1}{2}\sum_{j=1}^{d} \mu_j\, v_j^2 + O(|v|^3) \;=\; f(0) + \frac{1}{2}\sum_{j=1}^{d-1} |\mu_j|\, v_j^2 - \frac{1}{2}|\mu_d|\, v_d^2 + O(|v|^3)\,. \tag{61}$$

Therefore, up to choosing V_z again smaller, one can assume that

$$\arg\min_{\overline{\mathsf{V}_z}} \big(f(v) + |\mu_d| v_d^2\big) = \{z\}. \tag{62}$$

For $\delta_1 > 0$ and $\delta_2 > 0$ small enough, one defines the following neighborhood of z in $\partial\Omega$,

$$\mathsf{V}_{\partial\Omega}^{\delta_2}(z) := \{p \in \mathsf{V}_z,\, v_d(p) = 0 \text{ and } |v'(p)| \leq \delta_2\} \ \text{(see (58)-(59))}, \tag{63}$$

and the following neighbourhood of z in $\overline{\Omega}$,

$$\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z) = \big\{p \in \mathsf{V}_z, |v'(p)| \leq \delta_2 \text{ and } v_d(p) \in [-2\delta_1, 0]\big\}. \tag{64}$$

2. The case when $z \in \Omega$.

Let us recall that in this case z is a non degenerate saddle point of f in Ω. Let $(\mathsf{e}_1, \ldots, \mathsf{e}_d)$ be an orthonormal basis of eigenvectors of Hess $f(z)$ associated with its eigenvalues $(\mu_1, \ldots, \mu_d)$ with $\mu_d < 0$ and, for all $j \in \{1, \ldots, d-1\}$, $\mu_j > 0$. Then, since e_d is normal to $\mathsf{W}_+(z)$, as in the case when $z \in \partial\Omega$ and $|\nabla f(z)| = 0$ and up to replacing e_d by $-\mathsf{e}_d$, there exists a coordinate system

$$p \in \mathsf{V}_z \mapsto v = (v', v_d) \in \mathbb{R}^{d-1} \times \mathbb{R} \tag{65}$$

such that

$$v(z) = 0\,,\ \mathsf{C_j}(x) \cap \mathsf{V}_z \subset \{p \in \mathsf{V}_z,\, v_d(p) < 0\}\,,\ \{p \in \mathsf{V}_z,\, v_d(p) = 0\} = \mathsf{W}_+(z) \cap \mathsf{V}_z, \tag{66}$$

and

$$\forall i,j \in \{1,\dots,d\}\,, \quad g_z\big(\frac{\partial}{\partial v_i}(z), \frac{\partial}{\partial v_j}(z)\big) = \delta_{ij} \quad \text{and} \quad \frac{\partial}{\partial v_d}(z) = \mathsf{e}_d, \tag{67}$$

with moreover, in the v coordinates,

$$f(v) \;=\; f(0) + \frac{1}{2}\sum_{j=1}^{d} \mu_j\, v_j^2 + O(|v|^3) \;=\; f(0) + \frac{1}{2}\sum_{j=1}^{d-1} |\mu_j|\, v_j^2 - \frac{1}{2}|\mu_d|\, v_d^2 + O(|v|^3). \tag{68}$$

Then, up to choosing V_z smaller, one can assume that

$$\arg\min_{\overline{\mathsf{V}_z}} \big(f(v) + |\mu_d| v_d^2\big) = \{z\}. \tag{69}$$

Then, for $\delta_1 > 0$ and $\delta_2 > 0$ small enough, one defines the following neighbourhood of z in $\mathsf{W}^+(z)$ (see (65) and (66)),

$$\mathsf{V}^{\delta_2}_{\mathsf{W}^+}(z) := \{p \in \mathsf{V}_z,\, v_d(p) = 0 \text{ and } |v'(p)| \le \delta_2\} \subset \mathsf{W}^+(z), \tag{70}$$

and the following neighbourhood of z in Ω,

$$\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z) = \big\{p \in \mathsf{V}_z, |v'(p)| \le \delta_2 \text{ and } v_d \in [-2\delta_1, 2\delta_1]\big\}. \tag{71}$$

Notice that one has:

$$\arg\min_{\mathsf{V}^{\delta_2}_{\mathsf{W}^+}(z)} f = \{z\}. \tag{72}$$

Some properties of these coordinate systems.

The sets defined in (57), (64), and (71) are cylinders centred at z in the respective system of coordinates. Up to choosing $\delta_1 > 0$ and $\delta_2 > 0$ smaller, one can assume that all these cylinders are two by two disjoint. Schematic representations of these sets introduced in (56)–(71) are given in Figures 4, 5 and 6.

Let us conclude this section by giving several properties of the sets previously introduced which will be needed for upcoming computations. Let us recall that, from (44), when $z \in \mathbf{j}(x)$ for some $x \in \mathsf{U}_0$, it holds $f(z) > f(x)$. Moreover, by construction of the map $\mathbf{j}$ in Section 3.3, it obviously holds $\mathsf{U}_0 \cap \cup_{x\in\mathsf{U}_0}\mathbf{j}(x) = \emptyset$. Therefore, up to choosing $\delta_1 > 0$ and $\delta_2 > 0$ small enough, the following properties are satisfied:

1. When $z \in \partial\Omega \cap \mathbf{j}(x)$ for some $x \in \mathsf{U}_0$, it holds

$$\min_{\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z)} f > f(x), \quad \mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z) \cap \mathsf{U}_0 = \emptyset, \tag{73}$$

   and

$$\arg\min_{\mathsf{V}^{\delta_2}_{\partial\Omega}(z)} f = \{z\} \quad \text{(which follows from (51))}. \tag{74}$$

2. When $z \in \Omega \cap \mathbf{j}(x)$ for some $x \in \mathsf{U}_0$, it holds:

$$\min_{\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z)} f > f(x) \text{ and } \mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z) \cap \mathsf{U}_0 = \emptyset. \tag{75}$$

The parameter $\delta_2 > 0$ is now kept fixed. Finally, using (72), (74), and up to choosing $\delta_1 > 0$ smaller, there exists $r > 0$ such that (see Figures 4, 5 and 6):

1. For all $z \in \partial\Omega \cap \mathbf{j}(x)$ for some $x \in \mathsf{U}_0$,

$$\big\{p \in \mathsf{V}_z, |v'(p)| = \delta_2 \text{ and } v_d(p) \in [-2\delta_1, 0]\big\} \subset \{f \geq f(z) + r\}. \tag{76}$$

2. For all $z \in \Omega \cap \mathbf{j}(x)$ for some $x \in \mathsf{U}_0$,

$$\big\{p \in \mathsf{V}_z, |v'(p)| = \delta_2 \text{ and } v_d \in [-2\delta_1, 2\delta_1]\big\} \subset \{f \geq f(z) + r\}. \tag{77}$$

The parameter $\delta_1 > 0$ is now kept fixed.

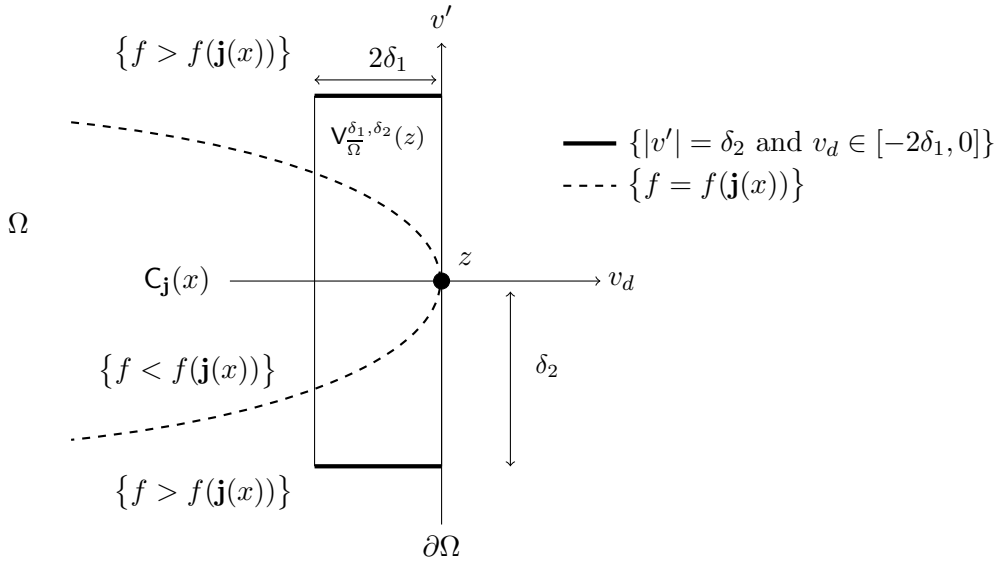

Figure 4: Schematic representation of the cylinder $\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)$, in the v-coordinates, when $z \in \mathbf{j}(x) \cap \partial\Omega$ (for some $x \in \mathsf{U}_0$) is such that $|\nabla f(z)| \neq 0$. One recalls that $\mathbf{j}(x) \subset \partial\mathsf{C}_{\mathbf{j}}(x)$ and that, in this case, z is a non degenerate local minimum of $f|_{\partial\Omega}$ and $\partial_{\mathsf{n}_\Omega} f(z) > 0$.

4.2 Quasi-modal construction near the elements of $\cup_{x\in\mathsf{U}_0}\mathbf{j}(x)$

Let us introduce an even cut-off function $\chi \in C^\infty(\mathbb{R}, [0,1])$ such that

$$\text{supp } \chi \subset [-\delta_1, \delta_1] \text{ and } \chi = 1 \text{ on } \Big[-\frac{\delta_1}{2}, \frac{\delta_1}{2}\Big]. \tag{78}$$

Let $z \in \bigcup_{x\in\mathsf{U}_0}\mathbf{j}(x)$. Then, the function φ_z associated with z and x is defined as follows:

1. Let us assume that $z \in \partial\Omega$.

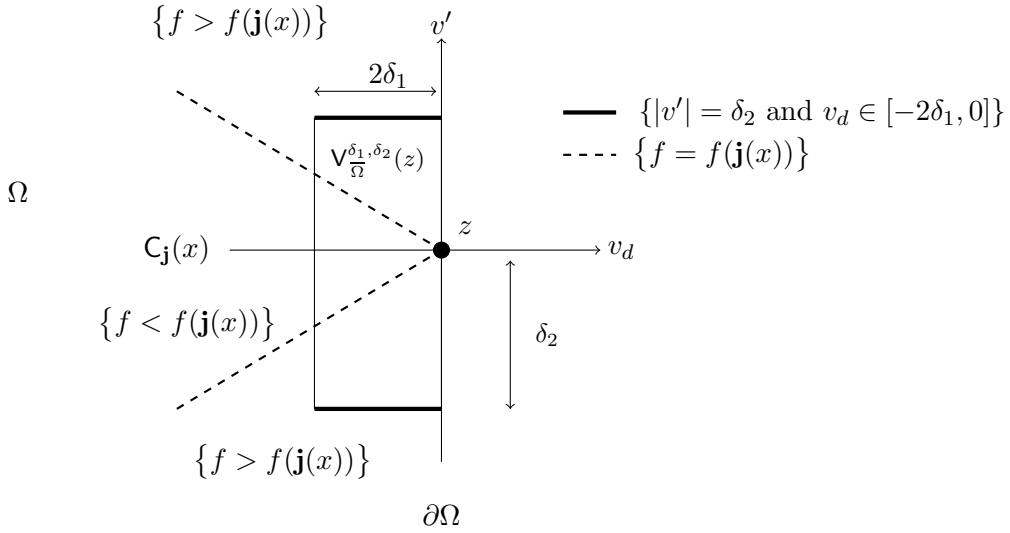

Figure 5: Schematic representation of the cylinder $\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)$, in the v-coordinates, when $z \in \mathbf{j}(x) \cap \partial\Omega$ (for some $x \in \mathsf{U}_0$) is such that $|\nabla f(z)| = 0$. One recalls that $\mathbf{j}(x) \subset \partial\mathsf{C}_{\mathbf{j}}(x)$ and that, in this case, z is a non degenerate saddle point of f and a non degenerate local minimum of $f|_{\partial\Omega}$.

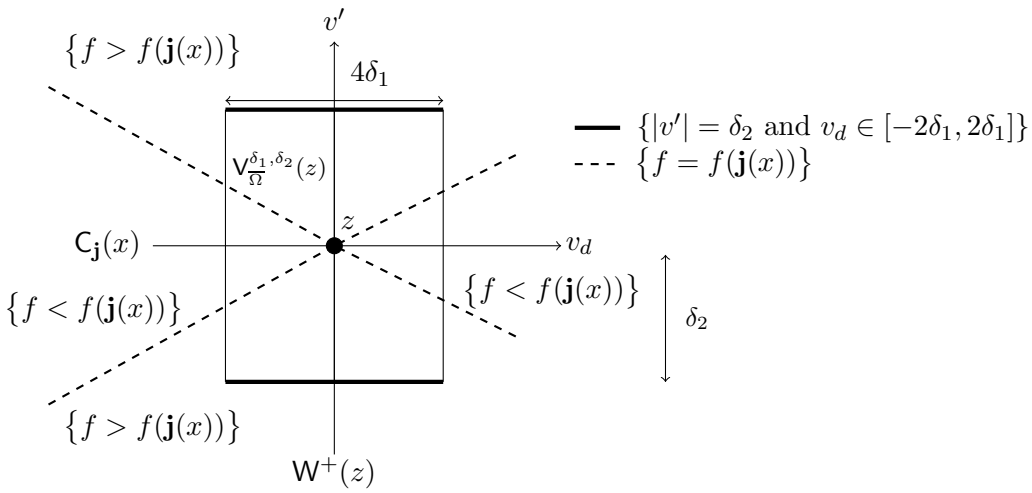

Figure 6: Schematic representation of the cylinder $\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)$, in the v-coordinates, when $z \in \mathbf{j}(x) \cap \Omega$ for some $x \in \mathsf{U}_0$. One recalls that $\mathbf{j}(x) \subset \partial\mathsf{C}_{\mathbf{j}}(x)$ and that, in this case, z is a separating saddle point of f in Ω (see Definition 10).

(a) When $|\nabla f(z)| \neq 0$, one defines (see (52), (53), and (57)):

$$\forall v = (v', v_d) \in v\big(\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)\big), \quad \varphi_z(v', v_d) := \frac{\int_{v_d}^0 \chi(t) e^{\frac{2}{h}\mu t} dt}{\int_{-2\delta_1}^0 \chi(t) e^{\frac{2}{h}\mu t} dt}, \tag{79}$$

where we recall that $\mu = \partial_{\mathsf{n}_\Omega} f(z) > 0$. Note that the function φ_z only

depends on the variable v_d. Moreover, it holds (see (78)),

$$\begin{cases} \varphi_z \in C^\infty\big(v\big(\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)\big), [0,1]\big) \text{ and} \\ \forall (v', v_d) \in v\big(\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)\big),\ \varphi_z(v', v_d) = 1 \text{ if } v_d \in [-2\delta_1, -\delta_1]. \end{cases} \tag{80}$$

(b) When $|\nabla f(z)| = 0$, one defines (see (58), (59), and (64)):

$$\forall v = (v', v_d) \in v\big(\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)\big), \quad \varphi_z(v', v_d) := \frac{\int_{v_d}^0 \chi(t) e^{-\frac{1}{h}|\mu_d|\, t^2} dt}{\int_{-2\delta_1}^0 \chi(t)\, e^{-\frac{1}{h}|\mu_d|\, t^2} dt}, \tag{81}$$

where we recall that $\mu_d < 0$ is the negative eigenvalue of Hess$f(z)$. The function φ_z thus only depends on the variable v_d and it holds

$$\begin{cases} \varphi_z \in C^\infty\big(v\big(\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)\big), [0,1]\big) \text{ and} \\ \forall (v', v_d) \in v\big(\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)\big),\ \varphi_z(v', v_d) = 1 \text{ if } v_d \in [-2\delta_1, -\delta_1]. \end{cases} \tag{82}$$

2. Let us assume that $z \in \Omega$. We recall that in this case, z is a separating saddle point of f in Ω (by construction of the map $\mathbf{j}$, see also Definition 10). Then, one defines the function (see (65), (66), and (71)):

$$\forall v = (v', v_d) \in v\big(\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)\big),\ \varphi_z(v', v_d) := \frac{\int_{v_d}^{2\delta_1} \chi(t)\, e^{-\frac{1}{h}|\mu_d|\, t^2} dt}{\int_{-2\delta_1}^{2\delta_1} \chi(t)\, e^{-\frac{1}{h}|\mu_d|\, t^2} dt}, \tag{83}$$

where μ_d is the negative eigenvalue of Hess $f(z)$. Again, φ_z only depends on the variable v_d and it holds:

$$\varphi_z \in C^\infty\Big(v\big(\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)\big), [0,1]\Big) \tag{84}$$

and for all $(v', v_d) \in v\big(\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)\big)$,

$$\varphi_z(v', v_d) = 1 \text{ if } v_d \in [-2\delta_1, -\delta_1] \text{ and } \varphi_z(v', v_d) = 0 \text{ if } v_d \in [\delta_1, 2\delta_1]. \tag{85}$$

4.3 Construction of m_0 quasi-modes for $\Delta_{f,h}^D$

In the following, one considers some arbitrary

$$x \in \mathsf{U}_0.$$

Let us recall the geometry of f near the boundary of the critical component $\partial\mathsf{C}_{\mathbf{j}}(x)$. Let us consider a point $p \in \partial\mathsf{C}_{\mathbf{j}}(x) \setminus \mathbf{j}(x)$. Since $\mathbf{j}(x) = \partial\mathsf{C}_{\mathbf{j}}(x) \cap \mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega})$ and $\partial\mathsf{C}_{\mathbf{j}}(x) \cap \partial\Omega \subset \mathbf{j}(x)$, $p \in \Omega \setminus \mathsf{U}_1^{\mathsf{ssp}}(\Omega)$. Thus, there are two possible cases:

- Either p is a saddle point of f in Ω. From Lemma 9, $\{f < f(\mathbf{j}(x))\} \cap B(p,r)$ has then, for $r > 0$ small enough, two connected components which are included in $\mathsf{C}_{\mathbf{j}}(x)$, since p is not separating (see Figure 8).

- Or p is not a saddle point of f in Ω. According to Lemma 9, $\{f < f(\mathbf{j}(x))\} \cap B(p,r)$ is then connected for $r > 0$ small enough and is thus included in $\mathsf{C}_{\mathbf{j}}(x)$.

In conclusion, when $p \in \partial \mathsf{C}_{\mathbf{j}}(x) \setminus \mathbf{j}(x)$, $\{f < f(\mathbf{j}(x))\} \cap B(p,r)$ is included in $\mathsf{C}_{\mathbf{j}}(x) \cap \Omega$ for $r > 0$ small enough. Moreover, one constructed in (57), (64), and (71), disjoint cylinders in neighborhoods of each $z \in \cup_{y \in \mathsf{U}_0} \mathbf{j}(y)$ which satisfy (73) and (75)–(77). This makes possible the construction used in the definition below.

Definition 21. *Let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ Morse function which satisfies* **(H1)** *and* **(H2)**. *Then $\mathsf{U}_0 \neq \emptyset$ and, for each $x \in \mathsf{U}_0$, there exist two C^∞ connected open sets $\Omega_1(x)$ and $\Omega_2(x)$ of Ω satisfying the following properties:*

1. *For all $x \in \mathsf{U}_0$, it holds*

$$\overline{\mathsf{C}_{\mathbf{j}}(x)} \subset \Omega_1(x) \cup \partial\Omega \quad \text{and} \quad \underset{\overline{\Omega_1(x)}}{\arg\min} f = \underset{\overline{\mathsf{C}_{\mathbf{j}}(x)}}{\arg\min} f.$$

2. *For all $x \in \mathsf{U}_0$, $\overline{\Omega_2(x)} \subset \Omega_1(x)$ and the strip $\overline{\Omega_1(x)} \setminus \Omega_2(x)$ equal:*

$$\overline{\Omega_1(x)} \setminus \Omega_2(x) = \bigcup_{z \in \mathbf{j}(x)} \mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z) \bigcup \mathsf{O}_1(x), \tag{86}$$

   where there exists $c > 0$ such that:

$$\forall q \in \mathsf{O}_1(x), \quad f(q) \geq f(\mathbf{j}(x)) + c. \tag{87}$$

   Notice that item 1, (86), (87), *and the first statements in* (73) *and in* (75) *imply that* $\underset{\overline{\Omega_1(x)}}{\arg\min} f = \underset{\overline{\Omega_2(x)}}{\arg\min} f = \underset{\mathsf{C}_{\mathbf{j}}(x)}{\arg\min} f$.

3. *For all $x, y \in \mathsf{U}_0$ such that $x \neq y$, it holds (depending on the two possible cases described in items 4.(i) and 4.(ii) in Section 3.3):*

   (i) If $\mathbf{j}(y) \cap \mathbf{j}(x) = \emptyset$:

$$\begin{cases} \text{either } \overline{\mathsf{C}_{\mathbf{j}}(y)} \cap \overline{\mathsf{C}_{\mathbf{j}}(x)} = \emptyset \text{ and } \overline{\Omega_1(x)} \cap \overline{\Omega_1(y)} = \emptyset, \\ \text{or, up to switching } x \text{ and } y, \ \overline{\mathsf{C}_{\mathbf{j}}(y)} \subset \mathsf{C}_{\mathbf{j}}(x) \text{ and } \overline{\Omega_1(y)} \subset \Omega_2(x). \end{cases}$$

   (ii) If $\mathbf{j}(y) \cap \mathbf{j}(x) \neq \emptyset$ (in this case, one recalls that $f(\mathbf{j}(y)) = f(\mathbf{j}(x))$ and thus, $\mathsf{C}_{\mathbf{j}}(y)$ and $\mathsf{C}_{\mathbf{j}}(x)$ are two connected components of $\{f < f(\mathbf{j}(x))\}$), then:

$$\overline{\Omega_1(x)} \cap \overline{\Omega_1(y)} = \bigcup_{z \in \mathbf{j}(y) \cap \mathbf{j}(x)} \mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z) \bigcup \mathsf{O}_2(x,y),$$

   where $\mathsf{O}_2(x,y) \subset \mathsf{O}_1(x)$ and $\mathsf{O}_2(x,y) \cap \mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z) = \emptyset$ for all $z \in \mathbf{j}(y) \cup \mathbf{j}(x)$.

For $x \in \mathsf{U}_0$, schematic representations of $\Omega_1(x)$, $\Omega_2(x)$, and $\mathsf{O}_1(x)$ are given in Figures 7 and 8. With the help of the sets $\Omega_1(x)$ and $\Omega_2(x)$ introduced in Definition 21, one defines a smooth function $\phi_x : \overline{\Omega} \to [0,1]$ associated with each $x \in \mathsf{U}_0$ as follows.

Definition 22. *Let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ Morse function which satisfies* **(H1)** *and* **(H2)**. *For each $x \in \mathsf{U}_0$, a function $\phi_x : \overline{\Omega} \to [0,1]$ is constructed as follows:*

1. *For every $z \in \mathbf{j}(x)$, ϕ_x is defined on the cylinder $\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)$ (see* (57), (64), *and* (71)*) by*

$$\forall p \in \mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z),\ \ \phi_x(p) := \varphi_z(v(p)), \quad \textit{see } (79), (81), \textit{ and } (83). \tag{88}$$

2. *From* (80), (82), (84), (85), *and the facts that $\overline{\Omega_2(x)} \subset \Omega_1(x)$ (see Definition 21) and* (86) *holds, ϕ_x can be extended to $\overline{\Omega}$ such that*

$$\phi_x = 0 \ \textit{on } \overline{\Omega} \setminus \Omega_1(x), \quad \phi_x = 1 \ \textit{on } \Omega_2(x), \ \textit{and } \phi_x \in C^\infty(\overline{\Omega}, [0,1]). \tag{89}$$

Notice that (89) *implies that:*

$$\operatorname{supp} d\phi_x \subset \overline{\Omega_1(x)} \setminus \Omega_2(x). \tag{90}$$

Finally, in view of (79), (81), (83), *and* (86), *ϕ_x can be chosen on O_1 such that for some $C > 0$ and for every h small enough (see indeed* (99), (105), *and* (109) *below):*

$$\forall \alpha \in \mathbb{N}^d,\ |\alpha| \in \{1,2\},\ \left\|\partial^\alpha \phi_x\right\|_{L^\infty(\mathsf{O}_1(x))} \leq \frac{C}{h^2}. \tag{91}$$

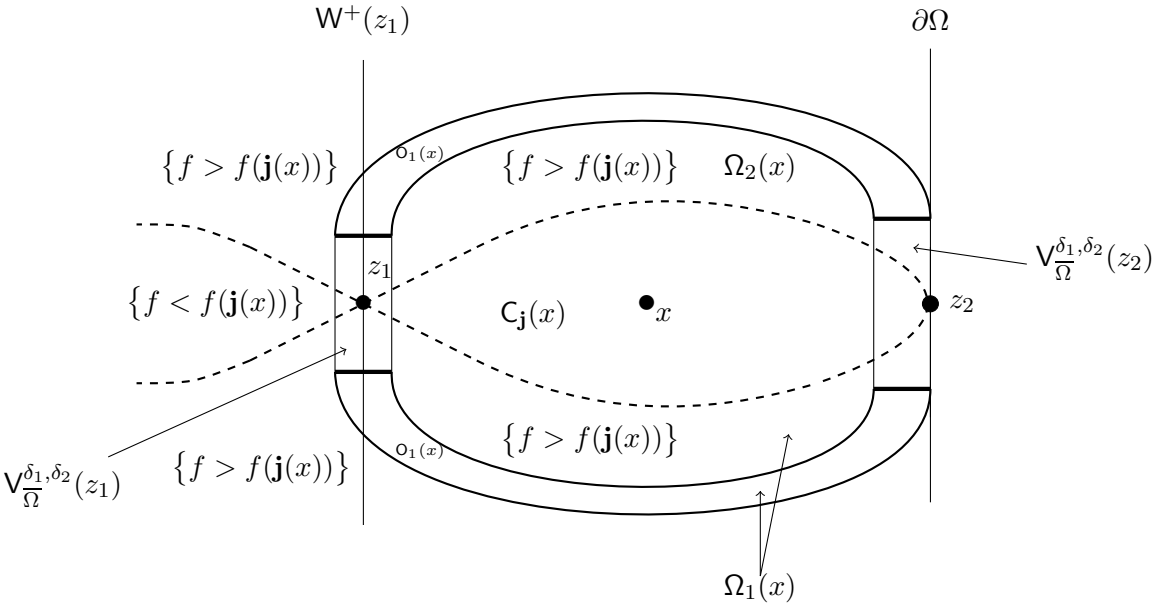

Figure 7: Schematic representation of $\Omega_2(x)$, $\Omega_1(x)$, and $\mathsf{O}_1(x)$ (see Definition 21). On the figure, $\mathbf{j}(x) = \{z_1, z_2\}$ with $z_1 \in \Omega$ and $z_2 \in \partial\Omega$ ($|\nabla f(z_2)| = 0$).

Let us now define, for each $x \in \mathsf{U}_0$, the quasi-mode $\psi_x : \overline{\Omega} \to \mathbb{R}^+$ of $\Delta_{f,h}^D$ as follows.

Definition 23. *Let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ Morse function which satisfies* **(H1)** *and* **(H2)**. *For every $x \in \mathsf{U}_0$, one defines*

$$\psi_x := \frac{\phi_x\, e^{-\frac{f}{h}}}{Z_x} \quad \textit{and} \quad Z_x := \left\|\phi_x\, e^{-\frac{f}{h}}\right\|_{L^2(\Omega)},$$

where ϕ_x is the function introduced in Definition 22.

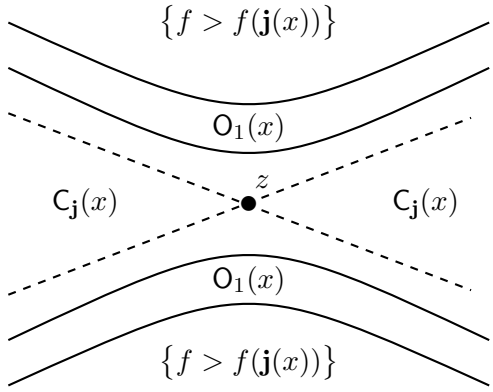

Figure 8: Schematic representation of $\mathsf{O}_1(x)$ (see (87)) in a neighborhood of a non separating saddle point z of f on $\partial\mathsf{C}_\mathbf{j}(x)$.

By construction of ϕ_x in Definition 22, $\psi_x \in C^\infty(\overline{\Omega}, \mathbb{R}^+)$ and $\psi_x = 0$ on $\partial\Omega$ (see indeed (89) together with the fact that $\Omega_1(x) \subset \Omega$, see Definition 21). In particular:

$$\psi_x \in D(\Delta^D_{f,h}) = H^2(\Omega) \cap H^1_0(\Omega). \tag{92}$$

5 Asymptotic equivalents of the small eigenvalues of $\Delta^D_{f,h}$

5.1 First quasi-modal estimates

Let us start with the following result which gives asymptotic estimates on the L^2-norms of $d_{f,h}(\psi_x)$ and of $\Delta_{f,h}(\psi_x)$ around the points $z \in \mathbf{j}(x)$ in the limit $h \to 0$.

Proposition 24. *Let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ Morse function which satisfies* **(H1)** *and* **(H2)**. *Let $x \in \mathsf{U}_0$, ψ_x be as introduced in Definition 23, and $z \in \mathbf{j}(x)$.*

1. *Let us assume that $z \in \partial\Omega$.*

   (a) *When $|\nabla f(z)| \neq 0$ (recall that in this case z is a non degenerate local minimum of $f|_{\partial\Omega}$ and $\partial_{\mathsf{n}_\Omega} f(z) > 0$, see item (a) in Corollary 14 and (49)), it holds in the limit $h \to 0$:*

$$\begin{cases} \displaystyle\int_{\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z)} \big|d_{f,h}\,\psi_x\big|^2 = \mathsf{c}_{x,z}\,\sqrt{h}\,e^{-\frac{2}{h}(f(\mathbf{j}(x))-f(x))}\big(1+O(h)\big), \\ \text{where } \mathsf{c}_{x,z} := \dfrac{2\,\partial_{\mathsf{n}_\Omega} f(z)}{\sqrt{\pi}}\,\dfrac{\big(\det \mathrm{Hess}\, f|_{\partial\Omega}(z)\big)^{-\frac{1}{2}}}{\displaystyle\sum_{q\in\arg\min_{\mathsf{C}_\mathbf{j}(x)} f}\big(\det \mathrm{Hess}\, f(q)\big)^{-\frac{1}{2}}}. \end{cases} \tag{93}$$

   Furthermore, one has when $h \to 0$:

$$\int_{\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z)} \big|\Delta_{f,h}\,\psi_x\big|^2 = O(h^2)\int_{\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z)} \big|d_{f,h}\,\psi_x\big|^2.$$

(b) *When* $|\nabla f(z)| = 0$ *(recall that in this case* z *is a saddle point of* f*, see item (b) in Corollary 14), it holds in the limit* $h \to 0$*:*

$$\begin{cases} \displaystyle\int_{\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)} \left|d_{f,h}\,\psi_x\right|^2 = \mathsf{c}_{x,z}\, h\, e^{-\frac{2}{h}(f(\mathsf{j}(x))-f(x))}\big(1+O(\sqrt{h})\big), \\ \text{where } \mathsf{c}_{x,z} := \dfrac{2\,|\mu_d|}{\pi}\dfrac{\big|\det \operatorname{Hess} f(z)\big|^{-\frac{1}{2}}}{\displaystyle\sum_{q\in\arg\min_{\mathsf{C}_{\mathsf{j}(x)}} f}\big(\det \operatorname{Hess} f(q)\big)^{-\frac{1}{2}}}, \end{cases} \tag{94}$$

where we recall that $\mu_d < 0$ *is the negative eigenvalue of* $\operatorname{Hess} f(z)$*. Moreover, when* $h \to 0$*, one has:*

$$\int_{\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)} \left|\Delta_{f,h}\,\psi_x\right|^2 = O(h^2)\int_{\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)} \left|d_{f,h}\,\psi_x\right|^2.$$

2. *Let us assume that* $z \in \Omega$ *(recall that in this case* z *is a saddle point of* f *in* Ω*). Then, it holds in the limit* $h \to 0$*:*

$$\begin{cases} \displaystyle\int_{\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)} \left|d_{f,h}\,\psi_x\right|^2 = \mathsf{c}_{x,z}\, h\, e^{-\frac{2}{h}(f(\mathsf{j}(x))-f(x))}\big(1+O(h)\big), \\ \text{where } \mathsf{c}_{x,z} := \dfrac{|\mu_d|}{\pi}\dfrac{\big|\det \operatorname{Hess} f(z)\big|^{-\frac{1}{2}}}{\displaystyle\sum_{q\in\arg\min_{\mathsf{C}_{\mathsf{j}(x)}} f}\big(\det \operatorname{Hess} f(q)\big)^{-\frac{1}{2}}}, \end{cases} \tag{95}$$

where we recall that $\mu_d < 0$ *is the negative eigenvalue of* $\operatorname{Hess} f(z)$*. Finally, when* $h \to 0$*, one has:*

$$\int_{\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)} \left|\Delta_{f,h}\,\psi_x\right|^2 = O(h^2)\int_{\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)} \left|d_{f,h}\,\psi_x\right|^2.$$

Remark 25. *The remainder term* $O(\sqrt{h})$ *in* (94) *follows from the Laplace method applied to* $\int_{\mathbb{R}^d_-\cap B(0,r)} \varphi_2\, e^{-\frac{1}{h}\varphi_1}$ *when* $|\nabla\varphi_1(0)| = 0$*,* $\operatorname{Hess}\varphi_1(0) > 0$*, and* 0 *is the unique minimum of* φ_1 *on* $\overline{B(0,r)}$*, see* (106) *and the lines below (when* $d = 1$*, this is also known as Watson's lemma). On the other hand, the* $O(h)$ *in* (95) *arises from the standard Laplace method, i.e. when considering* $\int_{B(0,r)} \varphi_2\, e^{-\frac{1}{h}\varphi_1}$*. In particular, these remainder terms are optimal.*

Proof. Let $x \in \mathsf{U}_0$. Then, according to Definitions 23 and 22, one has

$$Z_x^2 = \int_\Omega \phi_x^2\, e^{-\frac{2}{h}} = \int_{\Omega_1(x)} \phi_x^2\, e^{-\frac{2}{h}f} = \int_{\Omega_2(x)} \phi_x^2\, e^{-\frac{2}{h}f} + \int_{\Omega_1(x)\setminus\Omega_2(x)} \phi_x^2\, e^{-\frac{2}{h}f}.$$

Let us recall that by construction $0 \le \phi_x \le 1$ on Ω. Moreover, from the first statements in (73) and (75) together with (86) and (87), there exists $c > 0$ such that $f \ge f(x) + c$ on $\overline{\Omega_1(x)} \setminus \Omega_2(x)$. Thus, it holds, for some $C > 0$ independent of h:

$$\int_{\Omega_1(x)\setminus\Omega_2(x)} \phi_x^2\, e^{-\frac{2}{h}f} \le C e^{-\frac{2}{h}(f(x)+c)}.$$

In addition, since $\phi_x = 1$ on $\Omega_2(x)$ (see (89)) and

$$\underset{\overline{\Omega_1(x)}}{\arg\min} f = \underset{\overline{\Omega_2(x)}}{\arg\min} f = \underset{\mathsf{C}_{\mathbf{j}}(x)}{\arg\min} f \quad \text{(see item 2 in Definition 21)}$$

consists in a finite number of non degenerate local minima q of f in Ω such that $f(q) = f(x)$ (since by construction of $\mathsf{C}_{\mathbf{j}}$, $x \in \arg\min_{\mathsf{C}_{\mathbf{j}}(x)} f$), one has when $h \to 0$, using the Laplace method,

$$\int_{\Omega_2(x)} \phi_x^2 \, e^{-\frac{2}{h} f} = \sum_{q \in \underset{\mathsf{C}_{\mathbf{j}}(x)}{\arg\min} f} \frac{(\pi\, h)^{\frac{d}{2}}}{\sqrt{\det \operatorname{Hess} f(q)}} \, e^{-\frac{2}{h} f(x)} \big(1 + O(h)\big).$$

Therefore, when $h \to 0$,

$$Z_x = (\pi\, h)^{\frac{d}{4}} \Big(\sum_{q \in \arg\min_{\mathsf{C}_{\mathbf{j}}(x)} f} \big(\det \operatorname{Hess} f(q) \big)^{-\frac{1}{2}} \Big)^{\frac{1}{2}} \, e^{-\frac{1}{h} f(x)} \big(1 + O(h)\big). \tag{96}$$

Let now z belong to $\mathbf{j}(x)$. The rest of the proof of Proposition 24 is divided into two steps, whether $z \in \partial\Omega$ or $z \in \Omega$.

Step 1.a) The case when $z \in \partial\Omega$ and $|\nabla f(z)| \neq 0$.

In this case, from Definition 23, one has

$$\int_{\mathsf{V}_{\overline{\Omega}}^{\delta_1, \delta_2}(z)} \big| d_{f,h}\, \psi_x \big|^2 = h^2 \frac{\int_{\mathsf{V}_{\overline{\Omega}}^{\delta_1, \delta_2}(z)} \big| d\phi_x \big|^2 \, e^{-\frac{2}{h} f}}{Z_x^2}. \tag{97}$$

Moreover, according to (88) and to (79), it holds:

$$\int_{\mathsf{V}_{\overline{\Omega}}^{\delta_1, \delta_2}(z)} \big| d\phi_x \big|^2 \, e^{-\frac{2}{h} f} = \frac{\int_{|v'| \leq \delta_2} \int_{v_d = -2\delta_1}^{0} |dv_d|^2 \, \chi^2(v_d) \, e^{-\frac{2}{h}(f - 2\mu v_d)} \, d_g v}{\Big(\int_{-2\delta_1}^{0} \chi(t) e^{\frac{2}{h}\mu\, t} dt \Big)^2}, \tag{98}$$

where we recall that $\mu = \partial_{\mathsf{n}_\Omega} f(z) > 0$, and $d_g v = \sqrt{\det g}\, dv$ denotes the Riemannian volume form. A straightforward computation (see (78)) implies that there exists $c > 0$ such that in the limit $h \to 0$,

$$N_z := \int_{-2\delta_1}^{0} \chi(t) e^{\frac{2}{h}\mu\, t} dt = \frac{h}{2\mu} \big(1 + O(e^{-\frac{c}{h}})\big). \tag{99}$$

Moreover, from the Laplace method together with, (78), (55), and (54), one has when $h \to 0$:

$$\int_{|v'| \leq \delta_2} \int_{-2\delta_1}^{0} |dv_d|^2 \, \chi^2(v_d) \, e^{-\frac{2}{h}(f - 2\mu v_d)} \, d_g v = \frac{h}{2\mu} \frac{(\pi h)^{\frac{d-1}{2}} e^{-\frac{2}{h} f(0)}}{\big(\det \operatorname{Hess} f|_{\{v_d = 0\}}(0) \big)^{\frac{1}{2}}} \big(1 + O(h)\big), \tag{100}$$

where we recall that with our notation, $f(0) = f(z) = f(\mathbf{j}(x))$ since $z \in \mathbf{j}(x)$ (see item 4 in Section 3.3). The relations (97)–(100) and (96) lead to the first statement

of item 1.(a) in Proposition 24. Let us now prove the second statement of item 1.(a). Since $\Delta_{f,h} = 2he^{-\frac{f}{h}}\big(\frac{h}{2}\Delta_H + \nabla f\cdot\nabla\big)e^{\frac{f}{h}}$, one has

$$\Delta_{f,h}\psi_x \;=\; \frac{2he^{-\frac{f}{h}}}{Z_x}\Big(\frac{h}{2}\Delta_H + \nabla f\cdot\nabla\Big)\phi_x \;=\; \frac{2he^{-\frac{f}{h}}}{Z_x}\Big(\frac{h}{2}d^*d\phi_x + df(\nabla\phi_x)\Big). \quad (101)$$

Thus, according to (79) and to (54), (55), it holds on $\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)$,

$$\begin{aligned}
\Delta_{f,h}\psi_x &= \frac{2he^{-\frac{f}{h}}}{Z_x}\big(\frac{h}{2}d^*d\varphi_z \;+\; df(\nabla\varphi_z)\big)\\
&= \frac{2he^{-\frac{f}{h}}}{Z_xN_z}\Big(\frac{h}{2}d^*\big(-\chi(v_d)e^{\frac{2}{h}\mu v_d}dv_d\big) \;-\; \mu\, dv_d\big(\chi(v_d)e^{\frac{2}{h}\mu v_d}\nabla v_d\big) + O(|v|^2)\,e^{\frac{2}{h}\mu v_d}\Big)\\
&= \frac{2he^{-\frac{f}{h}}\,e^{\frac{2}{h}\mu v_d}}{Z_xN_z}\Big(O(h) + \frac{h}{2}\,\chi(v_d)\,dv_d\big(\frac{2}{h}\,\mu\,\nabla v_d\big) \;-\; \mu\, dv_d\big(\chi(v_d)\nabla v_d\big) + O(|v|^2)\Big)\\
&= \frac{h\,e^{-\frac{1}{h}(f-2\mu v_d)}}{Z_xN_z}\big(O(h) + O(|v|^2)\big)\,, \qquad (102)
\end{aligned}$$

where N_z is defined by (99). It then follows from (96) that for every h small enough, it holds

$$\int_{\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)} \big|\Delta_{f,h}\,\psi_x\big|^2 \;=\; O(h^2)\sqrt{h}\,e^{-\frac{2}{h}(f(z)-f(x))} \;=\; O(h^2)\int_{\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)} \big|d_{f,h}\,\psi_x\big|^2,$$

which concludes the proof of item 1.(a) in Proposition 24.

Step 1.b) The case when $z\in\partial\Omega$ and $|\nabla f(z)| = 0$.

From Definition 23, it holds

$$\int_{\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)} \big|d_{f,h}\,\psi_x\big|^2 = h^2\frac{\int_{\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)} \big|d\phi_x\big|^2\,e^{-\frac{2}{h}f}}{Z_x}\,, \qquad (103)$$

where, according to (88) and (81),

$$\int_{\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)} \big|d\phi_x\big|^2\,e^{-\frac{2}{h}f} = \frac{\int_{|v'|\le\delta_2}\int_{v_d=-2\delta_1}^{0} |dv_d|^2\,\chi^2(v_d)\,e^{-\frac{2}{h}(f+|\mu_d|v_d^2)}d_gv}{\Big(\int_{-2\delta_1}^{0}\chi(t)\,e^{-\frac{1}{h}|\mu_d|\,t^2}dt\Big)^2}, \qquad (104)$$

where we recall that μ_d is the negative eigenvalue of $\operatorname{Hess} f(z)$. A straightforward computation (see (78)) implies that there exists $c>0$ such that in the limit $h\to 0$,

$$N_z := \int_{-2\delta_1}^{0}\chi(t)\,e^{-\frac{1}{h}|\mu_d|\,t^2}dt = \frac{\sqrt{\pi h}}{2\sqrt{|\mu_d|}}\big(1 + O(e^{-\frac{c}{h}})\big). \qquad (105)$$

Furthermore, from, (78), (60), (61), and (62) together with the Laplace method, one has in the limit $h\to 0$:

$$\int_{|u'|\le\delta_2}\int_{-2\delta_1}^{0} |dv_d|^2\,\chi^2(v_d)\,e^{-\frac{2}{h}(f+|\mu_d|v_d^2)}d_gv = \frac{(\pi h)^{\frac{d}{2}}e^{-\frac{2}{h}f(0)}}{\sqrt{\mu_1\cdots\mu_{d-1}|\mu_d|}}\big(\frac{1}{2} + O(\sqrt{h})\big), \quad (106)$$

where $\mu_1, \dots, \mu_{d-1}$ are the positive eigenvalues of $\operatorname{Hess} f(z)$. Let us point out that the integral in (106) has the form $\int_{\mathbb{R}^d_- \cap B(0,r)} \varphi_2(v)\, e^{-\frac{1}{h}\varphi_1(v)} dv$. Hence, the terms of the type $\int_{\mathbb{R}^d_- \cap B(0,r)} v^\alpha\, e^{-\frac{1}{h}\, {}^t v \operatorname{Hess} \varphi_1(0)\, v} dv$ which appear when performing the Laplace method do not cancel (up to an exponentially small error term) when $|\alpha|$ is odd, contrary to the terms $\int_{B(0,r)} v^\alpha\, e^{-\frac{1}{h}\, {}^t v \operatorname{Hess} \varphi_1(0)\, v} dv$ appearing in the standard Laplace method (by a parity argument) as used to get (110). This justifies the optimality of the $O(\sqrt{h})$ in (106) (see Remark 25 above).

Equations (103)–(106) and (96) lead to the first statement in item 1.(b) of Proposition 24. Let us now prove the second statement in item 1.(b). Doing the same computations as to obtain (102), one deduces from (81), (60), and (61) that on $\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z)$,

$$\begin{aligned}
\Delta_{f,h}\psi_x &= \frac{2he^{-\frac{f}{h}}}{Z_x N_z}\Big(\frac{h}{2} d^*\big(-\chi(v_d) e^{-\frac{1}{h}|\mu_d| v_d^2} dv_d\big) \,+\, |\mu_d|\, v_d\, dv_d\big(\chi(v_d) e^{-\frac{1}{h}|\mu_d| v_d^2} \nabla v_d\big) + O(|v|^2)\, e^{-\frac{1}{h}|\mu_d| v_d^2} \Big) \\
&= \frac{2h\, e^{-\frac{1}{h}(f+|\mu_d| v_d^2)}}{Z_x N_z}\Big(O(h) - \frac{h}{2}\, \chi(v_d)\, dv_d\big(\frac{1}{h}\, |\mu_d|\, \nabla v_d^2\big) \,+\, |\mu_d|\, v_d\, dv_d\big(\chi(v_d) \nabla v_d\big) + O(|v|^2) \Big) \\
&= \frac{2h\, e^{-\frac{1}{h}(f+|\mu_d| v_d^2)}}{Z_x N_z}\Big(O(h) + O(|v|^2) \Big)\,,
\end{aligned}$$

where N_z is defined by (105). It then follows from (105), (96), and (62) that in the limit $h \to 0$,

$$\int_{\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z)} \big|\Delta_{f,h}\, \psi_x\big|^2 = O(h^3)\, e^{-\frac{2}{h}(f(z)-f(x))} = O(h^2) \int_{\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z)} \big|d_{f,h}\, \psi_x\big|^2.$$

This proves the second statement of item 1.(b) in Proposition 24.

Step 2. The case when $z \in \Omega$.

According to Definition 23, one has

$$\int_{\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z)} \big|d_{f,h}\, \psi_x\big|^2 = h^2 \frac{\int_{\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z)} \big|d\phi_x\big|^2\, e^{-\frac{2}{h}f}}{Z_x}, \tag{107}$$

where, from (88) and (83), one has:

$$\int_{\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z)} \big|d\phi_x\big|^2\, e^{-\frac{2}{h}f} = \frac{\int_{|v'|\le\delta_2} \int_{v_d=-2\delta_1}^{2\delta_1} |dv_d|^2\, \chi^2(v_d)\, e^{-\frac{2}{h}(f+|\mu_d| v_d^2)} d_g v}{\Big(\int_{-2\delta_1}^{2\delta_1} \chi(t)\, e^{-\frac{1}{h}|\mu_d|\, t^2} dt\Big)^2}, \tag{108}$$

where μ_d is the negative eigenvalue of $\operatorname{Hess} f(z)$. A straightforward computation (see (78)) implies the existence of $c > 0$ such that in the limit $h \to 0$,

$$N_z := \int_{-2\delta_1}^{2\delta_1} \chi(t)\, e^{-\frac{1}{h}|\mu_d|\, t^2} dt = \frac{\sqrt{\pi h}}{\sqrt{|\mu_d|}}\big(1 + O(e^{-\frac{c}{h}})\big). \tag{109}$$

Moreover, from, (78), (67), (68), (69) and the Laplace method, one has in the limit $h \to 0$:

$$\int_{|v'|\le\delta_2} \int_{v_d=-2\delta_1}^{2\delta_1} |dv_d|^2\, \chi^2(v_d)\, e^{-\frac{2}{h}(f+|\mu_d| v_d^2)} d_g v = \frac{(\pi h)^{\frac{d}{2}} e^{-\frac{2}{h}f(0)}}{\sqrt{\mu_1 \cdots \mu_{d-1} |\mu_d|}}\big(1 + O(h)\big), \tag{110}$$

where $\mu_1, \dots, \mu_{d-1}$ are the positive eigenvalues of Hess $f(z)$. The relations (107)–(110) and (96) imply the first statement of item 2 in Proposition 24. Let us lastly prove the second statement in item 2. From (83), (67), and (68), the same computations as those used to obtain (102) imply that on $\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)$,

$$\Delta_{f,h}\psi_x = \frac{2h\,\chi\, e^{-\frac{1}{h}(f+|\mu_d|v_d^2)}}{Z_x N_z}\Big(O(h) + O(|v|^2)\Big)$$

and the relations (69), (109), and (96) then lead to

$$\int_{\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)} \big|\Delta_{f,h}\,\psi_x\big|^2 = O(h^3)\, e^{-\frac{2}{h}(f(z)-f(x))} = O(h^2)\int_{\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)} \big|d_{f,h}\,\psi_x\big|^2.$$

This concludes the proof of Proposition 24. ∎

For every $x \in \mathsf{U}_0$, one defines the following constants:

$$\mathsf{K}_{1,x} := \sum_{\substack{z\in\mathbf{j}(x)\\ |\nabla f(z)|\neq 0}} \mathsf{c}_{x,z} \quad\text{and}\quad \mathsf{K}_{2,x} := \sum_{\substack{z\in\mathbf{j}(x)\\ |\nabla f(z)|= 0}} \mathsf{c}_{x,z}, \tag{111}$$

where the constants $\mathsf{c}_{x,z}$ are defined in (93), (94), and (95), with the convention $\sum_\emptyset = 0$. Let us recall that $\{z \in \mathbf{j}(x), |\nabla f(z)| \neq 0\} \subset \partial\Omega$. Finally, for $y \neq x \in \mathsf{U}_0$, one defines:

$$\mathsf{K}_{x,y} := \sum_{z\in\mathbf{j}(x)\cap\mathbf{j}(y)} \sqrt{\mathsf{c}_{x,z}}\sqrt{c_{y,z}}, \quad \text{see (93)–(95).} \tag{112}$$

Let us mention that since for all $x \in \mathsf{U}_0$, one has $\mathbf{j}(x) \neq \emptyset$, it holds $(\mathsf{K}_{1,x}, \mathsf{K}_{2,x}) \neq (0,0)$. Proposition 24 has the following consequence.

Proposition 26. *Let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ Morse function which satisfies* **(H1)** *and* **(H2)**. *Let $x \in \mathsf{U}_0$ and ψ_x be as introduced in Definition 23.*

1. *In the limit $h \to 0$, one has:*

$$\big\|d_{f,h}\psi_x\big\|^2_{\Lambda^1 L^2(\Omega)} = \Big(\sqrt{h}\,\mathsf{K}_{1,x}(1+O(h)) + h\,\mathsf{K}_{2,x}(1+O(\sqrt{h}))\Big)e^{-\frac{2}{h}(f(\mathbf{j}(x))-f(x))},$$

where the constants $\mathsf{K}_{1,x}$ and $\mathsf{K}_{2,x}$ are defined in (111). When $\mathbf{j}(x)\cap\partial\Omega$ does not contain any critical point of f, the term $O(\sqrt{h})$ is actually of order $O(h)$. Moreover, it holds in the limit $h \to 0$:

$$\big\|\Delta_{f,h}\psi_x\big\|^2_{L^2(\Omega)} = O(h^2)\big\|d_{f,h}\psi_x\big\|^2_{\Lambda^1 L^2(\Omega)}.$$

2. *Let $y \in \mathsf{U}_0$ be such that $y \neq x$. Then, for each of the two possible cases described in items 4.(i) and 4.(ii) in Section 3.3, it holds in the limit $h \to 0$:*

   (i) When $\mathbf{j}(x)\cap\mathbf{j}(y) = \emptyset$, $\big\langle d_{f,h}\psi_x, d_{f,h}\psi_y\big\rangle_{\Lambda^1 L^2(\Omega)} = 0$.

(ii) When $\mathbf{j}(x)\cap\mathbf{j}(y)\neq\emptyset$,

$$\big\langle d_{f,h}\psi_x, d_{f,h}\psi_y\big\rangle_{\Lambda^1 L^2(\Omega)} = -h\,\mathsf{K}_{x,y}\,e^{-\frac{1}{h}(2f(\mathbf{j}(x))-f(x)-f(y))}\big(1+O(h)\big),$$

where $\mathsf{K}_{x,y}$ *is defined in* (112).

Proof. Let $x\in\mathsf{U}_0$.

Let us first prove item 1 in Proposition 26. From Definition 23 and (90),

$$d_{f,h}\psi_x = Z_x^{-1}\,he^{-\frac{f}{h}}d\phi_x \text{ is supported in } \overline{\Omega_1(x)}\setminus\Omega_2(x). \tag{113}$$

Moreover, from (87), (91), and (96), there exists $c>0$ such that for h small enough, $h^2 Z_x^{-2}\int_{\mathsf{O}_1(x)}|d\,\phi_x|^2 e^{-\frac{2}{h}f} = O\big(e^{-\frac{2}{h}(f(\mathbf{j}(x))-f(x)+c)}\big)$. Thus, using in addition (113) and (86), there exists $c>0$ such that for h small enough,

$$\int_\Omega |d_{f,h}\,\psi_x|^2 = \sum_{z\in\mathbf{j}(x)}\int_{\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z)}|d_{f,h}\,\psi_x|^2 + O\big(e^{-\frac{2}{h}(f(\mathbf{j}(x))-f(x)+c)}\big).$$

The first statement in item 1 in Proposition 26 is then a direct consequence of Proposition 24. Let us now prove the second statement in Proposition 26. To this end, note first that according to (113),

$$\Delta_{f,h}\psi_x = d^*_{f,h}d_{f,h}\psi_x \text{ is supported in } \overline{\Omega_1(x)}\setminus\Omega_2(x).$$

Thus, from (86), (87), (91) together with (96), it holds for some $c>0$ and every h small enough,

$$\int_\Omega |\Delta_{f,h}\,\psi_x|^2 = \sum_{z\in\mathbf{j}(x)}\int_{\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z)}|\Delta_{f,h}\,\psi_x|^2 + O\big(e^{-\frac{2}{h}(f(\mathbf{j}(x))-f(x)+c)}\big).$$

Together with Proposition 24, this proves item 1 in Proposition 26.
Let us now prove item 2 in Proposition 26. Let us consider $y\in\mathsf{U}_0$ such that $y\neq x$. According to (113) and (90),

$$d_{f,h}\,\psi_x\cdot d_{f,h}\,\psi_y = \frac{h^2\,e^{-\frac{2}{h}f}d\,\phi_x\cdot d\,\phi_y}{Z_xZ_y} \text{ is supported in } \overline{\Omega_1(x)}\setminus\Omega_2(x)\bigcap\overline{\Omega_1(y)}\setminus\Omega_2(y).$$

Thus, using item 3 in Definition 21, it holds:

(i) When $\mathbf{j}(x)\cap\mathbf{j}(y)=\emptyset$, then, either $\overline{\Omega_1(x)}\cap\overline{\Omega_1(y)}=\emptyset$ or, up to switching x and y, $\overline{\Omega_1(y)}\subset\Omega_2(x)$. In any case, this implies $\int_\Omega d_{f,h}\,\psi_x\cdot d_{f,h}\,\psi_y=0$.

(ii) When $\mathbf{j}(x)\cap\mathbf{j}(y)\neq\emptyset$, one has,

$$\begin{aligned}\int_\Omega d_{f,h}\,\psi_x\cdot d_{f,h}\,\psi_y &= \frac{h^2}{Z_xZ_y}\sum_{z\in\mathbf{j}(y)\cap\mathbf{j}(x)}\int_{\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z)} d\,\phi_x\cdot d\,\phi_y\;e^{-\frac{2}{h}f}\\ &\quad+\frac{h^2}{Z_xZ_y}\int_{\mathsf{O}_2(x,y)} d\,\phi_x\cdot d\,\phi_y\;e^{-\frac{2}{h}f}.\end{aligned} \tag{114}$$

Since $\mathsf{O}_2(x,y) \subset \mathsf{O}_1(x)$, from (87), (91), and (96), there exists $c > 0$ such that for h small enough:

$$\frac{h^2}{Z_x Z_y} \int_{\mathsf{O}_2(x,y)} d\,\phi_x \cdot d\,\phi_y \; e^{-\frac{2}{h}f} = O\big(e^{-\frac{1}{h}(2f(\mathbf{j}(x))-f(x)-f(y)+c)}\big), \tag{115}$$

where we used $f(\mathbf{j}(y)) = f(\mathbf{j}(x))$. Moreover, using item 1 in Definition 22, for all $z \in \mathbf{j}(x) \cap \mathbf{j}(y)$ (recall that $\mathbf{j}(x) \cap \mathbf{j}(y) \subset \Omega$), $d\phi_x = -d\phi_y$ on $\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)$. Thus, from (113), for all $z \in \mathbf{j}(x) \cap \mathbf{j}(y)$, it holds:

$$\frac{h^2}{Z_x Z_y} \int_{\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)} d\,\phi_x \cdot d\,\phi_y \; e^{-\frac{2}{h}f} = -\frac{Z_x}{Z_y} \int_{\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z)} |d_{f,h}\,\psi_x|^2.$$

Then, item 2.(ii) in Proposition 26 is a consequence of (114) and (115) together with (96) and item 2 in Proposition 24.

This concludes the proof of Proposition 26. ∎

5.2 Linear independence of the quasi-modes

Let us recall that according to Theorem 1, there exists $c_0 > 0$ such that for every h small enough:

$$\dim \operatorname{Ran} \pi_{[0,c_0 h]}\big(\Delta_{f,h}^D\big) = \mathsf{m}_0.$$

In the following, for ease of notation, one denotes

$$\pi_h := \pi_{[0,c_0 h]}\big(\Delta_{f,h}^D\big). \tag{116}$$

In this section, one proves that for every h small enough, $\big(\pi_h \psi_x\big)_{x \in \mathsf{U}_0}$ is linearly independent, and hence a basis of $\operatorname{Ran} \pi_h$, and that $\big(d_{f,h}\pi_h\psi_x\big)_{x \in \mathsf{U}_0}$ is linearly independent in $\Lambda^1 L^2(\Omega)$. Let us start with the following result.

Proposition 27. *Let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ Morse function which satisfies* **(H1)** *and* **(H2)**. *Let $x \in \mathsf{U}_0$ and ψ_x be as introduced in Definition 23. Then, there exists $C > 0$ such that for every h small enough:*

$$\big\|(1-\pi_h)\psi_x\big\|_{L^2(\Omega)} \le C \, \big\|d_{f,h}\psi_x\big\|_{L^2(\Omega)}$$

and

$$\big\|d_{f,h}(\pi_h\psi_x)\big\|_{\Lambda^1 L^2(\Omega)} = \big\|d_{f,h}\psi_x\big\|_{\Lambda^1 L^2(\Omega)}\big(1 + O(h)\big).$$

Proof. Let $c_0 > 0$ be the constant used to define π_h in (116). According to Theorem 1, for every h small enough, $\Delta_{f,h}^D$ has m_0 eigenvalues smaller than $c_0 h$ which are moreover exponentially small. Let $C(\frac{c_0}{2}h) \subset \mathbb{C}$ be the circle centered at 0 of radius $\frac{c_0}{2}h$. Then, there exists $c > 0$ such that for every h small enough, all the points in $C(\frac{c_0}{2}h)$ are at a distance larger than ch of the spectrum of $\Delta_{f,h}^D$. Thus, by the spectral theorem, it holds:

$$\sup_{z \in C(\frac{c_0}{2}h)} \big\|(z - \Delta_{f,h}^D)^{-1}\big\|_{L^2(\Omega) \to L^2(\Omega)} \le \frac{1}{ch}. \tag{117}$$

Moreover, since $\psi_x \in D(\Delta^D_{f,h})$ for all $x \in \mathsf{U}_0$ (see (92)), it holds

$$\begin{aligned}(1-\pi_h)\psi_x &= \frac{1}{2\pi \mathrm{i}}\int_{C(\frac{c_0}{2}h)} \big(z^{-1} - (z-\Delta^D_{f,h})^{-1}\big)\psi_x\, dz \\ &= -\frac{1}{2\pi \mathrm{i}}\int_{C(\frac{c_0}{2}h)} z^{-1}(z-\Delta^D_{f,h})^{-1}\Delta^D_{f,h}\psi_x\, dz.\end{aligned}$$

Thus, using (117) and the second estimate in item 1 in Proposition 26, one obtains that

$$\big\|(1-\pi_h)\psi_x\big\|_{L^2(\Omega)} \leq C\|d_{f,h}\psi_x\|_{\Lambda^1 L^2(\Omega)},$$

for some $C > 0$ independent of h. Let us now prove the second asymptotic estimate of Proposition 27. Since the orthogonal projector π_h and $\Delta^D_{f,h}$ commute on $D(\Delta_{f,h})$ and $\psi_x \in D(\Delta^D_{f,h})$, one has

$$\begin{aligned}\big\|d_{f,h}(\pi_h\psi_x)\big\|^2_{\Lambda^1 L^2(\Omega)} &= \langle \pi_h\psi_x, \Delta_{f,h}\psi_x\rangle_{L^2(\Omega)} \\ &= \langle \psi_x, \Delta_{f,h}\psi_x\rangle_{L^2(\Omega)} - \langle (1-\pi_h)\psi_x, \Delta_{f,h}\psi_x\rangle_{L^2(\Omega)} \\ &= \big\|d_{f,h}\psi_x\big\|^2_{\Lambda^1 L^2(\Omega)} + O\big(\big\|(1-\pi_h)\psi_x\big\|_{L^2(\Omega)}\big\|\Delta_{f,h}\psi_x\big\|_{L^2(\Omega)}\big) \\ &= \big\|d_{f,h}\psi_x\big\|^2_{\Lambda^1 L^2(\Omega)} + O(h)\big\|d_{f,h}\psi_x\big\|^2_{\Lambda^1 L^2(\Omega)},\end{aligned}$$

where one used at the last line the second asymptotic estimate in item 1 in Proposition 26 and the first asymptotic estimate in Proposition 27. This concludes the proof of Proposition 27. ∎

Remark 28. *Note here that using the estimate* (14) *to obtain an upper bound on* $\big\|(1-\pi_h)\psi_x\big\|_{L^2(\Omega)}$, *one would obtain* $\big\|(1-\pi_h)\psi_x\big\|_{L^2(\Omega)} \leq \frac{1}{\sqrt{c_0 h}}\|d_{f,h}\psi_x\|_{\Lambda^1 L^2(\Omega)}$. *This would finally lead to a remainder term of order* $O(\sqrt{h})$ *instead of the* $O(h)$ *appearing in* (134) *in Theorem 3 below.*

Definition 29. *Let* $f : \overline{\Omega} \to \mathbb{R}$ *be a* C^∞ *Morse function which satisfies* **(H1)** *and* **(H2)**. *Let* $x \in \mathsf{U}_0$ *and* ψ_x *be as introduced in Definition 23. Then, one defines the* 1*-form:*

$$\Theta_x := \frac{d_{f,h}\psi_x}{\|d_{f,h}\psi_x\|_{\Lambda^1 L^2(\Omega)}},$$

which is C^∞ *on* $\overline{\Omega}$ *and supported in* $\overline{\Omega_1(x)}\backslash\Omega_2(x)$ *(see* (113)*). Notice that from item 1 in Proposition 26,* $\|d_{f,h}\psi_x\|_{\Lambda^1 L^2(\Omega)} \neq 0$ *for* h *small enough. Moreover, for every* h *small enough, one defines:*

$$\psi^\pi_x := \frac{\pi_h\,\psi_x}{\|\pi_h\,\psi_x\|_{L^2(\Omega)}} \quad \textit{and} \quad \Theta^\pi_x := \frac{d_{f,h}(\pi_h\psi_x)}{\|d_{f,h}(\pi_h\psi_x)\|_{\Lambda^1 L^2(\Omega)}},$$

which are well defined for every h *small enough (see indeed Proposition 27) and where we recall that the orthogonal projector* π_h *on* $L^2(\Omega)$ *is defined by* (116).

A consequence of Proposition 27 on the families $\big(\psi^\pi_x\big)_{x\in\mathsf{U}_0}$ and $(\Theta^\pi_x)_{x\in\mathsf{U}_0}$ introduced in Definition 29 is the following.

Proposition 30. *Let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ Morse function which satisfies* **(H1)** *and* **(H2)**. *Let $x, y \in \mathsf{U}_0$. Then, there exists $c > 0$ such that for every h small enough:*

$$\langle \psi_x^\pi, \psi_y^\pi \rangle_{L^2(\Omega)} = \langle \psi_x, \psi_y \rangle_{L^2(\Omega)} + O\big(e^{-\frac{c}{h}}\big),$$

and

$$\langle \Theta_x^\pi, \Theta_y^\pi \rangle_{\Lambda^1 L^2(\Omega)} = \langle \Theta_x, \Theta_y \rangle_{\Lambda^1 L^2(\Omega)} + O(h).$$

Proof. Let us recall that the orthogonal projector π_h and $\Delta_{f,h}^D$ commute on $D(\Delta_{f,h})$ and that $\psi_x \in D(\Delta_{f,h}^D)$. Then, for every $x, y \in \mathsf{U}_0$, it holds

$$\langle \pi_h \psi_x, \pi_h \psi_y \rangle_{L^2(\Omega)} = \langle \psi_x, \psi_y \rangle_{L^2(\Omega)} - \langle (1 - \pi_h)\psi_x, \psi_y \rangle_{L^2(\Omega)},$$

and

$$\langle d_{f,h}(\pi_h \psi_x), d_{f,h}(\pi_h \psi_y) \rangle_{\Lambda^1 L^2(\Omega)} = \langle d_{f,h}\psi_x, d_{f,h}\psi_y \rangle_{\Lambda^1 L^2(\Omega)} - \langle (1-\pi_h)\psi_x, \Delta_{f,h}\psi_y \rangle_{L^2(\Omega)}.$$

Proposition 30 is then a direct consequence of these identities together with Propositions 26 and 27 (see also (44)). ∎

The Gram matrices of the families $\big(\psi_x\big)_{x \in \mathsf{U}_0}$ and $(\Theta_x)_{x \in \mathsf{U}_0}$ are not necessarily quasi-unitary, i.e. of the form $\mathrm{Id} + o(1)$ when $h \to 0$. For the family $\big(\psi_x\big)_{x \in \mathsf{U}_0}$, this follows from the fact that a global minimum of f in $\operatorname{supp} \psi_x$ can also be a global minimum of f in $\operatorname{supp} \psi_y$ (this can only occur in the situation described in item 4.(i) in Section 3.3 when $\mathbf{j}(x) \cap \mathbf{j}(y) = \emptyset$ and, up to interchanging x with y, $\overline{\mathsf{C}_{\mathbf{j}}(y)} \subset \mathsf{C}_{\mathbf{j}}(x)$). For the family $(\Theta_x)_{x \in \mathsf{U}_0}$, this follows from the fact that $\langle d_{f,h}\psi_x, d_{f,h}\psi_y \rangle_{\Lambda^1 L^2(\Omega)}$ can be of the same order as both $\|d_{f,h}\psi_x\|^2_{\Lambda^1 L^2(\Omega)}$ and $\|d_{f,h}\psi_y\|^2_{\Lambda^1 L^2(\Omega)}$ (see item 2.(ii) in Proposition 26). However, according to Proposition 33 below, these families are, in the limit $h \to 0$, uniformly linearly independent in the sense of the following definition (see [19]).

Definition 31. *Let $\mathcal{H}$ be a Hilbert space, $n \geq 1$ be an integer smaller than $\dim \mathcal{H}$, and $\mathcal{B}'$ be a family of n elements of $\mathcal{H}$ depending on a parameter $h > 0$. The family $\mathcal{B}'$ is said to be uniformly linearly independent in the limit $h \to 0$ if there exists $C > 0$ and $h_0 > 0$ such that for all $h \in (0, h_0)$, the family $\mathcal{B}'$ is linearly independent and for some (and thus for any) orthonormal family $\mathcal{B}$ of $\operatorname{Span}\big(\mathcal{B}'\big)$ and for some (and thus for any) matrix norm $\|\cdot\|$ on $\mathbb{R}^{n \times n}$, it holds*

$$\Big\|\mathrm{Mat}_{\mathcal{B},\mathcal{B}'}(\mathrm{Id})\Big\| \leq C \quad \textit{and} \quad \Big\|\mathrm{Mat}_{\mathcal{B}',\mathcal{B}}(\mathrm{Id})\Big\| \leq C.$$

Remark 32. *Since the Gram matrix $G^{\mathcal{B}'}$ of $\mathcal{B}'$ writes $G^{\mathcal{B}'} = {}^t\mathrm{Mat}_{\mathcal{B}',\mathcal{B}}(\mathrm{Id})\,\mathrm{Mat}_{\mathcal{B}',\mathcal{B}}(\mathrm{Id})$, the family $\mathcal{B}'$ is uniformly linearly independent in the limit $h \to 0$ if and only if there exists a constant $C > 0$ independent of h such that, for every h small enough, $\frac{1}{C} \leq G^{\mathcal{B}'} \leq C$ in the sense of quadratic forms.*

Proposition 33. *Let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ Morse function which satisfies* **(H1)** *and* **(H2)**. *Then, the family of functions $\big(\psi_x^\pi\big)_{x \in \mathsf{U}_0}$ (resp. the family of 1-forms*

$(\Theta_x^\pi)_{x\in\mathsf{U}_0}$) *introduced in Definition 29 is uniformly linearly independent in* $L^2(\Omega)$ *(resp. in* $\Lambda^1 L^2(\Omega)$*) in the limit* $h\to 0$ *(see Definition 31). In particular,* $\big(\psi_x^\pi\big)_{x\in\mathsf{U}_0}$ *is a basis of* $\operatorname{Ran}\pi_h$ *for every* h *small enough.*

The following lemma, which is a direct consequence of Proposition 24, item 1 in Proposition 26, and Definition 29, will be used in the proof of Proposition 33.

Lemma 34. *Let* $f:\overline{\Omega}\to\mathbb{R}$ *be a* C^∞ *Morse function which satisfies* **(H1)** *and* **(H2)**, *and* $x\in\mathsf{U}_0$.

1. *When there exists* $z\in\mathbf{j}(x)$ *such that* $|\nabla f(z)|\neq 0$ *(in this case* $z\in\partial\Omega$*), one has in the limit* $h\to 0$*, for every* $z\in\mathbf{j}(x)$ *such that* $|\nabla f(z)|\neq 0$,

$$\|\Theta_x\|^2_{\Lambda^1 L^2\left(\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z)\right)}=\frac{\mathsf{c}_{x,z}}{\sum_{p\in\mathbf{j}(x),|\nabla f(p)|\neq 0}c_{x,p}}\big(1+O(\sqrt{h})\big),$$

where the constant $\mathsf{c}_{x,z}$ *is defined in* (93) *and* $\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z)$ *is defined in* (57).

2. *When* $|\nabla f(z)|=0$ *for every* $z\in\mathbf{j}(x)$*, one has in the limit* $h\to 0$*, for every* $z\in\mathbf{j}(x)$,

$$\|\Theta_x\|^2_{\Lambda^1 L^2(\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z)))}=\frac{\mathsf{c}_{x,z}}{\sum_{p\in\mathbf{j}(x)}c_{x,p}}\big(1+O(\sqrt{h})\big),$$

where the constants $\mathsf{c}_{x,z}$ *are defined in* (94) *and* (95) *and* $\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z)$ *is defined in* (64) *and* (71).

Proof of Proposition 33. In view of Proposition 30 and of Remark 32, Proposition 33 is equivalent to the fact that the family $\big(\psi_x\big)_{x\in\mathsf{U}_0}$ (resp. $(\Theta_x)_{x\in\mathsf{U}_0}$) is uniformly linearly independent in $L^2(\Omega)$ (resp. in $\Lambda^1L^2(\Omega)$), in the limit $h\to 0$. Moreover, the proof of this property for $\big(\psi_x\big)_{x\in\mathsf{U}_0}$ is exactly the same as the one made in [19, Section 4.2]. Let us now prove that $(\Theta_x)_{x\in\mathsf{U}_0}$ is uniformly linearly independent in $\Lambda^1L^2(\Omega)$ in the limit $h\to 0$. The following proof is inspired by the analysis done in [19, Section 4.2]. Let us recall that according to the construction of $\mathsf{C}_{\mathbf{j}}$ made in Section 3.3, one has:

$$(\mathsf{C}_{\mathbf{j}}(x))_{x\in\mathsf{U}_0}=\bigcup_{k\geq 1}\big\{\mathsf{C}_{\mathbf{j}}(x_{k,1}),\dots,\mathsf{C}_{\mathbf{j}}(x_{k,\mathsf{N}_k})\big\},$$

where the union over k is actually finite. For all $k\geq 1$, let us divide $\big\{\mathsf{C}_{\mathbf{j}}(x_{k,1}),\dots,\mathsf{C}_{\mathbf{j}}(x_{k,\mathsf{N}_k})\big\}$ into n_k groups ($n_k\leq\mathsf{N}_k$):

$$\big\{\mathsf{C}_{\mathbf{j}}(x_{k,1}),\dots,\mathsf{C}_{\mathbf{j}}(x_{k,\mathsf{N}_k})\big\}=\bigcup_{\ell=1}^{n_k}\{\mathsf{C}^1_{k,\ell},\dots,\mathsf{C}^{m_\ell}_{k,\ell}\}$$

which are such that for all $\ell\in\{1,\dots,n_k\}$,

$$\begin{cases}\text{the set }\bigcup_{j=1}^{m_\ell}\overline{\mathsf{C}^j_{k,\ell}}\text{ is connected, and}\\ \forall\mathsf{C}\in\big\{\mathsf{C}_{\mathbf{j}}(x_{k,1}),\dots,\mathsf{C}_{\mathbf{j}}(x_{k,\mathsf{N}_k})\big\}\setminus\{\mathsf{C}^1_{k,\ell},\dots,\mathsf{C}^{m_\ell}_{k,\ell}\},\ \overline{\mathsf{C}}\cap\bigcup_{j=1}^{m_\ell}\overline{\mathsf{C}^j_{k,\ell}}=\emptyset.\end{cases}\tag{118}$$

Let $x, y \in \mathsf{U}_0$. Let k, k', ℓ, and ℓ' be such that $\mathsf{C}_{\mathbf{j}}(x) \in \{\mathsf{C}^1_{k,\ell}, \dots, \mathsf{C}^{m_\ell}_{k,\ell}\}$ and $\mathsf{C}_{\mathbf{j}}(y) \in \{\mathsf{C}^1_{k',\ell'}, \dots, \mathsf{C}^{m_{\ell'}}_{k',\ell'}\}$. Let us recall that $\mathbf{j}(x) \cap \mathbf{j}(y) \neq \emptyset$ is equivalent to $f(\mathbf{j}(x)) = f(\mathbf{j}(y))$ (which implies $k = k'$) and $\overline{\mathsf{C}_{\mathbf{j}}(y)} \cap \overline{\mathsf{C}_{\mathbf{j}}(x)} \neq \emptyset$ (which implies $\ell = \ell'$). Therefore, when $\mathsf{C}_{\mathbf{j}}(x)$ and $\mathsf{C}_{\mathbf{j}}(y)$ belong to different groups, i.e. when $(k', \ell') \neq (k, \ell)$, it holds $\mathbf{j}(x) \cap \mathbf{j}(y) = \emptyset$. Thus, according to item 2.(i) in Proposition 26 and to Definition 29, it holds $\langle \Theta_x, \Theta_y \rangle_{\Lambda^1 L^2(\Omega)} = 0$. This implies that in $\Lambda^1 L^2(\Omega)$, it holds:

$$\mathrm{Span}\big(\,(\Theta_x)_{x \in \mathsf{U}_0}\,\big) = \bigoplus_{k \geq 1}^{\perp} \Big[\bigoplus_{\ell = 1, \dots, n_k}^{\perp} \mathrm{Span}\big(\Theta_x,\ x \text{ s.t. } \mathsf{C}_{\mathbf{j}}(x) \in \{\mathsf{C}^1_{k,\ell}, \dots, \mathsf{C}^{m_\ell}_{k,\ell}\}\big) \Big]. \quad (119)$$

According to Definition 31, in order to prove that $(\Theta_x)_{x \in \mathsf{U}_0}$ is uniformly linearly independent in the limit $h \to 0$, it then suffices to prove that for all $k \geq 1$ and $\ell \in \{1, \dots, n_k\}$, the family $\big(\Theta_x,\ x \text{ s.t. } \mathsf{C}_{\mathbf{j}}(x) \in \{\mathsf{C}^1_{k,\ell}, \dots, \mathsf{C}^{m_\ell}_{k,\ell}\}\big)$ is uniformly linearly independent in the limit $h \to 0$. To this end, let $k \geq 1$ and $\ell \in \{1, \dots, n_k\}$. For ease of notation, we denote m_ℓ by m, $\{\mathsf{C}^1_{k,\ell}, \dots, \mathsf{C}^{m_\ell}_{k,\ell}\}$ by $\{\mathsf{C}^1, \dots, \mathsf{C}^m\}$, and $\big(\Theta_x,\ x \text{ s.t. } \mathsf{C}_{\mathbf{j}}(x) \in \{\mathsf{C}^1_{k,\ell}, \dots, \mathsf{C}^{m_\ell}_{k,\ell}\}\big)$ by $(\Theta_1, \dots, \Theta_m)$. For h small enough, let us then consider some $\varphi = \varphi(h) \in \mathrm{Span}\{\Theta_1, \dots, \Theta_m\}$:

$$\varphi = \sum_{i=1}^{m} a_i(h)\, \Theta_i, \text{ where for all } i \in \{1, \dots, m\},\ a_i(h) \in \mathbb{R}. \quad (120)$$

From (118) and using Lemma 20, up to reordering $\{\mathsf{C}^1, \dots, \mathsf{C}^m\}$, there exists $z_1 \in \mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega})$ such that $z_1 \in \partial \mathsf{C}^1 \setminus \big(\cup_{i=2}^m \partial \mathsf{C}^i\big)$. Let us now choose such a point z_1 as follows:

- When $\{p \in \partial \mathsf{C}^1 \cap \mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega}) \text{ s.t.} |\nabla f(p)| \neq 0\} = \emptyset$, one chooses any z_1 in $\mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega}) \cap \partial \mathsf{C}^1 \setminus \big(\cup_{i=2}^m \partial \mathsf{C}^i\big)$ (and it holds $|\nabla f(z_1)| = 0$).
- When $\{p \in \partial \mathsf{C}^1 \cap \mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega}) \text{ s.t. } |\nabla f(p)| \neq 0\} \neq \emptyset$, then C^1 is a principal well of f (see (45)) and thus $\mathsf{C}^1, \dots, \mathsf{C}^m$ are principal wells of f. In this case, one chooses $z_1 \in \mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega}) \cap \{p \in \partial \mathsf{C}^1 \text{ s.t.} |\nabla f(p)| \neq 0\} \subset \partial \Omega$ and from (29), it holds $z_1 \notin \cup_{i=2}^m \partial \mathsf{C}^i$.

In both cases, according to Lemma 34, one has when $h \to 0$,

$$\|\Theta_1\|_{\Lambda^1 L^2(\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z_1))} = c_1(1 + o(1))\,,$$

where $c_1 \in (0, 1]$ is independent of h. Since $z_1 \in \partial \mathsf{C}^1 \setminus \big(\cup_{i=2}^m \partial \mathsf{C}^i\big)$ and since all the cylinders defined by (57), (64), and (71) are two by two disjoint, the cylinder $\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z_1)$ does not meet any of the cylinders associated with the $z \in \mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega}) \cap \cup_{i=2}^m \partial \mathsf{C}^i$. Therefore, by definition of Θ_i (see Definition 29) and item 3 in Definition 21, it holds $\Theta_i \equiv 0$ on $\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z_1)$ for all $i \in \{2, \dots, m\}$. Taking the $\Lambda^1 L^2$-norm of (120) in $\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z_1)$, one has for h small enough, $\|\varphi\|_{\Lambda^1 L^2(\Omega)} \geq \|\varphi\|_{\Lambda^1 L^2(\mathsf{V}^{\delta_1,\delta_2}_{\overline{\Omega}}(z_1))} \geq \frac{c_1}{2} |a_1(h)|$. Thus, for h small enough, it holds:

$$|a_1(h)| \leq \frac{2}{c_1} \|\varphi\|_{\Lambda^1 L^2(\Omega)}. \quad (121)$$

Let us now get a similar upper bound on $|a_2(h)|$. Since $\cup_{i=1}^m \overline{\mathsf{C}^i}$ is connected (see (118)), up to reordering $\{\mathsf{C}^2, \dots, \mathsf{C}^m\}$, it holds $\overline{\mathsf{C}^1} \cap \overline{\mathsf{C}^2} \neq \emptyset$, and one chooses $z_2 \in \mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega}) \cap \partial \mathsf{C}_2$ as follows:

- When $\{p \in \partial \mathsf{C}^2 \cap \mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega}) \text{ s.t.} |\nabla f(p)| \neq 0\} = \emptyset$, one chooses any $z_2 \in \partial \mathsf{C}^2 \cap \partial \mathsf{C}^1$.
- When $\{p \in \partial \mathsf{C}^2 \cap \mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega}) \text{ s.t.} |\nabla f(p)| \neq 0\} \neq \emptyset$, one chooses $z_2 \in \{p \in \partial \mathsf{C}^2 \cap \mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega}) \text{ s.t.} |\nabla f(p)| \neq 0\}$.

In both cases, $z_2 \in \mathsf{U}_1^{\mathsf{ssp}}(\overline{\Omega}) \cap \partial \mathsf{C}^2 \setminus \big(\cup_{i=3}^m \partial \mathsf{C}^i\big)$. Therefore, it holds $\Theta_i \equiv 0$ on $\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z_2)$ for all $i \in \{3, \dots, m\}$ while, from Lemma 34, $\|\Theta_2\|_{\Lambda^1 L^2(\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z_2))} = c_2(1 + o(1))$ in the limit $h \to 0$ and for some $c_2 \in (0, 1]$ independent of h. Taking the $\Lambda^1 L^2$-norm of (120) in $\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z_2)$ and using the fact that $\|\Theta_1\|_{\Lambda^1 L^2(\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z_2))} \leq 1$ lead to

$$\|\varphi\|_{\Lambda^1 L^2(\Omega)} \geq \|\varphi\|_{\Lambda^1 L^2(\mathsf{V}_{\overline{\Omega}}^{\delta_1,\delta_2}(z_2))} \geq -|a_1(h)| + \frac{c_2}{2}|a_2(h)|$$

for every h small enough. Using in addition (121), one obtains

$$|a_2(h)| \leq \frac{2}{c_2}\Big(1 + \frac{2}{c_1}\Big)\|\varphi\|_{\Lambda^1 L^2(\Omega)}.$$

Repeating this last procedure $m-2$ times leads to the existence of some $C > 0$ independent of h such that for every h small enough, it holds $\sum_{i=1}^m |a_i(h)| \leq C\,\|\varphi\|_{\Lambda^1 L^2(\Omega)}$. Using (120), it follows that the family $(\Theta_1, \dots, \Theta_m)$ is uniformly linearly independent in the limit $h \to 0$, which concludes the proof of Proposition 33. ∎

5.3 An accurate interaction matrix

Let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ Morse function which satisfies **(H1)** and **(H2)**. In the rest of this section, one chooses for ease of notation an arbitrary labeling of $\mathsf{U}_0 = \{x_1, \dots, x_{\mathsf{m}_0}\}$ and one assumes that $(\psi_x)_{x \in \mathsf{U}_0} = (\psi_1, \dots, \psi_{\mathsf{m}_0})$ and $(\Theta_x)_{x \in \mathsf{U}_0} = (\Theta_1, \dots, \Theta_{\mathsf{m}_0})$ (see Definitions 23 and 29) are ordered according to this labeling.

Let us recall from Proposition 33 that for every h small enough, $\big(\psi_j^\pi\big)_{j \in \{1,\dots,\mathsf{m}_0\}}$ and $(\Theta_i^\pi)_{i \in \{1,\dots,\mathsf{m}_0\}}$ are uniformly linearly independent (see Definitions 29 and 31), which implies in particular, according to Theorem 1, that

$$\mathrm{Span}\big(\psi_j^\pi\big)_{j \in \{1,\dots,\mathsf{m}_0\}} = \mathrm{Ran}\,\pi_h.$$

Let us now consider an orthonormal basis $\mathcal{B}_0$ of $\mathrm{Ran}(\pi_h)$ in $L^2(\Omega)$ and an orthonormal basis $\mathcal{B}_1$ of $\mathrm{Span}\,(\Theta_i^\pi)_{i \in \{1,\dots,\mathsf{m}_0\}}$ in $\Lambda^1 L^2(\Omega)$. The eigenvalues of $\Delta_{f,h}^D$ which are smaller than $c_0 h$ for h small enough are then the eigenvalues of the matrix $M^{\mathcal{B}_0}$ of $\Delta_{f,h}^D$ in the basis $\mathcal{B}_0$, and hence the squares of the singular values of the matrix $S^{\mathcal{B}_0,\mathcal{B}_1}$ defined by

$$S^{\mathcal{B}_0,\mathcal{B}_1} := \mathrm{Mat}_{\mathcal{B}_0,\mathcal{B}_1}(d_{f,h}), \tag{122}$$

which follows from the relation $M^{\mathcal{B}_0} = {}^t S^{\mathcal{B}_0,\mathcal{B}_1} S^{\mathcal{B}_0,\mathcal{B}_1}$. This reduces the analysis of the asymptotic behaviour of the m_0 smallest eigenvalues of $\Delta^D_{f,h}$ in the limit $h \to 0$ to the study of the asymptotic behaviour of the singular values of the matrix $S^{\mathcal{B}_0,\mathcal{B}_1}$.

Note moreover that according to Definition 29, the matrix $S^{\mathcal{B}_0,\mathcal{B}_1}$ defined by (122) has the form

$$S^{\mathcal{B}_0,\mathcal{B}_1} = {}^t C_1^\pi \, S^\pi \, C_0^\pi, \tag{123}$$

where

$$C_1^\pi := \mathrm{Mat}_{\mathcal{B}_1\,,\,(\Theta_i^\pi)_{i\in\{1,\dots,\mathsf{m}_0\}}}(\mathrm{Id}), \quad C_0^\pi := \mathrm{Mat}_{\mathcal{B}_0\,,\,\left(\psi_j^\pi\right)_{j\in\{1,\dots,\mathsf{m}_0\}}}(\mathrm{Id}), \tag{124}$$

and

$$\begin{aligned} \text{for all } i,j \in \{1,\dots,\mathsf{m}_0\}, \quad S^\pi_{i,j} &= \frac{\langle d_{f,h}\psi_j^\pi, d_{f,h}\psi_i^\pi\rangle_{\Lambda^1 L^2(\Omega)}}{\left\|d_{f,h}\psi_i^\pi\right\|_{\Lambda^1 L^2(\Omega)}} \\ &= \left\|d_{f,h}\psi_j^\pi\right\|_{\Lambda^1 L^2(\Omega)} \langle \Theta_j^\pi, \Theta_i^\pi\rangle_{\Lambda^1 L^2(\Omega)}. \end{aligned} \tag{125}$$

In order to give asymptotic estimates on the entries of the matrix S^π in the limit $h \to 0$, let us introduce the square matrix S defined by:

$$\begin{aligned} \text{for all } i,j \in \{1,\dots,\mathsf{m}_0\}, \quad S_{i,j} &:= \frac{\langle d_{f,h}\psi_j, d_{f,h}\psi_i\rangle_{\Lambda^1 L^2(\Omega)}}{\left\|d_{f,h}\psi_i\right\|_{\Lambda^1 L^2(\Omega)}} \\ &= \left\|d_{f,h}\psi_j\right\|_{\Lambda^1 L^2(\Omega)} \langle \Theta_j, \Theta_i\rangle_{\Lambda^1 L^2(\Omega)}. \end{aligned} \tag{126}$$

From Propositions 26, 27, and 30, one has the following asymptotic result on the entries of the matrices S and S^π.

Proposition 35. *Let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ Morse function which satisfies* **(H1)** *and* **(H2)**, *and $i,j \in \{1,\dots,\mathsf{m}_0\}$. We then have the following estimates when $h \to 0$:*

1. *When $\mathbf{j}(x_i) \cap \mathbf{j}(x_j) = \emptyset$, $S_{i,j} = 0$.*
2. *When $\mathbf{j}(x_i) \cap \mathbf{j}(x_j) \neq \emptyset$ and $i = j$,*

$$S_{j,j} = h^{\frac14}\left(\mathsf{K}_{1,x_j}(1+O(h)) + h^{\frac12}\,\mathsf{K}_{2,x_j}(1+O(\sqrt{h}))\right)^{\frac12} e^{-\frac1h(f(\mathbf{j}(x_j))-f(x_j))}$$

and, when $\mathbf{j}(x_i) \cap \mathbf{j}(x_j) \neq \emptyset$ and $i \neq j$,

$$S_{i,j} = -\frac{h^{\frac34}\mathsf{K}_{x_i,x_j}}{\left(\mathsf{K}_{1,x_i}(1+O(h)) + h^{\frac12}\mathsf{K}_{2,x_i}(1+O(\sqrt{h}))\right)^{\frac12}} e^{-\frac1h(f(\mathbf{j}(x_j))-f(x_j))},$$

where the constants K_{1,x_j}, K_{2,x_j}, and K_{x_i,x_j} are defined in (111) *and* (112).

3. *Finally, it holds in any case*

$$S^\pi_{i,j} = S_{i,j} + O(h) S_{j,j}.$$

In order to suitably factorize the matrix S^π, let us first write $S = TD$, where D and T are the following $\mathsf{m}_0 \times \mathsf{m}_0$ matrices (defined for every h small enough):

- the matrix D is the diagonal matrix such that for all $j \in \{1, \dots, \mathsf{m}_0\}$,

$$D_{j,j} := h^{p_j}\, e^{-\frac{1}{h}(f(\mathfrak{j}(x_j)) - f(x_j))}, \tag{127}$$

  where

$$p_j := \frac{1}{4} \text{ when } \mathsf{K}_{1,x_j} \neq 0 \;\text{ and }\; p_j := \frac{1}{2} \text{ when } \mathsf{K}_{1,x_j} = 0, \tag{128}$$

- the matrix T is the matrix SD^{-1}, i.e.

$$\text{for all } i, j \in \{1, \dots, \mathsf{m}_0\}, \quad T_{i,j} := \frac{S_{i,j}}{D_{j,j}}. \tag{129}$$

It then follows from (127)–(129) and Proposition 35 that in the limit $h \to 0$,

$$S^\pi \;=\; (T + R)D \quad \text{with} \quad R = S^\pi D^{-1} - T = (S^\pi - S)D^{-1} = O(h)$$

and $T = O(1)$. Moreover, according to Lemma 36 below, T is invertible and its inverse satisfies $T^{-1} = O(1)$. Thus, the matrix S^π factorizes as follows:

$$S^\pi = (T + O(h))D = (I_{\mathsf{m}_0} + O(h)T^{-1})TD = (I_{\mathsf{m}_0} + O(h))TD = (I_{\mathsf{m}_0} + O(h))S. \tag{130}$$

We conclude this section by stating and proving Lemma 36 which led to (130).

Lemma 36. *Let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ Morse function which satisfies* **(H1)** *and* **(H2)**. *Let $\|\cdot\|$ be a matrix norm on $\mathbb{R}^{\mathsf{m}_0 \times \mathsf{m}_0}$. Then, for every h small enough, the matrix T defined by* (129) *is invertible and there exists $C > 0$ independent of h such that*

$$\|T\| \leq C \text{ and } \|T^{-1}\| \leq C.$$

Proof. We already noticed the relation $\|T\| = O(1)$ in the limit $h \to 0$. To prove the relation $\|T^{-1}\| = O(1)$, let us first notice that from (126), (127), (129), and Definition 29, it holds

$$T = SD^{-1} = G^\Theta U D^{-1},$$

where

$$U = \mathrm{Diag}\,\left(\left\|d_{f,h}\psi_1\right\|_{\Lambda^1 L^2(\Omega)}, \dots, \left\|d_{f,h}\psi_{\mathsf{m}_0}\right\|_{\Lambda^1 L^2(\Omega)}\right) = \mathrm{Diag}\,\left(S_{1,1}, \dots, S_{\mathsf{m}_0,\mathsf{m}_0}\right)$$

and G^Θ is the Gram matrix of the family $(\Theta_1, \dots, \Theta_{\mathsf{m}_0})$ in $\Lambda^1 L^2(\Omega)$. Moreover, according to (127), (128), and Proposition 35, there exist positive constants $c_1, \dots, c_{\mathsf{m}_0}$ such that $\lim_{h\to 0} UD^{-1} = \mathrm{Diag}\,(c_1, \dots, c_{\mathsf{m}_0})$ and thus $DU^{-1} = O(1)$. Lastly, let us recall from Proposition 33 that the family $(\Theta_1, \dots, \Theta_{\mathsf{m}_0})$ is uniformly linearly independent in the limit $h \to 0$ and then, according to Remark 32, $(G^\Theta)^{-1} = O(1)$. It follows that $T^{-1} = DU^{-1}(G^\Theta)^{-1} = O(1)$, which concludes the proof of Lemma 36. ∎

5.4 Asymptotic behaviour of the small eigenvalues of $\Delta^D_{f,h}$

In this section, one states and proves the main results of this work, Theorems 2 and 3 below, on the precise asymptotic behaviour of the small eigenvalues of $\Delta^D_{f,h}$ in the limit $h \to 0$.

The proofs of these results make both use of a weak form of the Fan inequalities stated in the following lemma (see for instance [36, Theorem 1.6]).

Lemma 37. *Let A, B, and C be three $\mathsf{m}_0 \times \mathsf{m}_0$ matrices. It then holds:*

$$\forall j \in \{1, \dots, \mathsf{m}_0\},\ \eta_j(A\,B\,C) \leq \big\|A\big\|\,\big\|C\big\|\,\eta_j(B),$$

where, for any matrix $U \in \mathbb{R}^{\mathsf{m}_0 \times \mathsf{m}_0}$, $\eta_1(U) \geq \cdots \geq \eta_{\mathsf{m}_0}(U)$ denote the singular values of U and $\|U\| := \sqrt{\max \sigma({}^tUU)} = \eta_1(U)$ is the spectral norm of U.

Notice that the singular values are labeled in decreasing order whereas the eigenvalues are labeled in increasing order. In Theorem 2, one gives a precise lower and upper bound on every small eigenvalue of $\Delta^D_{f,h}$ in the limit $h \to 0$ under the sole assumptions **(H1)** and **(H2)**.

Theorem 2. *Let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ Morse function which satisfies* **(H1)** *and* **(H2)**, *and thus such that $\mathsf{U}_0 \neq \emptyset$. Let us order the set $\mathsf{U}_0 = \{x_1, \dots, x_{\mathsf{m}_0}\}$ such that*

- *the sequence $\big(f(\mathbf{j}(x_j)) - f(x_j)\big)_{j \in \{1,\dots,\mathsf{m}_0\}}$ is decreasing,*
- *and, on any $\mathcal{J} \subset \{1, \dots, \mathsf{m}_0\}$ such that $\big(f(\mathbf{j}(x_j)) - f(x_j)\big)_{j \in \mathcal{J}}$ is constant, the sequence $(p_j)_{j \in \mathcal{J}}$ is decreasing (see* (128)*).*

Finally, for $j \in \mathbb{N}^*$, let us denote by $\lambda_{j,h}$ the j-th eigenvalue of $\Delta^D_{f,h}$ counted with multiplicity. Then, there exist $C > 0$ and $h_0 > 0$ such that for every $j \in \big\{1, \dots, \mathsf{m}_0\big\}$ and every $h \in (0, h_0)$, it holds

$$\frac{1}{C}\, h^{2p_j}\, e^{-\frac{2}{h}(f(\mathbf{j}(x_j)) - f(x_j))} \;\leq\; \lambda_{j,h} \;\leq\; C\, h^{2p_j}\, e^{-\frac{2}{h}(f(\mathbf{j}(x_j)) - f(x_j))}\,.$$

Proof. For any matrix $U \in \mathbb{R}^{\mathsf{m}_0 \times \mathsf{m}_0}$, we will denote by $\|U\|$ the spectral norm of U and by $\|U\| = \eta_1(U) \geq \cdots \geq \eta_{\mathsf{m}_0}(U)$ the singular values of U. Let us recall from Section 5.3 that the m_0 smallest eigenvalues of $\Delta^D_{f,h}$ are squares of the singular values of the matrix $S^{\mathcal{B}_0,\mathcal{B}_1} = {}^tC^\pi_1 S^\pi C^\pi_0 \in \mathbb{R}^{\mathsf{m}_0 \times \mathsf{m}_0}$, where C^π_0, C^π_1, and S^π are defined in (124) and in (125). Moreover, using Proposition 33, there exists $c > 0$ such that for every h small enough, it holds

$$\max\Big(\big\|C^\pi_0\big\|, \big\|(C^\pi_0)^{-1}\big\|, \big\|C^\pi_1\big\|, \big\|(C^\pi_1)^{-1}\big\|\Big) \leq c. \tag{131}$$

Thus, using Lemma 37, there exists $c > 0$ such that for every h small enough, it holds

$$\forall j \in \{1, \dots, \mathsf{m}_0\},\ \frac{1}{c}\,\eta_j(S^\pi) \leq \eta_j(S^{\mathcal{B}_0,\mathcal{B}_1}) \leq c\,\eta_j(S^\pi). \tag{132}$$

Moreover, let us recall that $S^\pi = (I_{\mathsf{m}_0} + O(h))TD$ according to (130) and then, using Lemmata 36 and 37, there exists $c > 0$ such that for every h small enough,

$$\forall j \in \{1, \dots, \mathsf{m}_0\},\ \frac{1}{c}\,\eta_j(D) \le \eta_j(S^\pi) \le c\,\eta_j(D). \tag{133}$$

Finally, according to the ordering of the elements of U_0 considered in the statement of Theorem 2, the singular values of D satisfy (see indeed (127)),

$$\forall j \in \{1, \dots, \mathsf{m}_0\},\ \eta_{\mathsf{m}_0+1-j}(D) = D_{j,j} = h^{p_j} e^{-\frac{1}{h}(f(\mathbf{j}(x_j)) - f(x_j))}.$$

Together with (132) and (133), this implies the statement of Theorem 2. ∎

Lastly, in the main result of this work stated below, one gives asymptotic equivalents of the smallest eigenvalues of $\Delta^D_{f,h}$ under additional assumptions on the maps $\mathbf{j}$ and $\mathsf{C}_{\mathbf{j}}$ built in Section 3.3 which ensure that the wells $\mathsf{C}_{\mathbf{j}}(x)$, $x \in \mathsf{U}_0$, are adequately separated.

Theorem 3. *Let $f : \overline{\Omega} \to \mathbb{R}$ be a C^∞ Morse function which satisfies* **(H1)** *and* **(H2)**, *and thus such that $\mathsf{U}_0 \neq \emptyset$. Let us assume that there exists $\mathsf{m}^* \in \{1, \dots, \mathsf{m}_0\}$ and a labeling of $\mathsf{U}_0 = \{x_1, \dots, x_{\mathsf{m}_0}\}$ such that (see Section 3.3 for the constructions of the maps $\mathbf{j}$ and $\mathsf{C}_{\mathbf{j}}$):*

1. *It holds*

$$f(\mathbf{j}(x_1)) - f(x_1) \ge \dots \ge f(\mathbf{j}(x_{\mathsf{m}^*})) - f(x_{\mathsf{m}^*}) > \max_{i=\mathsf{m}^*+1,\dots,\mathsf{m}_0} f(\mathbf{j}(x_i)) - f(x_i),$$

   with the convention $\max_{i=\mathsf{m}_0+1,\mathsf{m}_0} f(\mathbf{j}(x_i)) - f(x_i) = 0$.

2. *For all $j \in \{1, \dots, \mathsf{m}^*\}$, $\mathbf{j}(x_j) \cap \bigcup_{i \in \{1,\dots,\mathsf{m}_0\}, i \neq j} \mathbf{j}(x_i) = \emptyset$ (i.e. $\partial \mathsf{C}_{\mathbf{j}}(x_j)$ does not contain any separating saddle point which belongs to another $\partial \mathsf{C}_{\mathbf{j}}(x_i)$, $i \neq j$).*

3. *For all $k, \ell \in \{1, \dots, \mathsf{m}^*\}$ such that $k \neq \ell$ and $\mathsf{C}_{\mathbf{j}}(x_\ell) \subset \mathsf{C}_{\mathbf{j}}(x_k)$ (notice that this implies $f(x_\ell) \ge f(x_k)$ by construction of $\mathsf{C}_{\mathbf{j}}$), it holds $f(x_\ell) > f(x_k)$.*

For $j \in \mathbb{N}^*$, let us denote by $\lambda_{j,h}$ the j-th eigenvalue of $\Delta^D_{f,h}$ counted with multiplicity. Then, there exists $c > 0$ such that in the limit $h \to 0$, it holds

$$\lambda_{\mathsf{m}^*+1,h} = O(e^{-\frac{c}{h}})\lambda_{\mathsf{m}^*,h}.$$

Moreover, there exists $h_0 > 0$ such that for every $h \in (0, h_0)$, there exists a bijection

$$\Lambda_h : \{x_1, \dots, x_{\mathsf{m}^*}\} \longrightarrow \sigma(\Delta^D_{f,h}) \cap [0, \lambda_{\mathsf{m}^*,h}],$$

where the spectrum is counted with multiplicity, such that, for every $j \in \{1, \dots, \mathsf{m}^*\}$, it holds when $h \to 0$:

$$\begin{aligned}\Lambda_h(x_j) &= \Big(\sqrt{h}\,\mathsf{K}_{1,x_j}\big(1 + O(h)\big) + h\,\mathsf{K}_{2,x_j}\big(1 + O(\sqrt{h})\big)\Big) e^{-\frac{2}{h}(f(\mathbf{j}(x_j)) - f(x_j))} \\ &= \Big(\frac{A_{j,1} + \sqrt{h}\,A_{j,2}}{B_j} + O(h)\Big)\sqrt{\frac{h}{\pi}}\ e^{-\frac{2}{h}(f(\mathbf{j}(x_j)) - f(x_j))},\end{aligned} \tag{134}$$

where K_{1,x_j} *and* K_{2,x_j} *are defined in* (111), $B_j := \sum_{q\in\arg\min_{\mathsf{C}_{\mathbf{j}}(x_j)} f} (\det \mathrm{Hess}\, f(q))^{-\frac{1}{2}}$,

$$A_{j,1} = \sum_{\substack{z\in\mathbf{j}(x_j)\\ |\nabla f(z)|\neq 0}} \frac{2\partial_{\mathsf{n}_\Omega} f(z)}{(\det \mathrm{Hess}\, f|_{\partial\Omega}(z))^{\frac{1}{2}}} \quad \textit{and} \quad A_{j,2} = \frac{1}{\sqrt{\pi}} \sum_{\substack{z\in\mathbf{j}(x_j)\\ |\nabla f(z)|= 0}} \frac{(1+\mathbf{1}_{\partial\Omega}(z))\,|\mu_d|}{|\det \mathrm{Hess}\, f(z)|^{\frac{1}{2}}},$$

where $\mathbf{1}_{\partial\Omega}(z) = 1$ *if* $z \in \partial\Omega$ *and* $\mathbf{1}_{\partial\Omega}(z) = 0$ *if not, and* μ_d *denotes the negative eigenvalue of* $\mathrm{Hess}\, f(z)$ *when* $z \in \mathbf{j}(x)$ *and* $|\nabla f(z)| = 0$.
Finally, when $\mathbf{j}(x_j)\cap\partial\Omega$ *does not contain any critical point of* f*, the above error term* $O(\sqrt{h})$ *is actually of order* $O(h)$ *in* (134).

Remark 38. *The first statement of Theorem 3 is a simple consequence of its first item together with Theorem 2 (or even of Theorem 1 when* $\mathsf{m}^* = \mathsf{m}_0$*). Moreover, when in addition* $f(\mathbf{j}(x_1)) - f(x_1) > \ldots > f(\mathbf{j}(x_{\mathsf{m}^*})) - f(x_{\mathsf{m}^*})$*, the eigenvalues* $\lambda_{1,h}, \ldots, \lambda_{\mathsf{m}^*,h}$ *are respectively* $\Lambda_h(x_1), \ldots, \Lambda_h(x_{\mathsf{m}^*})$*. They are then simple and, for every* $\ell \in \{1, \ldots, \mathsf{m}^* - 1\}$*, there exists* $c > 0$ *such that it holds* $\lambda_{\ell+1,h} = O(e^{-\frac{c}{h}})\lambda_{\ell,h}$ *in the limit* $h \to 0$*. In general, the situation is slightly more involved and, when for example Theorem 3 applies with* $\mathsf{m}^* = 2$ *and* $f(\mathbf{j}(x_1)) - f(x_1) = f(\mathbf{j}(x_2)) - f(x_2)$*, Theorem 3 permits to discriminate which eigenvalue among* $\Lambda_h(x_1)$ *and* $\Lambda_h(x_2)$ *is* $\lambda_{1,h}$ *if and only if* $(A_{1,1}/B_1, A_{1,2}/B_1) \neq (A_{2,1}/B_2, A_{2,2}/B_2)$*, even though* $\lambda_{1,h}$ *is simple (see [26] in this connection when* f *is a double-well potential).*

Remark 39. *The term* $O(\sqrt{h})$ *in* (134) *is in general optimal, see Remark 25 and item 1 in Proposition 26.*

Remark 40. *Note that under the hypotheses made in Corollary 3, the set of principal wells of* f *consists in the unique element* $\mathsf{C}(x_1) = \mathsf{C}_{\mathbf{j}}(x_1) = \{f < \min_{\partial\Omega} f\}$*, where* $x_1 \in \arg\min_{\overline{\Omega}} f$ *(see Definition 7 and Section 3.3). It holds moreover* $\mathbf{j}(x_1) = \{z_1, \ldots, z_N\}$ *and the hypotheses of Theorem 3 are satisfied for* $\mathsf{m}^* = 1$*. The statement of Corollary 3 follows easily.*

Proof. Let us work with the labeling of $\mathsf{U}_0 = \{x_1, \ldots, x_{\mathsf{m}_0}\}$ considered in the statement of Theorem 3. Note in passing that the labeling of $\{x_{\mathsf{m}^*+1}, \ldots, x_{\mathsf{m}_0}\}$ is actually arbitrary. Let us moreover order $(\psi_x)_{x\in\mathsf{U}_0} = (\psi_1, \ldots, \psi_{\mathsf{m}_0})$ and $(\Theta_x)_{x\in\mathsf{U}_0} = (\Theta_1, \ldots, \Theta_{\mathsf{m}_0})$ according to this labeling of U_0. The proof of Theorem 3 is divided into several steps and is partly inspired by the analysis led in [19, Section 7.4] which generalizes the procedure made in [16, 17] (see also [31, Section C.3.1.2]).

Step 1. Let us first choose an orthonormal basis $\mathcal{B}_0$ of $\mathrm{Ran}(\pi_h)$ in $L^2(\Omega)$ and an adapted orthonormal basis $\mathcal{B}_1$ of $\mathrm{Span}\,(\Theta_i^\pi)_{i\in\{1,\ldots,\mathsf{m}_0\}}$ in $\Lambda^1 L^2(\Omega)$.

Step 1.a) Choice of the basis $\mathcal{B}_0$.
Let us first prove that items 2 and 3 in Theorem 3 imply the existence of $c > 0$ such that for every h small enough,

$$\forall i, j \in \{1, \ldots, \mathsf{m}^*\}, \quad \langle \psi_i, \psi_j \rangle_{L^2(\Omega)} = \delta_{i,j} + O\big(e^{-\frac{c}{h}}\big). \tag{135}$$

To this end, let us recall that from (89) and Definition 23, one has

$$\forall i \in \{1, \dots, \mathsf{m}_0\}, \quad \text{supp } \psi_i \subset \overline{\Omega_1(x_i)} \tag{136}$$

and let us consider $i, j \in \{1, \dots, \mathsf{m}^*\}$. According to item 2 in Theorem 3, it thus holds $\mathbf{j}(x_i) \cap \mathbf{j}(x_j) = \emptyset$ and, according to item 4.(i) in Section 3.3, there are two possible cases which finally lead to (135):

- either $\overline{\mathsf{C}_{\mathbf{j}}(x_j)} \cap \overline{\mathsf{C}_{\mathbf{j}}(x_i)} = \emptyset$, in which case, according to item 3.(i) in Definition 21 and to (136), the supports of ψ_i and ψ_j are disjoint and thus $\langle \psi_i, \psi_j \rangle_{L^2(\Omega)} = 0$,
- or, up to switching i and j, $\overline{\mathsf{C}_{\mathbf{j}}(x_j)} \subset \mathsf{C}_{\mathbf{j}}(x_i)$, in which case, according to item 3.(i) in Definition 21, $\overline{\Omega_1(x_j)} \subset \Omega_2(x_i) \subset \Omega_1(x_i)$. In this case, it then follows from Definition 23, (89), and (96), that

$$\langle \psi_i, \psi_j \rangle_{L^2(\Omega)} = \frac{\int_{\Omega_1(x_j)} \phi_i \phi_j \, e^{-\frac{2}{h} f}}{Z_{x_j} Z_{x_i}} \leq C h^{-\frac{d}{2}} \, e^{-\frac{1}{h}(2f(x_j) - f(x_i) - f(x_j))},$$

  where we also used the relation $\min_{\overline{\Omega_1(x_j)}} f = \min_{\overline{\mathsf{C}_{\mathbf{j}}(x_j)}} f = f(x_j)$ arising from the construction of the map $\mathsf{C}_{\mathbf{j}}$ and item 1 in Definition 21. Moreover, using item 3 in Theorem 3, it holds $f(x_j) > f(x_i)$, and thus, there exists $c > 0$ such that when $h \to 0$:

$$\langle \psi_i, \psi_j \rangle_{L^2(\Omega)} = O\big(e^{-\frac{c}{h}}\big).$$

Then, according to (135) and to Proposition 30, there exists $c > 0$ such that for all $i, j \in \{1, \dots, \mathsf{m}^*\}$, it holds in the limit $h \to 0$:

$$\langle \psi_i^\pi, \psi_j^\pi \rangle_{\Lambda^1 L^2(\Omega)} = \delta_{i,j} + O\big(e^{-\frac{c}{h}}\big). \tag{137}$$

Let us now consider the Gram-Schmidt orthonormalization $\mathcal{B}_0 := (e_1, \dots, e_{\mathsf{m}_0})$ of the family $(\psi_1^\pi, \dots, \psi_{\mathsf{m}_0}^\pi)$ in $L^2(\Omega)$. According to (137), it thus holds, for all $k \in \{1, \dots, \mathsf{m}^*\}$,

$$e_k = \big(1 + O\big(e^{-\frac{c}{h}}\big)\big)\psi_k^\pi + \sum_{q=1}^{k-1} O\big(e^{-\frac{c}{h}}\big)\, \psi_q^\pi.$$

Thus, the matrix C_0^π defined by (124) has the block structure

$$C_0^\pi = \begin{bmatrix} I_{\mathsf{m}^*} + O\big(e^{-\frac{c}{h}}\big) & [C_0^\pi]_2 \\ 0 & [C_0^\pi]_4 \end{bmatrix}, \tag{138}$$

where I_{m^*} is the identity matrix of $\mathbb{R}^{\mathsf{m}^* \times \mathsf{m}^*}$, $[C_0^\pi]_4 \in \mathbb{R}^{(\mathsf{m}_0 - \mathsf{m}^*) \times (\mathsf{m}_0 - \mathsf{m}^*)}$ is an invertible matrix (since, according to Proposition 33, C_0^π is invertible), and $[C_0^\pi]_2 \in \mathbb{R}^{\mathsf{m}^* \times (\mathsf{m}_0 - \mathsf{m}^*)}$. One then defines the $\mathsf{m}_0 \times \mathsf{m}_0$ matrix C_0 by

$$C_0 := \begin{bmatrix} I_{\mathsf{m}^*} & [C_0^\pi]_2 \\ 0 & [C_0^\pi]_4 \end{bmatrix}, \tag{139}$$

so that, according to Proposition 33, C_0 is invertible and

$$C_0 = O(1),\ C_0^{-1} = \begin{bmatrix} I_{\mathsf{m}^*} & -[C_0^\pi]_2[C_0^\pi]_4^{-1} \\ 0 & [C_0^\pi]_4^{-1} \end{bmatrix} = O(1),\ \text{and}\ C_0^{-1}C_0^\pi = I_{\mathsf{m}_0} + O\big(e^{-\frac{c}{h}}\big). \quad (140)$$

Step 1.b) Choice of the basis $\mathcal{B}_1$.
According to Definition 29, item 2 in Theorem 3, and to item 2.(i) in Proposition 26, it holds, for every h small enough:

$$\forall j \in \{1, \dots, \mathsf{m}^*\},\ \forall i \in \{1, \dots, \mathsf{m}_0\}, \quad \langle \Theta_i, \Theta_j \rangle_{\Lambda^1 L^2(\Omega)} = \delta_{i,j}. \quad (141)$$

Thus, using in addition Proposition 30, it holds, for every h small enough:

$$\forall j \in \{1, \dots, \mathsf{m}^*\},\ \forall i \in \{1, \dots, \mathsf{m}_0\}, \quad \langle \Theta_i^\pi, \Theta_j^\pi \rangle_{\Lambda^1 L^2(\Omega)} = \delta_{i,j} + O(h). \quad (142)$$

Let us now consider the Gram-Schmidt orthonormalization $\mathcal{B}_1 := (\Upsilon_1, \dots, \Upsilon_{\mathsf{m}_0})$ of the family $(\Theta_1^\pi, \dots, \Theta_{\mathsf{m}_0}^\pi\}$ in $\Lambda^1 L^2(\Omega)$. It thus holds in the limit $h \to 0$,

$$\forall k \in \{1, \dots, \mathsf{m}^*\}, \quad \Upsilon_k = \big(1 + O(h)\big)\Theta_k^\pi + \sum_{q=1}^{k-1} O(h)\, \Theta_q^\pi$$

and, for some real numbers $a_{k,q}(h)$, where $k \in \{\mathsf{m}^* + 1, \dots, \mathsf{m}_0\}$ and $q \in \{\mathsf{m}^* + 1, \dots, k\}$,

$$\forall k \in \{\mathsf{m}^* + 1, \dots, \mathsf{m}_0\}, \quad \Upsilon_k = \sum_{q=1}^{\mathsf{m}^*} O(h)\, \Theta_q^\pi + \sum_{q=\mathsf{m}^*+1}^{k} a_{k,q}(h)\, \Theta_q^\pi.$$

Hence, with this choice of $\mathcal{B}_1$, the matrix C_1^π defined by (124) has the block structure

$$C_1^\pi = \begin{bmatrix} I_{\mathsf{m}^*} + O(h) & O(h) \\ 0 & [C_1^\pi]_4 \end{bmatrix}, \quad (143)$$

where $[C_1^\pi]_4 \in \mathbb{R}^{(\mathsf{m}_0 - \mathsf{m}^*) \times (\mathsf{m}_0 - \mathsf{m}^*)}$ is an invertible matrix (since C_1^π is invertible, see indeed Proposition 33) and, according to (131), $[C_1^\pi]_4 = O(1)$ and $[C_1^\pi]_4^{-1} = O(1)$ in the limit $h \to 0$. Finally, let us define the $\mathsf{m}_0 \times \mathsf{m}_0$ matrix C_1 by

$$C_1 := \begin{bmatrix} I_{\mathsf{m}^*} & 0 \\ 0 & [C_1^\pi]_4 \end{bmatrix}, \quad (144)$$

so that, in the limit $h \to 0$, it holds

$$C_1 = O(1) \ \text{ and } \ C_1^{-1} = O(1) \quad (145)$$

and

$$\|C_1^{-1}\,(I_{\mathsf{m}_0} + O(h))\, C_1^\pi\| = 1 + O(h) \ \text{ and } \ \|(C_1^\pi)^{-1}(I_{\mathsf{m}_0} + O(h))\, C_1\| = 1 + O(h). \quad (146)$$

Step 2. Let us recall that in the limit $h \to 0$, the m_0 smallest eigenvalues of $\Delta_{f,h}^D$ are the squares of the singular values of the matrix $S^{\mathcal{B}_0,\mathcal{B}_1} = {}^tC_1^\pi\, S^\pi\, C_0^\pi \in \mathbb{R}^{\mathsf{m}_0 \times \mathsf{m}_0}$,

where C_0^π, C_1^π, and S^π are defined in (124) and in (125). Moreover, the relation (130) leads to the factorization (see (126) for the definition of the matrix S)

$$S^{\mathcal{B}_0,\mathcal{B}_1} = {}^t\big(C_1^{-1}(I_{\mathsf{m}_0} + O(h))C_1^\pi\big)\,{}^tC_1\,S\,C_0\,\big(C_0^{-1}C_0^\pi\big).$$

Using (140), (146), and Lemma 37, it follows that

$$\forall j \in \{1,\dots,\mathsf{m}_0\}, \quad \eta_j(S^{\mathcal{B}_0,\mathcal{B}_1}) = \eta_j({}^tC_1\,S\,C_0)\,\big(1+O(h)\big). \tag{147}$$

Hence, the m_0 smallest eigenvalues of $\Delta_{f,h}^D$ are, up to a multiplicative term of order $\big(1+O(h)\big)$, the squares of the singular values of the matrix ${}^tC_1\,S\,C_0$.

In order to prepare the precise computation of these singular values made in the following step, let us first suitably decompose the matrices taking part into ${}^tC_1\,S\,C_0$. To this end, let us introduce

$$\mathsf{k}^* \in \{1,\dots,\mathsf{m}^*\}$$

and write the diagonal matrix D defined by (127) and (128) as follows:

$$D = \begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix}, \tag{148}$$

where D_1 is the square diagonal matrix of size k^* defined by

$$D_1 := \mathrm{Diag}\big(h^{p_1}\,e^{-\frac{1}{h}(f(\mathsf{j}(x_1))-f(x_1))},\dots,h^{p_{\mathsf{k}^*}}\,e^{-\frac{1}{h}(f(\mathsf{j}(x_{\mathsf{k}^*}))-f(x_{\mathsf{k}^*}))}\big) \tag{149}$$

and D_2 is the square diagonal matrix of size $\mathsf{m}_0-\mathsf{k}^*$ defined by

$$D_2 := \mathrm{Diag}\big(h^{p_{\mathsf{k}^*+1}}\,e^{-\frac{1}{h}(f(\mathsf{j}(x_{\mathsf{k}^*+1}))-f(x_{\mathsf{k}^*+1}))},\dots,h^{p_{\mathsf{m}_0}}\,e^{-\frac{1}{h}(f(\mathsf{j}(x_{\mathsf{m}_0}))-f(x_{\mathsf{m}_0}))}\big). \tag{150}$$

Moreover, according to (141), the matrices $S = \big(\|d_{f,h}\psi_j\|_{\Lambda^1L^2(\Omega)}\,\langle\Theta_i,\Theta_j\rangle_{\Lambda^1L^2(\Omega)}\big)_{i,j}$ and $T = SD^{-1}$ defined in (126) and in (129) have the block structure

$$S = \begin{bmatrix} S_1 & 0 \\ 0 & S_2 \end{bmatrix} \quad\text{and}\quad T = \begin{bmatrix} T_1 & 0 \\ 0 & T_2 \end{bmatrix}, \tag{151}$$

where:

– T_1 and S_1 are square diagonal matrices of size k^* defined by

$$S_1 := \mathrm{Diag}(S_{1,1},\dots,S_{\mathsf{k}^*,\mathsf{k}^*}) \quad\text{and}\quad T_1 := S_1\,D_1^{-1}, \tag{152}$$

– $T_2, S_2 \in \mathbb{R}^{(\mathsf{m}_0-\mathsf{k}^*)\times(\mathsf{m}_0-\mathsf{k}^*)}$ and, according to Lemma 36,

$$T_2 = S_2\,D_2^{-1} \text{ is invertible} \quad\text{and}\quad T_2^{-1} = O(1). \tag{153}$$

Using in addition (139) and (144), the matrices C_0, C_1 and thus ${}^tC_1SC_0$ have the block structures

$$C_0 = \begin{bmatrix} I_{\mathsf{k}^*} & U \\ 0 & V \end{bmatrix}, \quad C_1 = \begin{bmatrix} I_{\mathsf{k}^*} & 0 \\ 0 & W \end{bmatrix}, \quad\text{and thus}\quad {}^tC_1\,S\,C_0 = \begin{bmatrix} S_1 & S_1U \\ 0 & {}^tWS_2V \end{bmatrix}, \tag{154}$$

where, according to (140) and (145), it holds in the limit $h \to 0$:

$$U, V = O(1)\,,\ V^{-1} = O(1) \quad \text{and} \quad W, W^{-1} = O(1). \tag{155}$$

Note lastly that when $\mathsf{k}^* = \mathsf{m}^*$, one has $U = [C_0^\pi]_2$, $V = [C_0^\pi]_4$, and $W = [C_1^\pi]_4$.

Step 3. We are now in position to prove Theorem 3. To this end, we will compute the smallest singular values of the matrix ${}^tC_1\, S\, C_0$ that we have seen to be, up to a multiplicative error term of order $1+O(h)$, the square roots of the smallest eigenvalues of $\Delta^D_{f,h}$ (see indeed (147)).

In the following, one uses the block decompositions exhibited in (148)–(154) and, for $\ell \in \mathbb{N}$, one denotes by $\|\cdot\|_2$ the Euclidean norm on $\mathbb{R}^\ell$. Moreover, for every h small enough, one chooses the ordering of the set $\{x_1, \dots, x_{\mathsf{m}^*}\}$, depending on h, such that

$$\text{the sequence } \big(S_{j,j}\big)_{j\in\{1,\dots,\mathsf{m}^*\}} \text{ is increasing.}$$

According to (147), (152), and to Proposition 35, it then suffices to show that there exists $c > 0$ such that it holds in the limit $h \to 0$,

$$\forall \ell \in \{1, \dots, \mathsf{m}^*\}\,, \quad \eta_{\mathsf{m}_0-\ell+1}({}^tC_1\, S\, C_0) = S_{\ell,\ell}\,\big(1 + O(e^{-\frac{c}{h}})\big). \tag{156}$$

To this end, we recall that by the Max-Min principle, one has for every $\ell \in \{1, \dots, \mathsf{m}_0\}$,

$$\eta_{\mathsf{m}_0-\ell+1}({}^tC_1\, S\, C_0) = \max_{E\subset\mathbb{R}^{\mathsf{m}_0},\ \dim E=\ell-1}\ \min_{y\in E^\perp\,;\,\|y\|_2=1} \big\|{}^tC_1\, S\, C_0 y\big\|_2 \tag{157}$$

$$= \min_{E\subset\mathbb{R}^{\mathsf{m}_0},\ \dim E=\ell}\ \max_{y\in E\,;\,\|y\|_2=1} \big\|{}^tC_1\, S\, C_0 y\big\|_2. \tag{158}$$

To obtain the upper bound in (156) for some arbitrary $\ell \in \{1, \dots, \mathsf{m}^*\}$, we apply (158) which gives, according to (154) applied with $\mathsf{k}^* = \ell$ and to (152):

$$\begin{aligned}\eta_{\mathsf{m}_0-\ell+1}({}^tC_1\, S\, C_0) \ \le\ \max_{y\in\mathbb{R}^\ell\,;\,\|y\|_2=1} \big\|{}^tC_1\, S\, C_0\,(y, 0, \dots, 0)\big\|_2 \ &= \max_{y\in\mathbb{R}^\ell\,;\,\|y\|_2=1} \big\|S_1 y\big\|_2 \\ &= S_{\ell,\ell}. \end{aligned} \tag{159}$$

Let us now prove the lower bound in (156) for some arbitrary $\ell \in \{1, \dots, \mathsf{m}^*\}$. For that purpose, let us introduce $y^* \in \mathbb{R}^{\mathsf{m}_0}$ such that $\|y^*\|_2 = 1$, $y^* \in (\mathbb{R}^{\ell-1} \times \{0, \dots, 0\})^\perp$, and

$$\big\|{}^tC_1\, S\, C_0\, y^*\big\|_2 = \min_{y\in(\mathbb{R}^{\ell-1}\times\{0,\dots,0\})^\perp\,;\,\|y\|_2=1} \big\|{}^tC_1\, S\, C_0\, y\big\|_2.$$

Note that according to (157), it holds in particular

$$\eta_{\mathsf{m}_0-\ell+1}({}^tC_1\, S\, C_0) \ \ge\ \big\|{}^tC_1\, S\, C_0\, y^*\big\|_2. \tag{160}$$

Let us also introduce $\mathsf{k}^* \in \{\ell, \dots, \mathsf{m}^*\}$ such that

$$f(\mathbf{j}(x_\ell)) - f(x_\ell) = f(\mathbf{j}(x_{\mathsf{k}^*})) - f(x_{\mathsf{k}^*}) > \max_{j\in\{\mathsf{k}^*+1,\dots,\mathsf{m}_0\}} f(\mathbf{j}(x_j)) - f(x_j). \tag{161}$$

Note that this is indeed possible by the first item of Theorem 3. Let us then write $y^* = (y_a^*, y_b^*)$, where $y_a^* \in \mathbb{R}^{\mathsf{k}^*}$ and $y_b^* \in \mathbb{R}^{\mathsf{m}_0-\mathsf{k}^*}$, and let us prove that there exists $c > 0$ such that when $h \to 0$,

$$\|y_b^*\|_2 = O\big(e^{-\frac{c}{h}}\big). \tag{162}$$

According to (160), (154) applied with k^*, and to the triangular inequality, one has

$$\eta_{\mathsf{m}_0-\ell+1}({}^tC_1\, S\, C_0) \geq \big\|\, {}^tC_1\, S\, C_0\, (y_a^*, y_\beta^*)\big\|_2 \geq \big\|\, {}^tC_1\, S\, C_0\, (0, y_b^*)\big\|_2 - \big\|\, {}^tC_1\, S\, C_0\, (y_a^*, 0)\big\|_2$$
$$= \big\|\, {}^tC_1\, S\, C_0\, (0, y_b^*)\big\|_2 - \big\|S_1 y_a^*\big\|_2.$$

Using in addition (159) and (152) with k^*, it follows that in the limit $h \to 0$:

$$\big\|\, {}^tC_1\, S\, C_0\, (0, y_b^*)\big\|_2 \;\leq\; S_{\ell,\ell} + \|S_1\|\, \|y_a^*\|_2 \;\leq\; 2\, S_{\mathsf{k}^*,\mathsf{k}^*}. \tag{163}$$

Moreover, according to (154), one has

$$\big\|\, {}^tC_1\, S\, C_0\, (0, y_b^*)\big\|_2 = \Big(\big\|\, S_1 U\, y_b^*\big\|_2^2 + \big\|\, {}^tW S_2 V\, y_b^*\big\|_2^2\Big)^{\frac{1}{2}} \geq \big\|\, {}^tW S_2 V\, y_b^*\big\|_2,$$

where, using (153) and (155), it holds for some $C > 0$ in the limit $h \to 0$,

$$\big\|\, {}^tW S_2 V\, y_b^*\big\|_2 = \big\|\, {}^tW T_2 D_2 V\, y_b^*\big\|_2 \geq \frac{1}{C} \|D_2^{-1}\|^{-1} \|y_b^*\|_2.$$

It then follows from (163) that in the limit $h \to 0$, it holds

$$\|y_b^*\|_2 \leq 2\, C\, \|D_2^{-1}\|\, S_{\mathsf{k}^*,\mathsf{k}^*},$$

which leads to (162) according to item 2 in Proposition 35, (150), and to (161).

Then, using (160), (154) with k^*, and (162) together with the fact that $U = O(1)$ (see (155)), we obtain the existence of $c > 0$ such that it holds in the limit $h \to 0$,

$$\eta_{\mathsf{m}_0-\ell+1}({}^tC_1\, S\, C_0) \geq \big\|\, {}^tC_1\, S\, C_0\, y^*\big\|_2 \geq \big\|S_1 y_a^*\big\|_2 - \big\|S_1 U y_b^*\big\|_2$$
$$= \big\|S_1 y_a^*\big\|_2 - \|S_1\|\, O\big(e^{-\frac{c}{h}}\big).$$

Hence, using in addition $\|y_a^*\|_2 = 1 + O\big(e^{-\frac{c}{h}}\big)$ (which follows from (162) and $\|y^*\|_2 = 1$), $y_{a,1}^* = \cdots = y_{a,\ell-1}^* = 0$ (since $y^* \in (\mathbb{R}^{\ell-1} \times \{0, \ldots, 0\})^\perp$), (152), item 2 in Proposition 35, and (161), it holds in the limit $h \to 0$,

$$\eta_{\mathsf{m}_0-\ell+1}({}^tC_1\, S\, C_0) \geq S_{\ell,\ell}\big(1 + O(e^{-\frac{c}{h}})\big) - S_{\mathsf{k}^*,\mathsf{k}^*}\, O\big(e^{-\frac{c}{h}}\big) \geq S_{\ell,\ell}\, \big(1 + O(e^{-\frac{c}{2h}})\big),$$

which concludes the proof of (156). The proof of Theorem 3 is thus complete. ∎

Acknowledgements. This work was partially supported by the grant PHC AMADEUS 2018 PROJET N° 39452YK.

References

[1] N. Berglund. Kramers' law: validity, derivations and generalisations. *Markov Process. Related Fields*, 19(3):459–490, 2013.

[2] N. Berglund and S. Dutercq. The Eyring-Kramers law for Markovian jump processes with symmetries. *J. Theoret. Probab.*, 29(4):1240–1279, 2016.

[3] N. Berglund and B. Gentz. The Eyring-Kramers law for potentials with nonquadratic saddles. *Markov Process. Relat. Fields*, 16(3):549–598, 2010.

[4] D. Borisov and O. Sultanov. Asymptotic analysis of exit time for dynamical systems with a single well potential. *J. Differential Equations*, 269(8):78–116, 2020.

[5] A. Bovier, M. Eckhoff, V. Gayrard, and M. Klein. Metastability in reversible diffusion processes. I. Sharp asymptotics for capacities and exit times. *J. Eur. Math. Soc.*, 6(4):399–424, 2004.

[6] A. Bovier, V. Gayrard, and M. Klein. Metastability in reversible diffusion processes. II. Precise asymptotics for small eigenvalues. *J. Eur. Math. Soc.*, 7(1):69–99, 2005.

[7] M. Cameron. Computing the asymptotic spectrum for networks representing energy landscapes using the minimum spanning tree. *Netw. Heterog. Media*, 9(3):383–416, 2014.

[8] H.L. Cycon, R.G. Froese, W. Kirsch, and B. Simon. *Schrödinger operators with application to quantum mechanics and global geometry.* Texts and Monographs in Physics. Springer-Verlag, Berlin, study edition, 1987.

[9] G. Di Gesù and D. Le Peutrec. Small noise spectral gap asymptotics for a large system of nonlinear diffusions. *J. Spectr. Theory*, 7(4):939–984, 2017.

[10] G. Di Gesù, T. Lelièvre, D. Le Peutrec, and B. Nectoux. The exit from a metastable state: concentration of the exit point distribution on the low energy saddle points, 2019. Preprint available on `https://arxiv.org/abs/1902.03270`, 113 pages.

[11] G. Di Gesù, T. Lelièvre, D. Le Peutrec, and B. Nectoux. The exit from a metastable state: concentration of the exit point distribution on the low energy saddle points, part 1. *J. Math. Pures Appl.*, 138(9):242–306, 2020.

[12] L.C. Evans. *Partial differential equations*, volume 19 of *Graduate Studies in Mathematics.* American Mathematical Society, Providence, RI, second edition, 2010.

[13] Y. Fan, S. Yip, and B. Yildiz. Autonomous basin climbing method with sampling of multiple transition pathways: application to anisotropic diffusion of point defects in hcp Zr. *Journal of Physics: Condensed Matter*, 26:365402, 2014.

[14] M.I. Freidlin and A.D. Wentzell. *Random Perturbations of Dynamical Systems.* Springer-Verlag, 2012.

[15] D. Gilbarg and N.S. Trudinger. *Elliptic partial differential equations of second order.* Classics in Mathematics. Springer-Verlag, Berlin, 2001. Reprint of the 1998 edition.

[16] B. Helffer, M. Klein, and F. Nier. Quantitative analysis of metastability in reversible diffusion processes via a Witten complex approach. *Mat. Contemp.*, 26:41–85, 2004.

[17] B. Helffer and F. Nier. Quantitative analysis of metastability in reversible diffusion processes via a Witten complex approach: the case with boundary. *Mém. Soc. Math. Fr. (N.S.)*, (105):vi+89, 2006.

[18] B. Helffer and J. Sjöstrand. Puits multiples en mécanique semi-classique IV Etude du complexe de Witten. *Comm. Partial Differential Equations*, 10(3):245–340, 1985.

[19] F. Hérau, M. Hitrik, and J. Sjöstrand. Tunnel effect and symmetries for Kramers-Fokker-Planck type operators. *J. Inst. Math. Jussieu*, 10(3):567–634, 2011.

[20] R.A. Holley, S. Kusuoka, and D.W. Stroock. Asymptotics of the spectral gap with applications to the theory of simulated annealing. *J. Funct. Anal.*, 83(2):333–347, 1989.

[21] J. Jost. *Riemannian geometry and geometric analysis.* Universitext. Springer, Heidelberg, sixth edition, 2011.

[22] C. Landim, M. Mariani, and I. Seo. Dirichlet's and Thomson's principles for non-selfadjoint elliptic operators with application to non-reversible metastable diffusion processes. *Arch. Rational Mech. Anal.*, 231(2):887–938, 2019.

[23] D. Le Peutrec. Local WKB construction for Witten Laplacians on manifolds with boundary. *Anal. PDE*, 3(3):227–260, 2010.

[24] D. Le Peutrec. Small eigenvalues of the Neumann realization of the semiclassical Witten Laplacian. *Ann. Fac. Sci. Toulouse Math. (6)*, 19(3-4):735–809, 2010.

[25] D. Le Peutrec. Quelques résultats d'analyse et de probabilités autour du laplacien de Witten, 2019. Habilitation dissertation, Université Paris-Sud, available on `https://tel.archives-ouvertes.fr/tel-02379066`, 136 pages.

[26] D. Le Peutrec and B. Nectoux. Repartition of the quasi-stationary distribution and first exit point density for a double-well potential. *SIAM J. Math. Anal.*, 52(1):581–604, 2020.

[27] T. Lelièvre and F. Nier. Low temperature asymptotics for quasistationary distributions in a bounded domain. *Anal. PDE*, 8(3):561–628, 2015.

[28] P. Mathieu. Spectra, exit times and long time asymptotics in the zero-white-noise limit. *Stochastics*, 55(1-2):1–20, 1995.

[29] L. Michel. About small eigenvalues of the Witten Laplacian. *Pure Appl. Anal.*, 1(2):149–206, 2019.

[30] L. Miclo. Comportement de spectres d'opérateurs de Schrödinger à basse température. *Bulletin des sciences mathématiques*, 119(6):529–554, 1995.

[31] B. Nectoux. *Analyse spectrale et analyse semi-classique pour la métastabilité en dynamique moléculaire.* PhD thesis, Université Paris Est, 2017.

[32] B. Nectoux. Sharp estimate of the mean exit time of a bounded domain in the zero white noise limit. *Markov Process. Relat. Fields*, 26(3):403–422, 2020.

[33] C. Schütte. Conformational dynamics: modelling, theory, algorithm and application to biomolecules, 1998. Habilitation dissertation, Free University Berlin.

[34] C. Schütte and M. Sarich. *Metastability and Markov state models in molecular dynamics*, volume 24 of *Courant Lecture Notes.* American Mathematical Society, 2013.

[35] G. Schwarz. *Hodge decomposition – a method for solving boundary value problems*, volume 1607 of *Lecture Notes in Mathematics.* Springer-Verlag, Berlin, 1995.

[36] B. Simon. *Trace ideals and their applications*, volume 35. Cambridge University Press Cambridge, 1979.

[37] M.R. Sorensen and A.F. Voter. Temperature-accelerated dynamics for simulation of infrequent events. *J. Chem. Phys.*, 112(21):9599–9606, 2000.

[38] A.F. Voter. A method for accelerating the molecular dynamics simulation of infrequent events. *J. Chem. Phys.*, 106(11):4665–4677, 1997.

[39] A.F. Voter. Parallel replica method for dynamics of infrequent events. *Phys. Rev. B*, 57(22):R13 985, 1998.

[40] A.F. Voter. *Radiation Effects in Solids*, chapter Introduction to the Kinetic Monte Carlo Method. Springer, NATO Publishing Unit, 2005.

[41] D.J. Wales. *Energy landscapes.* Cambridge University Press, 2003.

[42] E. Witten. Supersymmetry and Morse theory. *J. Differential Geom.*, 17(4):661–692 (1983), 1982.