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EYRING-KRAMERS EXIT RATES FOR THE OVERDAMPED LANGEVIN DYNAMICS: THE CASE WITH SADDLE POINTS ON THE BOUNDARY

by Tony Lelièvre, Dorian Le Peutrec & Boris Nectoux

Abstract. — Let $(X_t)_{t\geqslant 0}$ be the stochastic process solution to the overdamped Langevin dynamics

$$dX_t = -\nabla f(X_t)\,dt + \sqrt{h}\,dB_t$$

and let $\Omega \subset \mathbb{R}^d$ be the basin of attraction of a local minimum of $f : \mathbb{R}^d \to \mathbb{R}$. Up to a small perturbation of Ω to make it smooth, we prove that the exit rates of $(X_t)_{t\geqslant 0}$ from Ω through each of the saddle points of f on $\partial\Omega$ can be parametrized by the celebrated Eyring-Kramers laws, in the limit $h \to 0$. This result provides firm mathematical grounds to jump Markov models which are used to model the evolution of molecular systems, as well as to some numerical methods which use these underlying jump Markov models to efficiently sample metastable trajectories of the overdamped Langevin dynamics.

Résumé (Taux de sortie d'Eyring-Kramers pour la dynamique de Langevin sur-amortie : le cas des points-selles sur la frontière)

On considère la dynamique de Langevin sur-amortie

$$dX_t = -\nabla f(X_t)\,dt + \sqrt{h}\,dB_t$$

et $\Omega \subset \mathbb{R}^d$, le bassin d'attraction d'un minimum local de $f : \mathbb{R}^d \to \mathbb{R}$. Quitte à légèrement perturber Ω pour en lisser le bord, nous montrons que les taux de sortie du processus $(X_t)_{t\geqslant 0}$ de Ω par chacun des points-selles de f sur $\partial\Omega$ peuvent être paramétrés par les lois d'Eyring-Kramers, dans la limite $h \to 0$. Ce résultat fournit une base mathématique solide aux modèles de sauts markoviens qui sont utilisés pour décrire l'évolution des systèmes moléculaires, ainsi qu'à certaines méthodes numériques qui s'appuient sur ces modèles pour échantillonner efficacement des trajectoires métastables de la dynamique de Langevin sur-amortie.

Contents

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1. Motivation and statements of the main results

1.1. An informal presentation of the results. — Let us first present in this section the motivation for this work, namely the modeling and the efficient simulation of metastable stochastic dynamics which are used in molecular dynamics, as well as an informal statement of the main results.

Overdamped Langevin dynamics and metastable exit. — Let us consider a potential energy function

$$f : \mathbb{R}^d \longrightarrow \mathbb{R},$$

which is assumed to be smooth and with non-degenerate critical points. A prototypical dynamics to describe the evolution of a molecular system in the energy landscape f at a fixed temperature is the overdamped Langevin dynamics:

$$dX_t = -\nabla f(X_t)\, dt + \sqrt{h}\, dB_t, \tag{1}$$

where $(X_t)_{t\geqslant 0}$ gives the positions of the atoms as a function of time, $h > 0$ is (proportional to) the temperature (and will be assumed to be small in the following), and $(B_t)_{t\geqslant 0}$ is a d-dimensional standard Brownian motion. Let us consider $\Omega \subset \mathbb{R}^d$ a basin of attraction(1) of a local minimum of f. In many cases of interest, the process spends a lot of time within Ω before leaving it, typically because the temperature h is small compared to the energy barriers which have to be overcome to leave Ω: this phenomenon is called metastability, and an exit which occurs after a long relaxation time within Ω is called a metastable exit (this will be formalized below using the notion of quasi-stationary distribution). We are interested in the so-called exit problem [34], which consists in precisely describing the exit event from Ω in the limit $h \to 0$, namely the law of the pair of random variables(2) (τ, X_τ), where

$$\tau = \inf\{t \geqslant 0,\ X_t \notin \Omega\} \tag{2}$$

is the first exit time from Ω, and X_τ is thus the first exit point. More precisely, we will show that for a metastable exit, in the limit $h \to 0$, the law of (τ, X_τ) can be approximated using a simple jump Markov model with exit rates from Ω parametrized by the celebrated Eyring-Kramers laws, a model which is sometimes called kinetic Monte Carlo in the physics literature [91]. These exit rates are associated with the local minima of f on $\partial\Omega$, which are saddle points of f (namely critical points of f of index 1) since Ω is a basin of attraction. These points are on the most probable exit pathways from Ω.

Before providing more details on this kinetic Monte Carlo model in the next paragraph, let us emphasize that this question is both important in terms of modeling,

(1) Actually, as will be discussed below, since we require Ω to be a smooth bounded domain, one may need to consider a small perturbation of a basin of attraction of f to apply our results, see Remark 5.

(2) Throughout this work, Ω is a fixed domain, and we therefore do not indicate explicitly the dependency of τ on Ω.

and in terms of numerical simulation of (1). In terms of modeling, it gives a rigorous framework to prove that a coarse-grained version of the overdamped Langevin dynamics is indeed the kinetic Monte Carlo dynamics (also known as Markov state model) parametrized by the Eyring-Kramers laws. Actually, if the states form a partition of $\mathbb{R}^d$ (which is indeed the case, up to a null set, if one defines the states as the basin of attractions of the local minima of f) and if all the exits are assumed to be metastable, one can even use a kinetic Monte Carlo model not only to sample the exit from a metastable state, but to actually describe the full evolution of the system, see for example [13, 79, 80, 91, 92, 76]. In terms of numerical simulations, metastability implies that the direct numerical simulation of (1) is prohibitive, because a lot of computational time is wasted in metastable states: using the simpler underlying kinetic Monte Carlo model, one can then accelerate the sampling of the exit event when the process $(X_t)_{t\geqslant 0}$ remains trapped in a metastable state. This is the cornerstone of the so-called accelerated dynamics algorithms such as temperature accelerated dynamics [83] or hyperdynamics [90, 88], see [26, 62, 77] for more details. These algorithms are widely used in practice with applications in material science, see for instance [2, 73, 84, 33]. In this context, the states are very often defined as basins of attractions of local minima of f: this is indeed numerically convenient since a simple steepest decent algorithm can be used to identify in which state the system is.

Kinetic Monte Carlo and the Eyring-Kramers law. — Let us recall that Ω is a basin of attraction of a local minimum of f. Thus, f has a unique critical point in Ω, which is also the global minimum of f in Ω, denoted by x_0. Moreover, the local minima of f on $\partial\Omega$ are saddle points of f, that we denote by $\{z_1,\dots,z_n\}\subset\partial\Omega$. The kinetic Monte Carlo algorithm models the exit event from Ω through a pair of random variables $(\tau_{\mathsf{kMC}},\mathsf{Y}_{\mathsf{kMC}})$, where τ_{kMC} is the exit time and $\mathsf{Y}_{\mathsf{kMC}}\in\{z_1,\dots,z_n\}$ is equal to z_i if the process exits Ω through a neighborhood of z_i in $\partial\Omega$. The law of $(\tau_{\mathsf{kMC}},\mathsf{Y}_{\mathsf{kMC}})$ requires a collection of rates $(\mathsf{k}_z)_{z\in\{z_1,\dots,z_n\}}$ associated with the saddle points, and is defined by the following three properties:

(i) the time τ_{kMC} is exponentially distributed with parameter $\sum_{z\in\{z_1,\dots,z_n\}}\mathsf{k}_z$

$$\tau_{\mathsf{kMC}}\sim\mathcal{E}\Big(\sum_{z\in\{z_1,\dots,z_n\}}\mathsf{k}_z\Big);\tag{3}$$

(ii) τ_{kMC} is independent of $\mathsf{Y}_{\mathsf{kMC}}$; and (iii) for all $z\in\{z_1,\dots z_n\}$,

$$\mathbb{P}[\mathsf{Y}_{\mathsf{kMC}}=z]=\frac{\mathsf{k}_z}{\sum_{z\in\{z_1,\dots,z_n\}}\mathsf{k}_z}.\tag{4}$$

Moreover, in the setting of the so-called harmonic transition state theory, the rates are defined using the famous Eyring-Kramers formula [38, 91]: for any $z\in\{z_1,\dots,z_n\}$,

$$\mathsf{k}_z=\mathsf{P}_z\,e^{-(2/h)(f(z)-f(x_0))},\tag{5}$$

where, we recall, $x_0 \in \Omega$ is the global minimum of f in Ω and the prefactor P_z is

$$\mathsf{P}_z = \frac{|\mu_z|}{\pi} \frac{\sqrt{\det \operatorname{Hess} f(x_0)}}{\sqrt{|\det \operatorname{Hess} f(z)|}}, \tag{6}$$

where μ_z is the negative eigenvalue of $\operatorname{Hess} f(z)$.

Remark 1. — The Eyring-Kramers formulas are sometimes defined with a prefactor which is the half of the right-hand-side in (6). This depends whether one considers exit rates (as in this work) or transition rates (as for example in the works [8, 9] where eigenvalues of the infinitesimal generator of the process $(X_t)_{t\geqslant 0}$ are identified with transition rates). The transition rates are half of the exit rates since, in the small temperature regime, once the process reaches a saddle point z, it has a probability $1/2$ to immediately come back to Ω, and a probability $1/2$ to actually make a transition to the neighboring state (see e.g. [63, Rem. 8] for further discussions).

The objective of this work is to show that, for a metastable exit, in the limit $h \to 0$, the law of $(\tau_{\mathsf{kMC}}, \mathsf{Y}_{\mathsf{kMC}})$ indeed approximates the law of (τ, X_τ), in a sense that will be made precise in the next paragraph. We will use the quasi-stationary distribution approach to metastability, which appears to be very useful to study the exit problem [55, 27, 6].

The quasi-stationary distribution approach to metastability. — As explained above, we will study metastable exits, namely exits which occur after the stochastic process $(X_t)_{t\geqslant 0}$ solution to (1) relaxes within Ω. The notion of quasi-stationary distribution gives a way to formalize mathematically this idea. Let us recall standard facts on the existence and uniqueness of a quasi-stationary distribution for a diffusion process (see for example [14, 18] for more details).

Definition 2. — Let us denote by $\mathcal{P}(\Omega)$ the set of probability measures supported in Ω. A quasi-stationary distribution in $\Omega \subset \mathbb{R}^d$ for a Markov process $(X_t)_{t\geqslant 0}$ with values in $\mathbb{R}^d$ is a probability measure $\mu \in \mathcal{P}(\Omega)$ such that:

$$\forall t \geqslant 0, \forall \text{ measurable } A \subset \Omega, \quad \mu(A) = \frac{\mathbb{P}_\mu\left[X_t \in A, t < \tau\right]}{\mathbb{P}_\mu\left[t < \tau\right]},$$

where $\tau = \inf\{t > 0, X_t \notin \Omega\}$, and the subscript μ in $\mathbb{P}_\mu$ indicates that $X_0 \sim \mu$.

It is well-known (see for example [55, 15]) that for a smooth potential f and a bounded smooth domain Ω, the process $(X_t)_{t\geqslant 0}$ solution to (1) admits a unique quasi-stationary distribution on Ω, denoted by ν_h in the following. Moreover, the previously cited works also show the following exponential convergence result:

$$\begin{aligned} &\exists c > 0, \forall \mu \in \mathcal{P}(\Omega), \exists C(\mu) > 0, \exists t(\mu) > 0, \\ &\forall t \geqslant t(\mu), \forall \text{ measurable } A \subset \Omega, \quad \left|\mathbb{P}_\mu\big[X_t \in A \big| t < \tau\big] - \nu_h(A)\right| \leqslant C(\mu) e^{-ct}. \end{aligned} \tag{7}$$

Therefore, if the process $(X_t)_{t\geqslant 0}$ remains trapped in Ω for a long-time, then X_t is approximately distributed according to the quasi-stationary distribution ν_h, which can thus be seen as a local equilibrium within Ω. A metastable exit is then an exit which occurs after this local equilibrium has been reached, namely (using the Markov property) an exit for the process $(X_t)_{t\geqslant 0}$ with initial condition $X_0 \sim \nu_h$.

If $X_0 \sim \nu_h$, the exit event satisfies the two fundamental properties (see for example [55, Prop. 2.4]):

$$\tau \sim \mathcal{E}(\lambda_h) \quad \text{and} \quad \tau \text{ is independent of } X_\tau. \tag{8}$$

With these two properties, one can use a kinetic Monte Carlo model to exactly sample the exit event. Indeed, assume again for simplicity that Ω is the basin of attraction of a local minimum of f, and let us denote by $\mathsf{W}_z^+ \subset \partial\Omega$ the stable manifold of the saddle point $z \in \{z_1, \dots, z_n\}$ (see (13) below for a precise definition). Up to a null set, the sets $(\mathsf{W}_z^+)_{z\in\{z_1,\dots,z_n\}}$ form a partition of the boundary $\partial\Omega$ of the basin of attraction. Let us now introduce the rates: for any $z \in \{z_1, \dots, z_n\}$,

$$\mathsf{k}_z^{o\ell} := \frac{\mathbb{P}_{\nu_h}\big[X_\tau \in \mathsf{W}_z^+\big]}{\mathbb{E}_{\nu_h}\big[\tau\big]}. \tag{9}$$

where the superscript $o\ell$ indicates that we consider the overdamped Langevin dynamics (1). Then the kinetic Monte Carlo model parametrized with these rates generates an exit event $(\tau_{\mathsf{kMC}}, \mathsf{Y}_{\mathsf{kMC}})$ which is exactly consistent with the exit event (τ, X_τ) of the original dynamics (1). Indeed, using (3)–(4) and (8), one has: (i) τ_{kMC} has the same law as τ, (ii) τ_{kMC} and $\mathsf{Y}_{\mathsf{kMC}}$ are independent, which is also the case for τ and X_τ, and finally (iii) $\mathbb{P}(Y_{\mathsf{kMC}} = z) = \mathbb{P}(X_\tau \in \mathsf{W}_z^+)$. The mathematical question, which is the focus of this work, is now to prove that the rates $\mathsf{k}_z^{o\ell}$ can indeed be accurately approximated by the Eyring-Kramers formulas (5).

As already mentioned above (see Footnote (1) and Remark 5 below), we will need to assume that Ω is smooth and bounded. The smoothness assumption may require to slightly modify the basin of attraction in the neighborhoods of the boundaries of W_z^+ where $\partial\Omega$ is not necessarily smooth (these are anyway typically high energy points which are thus visited with an exponentially small probability when $h \to 0$). Therefore, we will not consider exactly $\mathsf{k}_z^{o\ell}$ but the following rates: for any $z \in \{z_1, \dots, z_n\}$,

$$\mathsf{k}_z^{o\ell}(\Sigma_z) := \frac{\mathbb{P}_{\nu_h}\big[X_\tau \in \Sigma_z\big]}{\mathbb{E}_{\nu_h}\big[\tau\big]}, \tag{10}$$

where Σ_z is an open neighborhood of z in $\partial\Omega$ which is positively stable for the gradient dynamics $\dot{x} = -\nabla f(x)$ and can be chosen arbitrarily large in $\partial\Omega \cap \mathsf{W}_z^+$. We will prove that, under some geometric assumptions, these rates can indeed be accurately approximated by the Eyring-Kramers formulas in the small temperature regime $h \to 0$, see Corollary 8 below. This requires sharp estimates of the probabilities that $(X_t)_{t\geqslant 0}$ exits Ω through the neighborhoods Σ_z of the saddle points $z \in \{z_1, \dots, z_n\}$. These precise approximations of the exit rates are used in particular in the temperature accelerated dynamics algorithm [83] to extrapolate exit events observed at high temperature to low temperature (see Remark 9 for a discussion underlying the similarities between our mathematical analysis and this algorithm). Let us now leave this informal presentation and present the precise setting and the main mathematical results of this work.

1.2. Mathematical setting and statements of the main results

1.2.1. *Notation and definition*. — In the following, Ω is a smooth bounded domain of $\mathbb{R}^d$. The function $f:\overline{\Omega}\to\mathbb{R}$ is assumed to be a $\mathcal{C}^\infty$ function, i.e., it is the restriction to $\overline{\Omega}$ of a smooth function defined on $\mathbb{R}^d$. We still denote by f a smooth extension of $f:\overline{\Omega}\to\mathbb{R}$ to $\mathbb{R}^d$. Since the quantities of interest in this work only depends on the values of f in the bounded set $\overline{\Omega}$, we assume throughout this work without loss of generality that the extension of f is such that:

$$\sup_{x\in\mathbb{R}^d}|\nabla f(x)|+\sup_{x\in\mathbb{R}^d}|\mathrm{Hess}\, f(x)|<+\infty, \tag{11}$$

where $\mathrm{Hess}\, f(x)$ denotes the Hessian matrix of f at $x\in\mathbb{R}^d$.

Basic notation. — The open ball of radius $r>0$ centered at $x\in\mathbb{R}^d$ is denoted by $\mathsf{B}(x,r)$. The unit outward normal to Ω at $z\in\partial\Omega$ is denoted by $\mathsf{n}_\Omega(z)$. The normal derivative on $\partial\Omega$ of a smooth function $f:\overline{\Omega}\to\mathbb{R}$ is denoted by $\partial_{\mathsf{n}_\Omega}f$. Its tangential gradient on $\partial\Omega$ is denoted by $\nabla_{\mathbf{T}}f$. We will simply write $\{f<a\}$ for the set $\{x\in\overline{\Omega}, f(x)<a\}$.

Index of a critical point. — A point $x\in\overline{\Omega}$ is a critical point of f if $|\nabla f(x)|=0$. The critical point x is non-degenerate if furthermore $\mathrm{Hess}\, f(x)$ is invertible. The function f is a Morse function if all its critical points in $\overline{\Omega}$ are non degenerate. The non-degenerate critical point x is of index $p\in\{0,\dots,d\}$ if $\mathrm{Hess}\, f(x)$ admits p negative eigenvalues. A saddle point is a non degenerate critical point with index 1. Notice that the index of a critical point on $\partial\Omega$ does not depend on the extension of f outside $\overline{\Omega}$.

Stable and unstable manifolds. — Let $x\in\mathbb{R}^d$ and denote by $\varphi_x(t)$ the maximal solution to the ordinary differential equation (which is defined for all $t\in\mathbb{R}$ by (11)):

$$\frac{d}{dt}\varphi_x(t)=-\nabla f(\varphi_x(t))\quad\text{with } \varphi_x(0)=x. \tag{12}$$

When $z\in\mathbb{R}^d$ is a saddle point of f, we denote by W_z^+ and W_z^- respectively the stable and unstable manifolds of z for the dynamics (12), i.e.,

$$\mathsf{W}_z^{\pm}=\Big\{x\in\mathbb{R}^d,\ \lim_{t\to\pm\infty}\varphi_x(t)=z\Big\}. \tag{13}$$

Let us recall the stable manifold theorem (see [50, Cor. 6.4.1]).

Theorem (Stable manifold theorem). — *Let $f:\mathbb{R}^d\to\mathbb{R}$ satisfying* (11), *and let z be a saddle point of f. Then, W_z^+ and W_z^- are $\mathcal{C}^\infty$ embedded manifolds, with dimensions $d-1$ and* 1 *respectively. Moreover, the tangent spaces of W_z^+ and W_z^- at point z satisfy*

$$T_z\mathsf{W}_z^+=\mathrm{Span}(\mathsf{e}_1\dots,\mathsf{e}_{d-1})\quad\textit{and}\quad T_z\mathsf{W}_z^-=\mathrm{Span}(\mathsf{e}_d),$$

where $(\mathsf{e}_1, \ldots, \mathsf{e}_{d-1})$ *is a basis of eigenvectors associated with the* $d-1$ *positive eigenvalues of* $\operatorname{Hess} f(z)$ *and* e_d *is an eigenvector associated with the negative eigenvalue of* $\operatorname{Hess} f(z)$.

Agmon distance. — Let us introduce the Agmon distance on $\overline{\Omega}$ which will be used to state our main results below.

Definition 3. — Let $f : \overline{\Omega} \to \mathbb{R}$ be a $\mathcal{C}^\infty$ function. The Agmon pseudo-distance between two points $x \in \overline{\Omega}$ and $y \in \overline{\Omega}$ is defined by:

$$\mathsf{d}_a(x, y) = \inf_{\gamma \in \mathcal{C}^1(x,y)} \int_0^1 |\nabla f|(\gamma(t))\, |\gamma'(t)|\, dt,$$

where $\mathcal{C}^1(x, y)$ is the set of curve $\gamma : [0, 1] \to \overline{\Omega}$ which are $\mathcal{C}^1$ with $\gamma(0) = x$, $\gamma(1) = y$.

Since f has a finite number of critical points in $\overline{\Omega}$ (which is indeed the case if f is a Morse function on $\overline{\Omega}$), d_a is a distance since for all $x, y \in \overline{\Omega}$, $\mathsf{d}_a(x, y) = 0$ if and only if $x = y$.

1.2.2. *Assumptions.* — Let us now gather in the following assumption all the geometric requirements on Ω and f.

Assumption (Ω-f). — The set Ω is a $\mathcal{C}^\infty$ bounded domain of $\mathbb{R}^d$. The functions $f : \overline{\Omega} \to \mathbb{R}$ and $f|_{\partial\Omega}$ are $\mathcal{C}^\infty$ Morse functions. Moreover:

(1) The domain Ω is positively stable for (12): $\forall x \in \Omega$, $\forall t \geqslant 0$, $\varphi_x(t) \in \Omega$. Moreover, there exists $x_0 \in \Omega$ such that for all $x \in \Omega$, $\lim_{t \to +\infty} \varphi_x(t) = x_0$.

(2) For any critical point $z \in \partial\Omega$ of f, there exists an open subset Γ_z of $\partial\Omega$ containing z and satisfying the following:

(a) If z is a saddle point of f, then

$$\overline{\Gamma_z} \subset \mathsf{W}_z^+, \tag{14}$$

and Γ_z is positively stable for the dynamics (12): $\forall x \in \Gamma_z, \forall t \geqslant 0$, $\varphi_x(t) \in \Gamma_z$.

(b) If z is not a saddle point of f, then $\partial_{\mathsf{n}_\Omega} f = 0$ on Γ_z.

(3) All the local minima of $f|_{\partial\Omega}$ are saddle points of f.

Assumption (Ω-f) has simple consequences that will be used many times in the following (the proofs are standard, and provided in Section A.1 for completeness).

Lemma 4. — *The following holds:*

(1) *Assume that item* (1) *in* (Ω-f) *is satisfied. Then* $\partial_{\mathsf{n}_\Omega} f \geqslant 0$ *on* $\partial\Omega$ *and* x_0 *is the only critical point of the function* f *in* Ω. *There is no local minimum of* f *on* $\partial\Omega$. *Furthermore,* $f(x_0) = \min_{\overline{\Omega}} f < \min_{\partial\Omega} f$, $\{f < \min_{\partial\Omega} f\}$ *is connected and* $\partial\{f < \min_{\partial\Omega} f\} \cap \partial\Omega = \arg\min_{\partial\Omega} f$.

(2) *Assume that* (Ω-f) *is satisfied. For all* $z \in \partial\Omega$ *such that* $|\nabla f|(z) = 0$, $\mathsf{n}_\Omega(z)$ *is an eigenvector of* $\operatorname{Hess} f(z)$ *associated with a negative eigenvalue.*

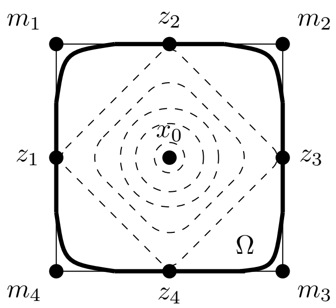

Figure 1. The basin of attraction $\mathcal{A}(0) = (-1,1)^2$ (for the dynamics (12)) of the local minimum $0 \in \mathbb{R}^2$ of the Morse function $f(x,y) = -\cos(\pi x) - \cos(\pi y)$. There are 8 critical points on $\partial\mathcal{A}(0)$: four saddle points (z_1, z_2, z_3, z_4) and four local maxima (m_1, m_2, m_3, m_4). Each edge of the square $(-1,1)^2$ is the stable manifold of the saddle point it contains. In thick lines, a domain Ω satisfying (Ω-f). In dashed lines, the level sets of f.

Other simple consequences of Assumption (Ω-f) are the following. If $z \neq x$ are saddle points of f, then $\Gamma_z \cap \Gamma_x = \varnothing$. For z a saddle point of f, the existence of a set Γ_z whose closure is arbitrarily large in W_z^+ and which is positively stable for the dynamics (12) is ensured by [27, Prop. 80], and Ω can then be defined such that $\Gamma_z \subset \partial\Omega$, see Remark 5. If z is a saddle point of f one can check that $\partial_{\mathsf{n}_\Omega} f = 0$ on Γ_z (since $\overline{\Gamma_z} \subset \mathsf{W}_z^+ \cap \partial\Omega$). Finally, all the saddle points of f in $\overline{\Omega}$ necessarily belong to $\partial\Omega$, and coincide with the local minima of f on $\partial\Omega$.

Remark 5. — Let $\mathcal{A}(x_0)$ be the basin of attraction of x_0 for the dynamics (12). As explained in the introduction, practitioners typically use as a definition of a bounded metastable domain the whole basin of attraction $\mathcal{A}(x_0)$, which indeed naturally satisfies all the Assumptions (Ω-f), except in some cases the smoothness assumption (Ω is indeed assumed to be $\mathcal{C}^\infty$ in (Ω-f)). More precisely, $\partial\mathcal{A}(x_0)$ is smooth on W_z^+ for all $z \in \{z_1, \dots, z_n\}$, $\partial\mathcal{A}(x_0) = \bigcup_{z \in \{z_1,\dots,z_n\}} \overline{\mathsf{W}_z^+}$ (see [69, Th. B.13]), but singularities may occur on the boundaries of W_z^+. In such a case, a domain $\Omega \subset \mathcal{A}(x_0)$ satisfying (Ω-f) can typically be obtained from $\mathcal{A}(x_0)$ by slightly modifying it in neighborhoods of the points of the boundary $\partial\mathcal{A}(x_0)$ where $\partial\mathcal{A}(x_0)$ is not smooth, see for example Figure 1 for a schematic illustration in dimension 2. This modification typically only concerns high energy points, which are anyway visited with an exponentially small probability by the dynamics (1) in the regime $h \to 0$.

Definition 6. — When (Ω-f) holds, the saddle points of f in $\overline{\Omega}$ are denoted by $\{z_1, \dots, z_n\} \subset \partial\Omega$ and ordered such that

$$\min_{\partial\Omega} f = f(z_1) = \cdots = f(z_{n_0}) < f(z_{n_0+1}) \leqslant \cdots \leqslant f(z_n). \tag{15}$$

The cardinal of $\arg\min f|_{\partial\Omega}$ is thus $n_0 \in \{1,\dots,n\}$. For all $k \in \{1,\dots,n\}$, μ_{z_k} is the negative eigenvalue of $\operatorname{Hess} f(z_k)$. For all $k \in \{1,\dots,n\}$, we denote by $\Sigma_{z_k} \subset \partial\Omega$ an open set such that

$$z_k \in \Sigma_{z_k} \quad \text{and} \quad \overline{\Sigma_{z_k}} \subset \Gamma_{z_k}. \tag{16}$$

A schematic representation of Ω, x_0, $\{z_1,\dots,z_n\}$, and $\{\Sigma_{z_1},\dots,\Sigma_{z_n}\}$ is given in Figure 2 when $n=4$.

1.2.3. *From stochastic processes to partial differential equations.* — In order to give sharp asymptotic estimates of the rates (10) when $h \to 0$, we will rewrite the law of the random variable (τ, X_τ) using the first eigenvalue and eigenvector of the infinitesimal generator of the process (1) with homogeneous Dirichlet boundary conditions on Ω. The small temperature regime then consists in analyzing the semi-classical limit of this eigenstate.

Let us denote by

$$\mathsf{L}^{(0)}_{f,h} = -\frac{h}{2}\Delta + \nabla f \cdot \nabla \tag{17}$$

the opposite of the infinitesimal generator of the process (1). Let $H^1_0(\Omega, e^{-(2/h)f}dx)$ be the set of functions $g \in H^1(\Omega, e^{-(2/h)f}dx)$ such that $g=0$ on $\partial\Omega$. The operator $\mathsf{L}^{(0)}_{f,h}$ on $L^2(\Omega, e^{-(2/h)f}dx)$ with domain

$$H^2(\Omega, e^{-(2/h)f}dx) \cap H^1_0(\Omega, e^{-(2/h)f}dx) = \big\{w \in H^2(\Omega, e^{-(2/h)f}dx),\ w=0 \text{ on } \partial\Omega\big\}.$$

is denoted by $\mathsf{L}^{\mathsf{Di},(0)}_{f,h}(\Omega)$. The superscripts Di and (0) respectively indicate that the operator is supplemented with Dirichlet boundary conditions, and acts on functions, namely 0-forms (operators on 1-forms will be also considered, see Section 2.5). The operator $\mathsf{L}^{\mathsf{Di},(0)}_{f,h}(\Omega)$ is the Friedrichs extension (see for instance [40, §4.3]) on $L^2(\Omega, e^{-(2/h)f}dx)$ of the closed quadratic form

$$\psi \in H^1_0(\Omega, e^{-(2/h)f}dx) \longmapsto \frac{h}{2}\int_\Omega |\nabla\psi|^2\, e^{-(2/h)f}. \tag{18}$$

The operator $\mathsf{L}^{\mathsf{Di},(0)}_{f,h}(\Omega)$ is thus a positive self-adjoint operator on $L^2(\Omega, e^{-(2/h)f}dx)$. In addition, it has a compact resolvent (as follows from the compact injection $H^1_0(\Omega, e^{-(2/h)f}dx) \subset L^2(\Omega, e^{-(2/h)f}dx)$). Then, by standard results on elliptic operators, its smallest eigenvalue λ_h is simple and any associated eigenfunction u_h is $\mathcal{C}^\infty$ on $\overline{\Omega}$ and has a sign on Ω (see for instance [31, §§6.3 & 6.5]). Without loss of generality, let us assume that:

$$u_h > 0 \text{ on } \Omega \quad \text{and} \quad \int_\Omega u_h^2\, e^{-(2/h)f} = 1. \tag{19}$$

Then, by the Hopf lemma (see for instance [31, §6.4.2]), one has $\partial_{\mathsf{n}_\Omega} u_h > 0$ on $\partial\Omega$.

Let us now go back to the probabilistic setting introduced in Section 1.1 and rewrite the rate (10) in terms of (λ_h, u_h) (see for example [55] for proofs of these results). The unique quasi-stationary distribution ν_h of the process $(X_t)_{t\geqslant 0}$ in Ω can be written in terms of u_h as follows:

$$\nu_h(dx) = \frac{u_h(x)e^{-(2/h)f(x)}}{\int_\Omega u_h(y)e^{-(2/h)f(y)}dy}\, dx. \tag{20}$$

Moreover, if $X_0 \sim \nu_h$ the parameter of the exponential random variable τ is λ_h (in particular $\mathbb{E}_{\nu_h}(\tau) = \lambda_h^{-1}$), and the law of X_τ can be written in terms of (λ_h, u_h) as follows: for any bounded measurable test function $\varphi : \partial\Omega \to \mathbb{R}$,

$$\mathbb{E}[\varphi(X_\tau)] = -\frac{h}{2\lambda_h}\frac{\int_{\partial\Omega}\varphi(x)\partial_{\mathsf{n}_\Omega}u_h(x)e^{-(2/h)f(x)}\sigma(dx)}{\int_\Omega u_h(y)e^{-(2/h)f(y)}dy}, \tag{21}$$

where σ is the Lebesgue measure on $\partial\Omega$. Using these properties, the rate (10) can thus be written in terms of u_h: for all $z \in \{z_1, \dots, z_n\}$,

$$\mathsf{k}_z^{o\ell}(\Sigma_z) = -\frac{h}{2}\frac{\int_{\Sigma_z}\partial_{\mathsf{n}_\Omega}u_h e^{-(2/h)f}d\sigma}{\int_\Omega u_h e^{-(2/h)f}}. \tag{22}$$

Proving that the transition rates (10) are accurately approximated by the Eyring-Kramers laws (5) in the limit $h \to 0$ thus requires in particular to get precise estimates of $\partial_{\mathsf{n}_\Omega}u_h$ on each Σ_z.

1.2.4. *Main results*. — We are now in position to precisely state our main results. Theorem 1 and Proposition 7 give precise asymptotic estimates on (λ_h, u_h) in the limit $h \to 0$.

Theorem 1. — *Let us assume that the assumption* (Ω-f) *is satisfied. Then, for all* $k \in \{1, \dots, n_0\}$ *it holds in the limit* $h \to 0$

$$\int_{\Sigma_{z_k}} \partial_{\mathsf{n}_\Omega}u_h\, e^{-(2/h)f}d\sigma = \frac{2|\mu_{z_k}|\big(\det \operatorname{Hess} f(x_0)\big)^{1/4}}{\pi^{3d/4}\big|\det \operatorname{Hess} f(z_k)\big|^{1/2}}\, h^{d/4-1}\, e^{-(1/h)(2f(z_1)-f(x_0))}\big(1+O(\sqrt{h})\big), \tag{23}$$

where u_h is the principal eigenfunction of $\mathsf{L}^{\mathsf{Di},(0)}_{f,h}(\Omega)$ *with the normalization* (19). *In addition, there exists $c > 0$ such that, when $h \to 0$*

$$\int_{\partial\Omega\smallsetminus\bigcup_{k=1}^{n_0}\Sigma_{z_k}} \partial_{\mathsf{n}_\Omega}u_h\, e^{-(2/h)f}d\sigma = O\big(e^{-(1/h)(2f(z_1)-f(x_0)+c)}\big). \tag{24}$$

Moreover, assume that:

$$\forall k \in \{1, \dots, n\}\,,\ \inf_{z\in\partial\Omega\smallsetminus\Gamma_{z_k}} \mathsf{d}_a(z, z_k) > \max[f(z_n) - f(z_k), f(z_k) - f(z_1)], \tag{25}$$

and

$$f(z_1) - f(x_0) > f(z_n) - f(z_1). \tag{26}$$

Then, for all $k \in \{n_0 + 1, \dots, n\}$, it holds in the limit $h \to 0$:

$$\int_{\Sigma_{z_k}} \partial_{\mathsf{n}_\Omega}u_h\, e^{-(2/h)f}d\sigma = \frac{2|\mu_{z_k}|\big(\det \operatorname{Hess} f(x_0)\big)^{1/4}}{\pi^{3d/4}\big|\det \operatorname{Hess} f(z_k)\big|^{1/2}}\, h^{d/4-1}\, e^{-(1/h)(2f(z_k)-f(x_0))}\big(1+O(\sqrt{h})\big). \tag{27}$$

Assumptions (25) and (26) are required to prove (27) with our analysis. In particular, Assumption (25) ensures that all the saddle points z_k, $k \in \{1, \dots, n\}$, are well separated in terms of the Agmon distance d_a, which measures the exponential decay of eigenforms away from critical points [41]. Without such an assumption, it has been numerically observed in [27, §1.6.2] that (27) does not hold, in a slightly different framework, namely when the normal derivative of f is strictly positive on $\partial\Omega$ (and thus the z_k's are so-called generalized saddle points, namely local minima of f on $\partial\Omega$).

Proposition 7. — *Let us assume that the assumption* (Ω-f) *is satisfied.*

$$\int_\Omega u_h \, e^{-(2/h)f} = (\pi h)^{d/4} \big(\det \operatorname{Hess} f(x_0)\big)^{-1/4} \, e^{-(1/h)\min_{\overline{\Omega}} f} (1 + O(h)). \tag{28}$$

Moreover, it holds in the limit $h \to 0$:

$$\lambda_h = \sum_{\ell=1}^{n_0} \frac{|\mu_{z_\ell}| \big(\det \operatorname{Hess} f(x_0)\big)^{1/2}}{\pi \big|\det \operatorname{Hess} f(z_\ell)\big|^{1/2}} \, e^{-(2/h)(f(z_1) - f(x_0))} (1 + O(\sqrt{h})). \tag{29}$$

Using the expression (21) for the law of the exit point X_τ, Theorem 1 and Proposition 7 yield the following sharp estimate of this law:

Theorem 2. — *Let us assume that the assumption* (Ω-f) *is satisfied. Then, for all $k \in \{1, \dots, n_0\}$, it holds in the limit $h \to 0$:*

$$\mathbb{P}_{\nu_h}[X_\tau \in \Sigma_{z_k}] = \frac{|\mu_{z_k}|}{\sqrt{|\det \operatorname{Hess} f(z_k)|}} \Bigg(\sum_{\ell=1}^{n_0} \frac{|\mu_{z_\ell}|}{\sqrt{|\det \operatorname{Hess} f(z_\ell)|}} \Bigg)^{-1} + O(\sqrt{h}), \tag{30}$$

In addition, there exists $c > 0$ such that in the limit $h \to 0$:

$$\mathbb{P}_{\nu_h}\big[X_\tau \in \partial\Omega \smallsetminus \textstyle\bigcup_{k=1}^{n_0} \Sigma_{z_k}\big] \leqslant e^{-c/h}. \tag{31}$$

Finally, if (25) *and* (26) *are satisfied, it holds for all $k \in \{n_0 + 1, \dots, n\}$, in the limit $h \to 0$:*

$$\mathbb{P}_{\nu_h}[X_\tau \in \Sigma_{z_k}] = \frac{|\mu_{z_k}|}{\sqrt{|\det \operatorname{Hess} f(z_k)|}} \Bigg(\sum_{\ell=1}^{n_0} \frac{|\mu_{z_\ell}|}{\sqrt{|\det \operatorname{Hess} f(z_\ell)|}} \Bigg)^{-1} \times e^{-(2/h)(f(z_k) - f(z_1))} \big(1 + O(\sqrt{h})\big). \tag{32}$$

As a corollary of Theorem 2 and Proposition 7, one immediately gets the following sharp estimates of the exit rates defined in (10):

Corollary 8. — *Let us assume that the assumption* (Ω-f) *is satisfied. Then, for all $k \in \{1, \dots, n_0\}$, it holds in the limit $h \to 0$:*

$$\mathsf{k}^{o\ell}_{z_k}(\Sigma_k) = \frac{|\mu_{z_k}|}{\pi} \frac{\sqrt{\det \operatorname{Hess} f(x_0)}}{\sqrt{|\det \operatorname{Hess} f(z_k)|}} \, e^{-(2/h)(f(z_1) - f(x_0))} \big(1 + O(\sqrt{h})\big). \tag{33}$$

In addition, if (25) *and* (26) *are satisfied, it holds for all $k \in \{n_0 + 1, \dots, n\}$, in the limit $h \to 0$:*

$$\mathsf{k}^{o\ell}_{z_k}(\Sigma_k) = \frac{|\mu_{z_k}|}{\pi} \frac{\sqrt{\det \operatorname{Hess} f(x_0)}}{\sqrt{|\det \operatorname{Hess} f(z_k)|}} \, e^{-(2/h)(f(z_k) - f(x_0))} \big(1 + O(\sqrt{h})\big). \tag{34}$$

As discussed in Section 1.1, Corollary 8 thus justifies the approximation of metastable exits of the overdamped Langevin dynamics (1) by a kinetic Monte Carlo model parametrized with the Eyring-Kramers formulas.

We will also show that Theorem 2 extends to deterministic initial conditions $x \in \Omega$ as follows (the subscript x in $\mathbb{P}_x$ indicates that $X_0 = x$).

Theorem 3. — *Let us assume that the assumption* $(\Omega\text{-}f)$ *is satisfied. Let* K *be a compact subset of* Ω. *Then, for all* $k \in \{1, \ldots, n_0\}$, *it holds in the limit* $h \to 0$*:*

$$\mathbb{P}_x[X_\tau \in \Sigma_{z_k}] = \frac{|\mu_{z_k}|}{\sqrt{|\det \operatorname{Hess} f(z_k)|}} \Big(\sum_{\ell=1}^{n_0} \frac{|\mu_{z_\ell}|}{\sqrt{|\det \operatorname{Hess} f(z_\ell)|}}\Big)^{-1} + O(\sqrt{h}), \tag{35}$$

uniformly in $x \in \mathsf{K}$. *In addition, there exists* $c > 0$ *such that in the limit* $h \to 0$*:*

$$\sup_{x \in \mathsf{K}} \mathbb{P}_x\big[X_\tau \in \partial\Omega \smallsetminus \textstyle\bigcup_{k=1}^{n_0} \Sigma_{z_k}\big] \leqslant e^{-c/h}. \tag{36}$$

Let us assume that (25) *and* (26) *are satisfied. Assume in addition there exists* $\ell_0 \in \{n_0 + 1, \ldots, n\}$ *such that*

$$2(f(z_{\ell_0}) - f(z_1)) < f(z_1) - f(x_0). \tag{37}$$

Let $k_0 \in \{n_0+1, \ldots, \ell_0\}$ *and* $\alpha_* \in \mathbb{R}$ *be such that* $f(x_0) < \alpha_* < 2f(z_1) - f(z_{k_0})$ *(notice that necessarily* $\alpha_* < f(z_1) = \min_{\partial\Omega} f$*). Then, it holds for* $k \in \{n_0 + 1, \ldots, k_0\}$ *in the limit* $h \to 0$*:*

$$\mathbb{P}_x[X_\tau \in \Sigma_{z_k}] = \frac{|\mu_{z_k}|}{\sqrt{|\det \operatorname{Hess} f(z_k)|}} \Big(\sum_{\ell=1}^{n_0} \frac{|\mu_{z_\ell}|}{\sqrt{|\det \operatorname{Hess} f(z_\ell)|}}\Big)^{-1} \times e^{-(2/h)(f(z_k)-f(z_1))}\big(1 + O(\sqrt{h})\big), \tag{38}$$

uniformly in $x \in \{f \leqslant \alpha_*\}$.

Before precisely discussing related results in the literature, let us provide some preliminary comments on the statements presented in this section. First, Equations (30)–(31) and (35)–(36) show that the most probable places of exit from Ω as $h \to 0$ are $\{z_1, \ldots, z_{n_0}\}$, and they provide the relative probabilities of exiting through (neighborhoods of) these points. Moreover, Equations (31) and (38) give precise asymptotic estimate of the probability to leave through higher energy saddle points. All these results can be seen as generalizations of those previously obtained in [27] and of some results in [28], where it is assumed that $\partial_{\mathsf{n}_\Omega} f > 0$ on $\partial\Omega$. In this case, the local minima of f on $\partial\Omega$ play the role of saddle points, and different prefactors than (6) appear in the asymptotic rates, for example. Let us finally emphasize that, as will become clear from the proofs, all the error terms $O(\sqrt{h})$ follow from the Laplace method applied to integrals on $\mathbb{R}^d_-$ and are optimal, see the computations leading to (201) (see also [58, Rem. 25 & 39] for more details).

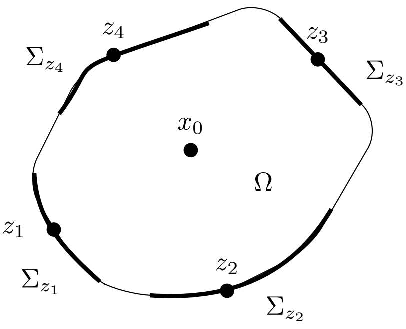

Figure 2. Example of a domain Ω with $n = 4$ saddle points $\{z_1, \ldots, z_4\}$.

1.2.5. *A short review on mathematical approaches to metastability.* — In this section, we succinctly present two aspects of metastability which have received attention from the mathematical community: the exit problem (which is the focus of this work) and the spectral analysis of the infinitesimal generator.

On the exit problem. — Even though the exit problem from a basin of attraction of a local minimum of f is a very natural question, this setting has not been considered up to now in the literature, at least to the best of our knowledge. This is essentially because of the mathematical difficulties induced by the presence of critical points of f on the boundary. Let us recall the main results which have been obtained.

Let us first mention that early inspiring formal computations were conducted by Z. Schuss and co-workers [67, 74, 68]. In terms of rigorous proofs, two techniques have then been developed, based on large deviations or the analysis of partial differential equations associated to the stochastic process.

From a probabilistic viewpoint, the exit problem has been studied a lot using large deviation techniques, pioneered by M.I. Friedlin and A.D. Wentzell [34]. Typically, results are only obtained on h-log limits of the mean exit time τ and of the law of the exit location X_τ, under the assumption that f does not have critical point on $\partial\Omega$, see also the developments by M.V. Day and M. Sugiura [21, 20, 23, 22, 86, 85]). A noteworthy exception is the work [24] by M.V. Day where large deviations principles are given for some conormally reflected processes with attractors on the boundary.

Techniques based on parabolic or elliptic partial differential equations associated with the stochastic process have also been developed in particular by S. Kamin [51, 52], H. Ishii and P.E. Souganidis [47, 48], B. Perthame [78], and more recently D. Borisov and D. Sultanov [7]. In particular, these articles study the concentration of the law of X_τ on the global minima of f on $\partial\Omega$ in the limit $h \to 0$. In these works, it is again assumed that f does not have critical points on the boundary. Let us mention [66] for early results on the h-log limits of the smallest eigenvalues of and [75] for sharp asymptotic equivalents on the mean exit time $\mathbb{E}[\tau]$ when f has critical points on $\partial\Omega$.

Notice that h-log limits cannot be used to compute the relative probabilities of exits through the lowest saddle points $\{z_1, \ldots, z_{n_0}\}$. Moreover, Equations (35) and (36) extend the results of [34, Th. 2.1] and [52, 51, 78, 22, 23, 64] to the case when f has critical points on $\partial\Omega$. Let us however acknowledge that even if the techniques mentioned above seem inherently limited to h-log limits, some of them are robust enough to apply to non reversible elliptic processes, or quasilinear parabolic equations (see [34, 21, 20, 23, 22, 47, 48]), whereas we only consider reversible dynamics here.

Spectral problem and the Eyring-Kramers laws. — The focus of the present work is on the exit problem (exit time, and first exit points), and we prove that the Eyring-Kramers laws precisely describe the exit rates from a basin of attraction of the potential energy function. In the mathematical literature, the Eyring-Kramers laws have also been obtained in a different context, namely when studying the smallest eigenvalues of the infinitesimal generator (seen as an operator on $\mathbb{R}^d$) of the overdamped Langevin process, see the definition (17) of $\mathsf{L}^{(0)}_{f,h}$. Two variational techniques have been used, based either on tools from potential theory or from spectral theory (see [3] for a nice review).

Let us first mention that sharp lower and upper bounds on the small eigenvalues were obtained in the pioneering works [71, 46]. Then, A. Bovier and collaborators developed in [8, 9] a potential theoretic approach [10] to obtain precise equivalents of the n_p smallest eigenvalues of $\mathsf{L}^{(0)}_{f,h}$, n_p being the number of local minima of f in $\mathbb{R}^d$. It is also proved that the non-zero eigenvalues coincide with the inverses of mean transition times to go from one local minimum of f to any of the other local minima with smaller energies. This potential theoretic approach have then been further developed by N. Berglund and co-workers [5, 4], and by C. Landim and I. Seo [53, 61], in particular for generalizations to non-reversible diffusions.

Using tools developed to analyze the semi-classical limit of the Schrödinger operator, similar results on the low-lying spectrum have been derived by B. Helffer, M. Klein and F. Nier in [41]. See also the recent works [57, 70, 60, 59] for generalizations, and [45] for asymptotic equivalents of the smallest eigenvalues of the kinetic Langevin operator. Let us mention the nice work [69] where it is proved that Poincaré and Logarithmic-Sobolev inequalities constants asymptotically satisfy an Eyring-Kramers law in the limit $h \to 0$.

Let us finally emphasize that the two problems we have discussed up to now in this section (the exit problem, and the low-lying spectrum of $\mathsf{L}^{(0)}_{f,h}$ in $\mathbb{R}^d$) are different in nature. In particular, the exit problem requires to precisely study the law of the first exit point in order to estimate all the the exit rates.

1.2.6. *Strategy of the proofs and mathematical novelties*

Strategy of the proofs and organization of the article. — Let us provide a concise presentation of the strategy of the proofs, together with an outline of this work. In view of Theorem 1 and (22), one needs precise asymptotic estimates of of $\nabla u_h \cdot \mathsf{n}_\Omega$ on $\partial\Omega$, as $h \to 0$. Recall that u_h is the principal eigenfunction of $\mathsf{L}^{\mathsf{Di},(0)}_{f,h}(\Omega)$: $\mathsf{L}^{\mathsf{Di},(0)}_{f,h}(\Omega)\, u_h = \lambda_h u_h$.

The cornerstone of the proof of Theorem 1 is that ∇u_h also satisfies an eigenvalue problem (with the same exponentially small eigenvalue λ_h), obtained by differentiating the previous equation:

$$\begin{cases} \mathsf{L}^{(1)}_{f,h}\nabla u_h = \lambda_h \nabla u_h \text{ in } \Omega, \\ \nabla_{\mathbf{T}} u_h = 0 \text{ on } \partial\Omega, \\ \Big(-\dfrac{h}{2}\operatorname{div} + \nabla f\cdot\Big)\nabla u_h = 0 \text{ on } \partial\Omega, \end{cases} \tag{39}$$

where $\mathsf{L}^{(1)}_{f,h} = -\frac{h}{2}\Delta + \nabla f\cdot\nabla + \operatorname{Hess} f$ is an operator acting on vector fields, trivially identified with 1-forms in this Euclidean setting, and where $\nabla_{\mathbf{T}} u_h$ denotes the tangential gradient of the function u_h on $\partial\Omega$. In the following, the operator $\mathsf{L}^{(1)}_{f,h}$ with tangential Dirichlet boundary conditions, as introduced in (39), is denoted by $\mathsf{L}^{\mathsf{Di},(1)}_{f,h}(\Omega)$. For $q\in\{0,1\}$, let us denote, by $\pi^{(q)}_h$ the orthogonal projector of $\mathsf{L}^{\mathsf{Di},(q)}_{f,h}(\Omega)$ on the eigenspace associated with the eigenvalues of $\mathsf{L}^{\mathsf{Di},(q)}_{f,h}(\Omega)$ smaller than a constant c_0 independent of h. From (39), it holds, in the limit $h\to 0$,

$$\nabla u_h \in \operatorname{Ran}\pi^{(1)}_h, \tag{40}$$

where $\operatorname{Ran}\pi^{(1)}_h$ stands for the image of the projector $\pi^{(1)}_h$. The first step of the analysis thus consists in studying the spectrum of the operators $\mathsf{L}^{\mathsf{Di},(q)}_{f,h}(\Omega)$, $q\in\{0,1\}$. This is done in Section 2 in a rather general setting (in particular without assuming that all the local minima of f on the boundary are necessary saddle points of f), since this study has its own interest. We will prove in particular (see Theorem 4 and Corollary 25) that for some c_0, and for all h sufficiently small,

$$\operatorname{Ran}\pi^{(0)}_h = \operatorname{Span} u_h \quad\text{and}\quad \dim\operatorname{Ran}\pi^{(1)}_h = n. \tag{41}$$

Then, in order to study the asymptotic behaviour of u_h and ∇u_h when $h\to 0$, we construct in Section 3 a suitable orthonormal basis of $\operatorname{Ran}\pi^{(1)}_h$ (in the weighted Sobolev space $L^2_w(\Omega)$, see Section 2.5.1) using so-called quasi-modes $\{\mathsf{f}^{(1)}_1,\dots,\mathsf{f}^{(1)}_n\}$ (see in particular Propositions 26 and 27). These quasi-modes $\{\mathsf{f}^{(1)}_1,\dots,\mathsf{f}^{(1)}_n\}$ are built such that for each $k\in\{1,\dots,n\}$, $\mathsf{f}^{(1)}_k$ is essentially the principal eigenform of the operator $\mathsf{L}^{(1)}_{f,h}$ defined on a domain $\Omega^{\mathrm{M}}_k\subset\Omega$, with mixed Dirichlet-Neumann boundary conditions, where the domain Ω^{M}_k is constructed in Proposition 30 (the superscript M refers to the fact that mixed Dirichlet-Neumann boundary conditions will be considered on $\partial\Omega^{\mathrm{M}}_k$). The only critical points of f in $\overline{\Omega^{\mathrm{M}}_k}$ are x_0 and z_k, so that $\mathsf{f}^{(1)}_k$ gather information on the exit through z_k. In particular, with these quasi-modes $\{\mathsf{f}^{(1)}_1,\dots,\mathsf{f}^{(1)}_n\}$, one has: for all $k\in\{1,\dots,n\}$,

$$\int_{\Sigma_{z_k}} \partial_{\mathsf{n}_\Omega} u_h\, e^{-(2/h)f} d\sigma \sim \langle \nabla \mathsf{u}^{(0)}, \mathsf{f}^{(1)}_k\rangle_{L^2_w(\Omega)} \int_{\Sigma_{z_k}} \mathsf{f}^{(1)}_k\cdot \mathsf{n}_\Omega\, e^{-(2/h)f} d\sigma, \quad \text{as } h\to 0, \tag{42}$$

and $\langle \nabla \mathsf{u}^{(0)}, \mathsf{f}^{(1)}_k\rangle_{L^2_w(\Omega)}$ and $\int_{\Sigma_{z_k}} \mathsf{f}^{(1)}_k\cdot\mathsf{n}_\Omega\ e^{-(2/h)f} d\sigma$ have the expected asymptotic behavior leading to Theorem 1. Here, the function $\mathsf{u}^{(0)}$ is an approximation of u_h (see Definition 41). More precisely, we construct Ω^{M}_k in a way that allows us to compute the asymptotic equivalent of the principal eigenvalue $\lambda(\Omega^{\mathrm{M}}_k)$ of the operator $\mathsf{L}^{(1)}_{f,h}$ defined with mixed Dirichlet-Neumann boundary conditions on Ω_k^{M}, with techniques recently used in [58]. We then show that the asymptotic equivalent of $\lambda(\Omega_k^{\mathrm{M}})$ provides the required asymptotic equivalent of the right-hand side in (42), for each $k \in \{1, \dots, n\}$. This method to estimate $\int_{\Sigma_{z_k}} \partial_{\mathsf{n}_\Omega} u_h \; e^{-(2/h)f} d\sigma$ is the main difference with the approach used previously in [27].

Finally, Section 4 builds on the two previous sections to prove the main results stated in Section 1.2.4: Section 4.1 is devoted to the proofs of Theorem 1, Proposition 7, Theorem 2, and Corollary 8; Section 4.2 contains the proof of Theorem 3.

The appendix gathers various technical results and additional comments.

Remark 9. — Interestingly enough, in the Temperature Accelerated Dynamics algorithm [83, 1, 26], the numerical method consists in sampling successive exits through the saddle points $(z_k)_{1 \leqslant k \leqslant n}$ at high temperature by imposing reflecting boundary conditions on the already visited transition pathways, and then to infer the exit event that would have been observed at low temperature using the Eyring-Kramers laws (see Corollary 8). Imposing reflecting boundary conditions on the dynamics is equivalent to introducing Neumann boundary conditions on the infinitesimal generator, and the sampled exits are thus very much related to the principal eigenforms $(\mathsf{f}_k^{(1)})_{1 \leqslant k \leqslant n}$ that we use as quasi-modes. For example, in the procedure outlined above, the exit through z_k is exponentially distributed with parameter $\lambda(\Omega_k^{\mathrm{M}})$ (in the regime $h \to 0$).

Mathematical novelties. — Let us finally emphasize the main mathematical novelties and difficulties of the present work, which is the first to precisely analyze the exit problem from a domain Ω when the local minima of f on $\partial\Omega$ are saddle points of f. We actually studied a similar problem in [27], but under the less natural assumption that $\partial_{\mathsf{n}_\Omega} f > 0$ on $\partial\Omega$. The presence of critical points of f on $\partial\Omega$ implies substantial difficulties from a mathematical viewpoint. First, to prove $\dim \operatorname{Ran} \pi_h^{(1)} = n$, we extend the analysis of [42] (see Remark 12 for more details), which is of independent interest. This is the purpose of Section 2 on the Witten complex, see more precisely Theorem 4. Second, we develop a new approach to compute the asymptotic equivalents as $h \to 0$ of the right-hand side of (42) without relying on WKB approximations which were used for example in [27]. Though WKB approximations are very powerful and central tools on which rely many works in semi-classical analysis (see for instance [44, 39, 29, 41, 42]), the fact that both $z_k \in \partial\Omega_k^{\mathrm{M}}$ and z_k is a critical point of f prevent us from using previously constructed WKB approximations for Witten Laplacians [44, 42] (this is explained in more details in Section A.2). Third, the proof of Theorem 3 uses other arguments than the one made to prove [27, Cor. 16] especially because the results of [30] (based on techniques from the large deviation theory) do not hold when f has critical points on $\partial\Omega$ (see the discussion after Corollary 47).

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2. Number of small eigenvalues of the Witten Laplacian

In all this section, the following general setting is assumed:

Assumption (M-f). — Let $\overline{\mathsf{M}}$ be a $\mathcal{C}^\infty$ oriented compact and connected Riemannian manifold of dimension d, with boundary $\partial\mathsf{M}$ and interior M. The metric tensor on $\overline{\mathsf{M}}$ is denoted by $\mathbf{g}_{\mathsf{M}}$. Let $f:\overline{\mathsf{M}}\to\mathbb{R}$ be a $\mathcal{C}^\infty$ function. The functions $f:\overline{\mathsf{M}}\to\mathbb{R}$ and $f|_{\partial\mathsf{M}}$ are assumed to be Morse functions. Finally, for all $x\in\partial\mathsf{M}$ such that $|\nabla f(x)|=0$, there exists a neighborhood $\mathsf{V}_x^{\partial\mathsf{M}}$ of x in $\partial\mathsf{M}$ such that:

$$\forall y\in \mathsf{V}_x^{\partial\mathsf{M}},\quad \partial_{\mathsf{n}_{\mathsf{M}}} f(y)=0.$$

Notice that (M-f) implies that f and $f|_{\partial\mathsf{M}}$ have a finite number of critical points. Since the normal derivative $\partial_{\mathsf{n}_{\mathsf{M}}} f$ is zero around critical points on $\partial\mathsf{M}$, $\partial\mathsf{M}$ is said to be characteristic (for the function f) in these regions. Let us recall that this condition is in particular natural when $\mathsf{M}\subset\mathbb{R}^d$ is the basin of attraction of a local minimum of f.

The objective of this section is to relate the number of critical points of index p of f, to the number of small eigenvalues of the Witten Laplacian acting on p-forms with tangential Dirichlet boundary conditions on $\partial\mathsf{M}$, see Theorem 4 below. This result is standard for manifolds without boundary [93, 44, 82, 45], and has been proved in [42, Th. 3.2.3] for manifolds with boundaries but when f does not have critical points on $\partial\mathsf{M}$ (see also [54, 56]). This section is organized as follows. The Witten Laplacian is introduced in Section 2.1. The main result is stated in Section 2.2 and proved in Section 2.4, after the study of model problems on the half space $\mathbb{R}^d_-$ in Section 2.3. Finally, consequences of these results to the particular problem of interest in this work are detailed in Section 2.5, with in particular the proof of (41).

2.1. Witten Laplacian with tangential Dirichlet boundary conditions

2.1.1. *Notation for Sobolev spaces*. — Let us introduce standard notation for Sobolev spaces on manifolds with boundaries (see [81] for details). For $q\in\{0,\dots,d\}$, one denotes by $\Lambda^q\mathcal{C}^\infty(\overline{\mathsf{M}})$ (respectively $\Lambda^q\mathcal{C}^\infty_c(\mathsf{M})$) the space of $\mathcal{C}^\infty$ q-forms on $\overline{\mathsf{M}}$ (respectively on M and with compact support in M). Moreover, the set $\Lambda^q\mathcal{C}^\infty_T(\overline{\mathsf{M}})$ is the set of $\mathcal{C}^\infty$ q-forms v such that $\mathbf{t}v=0$ on $\partial\mathsf{M}$, where $\mathbf{t}$ denotes the tangential trace on forms. For $q\in\{0,\dots,d\}$, $\Lambda^qL^2(\mathsf{M},\mathbf{g}_{\mathsf{M}})$ is the completion of the space $\Lambda^q\mathcal{C}^\infty(\overline{\mathsf{M}})$ for the norm

$$w\in\Lambda^q\mathcal{C}^\infty(\overline{\mathsf{M}})\longmapsto\Big(\int_{\mathsf{M}}|w|^2\Big)^{1/2}.$$

For $m\geqslant 0$, one denotes by $\Lambda^qH^m(\mathsf{M},\mathbf{g}_{\mathsf{M}})$ the Sobolev spaces of q-forms with regularity index m: $v\in\Lambda^qH^m(\mathsf{M},\mathbf{g}_{\mathsf{M}})$ if and only if for all multi-index α with $|\alpha|\leqslant m$, the α derivative of v is in $\Lambda^qL^2(\mathsf{M},\mathbf{g}_{\mathsf{M}})$. Let us recall for a multi-index $\alpha=(\alpha_1,\dots,\alpha_d)\in\mathbb{N}^d$, $|\alpha|=\sum_{i=1}^d\alpha_i$ and $\partial^\alpha v={}^t(\partial_{x_1}^{\alpha_1}v,\dots,\partial_{x_d}^{\alpha_d}v)$. We will denote by $\|.\|_{H^m(\mathsf{M},\mathbf{g}_{\mathsf{M}})}$ the norm on the space $\Lambda^qH^m(\mathsf{M},,\mathbf{g}_{\mathsf{M}})$. Moreover $\langle\cdot,\cdot\rangle_{L^2(\mathsf{M},\mathbf{g}_{\mathsf{M}})}$ denotes the scalar product in $\Lambda^qL^2(\mathsf{M},\mathbf{g}_{\mathsf{M}})$. For $q\in\{0,\dots,d\}$ and $m>1/2$, the set $\Lambda^qH^m_{\mathbf{T}}(\mathsf{M},\mathbf{g}_{\mathsf{M}})$ is defined by

$$\Lambda^qH^m_{\mathbf{T}}(\mathsf{M},\mathbf{g}_{\mathsf{M}}):=\{v\in\Lambda^qH^m(\mathsf{M},\mathbf{g}_{\mathsf{M}}),\ \mathbf{t}v=0\text{ on }\partial\mathsf{M}\}.$$

We will always explicitly indicate the dependency on the metric $\mathbf{g}_{\mathsf{M}}$ in the notation of the Witten Laplacians or associated quadratic forms, but often omit it in the notation of the Sobolev spaces and associated norms(3), to ease the notation.

2.1.2. *Tangential Dirichlet boundary conditions.* — In this section, we introduce the tangential Dirichlet Witten Laplacian and recall some of its properties. For $q \in \{0,\dots,d\}$, one defines the so-called distorted exterior derivative *à la Witten* $\mathsf{d}^{(q)}_{f,h}:\Lambda^q\mathcal{C}^\infty(\mathsf{M})\to\Lambda^{q+1}\mathcal{C}^\infty(\mathsf{M})$ and its formal adjoint $\mathsf{d}^{(q)}_{f,h}{}^{*}:\Lambda^{q+1}\mathcal{C}^\infty(\mathsf{M})\to\Lambda^{q}\mathcal{C}^\infty(\mathsf{M})$ by

$$\mathsf{d}^{(q)}_{f,h}:=e^{-(1/h)f}\,h\,\mathsf{d}^{(q)}\,e^{(1/h)f}\quad\text{ and }\quad \mathsf{d}^{(q)}_{f,h}{}^{*}:=e^{(1/h)f}\,h\,\mathsf{d}^{(q)\,*}\,e^{-(1/h)f},$$

where $\mathsf{d}^{(q)}$ is the differential operator on M and $\mathsf{d}^{(q)\,*}$ is the co-differential operator on the manifold M equipped with the metric tensor $\mathbf{g}_{\mathsf{M}}$. We may drop the superscript (q) when the index of the form is explicit from the context. The Witten Laplacian, firstly introduced in [93], is then defined similarly as the Hodge Laplacian $\Delta^{(q)}_{\mathbf{H}}(\mathsf{M},\mathbf{g}_{\mathsf{M}}):=(\mathsf{d}+\mathsf{d}^*)^2:\Lambda^q\mathcal{C}^\infty(\mathsf{M})\to\Lambda^q\mathcal{C}^\infty(\mathsf{M})$ by

$$\Delta^{(q)}_{f,h}(\mathsf{M},\mathbf{g}_{\mathsf{M}}):=(\mathsf{d}_{f,h}+\mathsf{d}^*_{f,h})^2=\mathsf{d}_{f,h}\mathsf{d}^*_{f,h}+\mathsf{d}^*_{f,h}\mathsf{d}_{f,h}\ :\ \Lambda^q\mathcal{C}^\infty(\mathsf{M})\longrightarrow\Lambda^q\mathcal{C}^\infty(\mathsf{M}).$$

Equivalently, one has

$$\Delta^{(q)}_{f,h}(\mathsf{M},\mathbf{g}_{\mathsf{M}})=h^2\Delta^{(q)}_{\mathbf{H}}(\mathsf{M},\mathbf{g}_{\mathsf{M}})+|\nabla f|^2_{\mathbf{g}_{\mathsf{M}}}+h(\mathcal{L}_{\nabla f}+\mathcal{L}^*_{\nabla f}),\tag{43}$$

where $\mathcal{L}_{\nabla f}$ is the Lie derivative associated with the vector field ∇f. Here and in the following $|.|_{\mathbf{g}_{\mathsf{M}}}$ stands for the norm in the tangent space associated with the metric tensor $\mathbf{g}_{\mathsf{M}}$. Let us now introduce the Dirichlet realization of $\Delta^{(q)}_{f,h}(\mathsf{M},\mathbf{g}_{\mathsf{M}})$ on $\Lambda^qL^2(\mathsf{M})$, following [42, §2.4].

Proposition 10. — *Let us assume that* $(\mathsf{M}\text{-}f)$ *is satisfied. Let* $q\in\{0,\dots,d\}$ *and* $h>0$. *The Friedrichs extension of the quadratic form*

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathsf{M},\mathbf{g}_{\mathsf{M}}):w\in\Lambda^qH^1_{\mathbf{T}}(\mathsf{M})\longmapsto\|\mathsf{d}_{f,h}w\|^2_{L^2(\mathsf{M})}+\|\mathsf{d}^*_{f,h}w\|^2_{L^2(\mathsf{M})}$$

on $\Lambda^qL^2(\mathsf{M})$ *is denoted by* $\Delta^{\mathsf{Di},(q)}_{f,h}(\mathsf{M},\mathbf{g}_{\mathsf{M}})$. *Its domain is*

$$\mathcal{D}\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathsf{M},\mathbf{g}_{\mathsf{M}})\big)=\big\{w\in\Lambda^qH^1_{\mathbf{T}}(\mathsf{M})\cap\Lambda^qH^2(\mathsf{M}),\ \mathbf{t}d^*_{f,h}w=0\ \text{on}\ \partial\mathsf{M}\big\}.$$

Moreover, $\Delta^{\mathsf{Di},(q)}_{f,h}(\mathsf{M},\mathbf{g}_{\mathsf{M}})$ *is a self-adjoint operator, with compact resolvent. Finally it holds, for all Borel set* $E\subset\mathbb{R}$ *and* $u\in\Lambda^qH^1_{\mathbf{T}}(\mathsf{M})$,

$$\pi_E\big(\Delta^{\mathsf{Di},(q+1)}_{f,h}(\mathsf{M},\mathbf{g}_{\mathsf{M}})\big)\,\mathsf{d}_{f,h}u=\mathsf{d}_{f,h}\,\pi_E\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathsf{M},\mathbf{g}_{\mathsf{M}})\big)\,u\tag{44}$$

and

$$\pi_E\big(\Delta^{\mathsf{Di},(q-1)}_{f,h}(\mathsf{M},\mathbf{g}_{\mathsf{M}})\big)\,\mathsf{d}^*_{f,h}u=\mathsf{d}^*_{f,h}\,\pi_E\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathsf{M},\mathbf{g}_{\mathsf{M}})\big)\,u.\tag{45}$$

(3)Of course, if M is a manifold satisfying $(\mathsf{M}\text{-}f)$ (in particular $\overline{\mathsf{M}}$ is compact), only the norms depend on the metric $\mathbf{g}_{\mathsf{M}}$, but not the Sobolev spaces. We will also use in the following Sobolev spaces on $\mathbb{R}^d_-$, which is not compact.

Here and in the following, for a Borel set $E \subset \mathbb{R}$ and T a non negative self-adjoint operator on a Hilbert space, $\pi_E(\mathsf{T})$ denotes the spectral projector associated with T and E.

The following standard lemma will be used several times throughout this work.

Lemma 11. — *Let $(\mathsf{T}, D(\mathsf{T}))$ be a non negative self-adjoint operator on a Hilbert space $(\mathcal{H}, \|\cdot\|)$ with associated quadratic form $q_{\mathsf{T}}(x) = (x, \mathsf{T}x)$ whose domain is $Q(\mathsf{T})$. It then holds:*

$$\forall b > 0,\ \forall u \in Q(\mathsf{T}), \quad \big\|\pi_{[b,+\infty)}(\mathsf{T})\, u\big\|^2 \leqslant \frac{q_{\mathsf{T}}(u)}{b}.$$

Generally speaking, a $\mathcal{H}$-normalized element $u \in D(\mathsf{T})$ such that $\|\pi_{[b,+\infty)}(\mathsf{T})\, u\|$ is small is called a quasi-mode for the spectrum in $[0, b]$ of T.

The objective of this section is to count the number of eigenvalues smaller than ch (for some $c > 0$) of $\Delta^{\mathsf{Di},(q)}_{f,h}(\mathsf{M}, \mathbf{g}_{\mathsf{M}})$, namely to identify the dimension of the range of $\pi_{[0,\mathsf{c}h]}\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathsf{M}, \mathbf{g}_{\mathsf{M}})\big)$, for h sufficiently small.

2.2. Number of small eigenvalues of $\Delta^{\mathsf{Di},(q)}_{f,h}(\mathsf{M}, \mathbf{g}_{\mathsf{M}})$. — Before stating the main result of Section 2, let us introduce a few more notation. Let us assume that (M-f) holds. Let $z \in \partial\mathsf{M}$ be a critical point of f (i.e., $|\nabla f(z)| = 0$). Then, z is a critical point of $f|_{\partial\mathsf{M}}$ and the unit outward normal $\mathsf{n}_{\mathsf{M}}(z)$ to M at z (see item (2) in Lemma 4) is an eigenvector with the associated eigenvalue:

$$\mu_z = {}^t\mathsf{n}_{\mathsf{M}}(z)\ \mathrm{Hess}\ f(z)\, \mathsf{n}_{\mathsf{M}}(z). \tag{46}$$

Let us now introduce the set of so-called generalized critical points of f for the operator $\Delta^{\mathsf{Di}}_{f,h}(\mathsf{M}, \mathbf{g}_{\mathsf{M}})$, which can be seen intuitively as critical points for the function f extended by $-\infty$ outside $\overline{\mathsf{M}}$. For $q \in \{0, \dots, d\}$, the standard critical points with index q in M are:

$$\mathsf{U}^{\mathsf{M}}_q = \big\{x \in \mathsf{M},\ x \text{ is a critical point of } f \text{ of index } q\big\},$$

with cardinal $\mathsf{m}^{\mathsf{M}}_q = \mathrm{Card}\big(\mathsf{U}^{\mathsf{M}}_q\big)$. Two additional sets of generalized critical points with index q on $\partial\mathsf{M}$ should be considered. First, let us introduce

$$\mathsf{U}^{\partial\mathsf{M},1}_q = \big\{z \in \partial\mathsf{M},\ z \text{ is a critical point of } f|_{\partial\mathsf{M}} \text{ of index } q-1 \text{ and } \partial_{\mathsf{n}_{\mathsf{M}}} f(z) > 0\big\}, \tag{47}$$

with cardinal $\mathsf{m}^{\partial\mathsf{M},1}_q = \mathrm{Card}\big(\mathsf{U}^{\partial\mathsf{M},1}_q\big)$, and with the convention that $\mathsf{U}^{\partial\mathsf{M},1}_0 = \varnothing$ for $q = 0$. Second, one defines,

$$\mathsf{U}^{\partial\mathsf{M},2}_q = \big\{z \in \partial\mathsf{M},\ |\nabla f(z)| = 0,\ z \text{ is a critical point of } f|_{\partial\mathsf{M}} \text{ of index } q-1 \text{ and } \mu_z < 0\big\}, \tag{48}$$

with cardinal $\mathsf{m}^{\partial\mathsf{M},2}_q = \mathrm{Card}\big(\mathsf{U}^{\partial\mathsf{M},2}_q\big)$, and with again the convention that $\mathsf{U}^{\partial\mathsf{M},2}_0 = \varnothing$ for $q = 0$. Finally, one defines the total number of generalized critical points with index q:

$$\mathsf{m}_q = \mathsf{m}^{\mathsf{M}}_q + \mathsf{m}^{\partial\mathsf{M},1}_q + \mathsf{m}^{\partial\mathsf{M},2}_q. \tag{49}$$

Let us now state the main result of this section.

Theorem 4. — *Let us assume that* $(\mathsf{M}\text{-}f)$ *holds. Then, for all* $q \in \{0, \dots, d\}$, *there exists* $\mathsf{c} > 0$ *and* $h_0 > 0$ *such that for all* $h \in (0, h_0)$:

$$\dim \operatorname{Ran} \pi_{[0,\mathsf{c}h]}\big(\Delta_{f,h}^{\mathsf{Di},(q)}(\mathsf{M}, \mathbf{g}_{\mathsf{M}})\big) = \mathsf{m}_q, \quad \textit{where } \mathsf{m}_q \textit{ is defined by } (49).$$

Let us mention that this result is proved in [58] for $q = 0$ under a weaker assumption than $(\mathsf{M}\text{-}f)$.

The proof of Theorem 4, inspired from [42, §3] and [19], consists in finding where the $L^2(\mathsf{M}, \mathbf{g}_{\mathsf{M}})$-norms of eigenforms associated with eigenvalues of order $o(h)$ concentrate in $\overline{\mathsf{M}}$, and in determining a finite dimensional linear space close to them. We first study in Section 2.3 model problems on $\mathbb{R}^d_-$ where

$$\mathbb{R}^d_- = \{x = (x', x_d), \quad x' = (x_1, \dots, x_{d-1}) \in \mathbb{R}^{d-1},\, x_d \in \mathbb{R},\, x_d < 0\},$$

before providing the proof of Theorem 4 in Section 2.4.

Remark 12. — Let us mention that the main difference with [42, Chap. 3] is that we cannot use a block-diagonalization of the metric $\mathbf{g}_{\mathsf{M}}$ and of the function f near the critical points in $\partial\mathsf{M}$, which would lead to an exact tensorization into a Witten Laplacian in a variable $x' \in \partial\mathsf{M}$ and a Witten Laplacian in a variable $x_d \in \mathbb{R}_-$. We actually only decompose the metric $\mathbf{g}_{\mathsf{M}}$ in a local system of coordinates near the critical point, constructed with the geodesic distance to the boundary. Then, using the fact that $\partial_{\mathsf{n}_{\mathsf{M}}} f = 0$ near critical points on $\partial\mathsf{M}$, it appears that a local asymptotic expansion of f in these coordinates is precise enough to count the number of small eigenvalues.

Remark 13. — A simple consequence of the above results is the following finite dimensional Dirichlet complex structures for Witten Laplacians on bounded domains under the assumption $(\mathsf{M}\text{-}f)$:

$$\{0\} \longrightarrow \operatorname{Ran} \pi_{[0,ch]}(\Delta_{f,h}^{\mathsf{Di},(0)}(\mathsf{M}, \mathbf{g}_{\mathsf{M}})) \xrightarrow{\mathsf{d}_{f,h}} \cdots$$
$$\cdots \xrightarrow{\mathsf{d}_{f,h}} \operatorname{Ran} \pi_{[0,ch]}(\Delta_{f,h}^{\mathsf{Di},(d)}(\mathsf{M}, \mathbf{g}_{\mathsf{M}})) \xrightarrow{\mathsf{d}_{f,h}} \{0\}$$

and

$$\{0\} \xleftarrow{\mathsf{d}^*_{f,h}} \operatorname{Ran} \pi_{[0,ch]}(\Delta_{f,h}^{\mathsf{Di},(0)}(\mathsf{M}, \mathbf{g}_{\mathsf{M}})) \xleftarrow{\mathsf{d}^*_{f,h}} \cdots$$
$$\cdots \xleftarrow{\mathsf{d}^*_{f,h}} \operatorname{Ran} \pi_{[0,ch]}(\Delta_{f,h}^{\mathsf{Di},(d)}(\mathsf{M}, \mathbf{g}_{\mathsf{M}})) \longleftarrow \{0\}.$$

These, combined with Theorem 4, yield strong Morse inequalities. This generalizes standard results for the Witten Laplacians in the full domain [44, 19, 93] or on bounded domain without critical points on the boundary [42, 56] (see also [54, 16]).

2.3. Number of small eigenvalues of Witten Laplacians in $\mathbb{R}^d_-$.

— The goal of this section is to count the number of small eigenvalues of $\Delta_{f,h}^{\mathsf{Di},(q)}(\mathbb{R}^d_-, \mathbf{g})$ in a simple geometric setting (in particular f has a single critical point, located at 0). The main result (Proposition 16) is stated in Section 2.3.1. The proof is done in three steps: we first recall well-known results for Witten Laplacians in $\mathbb{R}^{d-1}$ in Section 2.3.2; then we prove Proposition 16 in a simplified setting in Sections 2.3.3 and 2.3.4; and we finally conclude with the proof of Proposition 16 in Section 2.3.5.

2.3.1. *Witten Laplacian in $\mathbb{R}^d_-$ with tangential Dirichlet boundary conditions*. — Let us first introduce the tangential Dirichlet Witten Laplacian $\Delta^{(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})$ in $\mathbb{R}^d_-$, under two sets of assumptions.

Assumption (Metric-$\mathbb{R}^d_-$). — The space $\overline{\mathbb{R}^d_-}$ is endowed with a metric tensor $\mathbf{g}$ satisfying the following:

(i) $\mathbf{g}$ writes, for some $\mathcal{C}^\infty$ function $\mathbf{G}$ on $\overline{\mathbb{R}^d_-}$,

$$\mathbf{g}(x)=\mathbf{G}(x',x_d)dx'^2+dx_d^2, \tag{50}$$

with $\mathbf{G}(0,0)$ the identity matrix.

(ii) $\mathbf{G}$ and all its derivatives are bounded over $\overline{\mathbb{R}^d_-}$.

(iii) $\mathbf{G}$ is uniformly elliptic over $\overline{\mathbb{R}^d_-}$.

To ease the notation, we will not indicate explicitly the metric $\mathbf{G}$ in the functional spaces nor in the associated norm: we will simply write $\Lambda^qH^k(\mathbb{R}^d_-)$ (resp. $\Lambda^qH^1_{\mathbf{T}}(\mathbb{R}^d_-)$) for $\Lambda^qH^k(\mathbb{R}^d_-,\mathbf{g})$ (resp. $\Lambda^qH^1_{\mathbf{T}}(\mathbb{R}^d_-,\mathbf{g})$), and denote by $\|.\|_{H^k(\mathbb{R}^d_-)}$ the associated norm.

Notice that under (Metric-$\mathbb{R}^d_-$), the norm on $(\mathbb{R}^d_-,\mathbf{g})$ is uniformly equivalent to the norm on $(\mathbb{R}^d_-,\mathsf{I}_d\,dx^2)$ (where I_d is the identity matrix of size d), which is simply denoted by $|x|$: $|x|^2=\sum_{i=1}^d x_i^2$. Moreover, for all $q\in\{0,\dots,d\}$ and $k\geqslant 0$, the norm on $\Lambda^qH^k(\mathbb{R}^d_-,\mathbf{g})$ is equivalent to the norm on $\Lambda^qH^k(\mathbb{R}^d_-,\mathsf{I}_d dx^2)$, and $\Lambda^qH^1_{\mathbf{T}}(\mathbb{R}^d_-,\mathbf{g})=\Lambda^qH^1_{\mathbf{T}}(\mathbb{R}^d_-,\mathsf{I}_d\,dx^2)$.

Assumption (Potential-$\mathbb{R}^d_-$). — The function $f:\overline{\mathbb{R}^d_-}\to\mathbb{R}$ satisfies:

(i) f is a $\mathcal{C}^\infty$ function such that for all multi-index $\alpha\in\mathbb{N}^d$ with $|\alpha|\geqslant 1$, $\sup_{\overline{\mathbb{R}^d_-}}|\partial^\alpha_x f|<+\infty$.

(ii) The point 0 is the only critical point of f in $\overline{\mathbb{R}^d_-}$ and is a non degenerate critical point of f (this condition is independent of the metric tensor on $\mathbb{R}^d_-$). Moreover, there exist $R>0$ and $c>0$ such that:

$$\forall x\in\mathbb{R}^d_-,\ |x|\geqslant R\implies |\nabla f|(x)\geqslant c. \tag{51}$$

(iii) It holds:

$$\forall x'\in\mathbb{R}^{d-1},\quad \partial_{\mathsf{n}_{\mathbb{R}^d_-}}f(x',0)=0. \tag{52}$$

Notice that thanks to (50), for any $\phi\in\Lambda^0\mathcal{C}^1(\overline{\mathbb{R}^d_-})$, one has:

$$\forall x'\in\mathbb{R}^{d-1},\quad \partial_{\mathsf{n}_{\mathbb{R}^d_-}}\phi(x',0)=\partial_{x_d}\phi(x',0). \tag{53}$$

Moreover, under the above assumptions, up to an orthogonal transformation on x' (which preserves the fact that $\mathbf{G}(0,0)$ is the identity matrix), one can assume that the Hessian matrix of $f|_{\partial\mathbb{R}^d_-}$ at $0\in\mathbb{R}^{d-1}$ is diagonal. As a consequence, there exists a neighborhood V_0 of 0 in $\overline{\mathbb{R}^d_-}$ and $(\mu_1,\dots,\mu_d)\in(\mathbb{R}^*)^d$ such that:

$$\forall x=(x_1,\dots,x_d)\in\mathsf{V}_0,\quad f(x)=f(0)+\sum_{i=1}^d\frac{\mu_i}{2}\,x_i^2+O(|x|^3), \tag{54}$$

where $(\mu_1,\dots,\mu_d)$ are the eigenvalues of $\operatorname{Hess} f(0)$. More precisely, $\mu_d=\partial_{x_d,x_d}f(0)$, and $(\mu_1,\dots,\mu_{d-1})$ are the eigenvalues of $\operatorname{Hess} f|_{\partial\mathbb{R}^d_-}(0)$.

We will need the following standard results on the operator $\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})$.

Proposition 14. — *Let us assume that* (Metric-$\mathbb{R}^d_-$) *and item* (i) *in* (Potential-$\mathbb{R}^d_-$) *are satisfied. Let $q\in\{0,\dots,d\}$ and $h>0$ be fixed. The Friedrichs extension of the quadratic form*

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g}): w\in\Lambda^qH^1_{\mathbf{T}}(\mathbb{R}^d_-)\longmapsto \|\mathsf{d}_{f,h}w\|^2_{L^2(\mathbb{R}^d_-)}+\|\mathsf{d}^*_{f,h}w\|^2_{L^2(\mathbb{R}^d_-)} \tag{55}$$

on $\Lambda^qL^2(\mathbb{R}^d_-)$ is denoted by $\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})$. It is a self-adjoint operator with domain

$$\mathcal{D}\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})\big)=\big\{w\in\Lambda^qH^1_{\mathbf{T}}(\mathbb{R}^d_-)\cap\Lambda^qH^2(\mathbb{R}^d_-),\ \mathbf{t}\mathsf{d}^*_{f,h}w=0 \text{ on } \partial\mathbb{R}^d_-\big\}.$$

Moreover, it holds, for all Borel set $E\subset\mathbb{R}$ and $u\in\Lambda^qH^1_{\mathbf{T}}(\mathbb{R}^d_-)$,

$$\pi_E\big(\Delta^{\mathsf{Di},(q+1)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})\big)\,\mathsf{d}_{f,h}u=\mathsf{d}_{f,h}\,\pi_E\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})\big)\,u \tag{56}$$

and

$$\pi_E\big(\Delta^{\mathsf{Di},(q-1)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})\big)\,\mathsf{d}^*_{f,h}u=\mathsf{d}^*_{f,h}\,\pi_E\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})\big)\,u. \tag{57}$$

The following Green formula will be used many times in the sequel (it can be proved as in the compact case [42, Lem. 2.3.2] by density of $\Lambda^q\mathcal{C}^\infty_c(\overline{\mathbb{R}^d_-})$ in $\Lambda^qH^1(\mathbb{R}^d_-)$).

Lemma 15. — *Let $q\in\{0,\dots,d\}$. Let us assume that* (Metric-$\mathbb{R}^d_-$) *is satisfied. Then, for all $w\in\Lambda^qH^1_{\mathbf{T}}(\mathbb{R}^d_-)$, it holds:*

$$\begin{aligned}\|\mathsf{d}_{f,h}w\|^2_{L^2(\mathbb{R}^d_-)}+\|\mathsf{d}^*_{f,h}w\|^2_{L^2(\mathbb{R}^d_-)}&=h^2\|\mathsf{d}\,w\|^2_{L^2(\mathbb{R}^d_-)}+h^2\|\mathsf{d}^*\,w\|^2_{L^2(\mathbb{R}^d_-)}\\&\quad+\big\langle w,\big(|\nabla f|^2_{\mathbf{g}}+h(\mathcal{L}_{\nabla f}+\mathcal{L}^*_{\nabla f})\big)\,w\big\rangle_{L^2(\mathbb{R}^d_-)}\\&\quad-h\int_{\partial\mathbb{R}^d_-}\langle w,w\rangle_{T_{(x',0)}\partial\mathbb{R}^d_-}\,\partial_{\mathsf{n}_{\mathbb{R}^d_-}}f(x',0)\lambda(dx'),\end{aligned}$$

where $\lambda(dx')$ is of course the volume form on $\partial\mathbb{R}^d_-$ induced by the metric tensor $\mathbf{g}$.

Let us now state the main result of this section (recall the definition (54) of μ_d).

Proposition 16. — *Let us assume that* (Metric-$\mathbb{R}^d_-$) *and* (Potential-$\mathbb{R}^d_-$) *hold. Let $q\in\{0,\dots,d\}$. Then, there exist $C>0$, $c>0$, and $h_0>0$ such that for all $h\in(0,h_0)$, the following holds:*

(i) *If $q=0$, then:*

$$\forall w \in \Lambda^0 H^1_{\mathbf{T}}(\mathbb{R}^d_-),\ \ Q^{\mathsf{Di},(0)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(w) \geqslant Ch\,\|w\|^2_{L^2(\mathbb{R}^d_-)}. \tag{58}$$

Let $q\in\{1,\dots,d\}$. If the index of 0 as a critical point of $f|_{\partial\mathbb{R}^d_-}$ is not $q-1$ or if $\mu_d>0$, then:

$$\forall w \in \Lambda^q H^1_{\mathbf{T}}(\mathbb{R}^d_-),\quad Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(w) \geqslant Ch\,\|w\|^2_{L^2(\mathbb{R}^d_-)}. \tag{59}$$

If the index of 0 as a critical point of $f|_{\partial\mathbb{R}^d_-}$ is $q-1$ and $\mu_d<0$, then:

$$\operatorname{Ran}\pi_{[0,ch]}\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})\big) = \operatorname{Ker}\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g}) \text{ has dimension } 1. \tag{60}$$

(ii) *Assume that the index of 0 as a critical point of $f|_{\partial\mathbb{R}^d_-}$ is $q-1$ and $\mu_d<0$. Let $\chi:\overline{\mathbb{R}^d_-}\to[0,1]$ be a $\mathcal{C}^\infty$ function supported in a neighborhood of 0 which equals 1 in a neighborhood of 0. Let $\Psi_h\in\operatorname{Ker}\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})$ such that $\|\Psi_h\|_{L^2(\mathbb{R}^d_-)}=1$. Then, in the limit $h\to0$, it holds:*

$$\|\chi\Psi_h\|_{L^2(\mathbb{R}^d_-)} = 1+O(h^2) \quad\text{and}\quad Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(\chi\Psi_h)=O(h^2). \tag{61}$$

The next lemma shows that it is enough to prove (58)–(59) in Proposition 16 for forms w supported in a ball $\mathsf{B}(0,h^{2/5})$.

Lemma 17. — *Let us assume that* (Metric-$\mathbb{R}^d_-$) *and* (Potential-$\mathbb{R}^d_-$) *are satisfied. Let us assume that there exist $C>0$ and $h_0>0$ such that for all $h\in(0,h_0)$ and for all $v\in\Lambda^q H^1_{\mathbf{T}}(\mathbb{R}^d_-)$ supported in $\mathsf{B}(0,h^{2/5})$,*

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(v) \geqslant Ch\,\|v\|^2_{L^2(\mathbb{R}^d_-)}. \tag{62}$$

Then, there exist $c>0$ and $h_0>0$ such that for all $h\in(0,h_0)$ and for all $w\in\Lambda^q H^1_{\mathbf{T}}(\mathbb{R}^d_-)$,

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(w) \geqslant Ch\|w\|^2_{L^2(\mathbb{R}^d_-)}.$$

Proof. — Let us consider a quadratic partition of unity (χ_1,χ_2) such that $\chi_1\in\mathcal{C}^\infty_c(\overline{\mathbb{R}^d_-})$, $\chi_1=1$ on $\mathsf{B}(0,1/2)$, $\operatorname{supp}\chi_1\subset\mathsf{B}(0,1)$ and $\chi_1^2+\chi_2^2=1$. The IMS formula [19, 42] yields: for all $w\in\Lambda^q H^1_{\mathbf{T}}(\mathbb{R}^d_-)$,

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(w) = \sum_{k=1}^2 Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(\chi_k(h^{-2/5}.)w) - h^2\,\big\|\nabla\big[\chi_k(h^{-2/5}.)\big]w\big\|^2_{L^2(\mathbb{R}^d_-)}. \tag{63}$$

Using Lemma 15, $\partial_{\mathsf{n}_{\mathbb{R}^d_-}} f=0$ on $\partial\mathbb{R}^d_-$ (see (52)) and $\mathbf{t}(\chi_k(h^{-2/5}.)w)(x',0)=0$, one has:

$$\begin{aligned} Q^{\mathsf{Di},(q)}_{f,h}&(\mathbb{R}^d_-,\mathbf{g})(\chi_2(h^{-2/5}.)w)\\ &= h^2\big\|\mathsf{d}\big(\chi_2(h^{-2/5}.)w\big)\big\|^2_{L^2(\mathbb{R}^d_-)} + h^2\big\|\mathsf{d}^*\big(\chi_2(h^{-2/5}.)w\big)\big\|^2_{L^2(\mathbb{R}^d_-)}\\ &\quad + \big\langle \chi_2(h^{-2/5}.)w, \Big(|\nabla f|^2 - h\big(\mathcal{L}_{\nabla f}+\mathcal{L}^*_{\nabla f}\big)\Big)\chi_2(h^{-2/5}.)w\big\rangle_{L^2(\mathbb{R}^d_-)}. \end{aligned}$$

Moreover, using (Metric-$\mathbb{R}^d_-$) and item (ii) in (Potential-$\mathbb{R}^d_-$), there exists $C>0$ such that,

$$\forall x \in \mathbb{R}^d_- \setminus \mathsf{B}(0,h^{2/5}/2), \quad |\nabla f(x)|^2_{\mathbf{g}} \geqslant Ch^{4/5}, \tag{64}$$

for some $C>0$ independent of h. Thus, using the fact that $\mathcal{L}_{\nabla f}+\mathcal{L}^*_{\nabla f}$ is a 0th order operator and supp $\chi_2(h^{-2/5}.)\subset \mathbb{R}^d\setminus \mathsf{B}(0,h^{2/5}/2)$, one obtains that there exist $c>0$ and $h_0>0$ such that for all $h\in(0,h_0)$:

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(\chi_2(h^{-2/5}.)w) \geqslant Ch^{4/5}\|\chi_2(h^{-2/5}.)w\|^2_{L^2(\mathbb{R}^d_-)}. \tag{65}$$

This implies that there exist $c>0$ and $C>0$ such that

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(w) \geqslant Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(\chi_1(h^{-2/5}.)w) + Ch^{4/5}\|\chi_2(h^{-2/5}.)w\|^2_{L^2(\mathbb{R}^d_-)} - Ch^{6/5}\|w\|^2_{L^2(\mathbb{R}^d_-)}.$$

If (62) holds, one obtains (taking $v=\chi_1(h^{-2/5}.)w$ in (62)) for all h small enough:

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(w) \geqslant C\Big(h\|\chi_1(h^{-2/5}.)w\|^2_{L^2(\mathbb{R}^d_-)} + h^{4/5}\|\chi_2(h^{-2/5}.)w\|^2_{L^2(\mathbb{R}^d_-)} - h^{6/5}\|w\|^2_{L^2(\mathbb{R}^d_-)}\Big).$$

Thus, $Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(w)\geqslant Ch\|w\|^2_{L^2(\mathbb{R}^d_-)}$. This ends the proof of Lemma 17. ☐

The proof of Proposition 16 will be done in Section 16, after considering successively model problems on $\mathbb{R}^{d-1}$, and on $\mathbb{R}^d_-$ in a simplified setting.

2.3.2. *Witten Laplacian in* $\mathbb{R}^{d-1}$. — Let us first recall standard results on the number of eigenvalues of order $o(h)$ for the Witten Laplacian on $\mathbb{R}^{d-1}$ associated with a function $f_+:\mathbb{R}^{d-1}\to\mathbb{R}$ which has only one critical point in $\mathbb{R}^{d-1}$. Let us introduce the two sets of assumptions used to state this result.

Assumption (Metric-$\mathbb{R}^{d-1}$). — The space $\mathbb{R}^{d-1}$ is endowed with a $\mathcal{C}^\infty$ metric tensor denoted by $x'\in\mathbb{R}^{d-1}\mapsto \widetilde{\mathbf{G}}(x')\,dx'^2$. In addition,

(i) $\widetilde{\mathbf{G}}$ and all its derivatives are bounded over $\mathbb{R}^{d-1}$.
(ii) $\widetilde{\mathbf{G}}$ is uniformly elliptic over $\mathbb{R}^{d-1}$, i.e., $\widetilde{\mathbf{G}}\geqslant c$ over $\mathbb{R}^{d-1}$, for some $c>0$.

Again, we will not indicate explicitly the metric $\widetilde{\mathbf{G}}$ in the functional spaces nor in the associated norm: we will simply write $\Lambda^qH^k(\mathbb{R}^{d-1})$ for $\Lambda^qH^k(\mathbb{R}^{d-1},\widetilde{\mathbf{G}}\,dx'^2)$ and denote $\|\cdot\|_{H^k(\mathbb{R}^{d-1})}$ the associated norm.

Notice that, as above, under (Metric-$\mathbb{R}^{d-1}$), the norm on $(\mathbb{R}^{d-1},\widetilde{\mathbf{G}}\,dx'^2)$ is uniformly equivalent to the norm on $(\mathbb{R}^{d-1},\mathsf{I}_{d-1}\,dx'^2)$, the latter being simply denoted $|x'|$: $|x'|^2=\sum_{i=1}^{d-1}x_i^2$. In addition, for all $q\in\{0,\dots,d-1\}$ and $k\geqslant 0$, the norm on $\Lambda^qH^k(\mathbb{R}^{d-1},\widetilde{\mathbf{G}}\,dx'^2)$ is equivalent to the norm on $\Lambda^qH^k(\mathbb{R}^{d-1},\mathsf{I}_{d-1}\,dx'^2)$.

Assumption (Potential-$\mathbb{R}^{d-1}$). — The function $f_+:\mathbb{R}^{d-1}\to\mathbb{R}$ satisfies:

(i) f_+ is a $\mathcal{C}^\infty$ function such that for all multi-index $\beta\in\mathbb{N}^{d-1}$ with $|\beta|\geqslant 1$, $\sup_{\mathbb{R}^{d-1}}|\partial_x^\beta f_+|<+\infty$.

(ii) The point 0 is the only critical point of f_+ in $\mathbb{R}^{d-1}$ and is a non degenerate critical point, with an index denoted by $p \in \{0, \dots, d-1\}$ (the non-degeneracy and the index do not depend on the metric tensor on $\mathbb{R}^{d-1}$). Moreover, there exist $R > 0$ and $c > 0$ such that:

$$\forall x' \in \mathbb{R}^{d-1},\ |x'| \geqslant R \implies |\nabla f_+(x')| \geqslant c.$$

Under these assumptions, the following result holds (see [42, Prop. 3.3.2 & 3.3.3] and[41, Prop. 2.2] for proofs of very similar results).

Proposition 18. — *Let $d \geqslant 2$ and assume that* (Metric-$\mathbb{R}^{d-1}$) *and* (Potential-$\mathbb{R}^{d-1}$) *hold. Let $q \in \{0, \dots, d-1\}$ and $h > 0$. The Friedrichs extension of the quadratic form*

$$Q^{(q)}_{f_+,h}(\mathbb{R}^{d-1}, \widetilde{\mathbf{G}}\, dx'^2) : \begin{cases} \mathcal{D}\big(\Delta^{(q)}_{f_+,h}(\mathbb{R}^{d-1}, \widetilde{\mathbf{G}}\, dx'^2)\big) \longrightarrow \mathbb{R}_+ \\ w \longmapsto \|\mathsf{d}_{f,h} w\|^2_{L^2(\mathbb{R}^{d-1})} + \|\mathsf{d}^*_{f,h} w\|^2_{L^2(\mathbb{R}^{d-1})} \end{cases}$$

on $\Lambda^q L^2(\mathbb{R}^{d-1})$ is denoted by $\Delta^{(q)}_{f_+,h}(\mathbb{R}^{d-1}, \widetilde{\mathbf{G}} dx'^2)$. It is a self-adjoint operator with domain

$$\mathcal{D}\big(\Delta^{(q)}_{f_+,h}(\mathbb{R}^{d-1}, \widetilde{\mathbf{G}} dx'^2)\big) = \Lambda^q H^2(\mathbb{R}^{d-1}).$$

Moreover, there exist $C > 0$, $c > 0$ and $h_0 > 0$ such that for all $h \in (0, h_0)$:

(i) $\inf \sigma_{\mathrm{ess}}\big(\Delta^{(q)}_{f_+,h}(\mathbb{R}^{d-1}, \widetilde{\mathbf{G}}\, dx'^2)\big) \geqslant C$.

(ii) *When $p \neq q$,* $\dim \operatorname{Ran} \pi_{[0,ch]}\big(\Delta^{(q)}_{f_+,h}(\mathbb{R}^{d-1}, \widetilde{\mathbf{G}}\, dx'^2)\big) = 0$.

When $p = q$, $\operatorname{Ran} \pi_{[0,ch]}\big(\Delta^{(q)}_{f_+,h}(\mathbb{R}^{d-1}, \widetilde{\mathbf{G}}\, dx'^2)\big) = \operatorname{Ker} \Delta^{(q)}_{f_+,h}(\mathbb{R}^{d-1}, \widetilde{\mathbf{G}}\, dx'^2)$ *has dimension* 1.

2.3.3. *A simplified model in $\mathbb{R}^d_-$.* — We will first prove item (i) of Proposition 16 in the special case when $\mathbf{G}(x', x_d)$ in item (i) of (Metric-$\mathbb{R}^d_-$) is independent of the variable x_d.

Proposition 19. — *Assume that* (Metric-$\mathbb{R}^d_-$) *and* (Potential-$\mathbb{R}^d_-$) *are satisfied. Assume in addition that $\mathbf{G}$ is independent of x_d:*

$$\forall (x', x_d) \in \overline{\mathbb{R}^d_-},\ \mathbf{G}(x', x_d) = \widetilde{\mathbf{G}}(x'). \tag{66}$$

for some $\mathcal{C}^\infty$ function $\widetilde{\mathbf{G}}$ defined on $\mathbb{R}^{d-1}$. Then, item (i) *in Proposition* 16 *is satisfied.*

Before providing the proof of this proposition in Section 2.3.4, let us conclude this section with a few preliminary results. Notice first that when (Metric-$\mathbb{R}^d_-$) and (66), are satisfied, $\widetilde{\mathbf{G}}(x')dx'^2$ satisfies (Metric-$\mathbb{R}^{d-1}$). Moreover, we will need the following decomposition of the function f.

Definition 20. — Assume that (Potential-$\mathbb{R}^d_-$) is satisfied, and recall the expansion (54) of f around 0. Let us define f_+ and f_- by:

$$\forall x = (x', x_d) \in \mathsf{V}_0, \quad f_+(x') = \sum_{i=1}^{d-1} \frac{\mu_i}{2}\, x_i^2 \quad \text{and} \quad f_-(x_d) = -\frac{\mu_d}{2}\, x_d^2. \tag{67}$$

Let us then extend the function f_+ (resp. f_-) to a C^∞ function over $\mathbb{R}^{d-1}$ (resp. $\overline{\mathbb{R}_-}$) such that:

(1) All the derivatives of f_+ (resp. f_-) of order at least 1 are bounded over $\mathbb{R}^{d-1}$ (resp. $\overline{\mathbb{R}_-}$).

(2) The point 0 is the only critical point of f_+ (resp. f_-) on $\mathbb{R}^{d-1}$ (resp. $\overline{\mathbb{R}_-}$), and for some $c > 0$, $|\nabla f_+| \geqslant c$ (resp. $|\nabla f_-| \geqslant c$) outside a compact set of $\mathbb{R}^{d-1}$ (resp. of $\overline{\mathbb{R}_-}$).

In other words, f_+ satisfies (Potential-$\mathbb{R}^{d-1}$), and f_- satisfies (Potential-$\mathbb{R}^d_-$) for $d = 1$.

It is easy to check that, when $\mu_d < 0$, f_- satisfies

$$\forall h > 0, \quad e^{-(2/h)f_-} \in \Lambda^0 H^2(\mathbb{R}_-). \tag{68}$$

The following result is the key point to prove Proposition 19. It allows us to separate the variables x' and x_d in the Witten Laplacian $\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-, \mathbf{g})$, up to remainder terms of order $h^{6/5}$.

Lemma 21. — *Assume that* (Metric-$\mathbb{R}^d_-$), (Potential-$\mathbb{R}^d_-$), *and* (66) *are satisfied. Let us consider the functions f_+ and f_- as introduced in Definition* 20. *Let $q \in \{0, \dots, d\}$ and $w \in \mathcal{D}(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-, \mathbf{g}))$. Write $w = \mathsf{a} \wedge dx_d + \mathsf{b}$ where*

$$\mathsf{b} = \sum_{\substack{\mathsf{J}=\{j_1,\dots,j_q\},\\ j_1<\cdots<j_q,\, d\notin \mathsf{J}}} \mathsf{b}_\mathsf{J}\, dx_\mathsf{J} \quad \textit{and} \quad \mathsf{a} = \sum_{\substack{\mathsf{I}=\{i_1,\dots,i_{q-1}\},\\ i_1<\cdots<i_{q-1},\, d\notin \mathsf{I}}} \mathsf{a}_\mathsf{I}\, dx_\mathsf{I}.$$

It then holds, for some $\mathsf{c}_1 > 0$ and $\mathsf{c}_2 > 0$ independent of $h > 0$ and of w,

$$\begin{aligned} Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-, \mathbf{g})(w) \geqslant \mathsf{c}_1 \sum_\mathsf{I} \int_{x'\in\mathbb{R}^{d-1}} & Q^{\mathsf{Di},(1)}_{-f_-,h}(\mathbb{R}_-, dx_d^2)\big(\mathsf{a}_\mathsf{I}(x',.)dx_d\big)\mu(dx') \\ &+ \mathsf{c}_1 \sum_\mathsf{J} \int_{x'\in\mathbb{R}^{d-1}} Q^{\mathsf{Di},(0)}_{-f_-,h}(\mathbb{R}_-, dx_d^2)\big(\mathsf{b}_\mathsf{J}(x',.)\big)\mu(dx') \\ &+ \int_{x_d\in\mathbb{R}_-} Q^{(q-1)}_{f_+,h}(\mathbb{R}^{d-1}, \widetilde{\mathbf{G}}dx'^2)\big(\mathsf{a}(.,x_d)\big)dx_d \\ &+ \int_{x_d\in\mathbb{R}_-} Q^{(q)}_{f_+,h}(\mathbb{R}^{d-1}, \widetilde{\mathbf{G}}dx'^2)\big(\mathsf{b}(.,x_d)\big)dx_d - \mathsf{e}(h,w), \end{aligned}$$

where $|\mathsf{e}(h,w)| \leqslant \mathsf{c}_2 h^{6/5} \|w\|^2_{L^2(\mathbb{R}^d_-)}$ if $\operatorname{supp} w \subset \mathsf{B}(0, h^{2/5})$. The measure $\mu(dx')$ is the measure $\sqrt{\det \widetilde{\mathbf{G}}(x')}\, dx'$, where dx' is the Lebesgue measure on $\mathbb{R}^{d-1}$, and the measure dx_d is the Lebesgue measure on $\mathbb{R}_-$.

Proof. — One has from (54) and (67), in a neighborhood V_0 of 0 in $\overline{\mathbb{R}^d_-}$,

$$\forall x = (x', x_d) \in \mathsf{V}_0, \quad f(x) = f(0) + f_+(x') - f_-(x_d) + O(|x|^3) \tag{69}$$

and (using (66)),

$$|\nabla f(x)|^2_\mathbf{g} = |\nabla_{x'} f_+(x')|^2_{\widetilde{\mathbf{G}}dx'^2} + |\partial_{x_d} f_-(x_d)|^2 + O(|x|^3). \tag{70}$$

Moreover, one has:

$$\mathcal{L}_{\nabla f(x)} + \mathcal{L}^*_{\nabla f(x)} = \mathcal{L}_{\nabla (f_+(x)-f_-(x))} + \mathcal{L}^*_{\nabla (f_+(x)-f_-(x))} + O(|x|). \tag{71}$$

Let $w \in \mathcal{D}\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})\big)$. One has

$$\begin{aligned} Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(w) &= \langle w, \Delta^{(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})w\rangle_{L^2(\mathbb{R}^d_-)} \\ &= \langle w, \Delta^{(q)}_{f^+-f^-,h}(\mathbb{R}^d_-,\mathbf{g})w\rangle_{L^2(\mathbb{R}^d_-)} + \mathsf{e}(h,w), \end{aligned} \tag{72}$$

where, owing to (43), (69), (70), and (71), the remainder term $\mathsf{e}(h,w)$ satisfies: if w is supported in $\mathsf{B}(0,h^{2/5})$,

$$|\mathsf{e}(h,w)| \leqslant C(h^{6/5} + h\times h^{2/5})\|w\|^2_{L^2(\mathbb{R}^d_-)} \leqslant Ch^{6/5}\,\|w\|^2_{L^2(\mathbb{R}^d_-)}. \tag{73}$$

Let us now give a lower bound on $\langle w, \Delta^{(q)}_{f_+-f_-,h}(\mathbb{R}^d_-,\mathbf{g})w\rangle_{L^2(\mathbb{R}^d_-)}$. Algebraically, using (66), one has (see [42, Eq. (3.17)] or [56, Eq. (4.3.16)] for similar computations):

$$\begin{aligned} &\langle w, \Delta^{(q)}_{f_+-f_-,h}(\mathbb{R}^d_-,\mathbf{g})w\rangle_{L^2(\mathbb{R}^d_-)} \\ &\quad= \Big\langle \sum_{\mathsf{I}} dx_{\mathsf{I}}\wedge(\mathsf{a}_{\mathsf{I}}\,dx_d),\ \sum_{\mathsf{I}} dx_{\mathsf{I}}\wedge \Delta^{(1)}_{-f_-,h}(\mathbb{R}_-,dx_d^2)(\mathsf{a}_{\mathsf{I}}\,dx_d)\Big\rangle_{L^2(\mathbb{R}^d_-)} \\ &\qquad+ \Big\langle \sum_{\mathsf{J}} \mathsf{b}_{\mathsf{J}}\,dx_{\mathsf{J}},\ \sum_{\mathsf{J}} \Delta^{(0)}_{-f_-,h}(\mathbb{R}_-,dx_d^2)(\mathsf{b}_{\mathsf{J}})\,dx_{\mathsf{J}}\Big\rangle_{L^2(\mathbb{R}^d_-)} \\ &\qquad+ \big\langle \mathsf{a}\wedge dx_d, \Delta^{(q-1)}_{f_+,h}(\mathbb{R}^{d-1},\widetilde{\mathbf{G}}dx'^2)(\mathsf{a})\wedge dx_d\big\rangle_{L^2(\mathbb{R}^d_-)} \\ &\qquad+ \langle \mathsf{b}, \Delta^{(q)}_{f_+,h}(\mathbb{R}^{d-1},\widetilde{\mathbf{G}}dx'^2)\mathsf{b}\rangle_{L^2(\mathbb{R}^d_-)}. \end{aligned} \tag{74}$$

Since $\mathbf{t}w=0$ on $\partial\mathbb{R}^d_-$, it holds, for all J and for a.e. $x'\in\mathbb{R}^{d-1}$, $\mathsf{b}_{\mathsf{J}}(x',0)=0$. Thus (see Proposition 14 for the domain of $\Delta^{\mathsf{Di},(0)}_{-f_-,h}(\mathbb{R}_-,dx_d^2)$ and item (1) of Definition 20), for all J and a.e. $x'\in\mathbb{R}^{d-1}$,

$$\mathsf{b}_{\mathsf{J}}(x',.)\in\Lambda^0H^2(\mathbb{R}_-)\cap\Lambda^0H^1_{\mathbf{T}}(\mathbb{R}_-) = \mathcal{D}\big(\Delta^{\mathsf{Di},(0)}_{-f_-,h}(\mathbb{R}_-,dx_d^2)\big).$$

From (66), $\mathbf{t}\mathsf{d}^*_{f,h}w=0$ on $\partial\mathbb{R}^d_-$ (for the metric tensor $\mathbf{g}$) writes: for a.e. $x'\in\mathbb{R}^{d-1}$ and all I,

$$\partial_{x_d}(e^{-(1/h)f}\mathsf{a}_{\mathsf{I}})(x',0)=0. \tag{75}$$

Because $\partial_{x_d}f(x',0)=0$ for all $x'\in\mathbb{R}^{d-1}$, see (52) and (53), this condition thus writes $\partial_{x_d}\mathsf{a}_{\mathsf{I}}(x',0)=0$. On the other hand, $f_-'(0)=0$ and hence, $\partial_{x_d}(e^{-(1/h)f_-}\mathsf{a}_{\mathsf{I}})(x',0)=0$ for a.e. $x'\in\mathbb{R}^{d-1}$, i.e., $\mathbf{t}\mathsf{d}^*_{f_-,h}(\mathsf{a}_{\mathsf{I}}(x',x_d)dx_d)=0$ on $\partial\mathbb{R}_-$ for the metric tensor dx_d^2 (recall that $\mathsf{d}^*(\phi dx_d)=-\partial_{x_d}\phi$ for the metric tensor dx_d^2). Thus, because in addition $\mathsf{a}_{\mathsf{I}}(x',.)dx_d\in\Lambda^1H^2(\mathbb{R}_-)$, one has (see Proposition 14 for the domain of $\Delta^{\mathsf{Di},(1)}_{-f_-,h}(\mathbb{R}_-,dx_d^2)$), for all I and a.e. $x'\in\mathbb{R}^{d-1}$:

$$\mathsf{a}_{\mathsf{I}}(x',.)dx_d\in\mathcal{D}\big(\Delta^{\mathsf{Di},(1)}_{-f_-,h}(\mathbb{R}_-,dx_d^2)\big).$$

Furthermore, one has (see Proposition 18 for the domain of $\Delta^{(q-1)}_{f_+,h}(\mathbb{R}^{d-1},\widetilde{\mathbf{G}}dx'^2)$): for a.e. $x_d<0$,

$$\begin{aligned}\mathsf{a}(.,x_d)\in\Lambda^{q-1}H^2(\mathbb{R}^{d-1})&=\mathcal{D}\big(\Delta^{(q-1)}_{f_+,h}(\mathbb{R}^{d-1},\widetilde{\mathbf{G}}dx'^2)\big),\\ \mathsf{b}(.,x_d)\in\Lambda^{q}H^2(\mathbb{R}^{d-1},\widetilde{\mathbf{G}}dx'^2)&=\mathcal{D}\big(\Delta^{(q)}_{f_+,h}(\mathbb{R}^{d-1},\widetilde{\mathbf{G}}dx'^2)\big).\end{aligned}$$

Lemma 21 then follows from (73) and (72) together with two integration by parts in $\mathbb{R}^{d-1}$ and two integrations by parts in $\mathbb{R}_-$ in (74), the constant $\mathsf{c}_1>0$ being the minimum of the smallest eigenvalues of the matrices $(\Pi_{k=1}^{q-1}\widetilde{\mathbf{G}}_{i_k,i'_k})_{\mathsf{I},\mathsf{I}'}$ and $(\Pi_{k=1}^{q}\widetilde{\mathbf{G}}_{j_k,j'_k})_{\mathsf{J},\mathsf{J}'}$ on $\mathbb{R}^{d-1}$. □

2.3.4. *Proof of Proposition* 19. — We are now in position to prove Proposition 19. Let us assume that (Metric-$\mathbb{R}^d_-$), (Potential-$\mathbb{R}^d_-$), and (66) are satisfied. Let us recall that according to Lemma 17, it is enough to prove Proposition 19 for all $w\in\Lambda^qH^1_{\mathbf{T}}(\mathbb{R}^d_-)$ supported in $\mathsf{B}(0,h^{2/5})$. All along the proof, the constants $C>0$ and $c>0$ can change from one occurrence to another but do not depend on h and on the test function w. The proof of Proposition 19 is divided into three steps: the case $d=1$, the proof of (58) and (59) when $d>1$, and finally the proof of (60) when $d>1$.

Step 1: The case $d=1$ *(i.e.,* $\mathbb{R}^d_-=\mathbb{R}_-$*).* — Let us recall that according to item (i) in (Metric-$\mathbb{R}^d_-$), the space $\mathbb{R}_-=\{x_d\in\mathbb{R},\ x_d<0\}$ is endowed with the metric tensor $\mathbf{g}(x_d)=dx_d^2$. From (54), in a neighborhood V_0 of 0 in $\mathbb{R}_-$, one has

$$\forall x_d\in\mathsf{V}_0,\quad f(x_d)=f(0)+\frac{\mu_d}{2}\,x_d^2+O(|x|^3).$$

Notice that for $w\in\Lambda H^1_{\mathbf{T}}(\mathbb{R}_-)$ according to the decomposition $w=\mathsf{a}\wedge dx_d+\mathsf{b}$ in Lemma 21, $w=\mathsf{b}$ when w is a 0-form and $w=\mathsf{a}dx_d$ when w is a 1-form (a is a function, see (77) below). For all $\mathsf{b}\in\Lambda^0H^1_{\mathbf{T}}(\mathbb{R}_-)$, one has from Lemma 15 and since $\mathsf{b}(0)=0$,

$$Q^{\mathsf{Di},(0)}_{f,h}(\mathbb{R}_-,dx_d^2)(\mathsf{b})=h^2\|\partial_{x_d}\mathsf{b}\|^2_{L^2(\mathbb{R}_-)}+\|\mathsf{b}\,\partial_{x_d}f\|^2_{L^2(\mathbb{R}_-)}-h\langle\mathsf{b}\,\partial^2_{x_d}f,\,\mathsf{b}\rangle_{L^2(\mathbb{R}_-)}.\tag{76}$$

For all $\mathsf{a}\,dx_d\in\Lambda^1H^1_{\mathbf{T}}(\mathbb{R}_-)$ where we recall that

$$\Lambda^1H^1_{\mathbf{T}}(\mathbb{R}_-)=\Lambda^1H^1(\mathbb{R}_-)=\big\{\mathsf{a}\,dx_d,\ \mathsf{a}\in\Lambda^0H^1(\mathbb{R}_-)\big\},\tag{77}$$

one has, since $\partial_{x_d}f(0)=0$ (the boundary term vanishes in Lemma 15):

$$Q^{\mathsf{Di},(1)}_{f,h}(\mathbb{R}_-,dx_d^2)(\mathsf{a}\,dx_d)=h^2\big\|\partial_{x_d}\mathsf{a}\big\|^2_{L^2(\mathbb{R}_-)}+\big\|\mathsf{a}\,\partial_{x_d}f\big\|^2_{L^2(\mathbb{R}_-)}+h\langle\mathsf{a}\,\partial^2_{x_d}f,\,\mathsf{a}\rangle_{L^2(\mathbb{R}_-)}.$$

Let us now consider the two possibilities: $\mu_d>0$ or $\mu_d<0$.

Step 1a: The case $d=1$ *and* $\mu_d>0$ *(i.e.,* $\partial^2_{x_d}f(0)>0$*).* — Then, there exists $C>0$ such that $\partial^2_{x_d}f\geqslant C$ in a neighborhood of 0 in $\mathbb{R}_-$. Thus, for all $\mathsf{a}\,dx_d\in\Lambda^1H^1_{\mathbf{T}}(\mathbb{R}_-)$ such that a is supported in $\mathsf{B}(0,h^{2/5})$, one has $Q^{\mathsf{Di},(1)}_{f,h}(\mathbb{R}_-,dx_d^2)(\mathsf{a}\,dx_d)\geqslant Ch\,\|\mathsf{a}\|^2_{L^2(\mathbb{R}_-)}$. Thanks to Lemma 17, this inequality extends for all $\mathsf{a}\,dx_d\in\Lambda^1H^1_{\mathbf{T}}(\mathbb{R}_-)$: there exists $C>0$ such that for h small enough,

$$\forall\mathsf{a}\,dx_d\in\Lambda^1H^1_{\mathbf{T}}(\mathbb{R}_-),\quad Q^{\mathsf{Di},(1)}_{f,h}(\mathbb{R}_-,dx_d^2)(\mathsf{a}\,dx_d)\geqslant Ch\,\|\mathsf{a}\|^2_{L^2(\mathbb{R}_-)}.\tag{78}$$

Let us now prove that there exists $c>0$ such that for h small enough:

$$\forall \mathsf{b}\in \Lambda^0 H^1_{\mathbf{T}}(\mathbb{R}_-),\quad Q^{\mathsf{Di},(0)}_{f,h}(\mathbb{R}_-,dx_d^2)(\mathsf{b})\geqslant c\,h\,\|\mathsf{b}\|^2_{L^2(\mathbb{R}_-)}. \tag{79}$$

It is clear that $\operatorname{Ker}\Delta^{\mathsf{Di},(0)}_{f,h}(\mathbb{R}_-,dx_d^2)=\{0\}$ since $e^{-(1/h)f}$ is not in the domain of $\Delta^{\mathsf{Di},(0)}_{f,h}(\mathbb{R}_-,dx_d^2)$. Let us now consider ψ_h in $\operatorname{Ran}\pi_{[0,Ch/2]}\big(\Delta^{\mathsf{Di},(0)}_{f,h}(\mathbb{R}_-,dx_d^2)\big)$ (where C is the constant appearing in (78)). Then, $\mathsf{d}_{f,h}\psi_h$ is in $\operatorname{Ran}\pi_{[0,Ch/2]}\big(\Delta^{\mathsf{Di},(1)}_{f,h}(\mathbb{R}_-,dx_d^2)\big)$ (thanks to (56)). From (78), this implies that $\mathsf{d}_{f,h}\psi_h=0$. Thus, $\Delta^{(0)}_{f,h}(\mathbb{R}_-,dx_d^2)\psi_h=0$ and hence, $\psi_h=0$. This proves (79).

Step 1b: The case $d=1$ *and* $\mu_d<0$ *(i.e.,* $\partial^2_{x_d}f(0)<0$*).* — Then, there exists $C>0$ such that $\partial^2_{x_d}f\leqslant -C$ in a neighborhood of 0 in $\overline{\mathbb{R}_-}$. Thus, from (76), for h small enough, one has for all $\mathsf{b}\in\Lambda^0H^1_{\mathbf{T}}(\mathbb{R}_-)$ such that b is supported in $\mathsf{B}(0,h^{2/5})$: $Q^{\mathsf{Di},(0)}_{f,h}(\mathbb{R}_-,dx_d^2)(\mathsf{b})\geqslant Ch\,\|\mathsf{b}\|^2_{L^2(\mathbb{R}_-)}$. Using Lemma 17, this inequality extends for all $\mathsf{b}\in\Lambda^0H^1_{\mathbf{T}}(\mathbb{R}_-)$, i.e., for h small enough:

$$\forall \mathsf{b}\in \Lambda^0 H^1_{\mathbf{T}}(\mathbb{R}_-,dx_d^2),\quad Q^{\mathsf{Di},(0)}_{f,h}(\mathbb{R}_-,dx_d^2)(\mathsf{b})\geqslant Ch\,\|\mathsf{b}\|^2_{L^2(\mathbb{R}_-)}. \tag{80}$$

Let us now prove that there exists $c>0$ such that for h small enough

$$\operatorname{Ran}\pi_{[0,ch]}\big(\Delta^{\mathsf{Di},(1)}_{f,h}(\mathbb{R}_-,dx_d^2)\big)=\operatorname{Ker}\Delta^{\mathsf{Di},(1)}_{f,h}(\mathbb{R}_-,dx_d^2)=\operatorname{Span}(e^{f/h}dx_d). \tag{81}$$

From item (ii) in (Potential-$\mathbb{R}^d_-$) and using the same arguments as those to check (68), one has $f'>c$ on $[-\infty,-\varepsilon]$ for some $\varepsilon>0$. Hence, for $h>0$, $e^{f/h}\in\Lambda^0L^2(\mathbb{R}_-)$ and from item (i) in (Potential-$\mathbb{R}^d_-$), $e^{f/h}\in\Lambda^0H^2(\mathbb{R}_-)$. Consequently (see Proposition 14), $e^{f/h}dx_d\in\mathcal{D}(\Delta^{\mathsf{Di},(1)}_{f,h}(\mathbb{R}_-,dx_d^2))$. Therefore, since for all $\mathsf{a}\,dx_d\in\Lambda^1H^1_{\mathbf{T}}(\mathbb{R}_-)$, $Q^{\mathsf{Di},(1)}_{f,h}(\mathbb{R}_-,dx_d^2)(\mathsf{a}\,dx_d)=\|\mathsf{d}^*_{f,h}\mathsf{a}\|^2_{L^2(\mathbb{R}_-)}$, it holds:

$$\operatorname{Ker}\Delta^{\mathsf{Di},(1)}_{f,h}(\mathbb{R}_-,dx_d^2)=\operatorname{Span}\big(e^{f/h}dx_d\big).$$

Let us now consider an eigenform $\psi_h\in\operatorname{Ran}\pi_{[0,Ch/2]}\Delta^{\mathsf{Di},(1)}_{f,h}(\mathbb{R}_-,dx_d^2)$ (where C is the constant appearing in (80)). Then, $\mathsf{d}^*_{f,h}\psi_h\in\operatorname{Ran}\pi_{[0,Ch/2]}\Delta^{\mathsf{Di},(0)}_{f,h}(\mathbb{R}_-,dx_d^2)$ (thanks to (57)). From (80), this implies that for h small enough, $\mathsf{d}^*_{f,h}\psi_h=0$. Thus $\psi_h\in\operatorname{Span}(e^{f/h}dx_d)$. This proves (81).

Step 2: The case $d>1$*, proofs of inequalities* (58) *and* (59). — Remember that $\mathbb{R}^d_-$ is endowed with a metric tensor $\mathbf{g}$ satisfying (66). Thanks to Lemma 17, it is enough to consider

$$w\in\mathcal{D}\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})\big)\text{ with supp }w\subset\mathsf{B}(0,h^{2/5}).$$

Following Lemma 21, $w=\mathsf{b}+\mathsf{a}\wedge dx_d$, where:

$$\mathsf{b}=\sum_{\substack{\mathsf{J}=\{j_1,\dots,j_q\},\\ j_1<\dots<j_q,\,d\notin\mathsf{J}}}\mathsf{b}_{\mathsf{J}}\,dx_{\mathsf{J}}\quad\text{and}\quad \mathsf{a}=\sum_{\substack{\mathsf{I}=\{i_1,\dots,i_{q-1}\},\\ i_1<\dots<i_{q-1},\,d\notin\mathsf{I}}}\mathsf{a}_{\mathsf{I}}\,dx_{\mathsf{I}}.$$

We will use many times that, from (Metric-$\mathbb{R}^d_-$) and (66),

$$\|w\|^2_{L^2(\mathbb{R}^d_-)}=\|\mathsf{b}\|^2_{L^2(\mathbb{R}^d_-)}+\|\mathsf{a}\wedge dx_d\|^2_{L^2(\mathbb{R}^d_-)}$$

(because b is orthogonal to $\mathsf{a}\wedge dx_d$) with

$$\|\mathsf{b}\|^2_{L^2(\mathbb{R}^d_-)} \geqslant \mathsf{c}_1 \sum_{\mathsf{I}} \|\mathsf{b}_{\mathsf{J}}\|^2_{L^2(\mathbb{R}^d_-)} \quad \text{and} \quad \|\mathsf{a}\wedge dx_d\|^2_{L^2(\mathbb{R}^d_-)} = \|\mathsf{a}\|^2_{L^2(\mathbb{R}^d_-)} \geqslant \mathsf{c}_1 \sum_{\mathsf{J}} \|\mathsf{a}_{\mathsf{I}}\|^2_{L^2(\mathbb{R}^d_-)}$$

(where $\mathsf{c}_1>0$ is as in Lemma 21).

Step 2a: The case $d>1$ *and* $q=0$*, proof of* (58). — Assume that $q=0$ (i.e., $w=\mathsf{b}$ is a function). Then, using Lemma 21, one has:

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(w) \geqslant \mathsf{c}_1 \int_{x'\in\mathbb{R}^{d-1}} Q^{\mathsf{Di},(0)}_{-f_-,h}(\mathbb{R}_-,dx_d^2)\big(\mathsf{b}(x',.)\big)\mu(dx') - \mathsf{c}_2 h^{6/5}\|w\|^2_{L^2(\mathbb{R}^d_-)}. \tag{82}$$

Equations (79) and (80) imply that that there exists $C>0$ (independent of x') such that for all h small enough and a.e. $x'\in\mathbb{R}^{d-1}$:

$$Q^{\mathsf{Di},(0)}_{-f_-,h}(\mathbb{R}_-,dx_d^2)\big(\mathsf{b}(x',.)\big) \geqslant Ch\|\mathsf{b}(x',.)\|^2_{L^2(\mathbb{R}_-)}.$$

Thus, using (82), one obtains for all $w\in D\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-)\big)$ supported in $\mathsf{B}(0,h^{2/5})$:

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(w) \geqslant Ch\|w\|^2_{L^2(\mathbb{R}^d_-)} - \mathsf{c}_2 h^{6/5}\,\|w\|^2_{L^2(\mathbb{R}^d_-)} \geqslant ch\|w\|^2_{L^2(\mathbb{R}^d_-)}.$$

Together with Lemma 17, this proves (58).

Step 2b: The case $d>1$, $q\geqslant 1$ *and* $\mu_d>0$*, proof of* (59). — The analysis above in dimension 1 (see (78) and (79)) implies that there exists $C>0$ (again, independent of x') such that for h small enough, for all I and a.e. $x'\in\mathbb{R}^{d-1}$,

$$Q^{\mathsf{Di},(1)}_{-f_-,h}(\mathbb{R}_-,dx_d^2)(\mathsf{a}_{\mathsf{I}}(x',.)dx_d) \geqslant Ch\|\mathsf{a}_{\mathsf{I}}(x',.)\|^2_{L^2(\mathbb{R}_-)},$$

and for h small enough, for all J and a.e. $x'\in\mathbb{R}^{d-1}$,

$$Q^{\mathsf{Di},(0)}_{-f_-,h}(\mathbb{R}_-,dx_d^2)(\mathsf{b}_{\mathsf{J}}(x',.)) \geqslant Ch\|\mathsf{b}_{\mathsf{J}}(x',.)\|^2_{L^2(\mathbb{R}_-)}.$$

Thus, using Lemma 21, for all $w\in D\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})\big)$ supported in $\mathsf{B}(0,h^{2/5})$, one has:

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(w) \geqslant Ch\|w\|^2_{L^2(\mathbb{R}^d_-)} - \mathsf{c}_2 h^{6/5}\,\|w\|^2_{L^2(\mathbb{R}^d_-)} \geqslant ch\|w\|^2_{L^2(\mathbb{R}^d_-)}.$$

Using Lemma 17, this proves (59) when $q\geqslant 1$ and $\mu_d>0$.

Step 2c: The case $d>1$, $q\geqslant 1$, $\mu_d<0$ *and the index of* 0 *as a critical point of* $f|_{\partial\mathbb{R}^d_-}$ *is not* $q-1$*, proof of* (59). — Using (80), there exists C (again, independent of x') such that for h small enough, for all J and a.e. $x'\in\mathbb{R}^{d-1}$,

$$Q^{\mathsf{Di},(0)}_{-f_-,h}(\mathbb{R}_-,dx_d^2)\big(\mathsf{b}_{\mathsf{J}}(x',.)\big) \geqslant Ch\|\mathsf{b}_{\mathsf{J}}(x',.)\|^2_{L^2(\mathbb{R}_-)}. \tag{83}$$

Thus, using Lemma 21, one has:

$$\begin{aligned} Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(w) &\geqslant Ch\|\mathsf{b}\|^2_{L^2(\mathbb{R}^d_-)} \\ &\quad + \mathsf{c}_1 \int_{x_d\in\mathbb{R}_-} Q^{(q-1)}_{f_+,h}(\mathbb{R}^{d-1},\mathbf{g}dx'^2)\big(\mathsf{a}(.,x_d)\big)dx_d - \mathsf{c}_2 h^{6/5}\,\|w\|^2_{L^2(\mathbb{R}^d_-)}. \end{aligned} \tag{84}$$

Recall that 0 is not a critical point of index $q-1$ of $f|_{\partial\mathbb{R}^d_-}$. Then, 0 is not a critical point of index $q-1$ for f_+ (see (54) and Definition 20). Since a is a $q-1$ form, this implies from Proposition 18 (applied with the metric tensor $\widetilde{\mathbf{G}}dx'^{\,2}$), that there exists C (independent of x_d) such that for h small enough,

$$Q^{(q-1)}_{f_+,h}(\mathbb{R}^{d-1},\widetilde{\mathbf{G}}dx'^2)\big(\mathsf{a}(.,x_d)\big)\geqslant Ch\|\mathsf{a}(.,x_d)\|^2_{L^2(\mathbb{R}^{d-1})}.$$

Therefore, using (84), for h small enough, one has:

$$\begin{aligned}Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(w)&\geqslant Ch(\|\mathsf{b}\|^2_{L^2(\mathbb{R}^d_-)}+\|\mathsf{a}\|^2_{L^2(\mathbb{R}^d_-)})-\mathsf{c}_2h^{6/5}\,\|w\|^2_{L^2(\mathbb{R}^d_-)}\\&\geqslant ch\|w\|^2_{L^2(\mathbb{R}^d_-)}.\end{aligned}$$

Using Lemma 17, this proves (59) when $q\geqslant 1$, $\mu_d<0$ and the index of 0 as a critical point of $f|_{\partial\mathbb{R}^d_-}$ is not $q-1$.

Step 3: The case $d>1$, $q\geqslant 1$, $\mu_d<0$ *and the index of* 0 *as a critical point of* $f|_{\partial\mathbb{R}^d_-}$ *is* $q-1$, *proof of* (60). — Notice that in this case, the point 0 is a critical point of f_+ of index $q-1$ (see Definition 20).

Step 3a: Proof of (60) *when* $f=f_+-f_-$. — Let us first prove (60) for the potential (see Definition 20):

$$x=(x',x_d)\in\overline{\mathbb{R}^d_-}\longmapsto f_+(x')-f_-(x_d).$$

In view of Definition 20 and (53), f_+-f_- satisfies (Potential-$\mathbb{R}^d_-$). Thus, Proposition 14, (58), and (59) are valid for f_+-f_- and $\mathbf{g}$. Let us consider

$$\Psi_h\in\operatorname{Ker}\Delta^{(q-1)}_{f_+,h}(\mathbb{R}^{d-1},\widetilde{\mathbf{G}}dx'^2)$$

with $\Psi_h\neq 0$ (which exists thanks to item (ii) in Proposition 18). Let us prove that there exist $c>0$ and $h_0>0$ such that for all $h\in(0,h_0)$,

$$\begin{aligned}\operatorname{Ran}\pi_{[0,ch]}\big(\Delta^{\mathsf{Di},(q)}_{f_+-f_-,h}(\mathbb{R}^d_-,\mathbf{g})\big)&=\operatorname{Ker}\Delta^{\mathsf{Di},(q)}_{f_+-f_-,h}(\mathbb{R}^d_-,\mathbf{g})\\&=\operatorname{Span}\big(\Psi_h\wedge e^{-(1/h)f_-}dx_d\big).\end{aligned}\tag{85}$$

Let $c_0>0$ and $\phi_h\in\operatorname{Ran}\pi_{[0,c_0h]}\big(\Delta^{\mathsf{Di},(q)}_{f_+-f_-,h}(\mathbb{R}^d_-,\mathbf{g})\big)$ where the constant c_0 is strictly smaller than the constants $C>0$ in (58) and (59) applied to $f=f_+-f_-$. Hence, using (56) and (57), one has for h small enough

$$\mathsf{d}_{f,h}\phi_h=0\quad\text{and}\quad\mathsf{d}^*_{f,h}\phi_h=0.$$

Thus, $Q^{\mathsf{Di},(q)}_{f_+-f_-,h}(\mathbb{R}^d_-,\mathbf{g})(\phi_h)=0$. Using Lemma 21 with $f=f_+-f_-$ (in which case $\mathsf{e}(h,\phi_h)=0$) together with item (ii) in Proposition 18 and (81) with $f=-f_-$?, one obtains

$$\phi_h\in\operatorname{Span}\big(\Psi_h\wedge e^{-(1/h)f_-}dx_d\big).\tag{86}$$

To prove (85), it thus remains to show that:

$$\Psi_h\wedge e^{-(1/h)f_-}dx_d\in\operatorname{Ker}\Delta^{\mathsf{Di},(q)}_{f_+-f_-,h}(\mathbb{R}^d_-,\mathbf{g}).\tag{87}$$

It first holds, from Propositions 18 and 14, and (68), $\Psi_h \wedge e^{-(1/h)f_-} dx_d$ is in $\mathcal{D}(\Delta^{\mathsf{Di},(q)}_{f_+-f_-,h}(\mathbb{R}^d_-,\mathbf{g}))$ (recall that the boundary condition $\mathbf{t}\mathsf{d}^*_{f_+-f_-,h} w = 0$ is equivalent to $\partial_{x_d}(e^{-(1/h)(f_+-f_-)}\mathsf{a}_{\mathsf{I}})(x',0)=0$, see indeed (75)). Besides, one has:

$$\mathsf{d}_{f_+-f_-,h}\big(\Psi_h \wedge e^{-(1/h)f_-} dx_d\big) = \mathsf{d}_{f_+,h}(\Psi_h) \wedge e^{-(1/h)f_-} dx_d = 0.$$

Moreover, from (66) (see also item (i) in (Metric-$\mathbb{R}^d_-$)), it holds

$$\mathsf{d}^{*,\mathbf{g}}\big(\Psi_h \wedge e^{-(1/h)f_-} dx_d\big) = \mathsf{d}^{*,\widetilde{\mathbf{G}}dx'^2}\big(\Psi_h\big) \wedge e^{-(1/h)f_-(x_d)} dx_d + \Psi_h \mathsf{d}^{*,dx_d^2}\big(e^{-(1/h)f_-} dx_d\big),$$

where the superscript indicates in which metric the operator d^* is built. And one can check that

$$\begin{aligned}\mathbf{i}_{\nabla(f_+-f_-)}&\big(\Psi_h \wedge e^{-(1/h)f_-} dx_d\big)\\ &= \mathbf{i}_{\nabla_{x'} f_+}\big(\Psi_h\big) \wedge e^{-(1/h)f_-(x_d)} dx_d - \Psi_h \wedge \mathbf{i}_{\nabla_{x_d} f_-}\big(e^{-(1/h)f_-} dx_d\big)\\ &= \mathbf{i}_{\nabla_{x'} f_+}\big(\Psi_h\big) \wedge e^{-(1/h)f_-(x_d)} dx_d + h\, \Psi_h\, \partial_{x_d}\big(e^{-(1/h)f_-(x_d)}\big).\end{aligned}$$

Therefore, $\mathsf{d}^*_{f_+-f_-,h}\big(\Psi_h \wedge e^{-(1/h)f_-} dx_d\big) = 0$. This proves (87) and then (85). This concludes the proof of (60) when $f = f_+ - f_-$.

Step 3b: Proof of (60) *for a general function* f. — Let $c_0 > 0$ be strictly smaller than the constants $C > 0$ in (58) and (59). Assume that $\operatorname{Ran} \pi_{[0,c_0 h]}\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})\big) \neq \{0\}$ and let us consider a $L^2(\mathbb{R}^d_-)$-normalized form

$$\psi_h \in \operatorname{Ran} \pi_{[0,c_0 h]}\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})\big).$$

Then, using (56) and (57), one has for h small enough, $\mathsf{d}_{f,h}\psi_h = 0$, $\mathsf{d}^*_{f,h}\psi_h = 0$, and thus $Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})\psi_h = 0$. This proves that for h small enough:

$$\operatorname{Ran} \pi_{[0,c_0 h]}\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})\big) = \operatorname{Ker} \Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g}).$$

Let us now consider a quadratic partition of unity (χ_1,χ_2) such that $\chi_1 \in \mathcal{C}^\infty_c(\overline{\mathbb{R}^d_-})$, $\chi_1 = 1$ on $\mathsf{B}(0,1/2)$, $\operatorname{supp}\chi_1 \subset \mathsf{B}(0,1)$, and $\chi_1^2 + \chi_2^2 = 1$. The IMS formula (63) implies that there exists $C > 0$ such that:

$$\begin{aligned}(88)\quad 0 \geqslant Q^{\mathsf{Di},(q)}_{f,h}&(\mathbb{R}^d_-,\mathbf{g})(\chi_1(h^{-2/5}.)\psi_h)\\ &+ Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(\chi_2(h^{-2/5}.)\psi_h) - Ch^{6/5}\,\|\psi_h\|^2_{L^2(\mathbb{R}^d_-)}.\end{aligned}$$

From (65), one has:

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(\chi_2(h^{-2/5}.)\psi_h) \geqslant Ch^{4/5}\|\chi_2(h^{-2/5}.)\psi_h\|^2_{L^2(\mathbb{R}^d_-)}.$$

Thus, it holds for $h > 0$ small enough:

$$(89)\quad \|\chi_2(h^{-2/5}.)\psi_h\|^2_{L^2(\mathbb{R}^d_-)} = O(h^{2/5}) \quad\text{and}\quad \|\chi_1(h^{-2/5}.)\psi_h\|^2_{L^2(\mathbb{R}^d_-)} = 1 + O(h^{2/5}),$$

and then:

$$(90)\qquad Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(\chi_1(h^{-2/5}.)\psi_h) \leqslant Ch^{6/5}\|\chi_1(h^{-1/5}.)\psi_h\|^2_{L^2(\mathbb{R}^d_-)}.$$

Using (55), (70) and (71), and using twice Lemma 15 (once for f and once for $f_+ - f_-$) together with the fact that $\partial_{\mathsf{n}_{\mathbb{R}^d_-}} f = \partial_{\mathsf{n}_{\mathbb{R}^d_-}}(f_+ - f_-) = 0$ on $\partial\mathbb{R}^d_-$, one has for h small enough and for all $v \in \Lambda^q H^1_{\mathbf{T}}(\mathbb{R}^d_-, \mathbf{g})$ supported in $\mathsf{B}(0, h^{2/5})$:

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-, \mathbf{g})(v) = Q^{\mathsf{Di},(q)}_{f_+-f_-,h}(\mathbb{R}^d_-, \mathbf{g})(v) + O(h^{6/5})\|v\|^2_{L^2(\mathbb{R}^d_-)}. \tag{91}$$

Thus, one gets for h small enough:

$$\begin{aligned} Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-, \mathbf{g})(\chi_1(h^{-1/5}.)\psi_h) = Q^{\mathsf{Di},(q)}_{f_+-f_-,h}&(\mathbb{R}^d_-, \mathbf{g})(\chi_1(h^{-1/5}.)\psi_h) \\ &+ O(h^{6/5})\big\|\chi_1(h^{-1/5}.)\psi_h\big\|^2_{L^2(\mathbb{R}^d_-)}. \end{aligned}$$

Then, using (90), it holds for h small enough:

$$Q^{\mathsf{Di},(q)}_{f_+-f_-,h}(\mathbb{R}^d_-, \mathbf{g})(\chi_1(h^{-2/5}.)\psi_h) = O(h^{6/5})\,\big\|\chi_1(h^{-1/5}.)\psi_h\big\|^2_{L^2(\mathbb{R}^d_-)}.$$

For all $(x', x_d) \in \mathbb{R}^d_-$, let us define (see (85)),

$$\Theta_h(x', x_d) = \kappa_h\, \Psi_h(x') \wedge e^{-(1/h)f_-(x_d)} dx_d, \quad \text{where } \kappa_h = \|\Psi_h \wedge e^{-(1/h)f_-} dx_d\|^{-1}_{L^2(\mathbb{R}^d_-)}.$$

Using Lemma 11 and (85) (choosing c_0 smaller than $c > 0$ appearing in (85)), one has for h small enough,

$$\begin{aligned} \operatorname{dist}_{L^2(\mathbb{R}^d_-)}&\big(\chi_1(h^{-2/5}.)\psi_h, \operatorname{Span}\Theta_h\big) \\ &= \big\|\pi_{[0,ch]}\big(\Delta^{\mathsf{Di},(q)}_{f_+-f_-,h}(\mathbb{R}^d_-, \mathbf{g})\big)\big(\chi_1(h^{-2/5}.)\phi_h\big)\big\|_{L^2(\mathbb{R}^d_-)} \\ &\leqslant \frac{Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-, \mathbf{g})(\chi_1(h^{-1/5}.)\psi_h)^{1/2}}{\sqrt{ch}} \leqslant Ch^{1/10}. \end{aligned}$$

Using in addition (89), one obtains for h small enough:

$$\operatorname{dist}_{L^2(\mathbb{R}^d_-)}\big(\psi_h, \operatorname{Span}\Theta_h\big) \leqslant Ch^{1/10} + C\|\chi_2(h^{-2/5}.)\psi_h\|^2_{L^2(\mathbb{R}^d_-)} \leqslant 2Ch^{1/10}.$$

Therefore, since we assumed that $\operatorname{Ran}\pi_{[0,c_0h]}\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-, \mathbf{g})\big) \neq \{0\}$, it holds for h small enough:

$$\dim \operatorname{Ran}\pi_{[0,c_0h]}\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-, \mathbf{g})\big) = 1.$$

It thus remains to prove that $\operatorname{Ran}\pi_{[0,c_0h]}\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-, \mathbf{g})\big) \neq \{0\}$. To this end, let us show that $\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-, \mathbf{g})$ admits an eigenvalue which is $o(h)$ when $h \to 0$. Using the IMS formula (63) together with the fact that

$$Q^{\mathsf{Di},(q)}_{f_+-f_-,h}(\mathbb{R}^d_-, \mathbf{g})(\Theta_h) = 0,$$

and
$$Q^{\mathsf{Di},(q)}_{f_+-f_-,h}(\mathbb{R}^d_-, \mathbf{g})(\chi_2(h^{-2/5}.)\Theta_h) \geqslant ch^{4/5}\,\big\|\chi_2(h^{-2/5}.)\Theta_h\big\|^2_{L^2(\mathbb{R}^d_-)},$$

one obtains, when $h \to 0$,

$$Q^{\mathsf{Di},(q)}_{f_+-f_-,h}(\mathbb{R}^d_-, \mathbf{g})(\chi_1(h^{-2/5}.)\Theta_h) = O(h^{6/5})$$

and
$$\big\|\chi_1(h^{-2/5}.)\Theta_h\big\|^2_{L^2(\mathbb{R}^d_-)} = 1 + O(h^{2/5}).$$

Using (91) and the Min-Max principle, $\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})$ admits an eigenvalue of order $O(h^{6/5})$ when $h\to 0$. Therefore, $\operatorname{Ran}\pi_{[0,c_0h]}(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g}))$ is of dimension 1 for h small enough. This proves (60) and concludes the proof of Proposition 19.

2.3.5. *Proof of Proposition* 16. — We are now in position to prove Proposition 16. Let us first state a preliminary result.

Lemma 22. — *Let us assume that the space* $\overline{\mathbb{R}^d_-}$ *is endowed with a metric tensor* $\mathbf{g}$ *satisfying* (Metric-$\mathbb{R}^d_-$). *Assume that* f *satisfies item* (i) *in* (Potential-$\mathbb{R}^d_-$). *Define for all* $x'\in\mathbb{R}^{d-1}$, $\widetilde{\mathbf{G}}(x')=\mathbf{G}(x',0)$ *and let us introduce the metric on* $\mathbb{R}^d_-$*:*

$$\forall x=(x',x_d)\in\overline{\mathbb{R}^d_-},\quad \widetilde{\mathbf{g}}(x)=\widetilde{\mathbf{G}}(x')dx'^{\,2}+dx_d^2. \tag{92}$$

Let $(\mathbf{g}_1,\mathbf{g}_2)=(\mathbf{g},\widetilde{\mathbf{g}})$ *or* $(\mathbf{g}_1,\mathbf{g}_2)=(\widetilde{\mathbf{g}},\mathbf{g})$. *Then, there exist* $C>0$, $c>0$, $h_0>0$, $\eta:[0,h_0]\to\mathbb{R}_+$, *such that for* $h\in(0,h_0)$, $\eta(h)=O(h^{2/5})$ *and for all* $w\in\Lambda^qH^1_{\mathbf{T}}(\mathbb{R}^d_-)$ *such that* $\operatorname{supp} w\subset\mathsf{B}(0,h^{2/5})$, *it holds,*

$$\|w\|_{L^2(\mathbb{R}^d_-,\mathbf{g}_2)}=\|w\|_{L^2(\mathbb{R}^d_-,\mathbf{g}_1)}\big(1+\eta(h)\big), \tag{93}$$

and for all $q\in\{0,\dots,d\}$,

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g}_1)(w)\geqslant C\,Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g}_2)(w)-Ch^{7/5}\,\|w\|^2_{L^2(\mathbb{R}^d_-,\mathbf{g}_2)}. \tag{94}$$

Equation (93) is a simple consequence of the two metric tensors are smooth and coincide at $x_d=0$. Equation (94) is easily obtained following the proof of [42, Lem. 3.3.7].

Let us now prove Proposition 16.

Proof. — Let us assume that (Metric-$\mathbb{R}^d_-$) and (Potential-$\mathbb{R}^d_-$) are satisfied. The proof is divided into three steps.

Step 1: Proofs of (58) *and* (59). — Let us recall that according to Lemma 17, it is sufficient to prove (58) and (59) for forms $w\in\Lambda^qH^1_{\mathbf{T}}(\mathbb{R}^d_-,\mathbf{g})$ supported in $\mathsf{B}(0,h^{2/5})$. Because the metric tensor $\widetilde{\mathbf{g}}$ defined in (92) satisfies (Metric-$\mathbb{R}^d_-$) Proposition 19 implies that (58) and (59) hold for $\widetilde{\mathbf{g}}$ and f. From those estimates and (93) and (94), one gets (58) and (59) for $\mathbf{g}$ and f.

Step 2: Proof of (60). — Let us assume that 0 is a critical point of index $q-1$ of $f|_{\partial\mathsf{M}}$ and $\mu_d<0$. Let $c>0$ be strictly smaller than the constants $C>0$ in (58) and (59). Assume that $\operatorname{Ran}\pi_{[0,ch]}\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})\big)\neq\{0\}$ and let us consider a $L^2(\mathbb{R}^d_-,\mathbf{g})$-normalized form $\phi_h\in\operatorname{Ran}\pi_{[0,ch]}\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})\big)$. This implies, using (56), (57), and the results of Step 1, that $\mathsf{d}_{f,h}\phi_h=0$ and $\mathsf{d}^*_{f,h}\phi_h=0$. Thus, it holds $Q^{\mathsf{Di},(0)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(\phi_h)=0$. Consequently, for $h>0$ small enough,

$$\operatorname{Ran}\pi_{[0,ch]}\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})\big)=\operatorname{Ker}\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g}).$$

Now, let (χ_1,χ_2) be a quadratic partition of unity such that $\chi_1\in\mathcal{C}^\infty_c(\overline{\mathbb{R}^d_-})$, $\chi_1=1$ on $\mathsf{B}(0,1/2)$, $\operatorname{supp}\chi_1\subset\mathsf{B}(0,1)$, and $\chi_1^2+\chi_2^2=1$. Using the IMS formula (63), there exists $C>0$ such that:

$$0\geqslant Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(\chi_1(h^{-2/5}.)\phi_h)+Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(\chi_2(h^{-2/5}.)\phi_h)-Ch^{6/5}\left\|\phi_h\right\|^2_{L^2(\mathbb{R}^d_-,\mathbf{g})}.$$

Therefore, one has $Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(\chi_2(h^{-2/5}.)\phi_h)=O(h^{6/5})$ and

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(\chi_1(h^{-2/5}.)\phi_h)=O(h^{6/5}). \tag{95}$$

In addition, let us recall that (see indeed (65)),

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})(\chi_2(h^{-2/5}.)\phi_h)\geqslant Ch^{4/5}\big\|\chi_2(h^{-2/5}.)\phi_h\big\|^2_{L^2(\mathbb{R}^d_-,\mathbf{g})}.$$

Therefore, one obtains in the limit $h\to 0$:

$$\begin{aligned}\big\|\chi_2(h^{-2/5}.)\phi_h\big\|^2_{L^2(\mathbb{R}^d_-,\mathbf{g})}&=O(h^{2/5}),\\ \big\|\chi_1(h^{-2/5}.)\phi_h\big\|^2_{L^2(\mathbb{R}^d_-,\mathbf{g})}&=1+O(h^{2/5}).\end{aligned} \tag{96}$$

Then, using (94) with $\mathbf{g}_1=\mathbf{g}$ and $\mathbf{g}_2=\widetilde{\mathbf{g}}$, one gets for all h small enough:

$$h^{6/5}\geqslant C\,Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\widetilde{\mathbf{g}})(\chi_1(h^{-2/5}.)\phi_h)-Ch^{7/5}\left\|\chi_1(h^{-2/5}.)\phi_h\right\|^2_{L^2(\mathbb{R}^d_-,\widetilde{\mathbf{g}})}.$$

Notice that from (93) and (96), one has for h small enough $\|\chi_1(h^{-2/5}.)\phi_h\|^2_{L^2(\mathbb{R}^d_-,\widetilde{\mathbf{g}})}=1+O(h^{2/5})$. Therefore, one obtains:

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\widetilde{\mathbf{g}})(\chi_1(h^{-2/5}.)\phi_h)\leqslant C\,h^{6/5}\left\|\chi_1(h^{-2/5}.)\phi_h\right\|^2_{L^2(\mathbb{R}^d_-,\widetilde{\mathbf{g}})}. \tag{97}$$

Recall (since f and $\widetilde{\mathbf{g}}$ satisfy (Potential-$\mathbb{R}^d_-$) and (Metric-$\mathbb{R}^d_-$)) that according to Proposition 19, there exist $c_0>0$ and $h_0>0$ such that for all $h\in(0,h_0)$, there exists a $L^2(\mathbb{R}^d_-,\widetilde{\mathbf{g}})$-normalized q-form Φ_h such that

$$\operatorname{Ran}\pi_{[0,c_0h]}\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\widetilde{\mathbf{g}})\big)=\operatorname{Span}(\Phi_h)=\operatorname{Ker}\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\widetilde{\mathbf{g}}). \tag{98}$$

Using Lemma 11 and (97), one obtains that for h small enough:

$$\operatorname{dist}_{L^2(\mathbb{R}^d_-,\widetilde{\mathbf{g}})}\big(\chi_1(h^{-2/5}.)\phi_h,\,\operatorname{Span}\Phi_h\big)=O(h^{1/10}).$$

This implies together with (96) and (93), and since we assume that

$$\operatorname{Ran}\pi_{[0,ch]}\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})\big)\neq\{0\},$$

that for h small enough:

$$\dim\operatorname{Ran}\pi_{[0,ch]}\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})\big)=1.$$

It remains to prove that $\operatorname{Ran}\pi_{[0,ch]}\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})\big)\neq\{0\}$. To this end, let us prove that $\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\mathbf{g})$ admits an eigenvalue of order $o(h)$ when $h\to 0$. Let us consider a $L^2(\mathbb{R}^d_-,\widetilde{\mathbf{g}})$-normalized q-form Φ_h which satisfies (98). Recall that from (89) and (90), one has when $h\to 0$:

$$\big\|\chi_2(h^{-2/5}.)\Phi_h\big\|^2_{L^2(\mathbb{R}^d_-,\widetilde{\mathbf{g}})}=O(h^{2/5})\quad\text{and}\quad\big\|\chi_1(h^{-2/5}.)\Phi_h\big\|^2_{L^2(\mathbb{R}^d_-,\widetilde{\mathbf{g}})}=1+O\big(h^{2/5}\big)$$

$$\text{and}\qquad Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-,\widetilde{\mathbf{g}})(\chi_1(h^{-2/5}.)\Phi_h)\leqslant Ch^{6/5}\left\|\chi_1(h^{-2/5}.)\Phi_h\right\|^2_{L^2(\mathbb{R}^d_-,\widetilde{\mathbf{g}})}.$$

From (93) and (94) (applied with $\mathbf{g}_1 = \widetilde{\mathbf{g}}$ and $\mathbf{g}_2 = \mathbf{g}$), one deduces that:

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-, \mathbf{g})(\chi_1(h^{-2/5}.)\Phi_h) \leqslant C\, h^{6/5}\, \big\|\chi_1(h^{-2/5}.)\Phi_h\big\|^2_{L^2(\mathbb{R}^d_-,\mathbf{g})}. \tag{99}$$

Then, using the Min-Max principle, for h small enough, $\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-, \mathbf{g})$ admits an eigenvalue of order $h^{6/5}$ when $h \to 0$. Thus, $\operatorname{Ran} \pi_{[0,ch]}\big(\Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-, \mathbf{g})\big) \neq \{0\}$. This ends the proof of (60).

Step 3: Proof of (61). — Let $\Psi_h \in \operatorname{Ker} \Delta^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-, \mathbf{g})$ such that $\|\Psi_h\|_{L^2(\mathbb{R}^d_-,\mathbf{g})} = 1$. Let $\chi : \overline{\mathbb{R}^d_-} \to [0,1]$ be a $\mathcal{C}^\infty$ function supported in a neighborhood of 0 which equals 1 in a neighborhood of 0 in $\overline{\mathbb{R}^d_-}$. Let us define $\widetilde{\chi} = \sqrt{1-\chi^2}$. Then, using Lemma 15 (and the fact that $\partial_{\mathsf{n}_{\mathbb{R}^d_-}} f(x',0) = 0$ for all $x' \in \mathbb{R}^{d-1}$), since there exists $c_1 > 0$ such that $\inf_{\operatorname{supp}\widetilde{\chi}} |\nabla f| \geqslant c_1$, it holds

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-, \mathbf{g})(\widetilde{\chi}\Psi_h) \geqslant C \big\|\widetilde{\chi}\Psi_h\big\|^2_{L^2(\mathbb{R}^d_-,\mathbf{g})}.$$

Using in addition the fact that $Q^{\mathsf{Di},(q)}_{f,h}(\mathbb{R}^d_-, \mathbf{g})(\Psi_h) = 0$ together with the IMS formula (63), one obtains (61) using a similar reasoning as in (96) and (95). This ends the proof of Proposition 16. □

2.4. Proof of Theorem 4. — Let us assume that (M-f) holds. For a fixed $q \in \{0, \ldots, d\}$, let us consider the operator $\Delta^{\mathsf{Di},(q)}_{f,h}(\mathsf{M}, \mathbf{g}_{\mathsf{M}})$. We will identify the number of eigenvalues smaller than $\mathsf{c}h$ for this operator, for some $\mathsf{c} > 0$ and for all sufficiently small h.

According to the analysis made in [42, Chap. 3] and [44], it is already known that one can build linearly independent quasi-modes associated with the (generalized) critical points in $\mathsf{U}^{\mathsf{M}}_q \cup \mathsf{U}^{\partial\mathsf{M},1}_q$ which thus yield at least $\mathsf{m}^{\mathsf{M}}_q + \mathsf{m}^{\partial\mathsf{M},1}_q$ small eigenvalues. The main novelty compared to [42, Chap. 3] is that we also have to consider critical points of f located on $\partial\mathsf{M}$:

$$\mathsf{B}^{\partial\mathsf{M},2} := \big\{z \in \partial\mathsf{M},\ |\nabla f(z)| = 0\big\}. \tag{100}$$

In the proof, we will thus consider all the critical points in

$$\mathsf{P}_q = \mathsf{U}^{\mathsf{M}}_q \cup \mathsf{U}^{\partial\mathsf{M},1}_q \cup \mathsf{B}^{\partial\mathsf{M},2}$$

as potential candidates to generate small eigenvalues, and we will prove that only those critical points in $\mathsf{Q}_q \subset \mathsf{P}_q$ where

$$\mathsf{Q}_q = \mathsf{U}^{\mathsf{M}}_q \cup \mathsf{U}^{\partial\mathsf{M},1}_q \cup \mathsf{U}^{\partial\mathsf{M},2}_q$$

will actually contribute to the spectrum of $\Delta^{\mathsf{Di},(q)}_{f,h}(\mathsf{M}, \mathbf{g}_{\mathsf{M}})$ in $[0, \mathsf{c}h]$.

By assumption (M-f), for all $z \in \mathsf{B}^{\partial\mathsf{M},2}$, $\partial_{\mathsf{n}_{\mathsf{M}}} f = 0$ in a neighborhood of z in $\partial\mathsf{M}$. Let us thus introduce a family $(\mathsf{V}_y)_{y\in\mathsf{P}_q}$ of neighborhoods in $\overline{\mathsf{M}}$ of $y \in \mathsf{P}_q$ such that:

– For all $y \in \mathsf{U}^{\mathsf{M}}_q$, $\overline{\mathsf{V}_y} \subset \mathsf{M}$ and y is the only critical point of f in $\overline{\mathsf{V}_y}$.

– For all $y \in \mathsf{U}^{\partial\mathsf{M},1}_q$, $\partial_{\mathsf{n}_{\mathsf{M}}} f > 0$ on $\partial\mathsf{M} \cap \overline{\mathsf{V}_y}$ and y is the only critical point of $f|_{\partial\mathsf{M}}$ in $\partial\mathsf{M} \cap \overline{\mathsf{V}_y}$.

– For all $y \in \mathsf{B}^{\partial\mathsf{M},2}$, $\partial_{\mathsf{n}_\mathsf{M}} f = 0$ on $\partial\mathsf{M} \cap \overline{\mathsf{V}_y}$ and y is the only critical point of f in $\overline{\mathsf{V}_y}$.

– The sets $(\overline{\mathsf{V}_y})_{y\in\mathsf{P}_q}$ are pairwise disjoint.

The neighborhoods $(\mathsf{V}_y)_{y\in\mathsf{P}_q}$ may be shrunk in the following in order to introduce local coordinates on V_y, this will be made precise below. In order to use an IMS localization formula, let us now introduce a quadratic partition of unity $(\chi_y)_{y\in\mathsf{P}_q} \cup \widetilde{\chi}$ such that $\widetilde{\chi}^2 + \sum_{y\in\mathsf{P}_q} \chi_y^2 = 1$ on $\overline{\mathsf{M}}$, and for all $y \in \mathsf{P}_q$, $\chi_y : \overline{\mathsf{M}} \to [0,1]$ is $\mathcal{C}^\infty$, supported in V_y, and $\chi_y = 1$ in a neighborhood of y in $\overline{\mathsf{M}}$. Let $w \in \Lambda^q H^1_{\mathbf{T}}(\mathsf{M}, \mathbf{g}_\mathsf{M})$. The IMS formula [19, 42] reads:

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathsf{M}, \mathbf{g}_\mathsf{M})(w) = \sum_{y\in\mathsf{P}_q} Q^{\mathsf{Di},(q)}_{f,h}(\mathsf{M}, \mathbf{g}_\mathsf{M})(\chi_y w) - \sum_{y\in\mathsf{P}_q} h^2 \left\| w\,\nabla\chi_y \right\|^2_{L^2(\mathbb{R}^d_-, \mathbf{g}_\mathsf{M})} + Q^{\mathsf{Di},(q)}_{f,h}(\mathsf{M}, \mathbf{g}_\mathsf{M})(\widetilde{\chi} w) - h^2 \left\| w\,\nabla\widetilde{\chi} \right\|^2_{L^2(\mathbb{R}^d_-, \mathbf{g}_\mathsf{M})}.$$

Thus, there exists $C > 0$ such that

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathsf{M}, \mathbf{g}_\mathsf{M})(w) \geqslant Q^{\mathsf{Di},(q)}_{f,h}(\mathsf{M}, \mathbf{g}_\mathsf{M})(\widetilde{\chi} w) - C\,h^2 \|w\|^2_{L^2(\mathbb{R}^d_-, \mathbf{g}_\mathsf{M})} + \sum_{y\in\mathsf{P}_q} Q^{\mathsf{Di},(q)}_{f,h}(\mathsf{M}, \mathbf{g}_\mathsf{M})(\chi_y w). \tag{101}$$

To prove Theorem 4, we will study separately the quantities $Q^{\mathsf{Di},(q)}_{f,h}(\mathsf{M}, \mathbf{g}_\mathsf{M})(\widetilde{\chi} w)$ and $Q^{\mathsf{Di},(q)}_{f,h}(\mathsf{M}, \mathbf{g}_\mathsf{M})(\chi_y w)$ for $y \in \mathsf{P}_q$. The latter will be estimated using Proposition 16, after having introduced coordinates on V_y in which the metric has the block structure assumed in item (i) of (Metric-$\mathbb{R}^d_-$), and f satisfies (54). The proof of Theorem 4 is divided into four steps.

Step 1: Results from [42, Chap. 3] *and* [44].

Step 1a: Quasi-modes associated with points in $\mathsf{U}^\mathsf{M}_q \cup \mathsf{U}^{\partial\mathsf{M},1}_q$. — Let $y \in \mathsf{U}^\mathsf{M}_q \cup \mathsf{U}^{\partial\mathsf{M},1}_q$. Let us introduce the set E defined as follows:

$$\mathsf{E} = \mathbb{R}^d \text{ if } y \in \mathsf{U}^\mathsf{M}_q \quad \text{and} \quad \mathsf{E} = \mathbb{R}^d_- \text{ if } y \in \mathsf{U}^{\partial\mathsf{M},1}_q.$$

Up to reducing the neighborhood V_y of y in $\overline{\mathsf{M}}$, the following results hold according to the analysis in [42, Chap. 3] (see also [44] and [41] for the case when $\mathsf{E} = \mathbb{R}^d$). There exists a $\mathcal{C}^\infty$ system of coordinates

$$v \in \mathsf{V}_y \longmapsto x(v) \in \overline{\mathsf{E}},$$

and a metric tensor $\mathbf{g}_y$ and a function f_y on $\overline{\mathsf{E}}$ which coincide on $x(\mathsf{V}_y)$ respectively with $\mathbf{g}_\mathsf{M}$ and f expressed in the x-coordinates, such that the following holds:

$$\exists \mathsf{c}_y > 0, \exists h_0 > 0, \forall h \in (0, h_0), \quad \operatorname{Ran} \pi_{[0,\mathsf{c}_y h]}\big(\mathsf{T}_y\big) = \operatorname{Ker} \mathsf{T}_y \text{ has dimension } 1, \tag{102}$$

where $\mathsf{T}_y = \Delta^{(q)}_{f_y,h}(\mathbb{R}^d, \mathbf{g}_y)$ if $y \in \mathsf{U}^\mathsf{M}_q$ and $\mathsf{T}_y = \Delta^{\mathsf{Di},(q)}_{f_y,h}(\mathbb{R}^d_-, \mathbf{g}_y)$ if $y \in \mathsf{U}^{\partial\mathsf{M},1}_q$. Moreover, let $\chi : \overline{\mathsf{E}} \to [0,1]$ be a $\mathcal{C}^\infty$ function supported in $x(\mathsf{V}_y)$ which equals 1 in a neighborhood of 0 in $x(\mathsf{V}_y)$. Let $\Psi^y_h \in \operatorname{Ker} \mathsf{T}_y$ such that $\|\Psi^y_h\|_{L^2(\mathsf{E}, \mathbf{g}_y)} = 1$, then, in the limit $h \to 0$, it holds:

$$\|\chi \Psi^y_h\|_{L^2(\mathsf{M}, \mathbf{g}_\mathsf{M})} = 1 + O(h^2) \quad \text{and} \quad Q^{\mathsf{Di},(q)}_{f,h}(\mathsf{M}, \mathbf{g}_\mathsf{M})(\chi \Psi^y_h) = O(h^2). \tag{103}$$

Step 1b: Lower bound on $Q^{\mathsf{Di},(q)}_{f,h}(\mathsf{M},\mathbf{g}_{\mathsf{M}})(\widetilde{\chi}w)$. — Moreover, it is proved in [42, §3.4] that there exist $\widetilde{C}>0$ and $h_0>0$ such that for all $h\in(0,h_0)$ and all $w\in\Lambda^q H^1_{\mathbf{T}}(\mathsf{M},\mathbf{g}_{\mathsf{M}})$:

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathsf{M},\mathbf{g}_{\mathsf{M}})(\widetilde{\chi}w)\geqslant \widetilde{C}h\,\|\widetilde{\chi}w\|^2_{L^2(\mathsf{M},\mathbf{g}_{\mathsf{M}})}. \tag{104}$$

More precisely, by [42, §3.4], one has for any $x\in\overline{\mathsf{M}}\setminus\mathsf{P}_q$:

(1) either $x\in\mathsf{M}$ with $|\nabla f(x)|\neq 0$, in which case there exist $c>0$ and a neighborhood V_x of x in M such that $Q^{\mathsf{Di},(q)}_{f,h}(\mathsf{M},\mathbf{g}_{\mathsf{M}})(\chi_x w)\geqslant c\,\|\chi_x w\|^2_{L^2(\mathsf{M},\mathbf{g}_{\mathsf{M}})}$ for any smooth function χ_x supported in V_x;

(2) or $x\in\mathsf{M}$ with $|\nabla f(x)|=0$ and $x\notin\mathsf{U}^{\mathsf{M}}_q$, in which case there exist $c>0$ and a neighborhood V_x of x in M such that $Q^{\mathsf{Di},(q)}_{f,h}(\mathsf{M},\mathbf{g}_{\mathsf{M}})(\chi_x w)\geqslant ch\,\|\chi_x w\|^2_{L^2(\mathsf{M},\mathbf{g}_{\mathsf{M}})}$ for any smooth function χ_x supported in V_x;

(3) or $x\in\partial\mathsf{M}$ with $|\nabla f(x)|\neq 0$ and $x\notin\mathsf{U}^{\partial\mathsf{M},1}_q$, in which case there exist $c>0$ and a neighborhood V_x of x in $\overline{\mathsf{M}}$ such that $Q^{\mathsf{Di},(q)}_{f,h}(\mathsf{M},\mathbf{g}_{\mathsf{M}})(\chi_x w)\geqslant ch\,\|\chi_x w\|^2_{L^2(\mathsf{M},\mathbf{g}_{\mathsf{M}})}$ for any smooth function χ_x supported in V_x.

Equation (104) then follows from the fact that $\widetilde{\chi}=0$ in a neighborhood of all the points in P_q.

Step 2: Change of coordinates near $y\in\mathsf{B}^{\partial\mathsf{M},2}$. — For $\varepsilon>0$ small enough, for all $v\in\overline{\mathsf{M}}$ such that $\mathsf{d}_{\overline{\mathsf{M}}}(v,\partial\mathsf{M})<\varepsilon$, there exists a unique point $\mathsf{z}(v)\in\partial\mathsf{M}$ such that

$$x_d(v):=-\mathsf{d}_{\overline{\mathsf{M}}}(v,\partial\mathsf{M})=-\mathsf{d}_{\overline{\mathsf{M}}}(v,\mathsf{z}(v)),$$

where we recall $\mathsf{d}_{\overline{\mathsf{M}}}$ denotes the geodesic distance in $\overline{\mathsf{M}}$. Moreover the function $v\mapsto\mathsf{d}_{\overline{\mathsf{M}}}(v,\partial\mathsf{M})$ is smooth on the set $\{v\in\overline{\mathsf{M}},\mathsf{d}_{\overline{\mathsf{M}}}(v,\partial\mathsf{M})<\varepsilon\}$.

Let us now consider a fixed $y\in\mathsf{B}^{\partial\mathsf{M},2}\subset\partial\mathsf{M}$ and let x' be a local system of coordinates in $\partial\mathsf{M}$ centered at y. Then there exists a neighborhood U_y of y in $\overline{\mathsf{M}}$ such that the mapping

$$v\in\mathsf{U}_y\longmapsto x(v):=(x'(\mathsf{z}(v)),x_d(v))\in\mathbb{R}^{d-1}\times\overline{\mathbb{R}_-} \tag{105}$$

is a system of coordinates near $y\in\partial\mathsf{M}$, centered at y: this is the so-called tangential-normal system of coordinates. Then, up to choosing V_y smaller, one can assume that:

$$\mathsf{U}_y=\mathsf{V}_y.$$

It holds, by construction of $v\mapsto x(v)$:

$$x(y)=0,\quad \{v\in\mathsf{V}_y,\,x_d(v)<0\}=\mathsf{M}\cap\mathsf{V}_y,\quad \{v\in\mathsf{V}_y,\,x_d(v)=0\}=\partial\mathsf{M}\cap\mathsf{V}_y,$$

and for all $(x',0)\in x(\mathsf{V}_y)$,

$$\partial_{x_d}v(x',0)=\mathsf{n}_{\mathsf{M}}(v(x',0)).$$

Moreover, by construction, the metric tensor $\mathbf{g}_{\mathsf{M}}$ in the x-coordinates has the desired block structure of item (i) in (Metric-$\mathbb{R}^d_-$), i.e.,

$$\forall(x',x_d)\in x(\mathsf{V}_y),\quad \mathbf{g}_{\mathsf{M}}(x',x_d)=\mathbf{G}_{\mathsf{M}}(x',x_d)dx'^{\,2}+dx_d^2, \tag{106}$$

where it is assumed, without loss of generality, that $\mathbf{G}_{\mathsf{M}}(0,0)$ is the identity matrix. In the following and with a slight abuse of notation, one still denotes by f the function f in the x-coordinates. Since $\mathbf{g}_{\mathsf{M}}(0,0) = dx'^{\,2} + dx_d^2$, the Hessian matrix of f (resp. the Hessian matrix of $f|_{\partial\mathbb{R}^d_-}$) at 0 in this new coordinates is unitarily equivalent to $\operatorname{Hess} f(y)$ (resp. $\operatorname{Hess} f|_{\partial\mathsf{M}}(y)$). In particular, they have the same eigenvalues. Let us recall that according to (M-f), $\mathsf{n}_{\mathsf{M}}(y)$ is an eigenvector of $\operatorname{Hess} f(y)$ for the eigenvalue μ_y, see (46), also denoted by μ_d in the following. Let us denote by $\mu_1,\dots,\mu_{d-1}$ the $d-1$ remaining eigenvalues of $\operatorname{Hess} f(y)$, the associated eigenspace being $T_y\partial\mathsf{M}$. These are also the eigenvalues of $\operatorname{Hess} f|_{\partial\mathsf{M}}(y)$. Let us recall that, up to an orthogonal transformation on $x' = (x_1,\dots,x_{d-1})$, it holds, in a neighborhood of 0 and in the x-coordinates,

$$f(x) \;=\; f(0) + \sum_{j=1}^{d} \frac{\mu_j}{2}\, x_j^2 + O(|x|^3), \tag{107}$$

which is precisely (54).

Remark 23. — Let us mention that (107) only requires that $\mathsf{n}_{\mathsf{M}}(y)$ is an eigenvector of $\operatorname{Hess} f(y)$. The stronger assumption that $\partial_{\mathsf{n}_{\mathsf{M}}} f = 0$ on $\partial\mathsf{M}\cap\mathsf{V}_y$ will be necessary to use the results of Proposition 16.

In addition, it holds:

$$\forall x' \in \mathbb{R}^{d-1}\cap x(\mathsf{V}_y), \quad \partial_{\mathsf{n}_{\mathbb{R}^d_-}} f(x',0) = 0. \tag{108}$$

In order to use Proposition 16, we extend the function f and the metric $\mathbf{g}_{\mathsf{M}}$ from $x(\mathsf{V}_y)$ to $\overline{\mathbb{R}^d_-}$ so that they satisfy respectively (Potential-$\mathbb{R}^d_-$) and (Metric-$\mathbb{R}^d_-$). We denote by f_y and $\mathbf{g}_y$ these extensions, defined on $\overline{\mathbb{R}^d_-}$. Notice that it holds since χ_y is supported in V_y,

$$Q^{\mathsf{Di},(q)}_{f_y,h}(\mathbb{R}^{d-1},\mathbf{g}_y)(\chi_y w) = Q^{\mathsf{Di},(q)}_{f,h}(\mathsf{M},\mathbf{g}_{\mathsf{M}})(\chi_y w)$$

and

$$\|\chi_y w\|_{L^2(\mathbb{R}^{d-1},\mathbf{g}_y)} = \|\chi_y w\|_{L^2(\mathsf{M},\mathbf{g}_{\mathsf{M}})},$$

where with a slight abuse of notation $\chi_y w$ both denotes the q-form defined on M and in the x-coordinates. These equalities will be used many times in the rest of the proof.

Step 3: Contributions of the points in $\mathsf{B}^{\partial\mathsf{M},2}$. — According to Step 2, one can use Proposition 16 to study $Q^{\mathsf{Di},(q)}_{f,h}(\mathsf{M},\mathbf{g}_{\mathsf{M}})(\chi_y w)$ when $y \in \mathsf{B}^{\partial\mathsf{M},2}$, where, we recall, $w \in \Lambda^0 H^1_{\mathbf{T}}(\mathsf{M},\mathbf{g}_{\mathsf{M}})$. There are thus three possible cases:

(1) By (58), if $q=0$, there exists $C>0$ such that for all h small enough:

$$Q^{\mathsf{Di},(0)}_{f,h}(\mathsf{M},\mathbf{g}_{\mathsf{M}})(\chi_y w) \geqslant Ch\,\|\chi_y w\|^2_{L^2(\mathsf{M},\mathbf{g}_{\mathsf{M}})}. \tag{109}$$

(2) By (59), for $q\in\{1,\dots,d\}$, if the index of y as a critical point of $f|_{\partial\mathsf{M}}$ is not $q-1$, or if $\mu_d>0$, then, there exists $C>0$ such that for all h small enough:

$$Q^{\mathsf{Di},(q)}_{f,h}(\mathsf{M},\mathbf{g}_{\mathsf{M}})(\chi_y w) \geqslant Ch\,\|\chi_y w\|^2_{L^2(\mathsf{M},\mathbf{g}_{\mathsf{M}})}. \tag{110}$$

(3) For $q \in \{1, \dots, d\}$, if the index of y as a critical point of $f|_{\partial \mathsf{M}}$ is $q-1$ and $\mu_d < 0$ (namely if $y \in \mathsf{U}_q^{\partial \mathsf{M},2}$), from (60) there exists $\mathsf{c}_y > 0$ such that for all h small enough:

$$\operatorname{Ran} \pi_{[0,\mathsf{c}_y h]}\big(\Delta_{f_y,h}^{\mathsf{Di},(q)}(\mathbb{R}^d_-, \mathbf{g}_y)\big) = \operatorname{Ker} \Delta_{f_y,h}^{\mathsf{Di},(q)}(\mathbb{R}^d_-, \mathbf{g}_y) \quad \text{has dimension 1.} \tag{111}$$

Moreover, let $\chi : \overline{\mathbb{R}^d_-} \to [0,1]$ be a $\mathcal{C}^\infty$ function supported in V_y which equals 1 in a neighborhood of y in V_y. Let $\Psi_h^y \in \operatorname{Ker} \Delta_{f_y,h}^{\mathsf{Di},(q)}(\mathbb{R}^d_-, \mathbf{g}_y)$ such that $\|\Psi_h^y\|_{L^2(\mathbb{R}^d_-, \mathbf{g}_y)} = 1$, then, in the limit $h \to 0$, it holds (by (61)):

$$\|\chi \Psi_h^y\|_{L^2(\mathsf{M}, \mathbf{g}_\mathsf{M})} = 1 + O(h^2) \quad \text{and} \quad Q_{f,h}^{\mathsf{Di},(q)}(\mathsf{M}, \mathbf{g}_\mathsf{M})(\chi \Psi_h^y) = O(h^2). \tag{112}$$

Let us insist again on the fact that in (109)–(110), the constants C and the interval $(0, h_0) \ni h$ do not depend on w.

Step 4: End of the proof of Theorem 4. — Let us consider $\eta_1 > 0$. Using the Min-Max principle, Equations (112), (103) together with the fact that the supports of $(\chi_y)_{y \in \mathsf{Q}_q}$ are pairwise disjoint, one gets that $\Delta_{f,h}^{\mathsf{Di},(q)}(\mathsf{M}, \mathbf{g}_\mathsf{M})$ admits at least m_q eigenvalues of order $O(h^2)$ when $h \to 0$. Thus, for h sufficiently small,

$$\dim \operatorname{Ran} \pi_{[0,\eta_1 h]}\big(\Delta_{f,h}^{\mathsf{Di},(q)}(\mathsf{M}, \mathbf{g}_\mathsf{M})\big) \geqslant \mathsf{m}_q.$$

Let us now prove the reverse inequality holds if η_1 is small enough. To this end, let us consider $w \in \Lambda^q H^1_{\mathbf{T}}(\mathsf{M}, \mathbf{g}_\mathsf{M})$ such that $\|w\|_{L^2(\mathsf{M}, \mathbf{g}_\mathsf{M})} = 1$ and

$$Q_{f,h}^{\mathsf{Di},(q)}(\mathsf{M}, \mathbf{g}_\mathsf{M})(w) \leqslant \eta_1 h,$$

and let us prove that the distance between w and $\operatorname{Span}\big(\chi_y \Psi_h^y,\, y \in \mathsf{Q}_q\big)$ (which, we recall, is of dimension m_q because $(\chi_y)_{y \in \mathsf{Q}_q}$ have supports which are pairwise disjoint) goes to 0 when $h \to 0$, for a sufficiently small η_1. Using (101), it holds for some $C_0 > 0$ independent of h:

$$\eta_1 h \geqslant Q_{f,h}^{\mathsf{Di},(q)}(\mathsf{M}, \mathbf{g}_\mathsf{M})(\widetilde{\chi} w) - C_0 h^2 + \sum_{y \in \mathsf{P}_q} Q_{f,h}^{\mathsf{Di},(q)}(\mathsf{M}, \mathbf{g}_\mathsf{M})(\chi_y w). \tag{113}$$

In the following $\widetilde{c} > 0$ is a constant independent of h, η_1 and w, which can change from one occurrence to another. Then (113) together with (110) and (109) yields that for all $y \in \mathsf{B}^{\partial \mathsf{M},2} \smallsetminus \mathsf{U}_q^{\partial \mathsf{M},2} = \mathsf{P}_q \smallsetminus \mathsf{Q}_q$, for all h small enough:

$$\|\chi_y w\|_{L^2(\mathsf{M})} \leqslant \sqrt{\eta_1 h + C_0 h^2} / \sqrt{Ch} \leqslant \widetilde{c}\, \sqrt{\eta_1}. \tag{114}$$

In addition, from Equations (113) and (104), one has for h small enough:

$$\|\widetilde{\chi} w\|_{L^2(\mathsf{M})} \leqslant \sqrt{\eta_1 h + C_0 h^2} / \sqrt{\widetilde{C} h} \leqslant \widetilde{c}\, \sqrt{\eta_1}. \tag{115}$$

Furthermore, one deduces from (113) that for all $y \in \mathsf{P}_q$, for h small enough:

$$Q_{f,h}^{\mathsf{Di},(q)}(\mathsf{M}, \mathbf{g}_\mathsf{M})(\chi_y w) \leqslant 2\, \eta_1\, h. \tag{116}$$

For $y \in \mathsf{Q}_q = \mathsf{U}_q^{\mathsf{M}} \cup \mathsf{U}_q^{\partial \mathsf{M},1} \cup \mathsf{U}_q^{\partial \mathsf{M},2}$, set (see the quasi-modes introduced in (102)–(103) and (111)–(112))

$$\Phi_h^y := \chi_y \Psi_h^y \,/\, \|\chi_y \Psi_h^y\|_{L^2(\mathsf{M})}. \tag{117}$$

It holds:

$$\operatorname{dist}_{L^2(\mathsf{M})}\Big(w, \operatorname{Span}\big(\Phi_h^y,\, y\in \mathsf{Q}_q\big)\Big)^2 = \Big\| w - \sum_{y\in\mathsf{Q}_q} \langle w, \Phi_h^y\rangle_{L^2(\mathsf{M})}\Phi_h^y\Big\|_{L^2(\mathsf{M})}^2$$

$$= \sum_{z\in\mathsf{P}_q}\Big\|\chi_z\Big(w - \sum_{y\in\mathsf{Q}_q} \langle w, \Phi_h^y\rangle_{L^2(\mathsf{M})}\Phi_h^y\Big)\Big\|_{L^2(\mathsf{M})}^2 + \Big\|\widetilde{\chi}\Big(w - \sum_{y\in\mathsf{Q}_q} \langle w, \Phi_h^y\rangle_{L^2(\mathsf{M})}\Phi_h^y\Big)\Big\|_{L^2(\mathsf{M})}^2.$$

The first inequalities in (112) and (103) imply that for all $y\in\mathsf{Q}_q$, as $h\to 0$:

$$\|(1-\widetilde{\chi})\chi_y\Psi_h^y\|_{L^2(\mathsf{M})} = 1 + O(h^2).$$

Therefore, using in addition (115), one deduces that:

$$\begin{aligned}\Big\|\widetilde{\chi}\Big(w - \sum_{y\in\mathsf{Q}_q} \langle w, \Phi_h^y\rangle_{L^2(\mathsf{M})}\Phi_h^y\Big)\Big\|_{L^2(\mathsf{M})}^2 &\leqslant \rho\Big(\|\widetilde{\chi}w\|_{L^2(\mathsf{M})}^2 + \sum_{y\in\mathsf{Q}_q}\|\widetilde{\chi}\Phi_h^y\|_{L^2(\mathsf{M})}^2\Big)\\ &\leqslant \widetilde{c}\big(\eta_1 + h^2\big),\end{aligned}$$

where $\rho>0$ is independent of h, η_1 and w, and since the supports of $(\chi_y)_{y\in\mathsf{P}_q}$ are pairwise disjoint,

$$\sum_{z\in\mathsf{P}_q\smallsetminus\mathsf{Q}_q}\Big\|\chi_z\Big(w - \sum_{y\in\mathsf{Q}_q} \langle w, \Phi_h^y\rangle_{L^2(\mathsf{M})}\Phi_h^y\Big)\Big\|_{L^2(\mathsf{M})}^2 \leqslant \widetilde{c}\,\eta_1.$$

On the other hand, when $z\in\mathsf{Q}_q$, one has since the supports of $(\chi_y)_{y\in\mathsf{P}_q}$ are pairwise disjoint and using Lemma 11, (116), (111), and (102),

$$\begin{aligned}&\Big\|\chi_z\Big(w - \sum_{y\in\mathsf{Q}_q} \langle w, \Phi_h^y\rangle_{L^2(\mathsf{M})}\Phi_h^y\Big)\Big\|_{L^2(\mathsf{M})}^2\\ &\qquad= \Big\|\chi_z w - \langle w, \chi_z\Psi_h^z\rangle_{L^2(\mathsf{M})}\frac{\chi_z^2\Psi_h^z}{\|\chi_z\Psi_h^z\|_{L^2(\mathsf{M})}^2}\Big\|_{L^2(\mathsf{M})}^2\\ &\qquad\leqslant \big\|(1-\pi_{[0,\mathsf{c}_z h]}(\mathsf{T}_z))(\chi_z w)\big\|_{L^2(\mathsf{E},\mathbf{g}_z)}^2 + \widetilde{c}h^2 \leqslant \widetilde{c}\big(\eta_1/\mathsf{c}_z + h^2\big),\end{aligned}$$

where $\mathsf{T}_z = \Delta_{f,h}^{\mathsf{Di},(q)}(\mathbb{R}^d_-, \mathbf{g}_z)$ if $z\in\partial\mathsf{M}$ and $\mathsf{T}_z = \Delta_{f,h}^{(q)}(\mathbb{R}^d, \mathbf{g}_z)$ if $z\in\mathsf{M}$ (recall that $\mathsf{E}=\mathbb{R}^d_-$ if $y\in\partial\mathsf{M}$ and $\mathsf{E}=\mathbb{R}^d$ if $y\in\mathsf{M}$). In conclusion, as $\eta_1\to 0$ and $h\to 0$,

$$\operatorname{dist}_{L^2(\mathsf{M})}\big(w, \operatorname{Span}(\Phi_h^y,\, y\in\mathsf{Q}_q)\big) \longrightarrow 0.$$

This implies that there exist $\eta>0$ and $h_0>0$ such that for all $\eta_1\in(0,\eta)$ and $h\in(0,h_0)$, $\dim\operatorname{Ran}\pi_{[0,\eta_1 h]}\big(\Delta_{f,h}^{\mathsf{Di},(q)}(\mathsf{M},\mathbf{g}_\mathsf{M})\big)\leqslant \mathsf{m}_q$. This concludes the proof of Theorem 4.

2.5. Application of Theorem 4 to the infinitesimal generator of the diffusion (1)

Let us go back to the setting introduced in Section 1. Recall that Ω is a smooth bounded domain of $\mathbb{R}^d$, and let us apply the results stated above to $\mathsf{M}=\Omega$ endowed with the standard Euclidean metric tensor: $\mathbf{g}_\mathsf{M} = (\delta_{i,j}\,dx_i\,dx_j)_{i,j=1,\dots,d}$. For the ease of notation, we henceforth omit the reference to the metric tensor in the notation of the Witten Laplacian and the Sobolev spaces.

2.5.1. *Notation for weighted Sobolev spaces.* — For $q \in \{0, \dots, d\}$ and $m \in \mathbb{N}$, one denotes by $\Lambda^q H_w^m(\Omega)$ the weighted Sobolev spaces of q-forms with regularity index m, for the weight $e^{-(2/h)f(x)}dx$ on Ω (hence the subscript w in $\Lambda^q H_w^m(\Omega)$). We refer again for example to [81] for an introduction to Sobolev spaces on manifolds with boundaries. For $q \in \{0, \dots, d\}$ and $m > 1/2$, the set $\Lambda^q H_{w,\mathbf{T}}^m(\Omega)$ is defined by

$$\Lambda^q H_{w,\mathbf{T}}^m(\Omega) := \{v \in \Lambda^q H_w^m(\Omega),\ \mathbf{t}v = 0 \text{ on } \partial\Omega\}.$$

The space $\Lambda^q H_w^0(\Omega)$ is denoted by $\Lambda^q L_w^2(\Omega)$. Let us mention that the space $\Lambda^0 H_{w,\mathbf{T}}^1(\Omega)$ (resp. $\Lambda^0 L_w^2(\Omega)$) is the space $H_0^1(\Omega, e^{-(2/h)f}dx)$ (resp. $L^2(\Omega, e^{-(2/h)f}dx)$) that we introduced in Section 1.2.3 to define the domain of $\mathsf{L}_{f,h}^{\mathsf{Di},(0)}(\Omega)$. We will denote by $\|.\|_{H_w^q}$ the norm on the weighted space $\Lambda^q H_w^m(\Omega)$ (without referring to the degree of the forms). Moreover $\langle\cdot,\cdot\rangle_{L_w^2}$ denotes the scalar product in $\Lambda^q L_w^2(\Omega)$. We will also simply denote $\Lambda^0 H_w^q(\Omega)$ by $H_w^q(\Omega)$ if there is no possibility for confusion.

2.5.2. *Link between* $\mathsf{L}_{f,h}^{\mathsf{Di},(0)}(\Omega)$ *and* $\Delta_{f,h}^{\mathsf{Di},(0)}(\Omega)$, *and proof of* (41). — The infinitesimal generator $-\mathsf{L}_{f,h}^{(0)}$ of the diffusion (1) (see Section 1.2.3) is linked to the Witten Laplacian $\Delta_{f,h}^{(0)} = \Delta_{\mathbf{H}}^{(0)} + |\nabla f|^2 + h\Delta_{\mathbf{H}}^{(0)} f$ (where we recall that the Hodge Laplacian writes here: $\Delta_{\mathbf{H}}^{(0)} = -\operatorname{div}\nabla = -\Delta$) through the unitary transformation:

$$\phi \in L_w^2(\Omega) \longmapsto e^{-f/h}\phi \in L^2(\Omega).$$

Indeed, one can check that

$$\Delta_{f,h}^{(0)} = 2\,h\,e^{-f/h}\,\mathsf{L}_{f,h}^{(0)}\,e^{f/h}. \tag{118}$$

Let us now generalize this to q-forms, using extensions of $\mathsf{L}_{f,h}^{(0)}$ to q-forms.

Proposition 24. — *Let $q \in \{0, \dots, d\}$. The Friedrichs extension of the quadratic form*

$$Q_{f,h}^{\mathsf{Di},(q)}(\Omega) : v \in \Lambda^q H_{w,\mathbf{T}}^1(\Omega) \longmapsto \frac{h}{2}\big\|\mathsf{d}^{(q)}v\big\|_{L_w^2(\Omega)}^2 + \frac{h}{2}\big\|e^{2f/h}\big(\mathsf{d}^{(q)}\big)^* e^{-2f/h}v\big\|_{L_w^2(\Omega)}^2$$

on $\Lambda^q L_w^2(\Omega)$, is denoted $\big(\mathsf{L}_{f,h}^{\mathsf{Di},(q)}(\Omega),\ \mathcal{D}\big(L_{f,h}^{\mathsf{Di},(q)}(\Omega)\big)\big)$. The operator $\mathsf{L}_{f,h}^{\mathsf{Di},(q)}(\Omega)$ is a positive unbounded self-adjoint operator on $\Lambda^q L_w^2(\Omega)$. Besides, one has

$$\mathcal{D}\big(\mathsf{L}_{f,h}^{\mathsf{Di},(q)}(\Omega)\big) = \big\{v \in \Lambda^q H_w^2(\Omega),\ \mathbf{t}v = 0,\ \mathbf{t}\mathsf{d}^*\big(e^{-2f/h}v\big) = 0\big\}.$$

Proposition 24 is proved in [42, §2.4]. For $p = 0$, the operator $\mathsf{L}_{f,h}^{\mathsf{Di},(0)}(\Omega)$ is the one introduced in Section 1.2.3. In particular, for $v \in \mathcal{D}\big(\mathsf{L}_{f,h}^{\mathsf{Di},(0)}(\Omega)\big)$, $\mathsf{L}_{f,h}^{\mathsf{Di},(0)}(\Omega)v = \mathsf{L}_{f,h}^{(0)}v$. For $p = 1$ the operator $\mathsf{L}_{f,h}^{\mathsf{Di},(1)}(\Omega)$ is the one introduced in Section 1.2.6. In particular, for $v \in \mathcal{D}\big(\mathsf{L}_{f,h}^{\mathsf{Di},(1)}(\Omega)\big)$, $\mathsf{L}_{f,h}^{\mathsf{Di},(1)}(\Omega)v = \mathsf{L}_{f,h}^{(1)}v$ where we recall that

$$\mathsf{L}_{f,h}^{(1)} = \frac{h}{2}\,\Delta_{\mathbf{H}}^{(1)} + \nabla f\cdot\nabla + \operatorname{Hess} f,$$

see (39).

As a generalization of (118), one gets:

$$\Delta_{f,h}^{\mathsf{Di},(q)}(\Omega) = 2\,h\,e^{-f/h}\big(\mathsf{L}_{f,h}^{\mathsf{Di},(q)}(\Omega)\big)\,e^{f/h}. \tag{119}$$

The intertwining relations (44) and (45) write on $\mathsf{L}^{\mathsf{Di},(q)}_{f,h}(\Omega)$: $\forall v\in\Lambda^q H^1_{w,\mathbf{T}}(\Omega)$,

$$\pi_E\big(\mathsf{L}^{\mathsf{Di},(q+1)}_{f,h}(\Omega)\big)\mathsf{d}v=\mathsf{d}\pi_E\big(\mathsf{L}^{\mathsf{Di},(q)}_{f,h}(\Omega)\big)v \tag{120}$$

and

$$\pi_E\big(\mathsf{L}^{\mathsf{Di},(q-1)}_{f,h}(\Omega)\big)\mathsf{d}^*_{2f,h}v=\mathsf{d}^*_{2f,h}\pi_E\big(L^{\mathsf{Di},(q)}_{f,h}(\Omega)\big)v, \tag{121}$$

Thanks to the relation (119), the operators $\mathsf{L}^{\mathsf{Di},(q)}_{f,h}(\Omega)$ and $\Delta^{\mathsf{Di},(q)}_{f,h}(\Omega)$ have the same spectral properties. In particular the operators $\mathsf{L}^{\mathsf{Di},(q)}_{f,h}(\Omega)$ and $\Delta^{\mathsf{Di},(q)}_{f,h}(\Omega)$ both have compact resolvents, and thus a discrete spectrum (see Proposition 10).

Equation (41) is a consequence of Theorem 4 as stated in the following results, which also gives a first estimate of λ_h.

Corollary 25. — *Let us assume that* (Ω-f) *is satisfied. Then, there exists* $\mathsf{c}>0$ *and* $h_0>0$ *such that for all* $h\in(0,h_0)$,

$$\dim\operatorname{Ran}\pi_{[0,\mathsf{c}]}\big(\mathsf{L}^{\mathsf{Di},(0)}_{f,h}(\Omega)\big)=1\quad\text{and}\quad\dim\operatorname{Ran}\pi_{[0,\mathsf{c}]}\big(\mathsf{L}^{\mathsf{Di},(1)}_{f,h}(\Omega)\big)=n.$$

Moreover, λ_h*, the principal eigenvalue of* $\mathsf{L}^{\mathsf{Di},(0)}_{f,h}(\Omega)$*, is exponentially small as* $h\to 0$.

For ease of notation, we set

$$\pi^{(q)}_h=\pi_{[0,\mathsf{c}]}\big(\mathsf{L}^{\mathsf{Di},(q)}_{f,h}(\Omega)\big),\ \text{for } q\in\{0,1\}, \tag{122}$$

where $\mathsf{c}>0$ is the constant introduced in Corollary 25.

Proof. — First of all, by item (2) in (Ω-f), for any $x\in\partial\Omega$ such that $|\nabla f(x)|=0$, there exists a neighborhood $\mathsf{V}^{\partial\Omega}_x$ of x in $\partial\Omega$ such that $\partial_{\mathsf{n}_\Omega}f=0$ on $\mathsf{V}^{\partial\Omega}_x$. Therefore, $\mathsf{M}=\Omega$ and f satisfy (M-f). By Theorem 4 and (119), for all $q\in\{0,\dots,d\}$, there exists $\mathsf{c}>0$ and $h_0>0$ such that for all $h\in(0,h_0)$:

$$\dim\operatorname{Ran}\pi_{[0,\mathsf{c}]}\big(\mathsf{L}^{\mathsf{Di},(q)}_{f,h}(\Omega)\big)=\mathsf{m}_q,\ \text{where by (49)},\ \mathsf{m}_q=\operatorname{Card}\big(\mathsf{U}^{\Omega}_q\cup\mathsf{U}^{\partial\Omega,1}_q\cup\mathsf{U}^{\partial\Omega,2}_q\big).$$

Let us first consider the case $q=0$. Recall that $\mathsf{U}^{\partial\Omega,1}_0\cup\mathsf{U}^{\partial\Omega,2}_0=\varnothing$. Thus $\mathsf{m}_0=\operatorname{Card}\big(\mathsf{U}^{\Omega}_0\big)=1$, since by Lemma 4, f has only one local minimum in Ω which is x_0.

Let us now consider the case $q=1$. Notice that $\mathsf{U}^{\Omega}_1=\varnothing$ since the minimum x_0 is the only critical point of f in Ω. One then has $\mathsf{m}_1=\operatorname{Card}\big(\mathsf{U}^{\partial\Omega,1}_1\cup\mathsf{U}^{\partial\Omega,2}_1\big)$. By item (3) in ($\Omega$-$f$) and by the definition (47) of $\mathsf{U}^{\partial\Omega,1}_1$, it holds $\mathsf{U}^{\partial\Omega,1}_1=\varnothing$. By (48), $\mathsf{U}^{\partial\Omega,2}_1$ is the set of saddle points of f on $\partial\Omega$. Thus, from Definition 6, $\mathsf{U}^{\partial\Omega,2}_1=\{z_1,\dots,z_n\}$. In conclusion, $\mathsf{m}_1=n$.

It remains to prove that λ_h is exponentially small when $h\to 0$. Let us recall the proof of this well-known result. Let $\chi:\mathbb{R}^d\to[0,1]$ be a $\mathcal{C}^\infty$ function supported in Ω such that $\chi=1$ in a neighborhood of x_0 in Ω. Then, since x_0 is the only global minimum of f in $\overline{\Omega}$ (see Lemma 4), there exists $\delta>0$ such that $f\geqslant f(x_0)+\delta$ on $\operatorname{supp}\nabla\chi$. In addition, because $\operatorname{Hess}f(x_0)>0$,

$$\int_\Omega\chi^2e^{-(2/h)f}=(\pi h)^{d/2}(1+O(h))e^{-(2/h)f(x_0)}/\sqrt{\det\operatorname{Hess}f(x_0)},$$

in the limit $h \to 0$. Thus, for h small enough, it holds:

$$\lambda_h \leqslant \langle \mathsf{L}^{\mathsf{Di},(0)}_{f,h}(\Omega)\chi, \chi\rangle_{L^2_w} = \frac{h}{2}\frac{\int_\Omega |\nabla \chi|^2 e^{-(2/h)f}}{\int_\Omega \chi^2 e^{-(2/h)f}} \leqslant Ce^{-\delta/h},$$

where $\delta > 0$ is independent of h. This ends the proof of Corollary 25. □

3. Quasi-modes associated with $(z_k)_{k=1,\dots,n}$

By Corollary 25, for h small enough, the rank of the spectral projector $\pi_h^{(1)}$ (defined by (122)) is the number n of saddle points of f and the rank of the spectral projector $\pi_h^{(0)}$ is 1 (the number of local minima of f). To prove Theorem 1, we will construct n quasi-modes $\{\mathsf{f}_1^{(1)}, \dots, \mathsf{f}_n^{(1)}\}$ for $\mathsf{L}^{\mathsf{Di},(1)}_{f,h}(\Omega)$ and a quasi-mode $\mathsf{u}^{(0)}$ for $\mathsf{L}^{\mathsf{Di},(0)}_{f,h}(\Omega)$ which form respectively a basis of Ran $\pi_h^{(1)}$ and of Ran $\pi_h^{(0)}$. We will build quasi-modes which satisfy appropriate estimates, listed in Section 3.1, in order to get the results of Theorem 1.

As already outlined in Section 1.2.6, the strategy to build the quasimode $\mathsf{f}_k^{(1)}$ consists in constructing a quasi-mode $\mathsf{v}_k^{(1)} \in \Lambda^1\mathcal{C}^\infty(\overline{\Omega})$ for $\Delta^{\mathsf{Di},(1)}_{f,h}(\Omega)$ associated with the saddle point $z_k \in \partial\Omega$ for each $k \in \{1, \dots, n\}$, from which a quasi-mode $\mathsf{f}_k^{(1)} = e^{f/h}\mathsf{v}_k^{(1)}$ for $\mathsf{L}^{\mathsf{Di},(1)}_{f,h}(\Omega)$ is deduced. This quasi-mode $\mathsf{v}_k^{(1)}$ is built as follows. We first introduce in Section 3.2 a subdomain Ω_k^{M} of Ω which satisfies some geometric conditions (in particular, z_k is the only saddle point of f in $\overline{\Omega_k^{\mathrm{M}}}$, and $\nabla f \cdot \mathsf{n}_{\Omega_k^{\mathrm{M}}} \geqslant 0$ on $\partial\Omega_k^{\mathrm{M}}$). Then, we introduce in Section 3.3 an auxiliary Witten Laplacian on Ω_k^{M} with mixed Dirichlet-Neumann boundary conditions, and we prove that it has only one eigenvalue $\lambda(\Omega_k^{\mathrm{M}})$ smaller than $\mathsf{c}h$ when considered on functions and 1-forms. The quasi-mode $\mathsf{v}_k^{(1)}$ is then defined as the principal 1-eigenform of this Witten Laplacian (denoted by $\mathsf{u}_k^{(1)}$) multiplied by a suitable cut-off function, see Section 3.4.

Let us emphasize that since $|\nabla f(z_k)| = 0$, the constructions of the quasi-mode $\mathsf{v}_k^{(1)}$ are very different from those done previously in the literature [27, 42, 28, 41]. In particular, WKB approximations of $\mathsf{v}_k^{(1)}$ are not sufficient to prove the required estimates (see Section A.2 for more details). Instead of using a WKB-approximation, we will use an asymptotic equivalent of $\lambda(\Omega_k^{\mathrm{M}})$ in the limit $h \to 0$, inspired by [58]. For $\lambda(\Omega_k^{\mathrm{M}})$ to be different from 0, we require in particular that Ω_k^{M} contains x_0, which was not the case in [27].

3.1. Sufficient estimates on the quasi-modes for $\mathsf{L}^{\mathsf{Di},(0)}_{f,h}(\Omega)$ and $\mathsf{L}^{\mathsf{Di},(1)}_{f,h}(\Omega)$

Let us exhibit sufficient conditions on the quasi-modes to get the results of Theorem 1 (recall that n_0 is the cardinal of $\arg\min f|_{\partial\Omega}$, see (15)).

Proposition 26. — *Let us assume that* (Ω-f) *is satisfied. Assume that there exists a family* $\{\mathsf{f}_1^{(1)}, \dots, \mathsf{f}_n^{(1)}\}$ *of smooth* 1*-forms on* $\overline{\Omega}$*, and a smooth function* $\mathsf{u}^{(0)}$ *on* $\overline{\Omega}$ *such that:*

(1) *The function* $\mathsf{u}^{(0)}$ *belongs to* $H^1_w(\Omega)$ *and is normalized in* $L^2_w(\Omega)$*. For all* $k \in \{1, \dots, n\}$*,* $\mathsf{f}_k^{(1)}$ *belongs to* $\Lambda^1 H^1_{w,\mathbf{T}}(\Omega)$ *and is normalized in* $\Lambda^1 L^2_w(\Omega)$*.*

(2)

(a) *There exists* $\varepsilon_1>0$ *such that for all* $k\in\{1,\dots,n\}$*, in the limit* $h\to 0$*:*

$$\big\|\big(1-\pi_h^{(1)}\big)\mathsf{f}_k^{(1)}\big\|^2_{H^1_w(\Omega)}\leqslant e^{-\varepsilon_1/h}. \tag{123}$$

(b) *For any* $r>0$*,* $\mathsf{u}^{(0)}$ *can be chosen such that there exist* $C_r>0$ *such that for* h *small enough:*

$$\|\nabla \mathsf{u}^{(0)}\|^2_{L^2_w(\Omega)}\leqslant C_r e^{-(2/h)(f(z_1)-f(x_0)-r)}.$$

(3) *There exists* $\varepsilon_0>0$ *such that for* h *small enough,* $\forall (k,\ell)\in\{1,\dots,n\}^2$ *with* $k\neq\ell$*:*

$$\big|\big\langle \mathsf{f}_k^{(1)},\mathsf{f}_\ell^{(1)}\big\rangle_{L^2_w(\Omega)}\big|\leqslant e^{-\varepsilon_0/h}.$$

(4)

(a) *There exist constants* $(\mathsf{K}_k)_{k=1,\dots,n_0}$ *and* p *which do not depend on* h *such that for all* $k\in\{1,\dots,n_0\}$*, in the limit* $h\to 0$*:*

$$\big\langle \nabla\mathsf{u}^{(0)},\mathsf{f}_k^{(1)}\big\rangle_{L^2_w(\Omega)}=\mathsf{K}_k\ h^{\mathsf{p}}e^{-(1/h)(f(z_1)-f(x_0))}\ (1+O(\sqrt{h})),$$

where we recall $f(z_k)=f(z_1)$ *for* $k=1,\dots,n_0$*. If* $k>n_0$*, it holds for* h *small enough:*

$$\big|\big\langle \nabla\mathsf{u}^{(0)},\mathsf{f}_k^{(1)}\big\rangle_{L^2_w(\Omega)}\big|\leqslant e^{-(1/h)(f(z_1)-f(x_0)+\varepsilon)}.$$

(b) *There exist constants* $(\mathsf{b}_k)_{k=1,\dots,n_0}$ *and* m *which do not depend on* h *such that for all* $(k,\ell)\in\{1,\dots,n\}^2$*, in the limit* $h\to 0$*:*

$$\int_{\Sigma_{z_\ell}}\mathsf{f}_k^{(1)}\cdot\mathsf{n}_\Omega\ e^{-(2/h)f}d\sigma=\begin{cases}0 & \text{if } k\neq\ell,\\ -\mathsf{b}_k\, h^{\mathsf{m}}\ e^{-(1/h)f(z_1)}(1+O(\sqrt{h})) & \text{if } k=\ell\in\{1,\dots,n_0\},\\ O(e^{-(1/h)(f(z_1)+c)}) & \text{if } k=\ell\in\{n_0+1,\dots,n\},\end{cases}$$

where all the Σ_{z_ℓ}*'s are such that* (16) *holds.*

Then, in the limit $h\to 0$*:*

$$\lambda_h=\frac{h^{2\mathsf{p}+1}}{2}\,e^{-(2/h)(f(z_1)-f(x_0))}\sum_{k=1}^{n_0}\mathsf{K}_k^2\ (1+O(\sqrt{h})),$$

where λ_h *is the principal eigenvalue of* $\mathsf{L}^{\mathsf{Di},(0)}_{f,h}(\Omega)$*. In addition, for all* $k\in\{1,\dots,n_0\}$*, in the limit* $h\to 0$*:*

$$\int_{\Sigma_{z_k}}(\partial_{\mathsf{n}_\Omega}u_h)\,e^{-(2/h)f}d\sigma=-\mathsf{K}_k\mathsf{b}_k\ h^{\mathsf{p}+\mathsf{m}}\,e^{-(1/h)(2f(z_1)-f(x_0))}\ (1+O(\sqrt{h})),$$

where u_h *is the principal eigenfunction of* $\mathsf{L}^{\mathsf{Di},(0)}_{f,h}(\Omega)$ *which satisfies* (19)*. Finally, there exists* $c>0$ *such that, when* $h\to 0$

$$\int_{\partial\Omega\smallsetminus\bigcup_{k=1}^{n_0}\Sigma_{z_k}}\partial_{\mathsf{n}_\Omega}u_h\,e^{-(2/h)f}d\sigma=O\big(e^{-(1/h)(2f(z_1)-f(x_0)+c)}\big).$$

Let us emphasize that, even if this is not explicitly indicated, the family $\{\mathsf{f}_1^{(1)}, \dots, \mathsf{f}_n^{(1)}\}$ depends on $h > 0$, and the function $\mathsf{u}^{(0)}$ depends on $h > 0$ and $r > 0$. The proof of Proposition 26 is based on finite dimensional linear algebra computations, and is similar to the proof of [28, Th. 5]. It is therefore not reproduced here. Notice that Equations (23) and (24) in Theorem 1 and Equation (29) in Proposition 7 will follow from the construction of quasi-modes $\{\mathsf{f}_1^{(1)}, \dots, \mathsf{f}_n^{(1)}\}$ and $\mathsf{u}^{(0)}$ satisfying all the assumptions of Proposition 26. This construction is made in the rest of Section 3 (see the formulas (186) and (237) for the constants b_k, m, K_k, and p, and Section 4.1 for more details).

To prove Equation (27) in Theorem 1 (i.e., to get an asymptotic equivalent of $\int_{\Sigma_{z_k}} (\partial_{\mathsf{n}_\Omega} u_h)\, e^{-(2/h)f} d\sigma$ for $k > n_0$, as $h \to 0$), one needs stronger assumptions on these quasi-modes.

Proposition 27. — *Let us assume that* $(\Omega\text{-}f)$ *is satisfied. Assume that there exists a family* $\{\mathsf{f}_1^{(1)}, \dots, \mathsf{f}_n^{(1)}\}$ *of smooth* 1*-forms on* $\overline{\Omega}$, *and a smooth function* $\mathsf{u}^{(0)}$ *on* $\overline{\Omega}$ *satisfying all the assumptions of Proposition* 26 *with the following additional requirements:*

(1) *Concerning item* (2a) *in Proposition* 26, *there exists* $\varepsilon_2 > 0$ *such that for all* $k \in \{1, \dots, n\}$, *in the limit* $h \to 0$*:*

$$\big\| (1 - \pi_h^{(1)}) \mathsf{f}_k^{(1)} \big\|^2_{H^1_w(\Omega)} \leqslant e^{-(2/h)(\max[f(z_n) - f(z_k), f(z_k) - f(z_1)] + \varepsilon_2)}. \tag{124}$$

(2) *Concerning item* (3) *in Proposition* 26, *there exists* $\varepsilon_3 > 0$ *such that* $\forall (k, \ell) \in \{1, \dots, n\}^2$ *with* $k > \ell$, *in the limit* $h \to 0$*:*

$$\big| \big\langle \mathsf{f}_k^{(1)}, \mathsf{f}_\ell^{(1)} \big\rangle_{L^2_w(\Omega)} \big| \leqslant e^{-(1/h)(f(z_k) - f(z_\ell) + \varepsilon_3)}.$$

(3) *Concerning item* (4a) *in Proposition* 26, *there exist* $(\mathsf{K}_k)_{k = n_0 + 1, \dots, n}$ *and* p *which do not depend on* h *such that for all* $k > n_0$, *in the limit* $h \to 0$*:*

$$\big\langle \nabla \mathsf{u}^{(0)}, \mathsf{f}_k^{(1)} \big\rangle_{L^2_w(\Omega)} = \mathsf{K}_k \; h^{\mathsf{p}} e^{-(1/h)(f(z_k) - f(x_0))} \; (1 + O(\sqrt{h})).$$

(4) *Concerning item* (4b) *in Proposition* 26, *there exist constants* $(\mathsf{b}_k)_{k = n_0 + 1, \dots, n}$ *and* m *which do not depend on* h *such that for all* $k \in \{n_0 + 1, \dots, n\}$, *in the limit* $h \to 0$*:*

$$\int_{\Sigma_{z_k}} \mathsf{f}_k^{(1)} \cdot \mathsf{n}_\Omega \; e^{-(2/h)f} d\sigma = -\mathsf{b}_k \; h^{\mathsf{m}} \; e^{-(1/h)f(z_k)} \; (1 + O(\sqrt{h})),$$

where all the Σ_{z_k}*'s are such that* (16) *holds.*

Then, for all $k \in \{n_0 + 1, \dots, n\}$, *in the limit* $h \to 0$*:*

$$\int_{\Sigma_{z_k}} (\partial_{\mathsf{n}_\Omega} u_h)\, e^{-(2/h)f} d\sigma = -\mathsf{K}_k \mathsf{b}_k \; h^{\mathsf{p}+\mathsf{m}} \, e^{-(1/h)(2f(z_k) - f(x_0))} \; (1 + O(\sqrt{h})).$$

Notice that the assumptions of Proposition 27 on the quasi-modes are stronger than those of Proposition 26 (see indeed (15)). Again, the proof of Proposition 27 is similar to the proof of [27, Prop. 25], and is therefore not reproduced here. Notice that Equation (27) in Theorem 1 will follow from the construction of quasi-modes satisfying the assumptions of Proposition 27. To construct such quasi-modes, the assumptions (25) on the Agmon distance and (26) on $f(x_0)$ will be used.

Let us finally mention that once Theorem 1 and Proposition 7 are proved, Theorem 2 and Corollary 8 are direct consequences of Theorem 1 together with (21), (22), and Proposition 7.

3.2. Construction of the subdomains $(\Omega_k^{\mathrm{M}})_{k=1,\dots,n}$ of Ω. — Let us recall that Ω is a smooth bounded domain of $\mathbb{R}^d$. In this section, we construct a Lipschitz subdomain Ω_k^{M} of Ω associated with each saddle point z_k of f in $\partial\Omega$, $k=1,\dots,n$. This subdomain will then be used to define in the next section a Witten Laplacian with mixed Dirichlet-Neumann boundary conditions on $\partial\Omega_k^{\mathrm{M}}$. We construct Ω_k^{M} such that:

(i) there exist two disjoint open subsets $\Gamma_{k,\mathbf{D}}^{\mathrm{M}}$ and $\Gamma_{k,\mathbf{N}}^{\mathrm{M}}$ of $\partial\Omega_k^{\mathrm{M}}$ such that $\partial\Omega_k^{\mathrm{M}} = \overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}} \cup \overline{\Gamma_{k,\mathbf{N}}^{\mathrm{M}}}$,

(ii) $\partial_{\mathsf{n}_{\Omega_k^{\mathrm{M}}}} f = 0$ on $\Gamma_{k,\mathbf{D}}^{\mathrm{M}}$ and $\partial_{\mathsf{n}_{\Omega_k^{\mathrm{M}}}} f > 0$ on $\Gamma_{k,\mathbf{N}}^{\mathrm{M}}$,

(iii) $x_0 \in \Omega_k^{\mathrm{M}}$, and finally

(iv) $\Gamma_{k,\mathbf{D}}^{\mathrm{M}}$ and $\Gamma_{k,\mathbf{N}}^{\mathrm{M}}$ meet at an angle strictly smaller than π (see Definition 31 below).

Conditions (ii) and (iii) will then be used to deduce in Section 3.3 the number of small eigenvalues of this Witten Laplacian on Ω_k^{M}, and the condition (iv) will be necessary to have existence of traces and regularity estimates for forms in the domain of this Witten Laplacian.

3.2.1. *Preliminary results*. — Before going through the construction of Ω_k^{M} (see Proposition 30), we need preliminary results stated in Propositions 28 and 29.

Proposition 28. — *Let us assume that the assumption* $(\Omega\text{-}f)$ *is satisfied. Consider* $k \in \{1,\dots,n\}$ *and* F *a compact subset of the open set* Γ_{z_k}*. Then, there exists a* $\mathcal{C}^\infty$ *simply connected subdomain* Γ_{F} *of* $\partial\Omega$ *containing* z_k *such that* $\overline{\Gamma_{\mathsf{F}}} \subset \Gamma_{z_k}$, $\mathsf{F} \subset \Gamma_{\mathsf{F}}$, *and*

$$\nabla f \cdot \mathsf{n}_{\Gamma_{\mathsf{F}}} > 0 \quad \text{on } \partial\Gamma_{\mathsf{F}}, \tag{125}$$

where $\mathsf{n}_{\Gamma_{\mathsf{F}}} \in T\partial\Omega$ *is the unit outward normal to* Γ_{F}.

Since Ω is a stable domain for the dynamics (12), one can prove a similar result on x_0 and Ω, as the one obtained in Proposition 28 on z_k and Γ_{z_k}.

Proposition 29. — *Let us assume that* $(\Omega\text{-}f)$ *is satisfied. Then, for any compact subset* K *of* Ω *there exists a* $\mathcal{C}^\infty$ *simply connected subdomain* Ω_{K} *of* Ω *containing* x_0 *such that* $\mathsf{K} \subset \Omega_{\mathsf{K}}$, $\overline{\Omega_{\mathsf{K}}} \subset \Omega$, *and*

$$\nabla f \cdot \mathsf{n}_{\Omega_{\mathsf{K}}} > 0 \quad \text{on } \partial\Omega_{\mathsf{K}}.$$

The proofs of Propositions 28 and 29 are tedious, and we therefore postpone them to Section A.3, in the appendix.

3.2.2. *Construction of* Ω_k^M. — We are now in position to construct, for each $k \in \{1,\dots,n\}$, the subdomain Ω_k^{M} of Ω associated with the saddle point z_k and its neighborhood Σ_{z_k} (see (16)).

Proposition 30. — *Let us assume that* $(\Omega\text{-}f)$ *is satisfied and consider* $k \in \{1,\dots,n\}$. *Then, there exists a Lipschitz subdomain* Ω_k^M *of* Ω *containing* x_0 *and such that:*

(1) *It holds* $\partial\Omega_k^M \cap \partial\Omega = \overline{\Gamma_{k,\mathbf{D}}^M}$ *where* $\Gamma_{k,\mathbf{D}}^M$ *is a* $\mathcal{C}^\infty$ *subdomain of* Γ_{z_k} *containing* $\overline{\Sigma_{z_k}}$ *which satisfies:*

(a) $\nabla f \cdot \mathsf{n}_{\Gamma_{k,\mathbf{D}}^M} > 0$ *on* $\partial\Gamma_{k,\mathbf{D}}^M$ *(recall that* $\mathsf{n}_{\Gamma_{k,\mathbf{D}}^M} \in T\partial\Omega \cap (T\partial\Gamma_{k,\mathbf{D}}^M)^\perp$ *is the unit outward normal to* $\Gamma_{k,\mathbf{D}}^M$*) and*

(b) *a.e. on* $\overline{\Gamma_{k,\mathbf{D}}^M}$,
$$\nabla f \cdot \mathsf{n}_{\Omega_k^M} = 0,$$
where, here and in the following, a.e. is with respect to the surface measure on $\partial\Omega_k^M$.

(2) *On* $\Gamma_{k,\mathbf{N}}^M := \partial\Omega_k^M \cap \Omega$ *it holds a.e.:*
$$\nabla f \cdot \mathsf{n}_{\Omega_k^M} > 0.$$

(3) *The sets* $\Gamma_{k,\mathbf{D}}^M$ *and* $\Gamma_{k,\mathbf{N}}^M$ *meet at an angle smaller than* π *(see Definition* 31 *below). This angle will be actually* $\pi/2$ *from the construction below.*

(4) *For all* $\delta > 0$, Ω_k^M *can be chosen such that*
$$\sup_{x \in \Gamma_{k,\mathbf{N}}^M} \mathsf{d}_{\overline{\Omega}}(x, \partial\Omega \smallsetminus \Gamma_{z_k}) \leqslant \delta, \tag{126}$$
where $\mathsf{d}_{\overline{\Omega}}$ *denotes the geodesic distance in* $\overline{\Omega}$.

Schematic representations of Ω_k^{M}, $\Gamma_{k,\mathbf{D}}^{\mathrm{M}}$, and $\Gamma_{k,\mathbf{N}}^{\mathrm{M}}$ are given in Figure 4 below. The subscript $\mathbf{D}$ (resp. $\mathbf{N}$) in $\Gamma_{k,\mathbf{D}}^{\mathrm{M}}$ (resp. in $\Gamma_{k,\mathbf{N}}^{\mathrm{M}}$) refers to the fact that Dirichlet (resp. Neumann) boundary conditions will be applied on $\Gamma_{k,\mathbf{D}}^{\mathrm{M}}$ (resp. on $\Gamma_{k,\mathbf{N}}^{\mathrm{M}}$) when defining the Witten Laplacian with mixed Dirichlet-Neumann boundary conditions on Ω_k^{M}, see Section 3.3.1 below. Let us recall the definition of an angle between two hypersurfaces used in item (3) of Proposition 30 (see [12, 49]).

Definition 31. — Let D be a bounded Lipschitz domain of $\mathbb{R}^d$. Let $\Gamma_{\mathbf{D}}$ and $\Gamma_{\mathbf{N}}$ be two open disjoint subsets of $\partial\mathsf{D}$ such that $\overline{\Gamma_{\mathbf{D}}} \cup \overline{\Gamma_{\mathbf{N}}} = \partial\mathsf{D}$. The sets $\Gamma_{\mathbf{D}}$ and $\Gamma_{\mathbf{N}}$ meet at an angle smaller than π (in D) if locally around any point $\mathsf{y} \in \overline{\Gamma_{\mathbf{D}}} \cap \overline{\Gamma_{\mathbf{N}}}$, there exists a local system of coordinates $(y_1, y'', y_d) \in \mathbb{R} \times \mathbb{R}^{d-2} \times \mathbb{R}$ on a neighborhood V_{y} of y, and two Lipschitz functions $\varphi_{\mathsf{y}} : \mathbb{R}^{d-1} \to \mathbb{R}$ and $\psi_{\mathsf{y}} : \mathbb{R}^{d-2} \to \mathbb{R}$ such that $\mathsf{D} \cap \mathsf{V}_{\mathsf{y}} = \{y_d > \varphi_{\mathsf{y}}(y_1, y'')\}$, $\Gamma_{\mathbf{D}} \cap \mathsf{V}_{\mathsf{y}} = \{y_d = \varphi_{\mathsf{y}}(y_1, y'') \text{ and } y_1 > \psi_{\mathsf{y}}(y'')\}$, $\Gamma_{\mathbf{N}} \cap \mathsf{V}_{\mathsf{y}} = \{y_d = \varphi_{\mathsf{y}}(y_1, y'') \text{ and } y_1 < \psi_{\mathsf{y}}(y'')\}$, and
$$\begin{aligned} \partial_{y_1}\varphi_{\mathsf{y}}(y_1, y'') &\geqslant \kappa \quad \text{on } y_1 > \psi_{\mathsf{y}}(y''), \\ \partial_{y_1}\varphi_{\mathsf{y}}(y_1, y'') &\leqslant -\kappa \quad \text{on } y_1 < \psi_{\mathsf{y}}(y''), \end{aligned}$$
for some $\kappa > 0$.

From a geometric viewpoint, the fact that $\Gamma_{\mathbf{D}}$ and $\Gamma_{\mathbf{N}}$ meet at an angle smaller than π is equivalent to the existence of a smooth vector field θ on $\partial\mathsf{D}$ such that $\langle\theta, \mathsf{n}_{\mathsf{D}}\rangle < 0$ on $\Gamma_{\mathbf{D}}$ and $\langle\theta, \mathsf{n}_{\mathsf{D}}\rangle > 0$ on $\Gamma_{\mathbf{N}}$. Let us now prove Proposition 30.

Proof of Proposition 30. — Let $k \in \{1, \ldots, n\}$. The domain Ω_k^{M} will be defined as the union of two intersecting subdomains of Ω. The proof of Proposition 30 is divided into several steps.

Step 1: Definition of Ω_k^M

Step 1a: Adapted system of coordinates and preliminary constructions

The set $\Gamma_{k,\mathbf{D}}^M$. — Recall (see (16)) that $z \in \Sigma_{z_k}$ and $\overline{\Sigma_{z_k}} \subset \Gamma_{z_k}$. Using Proposition 28, there exists a $\mathcal{C}^\infty$ subdomain $\Gamma_{k,\mathbf{D}}^{\mathrm{M}}$ of Γ_{z_k} such that $\overline{\Sigma_{z_k}} \subset \Gamma_{k,\mathbf{D}}^{\mathrm{M}}$, $\overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}} \subset \Gamma_{z_k}$, which can be as large as needed in Γ_{z_k}, and such that

$$\nabla f \cdot \mathsf{n}_{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}} > 0 \text{ on } \partial\Gamma_{k,\mathbf{D}}^{\mathrm{M}}. \tag{127}$$

In step 1b below (see indeed (147)), we will check that, from the definition (141) of Ω_k^{M}, $\overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}} = \partial\Omega_k^{\mathrm{M}} \cap \partial\Omega$, and this will therefore prove item (1a) of Proposition 30.

Systems of coordinates near $\partial\Omega$ and $\partial\Gamma_{k,\mathbf{D}}^M$. — In the following we introduce two systems of coordinates: one around $z \in \partial\Omega$ in $\overline{\Omega}$ (see (x', x_d) and one around $z \in \partial\Gamma_{k,\mathbf{D}}^{\mathrm{M}}$ in $\partial\Omega$ (see x' in (131) and (132)). They will be used to define Ω_k^{M}.

Recall that, for $\varepsilon > 0$ small enough, for all $x \in \overline{\Omega}$ such that $\mathsf{d}_{\overline{\Omega}}(x, \partial\Omega) < \varepsilon$, there exists a unique point $\mathsf{z}(x) \in \partial\Omega$ such that

$$x_d(x) := \mathsf{d}_{\overline{\Omega}}(x, \partial\Omega) = \mathsf{d}_{\overline{\Omega}}(x, \mathsf{z}(x)), \tag{128}$$

where we recall $\mathsf{d}_{\overline{\Omega}}$ denotes the geodesic distance in $\overline{\Omega}$. Moreover the function $x \mapsto \mathsf{d}_{\overline{\Omega}}(x, \partial\Omega)$ is smooth on the set $\{x \in \overline{\Omega},\ \mathsf{d}_{\overline{\Omega}}(x, \partial\Omega) < \varepsilon\}$. Let $z \in \partial\Omega$ and x' be a system of coordinates in $\partial\Omega$ centered at z. Then, there exists a neighborhood V_z of z in $\overline{\Omega}$ such that the function

$$v \in \mathsf{V}_z \longmapsto (x'(\mathsf{z}(v)), x_d(v)) \in \mathbb{R}^{d-1} \times \mathbb{R}_+ \tag{129}$$

is a system of coordinates in V_z (this is the tangential-normal system of coordinates already introduced above in (105)). For ease of notation, we omitted to write the dependency on z when writing (x', x_d), and we write with a slight abuse of notation, $x'(v)$ instead of $x'(\mathsf{z}(v))$. Let us assume, up to choosing V_z smaller that for $\varepsilon_z > 0$ small enough, V_z is a cylinder in the (x', x_d)-coordinates:

$$\mathsf{V}_z = \big\{v \in \mathsf{V}_z,\ |x'(v)| < \varepsilon_z \text{ and } x_d(v) \in [0, \varepsilon_z)\big\}. \tag{130}$$

Let us now be more precise on x' when $z \in \overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}}$. If $z \in \Gamma_{k,\mathbf{D}}^{\mathrm{M}}$, we choose $\varepsilon_z > 0$ small enough such that

$$\partial\Omega \cap \mathsf{V}_z = \big\{v \in \mathsf{V}_z,\ |x'(v)| \leqslant \varepsilon_z \text{ and } x_d(v) = 0\big\} \subset \Gamma_{k,\mathbf{D}}^{\mathrm{M}}. \tag{131}$$

If $z \in \partial\Gamma_{k,\mathbf{D}}^{\mathrm{M}}$, the system $x' = (x_1, \ldots, x_{d-1})$ in $\partial\Omega$ is chosen such that:

$$\Gamma_{k,\mathbf{D}}^{\mathrm{M}} \cap (\partial\Omega \cap \mathsf{V}_z) = \{v \in \partial\Omega \cap \mathsf{V}_z,\ x_1(v) > 0\}, \tag{132}$$

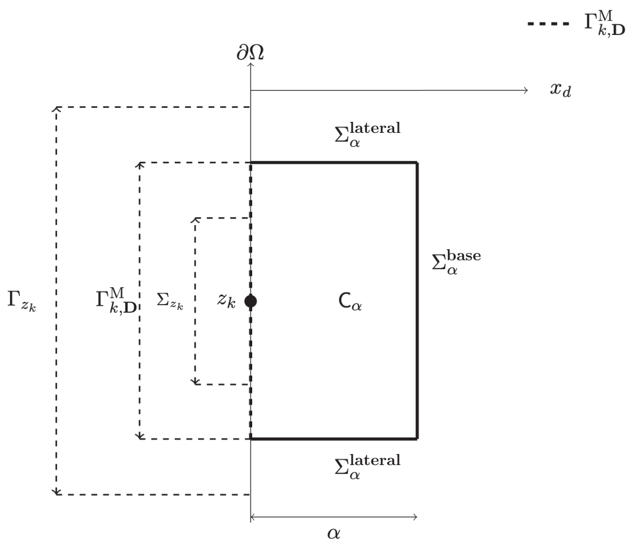

Figure 3. The cylinder C_α.

and

$$\partial\Gamma^{\mathrm{M}}_{k,\mathbf{D}} \cap (\partial\Omega \cap \mathsf{V}_z) = \{v \in \partial\Omega \cap \mathsf{V}_z,\ x_1(v) = 0\}. \tag{133}$$

This implies that for all $z \in \partial\Gamma^{\mathrm{M}}_{k,\mathbf{D}}$,

$$\mathsf{n}_{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}}(z) = -\frac{\nabla x_1(z)}{|\nabla x_1|(z)} \in T_z\partial\Omega. \tag{134}$$

Constructions of two subdomains of Ω*:* C_α *and* $\Omega_{\mathsf{K}_{\alpha/2}}$. — Define, for $\alpha > 0$ small enough, the open cylinder

$$\mathsf{C}_\alpha = \big\{x \in \overline{\Omega},\ \mathsf{z}(x) \in \Gamma^{\mathrm{M}}_{k,\mathbf{D}},\ x_d(x) \in (0,\alpha)\big\}, \tag{135}$$

(see Figure 3 for a schematic representation of C_α), and the compact set

$$\mathsf{K}_{\alpha/2} = \big\{v \in \overline{\Omega},\ \mathsf{d}_{\overline{\Omega}}(v, \partial\Omega) \geqslant \alpha/2\big\} \subset \Omega.$$

From Proposition 29, there exists a $\mathcal{C}^\infty$ subdomain $\Omega_{\mathsf{K}_{\alpha/2}}$ of Ω containing x_0 such that $\mathsf{K}_{\alpha/2} \subset \Omega_{\mathsf{K}_{\alpha/2}}$, $\overline{\Omega_{\mathsf{K}_{\alpha/2}}} \subset \Omega$, and

$$\nabla f \cdot \mathsf{n}_{\Omega_{\mathsf{K}_{\alpha/2}}} > 0 \quad \text{on } \partial\Omega_{\mathsf{K}_{\alpha/2}}. \tag{136}$$

A schematic representation of $\Omega_{\mathsf{K}_{\alpha/2}}$ and C_α is given in Figure 4.

Moreover it holds (see Figure 3):

$$\partial\mathsf{C}_\alpha = \overline{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}} \cup \Sigma^{\mathrm{lateral}}_{\alpha} \cup \overline{\Sigma^{\mathrm{base}}_{\alpha}}, \tag{137}$$

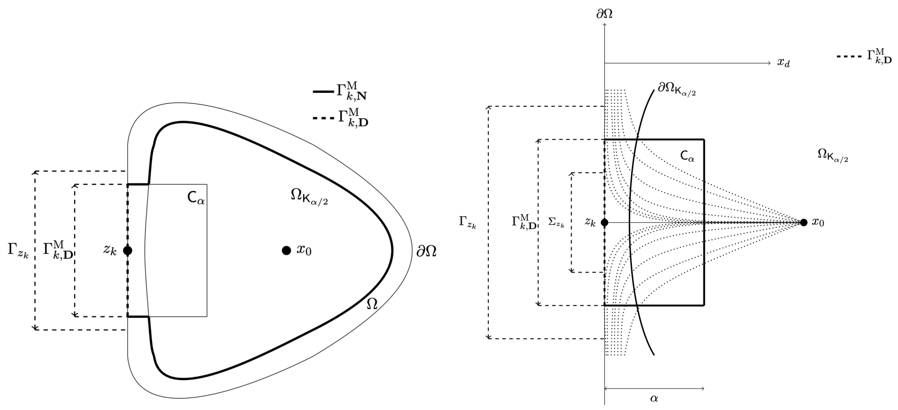

Figure 4. Schematic representations of $\Omega_k^{\mathrm{M}} = \mathsf{C}_\alpha \cup \Omega_{\mathsf{K}_{\alpha/2}}$, $\Gamma^{\mathrm{M}}_{k,\mathbf{D}}$, and $\Gamma^{\mathrm{M}}_{k,\mathbf{N}}$. On the right, a zoom in the neighborhood of Γ_{z_k}, where the dotted lines represent the flows of φ_x near the saddle point z_k of f (see (12) and item (1) in (Ω-f)).

where

$$\Sigma_\alpha^{\mathrm{lateral}} = \big\{x \in \overline{\Omega},\, \mathsf{z}(x) \in \partial\Gamma^{\mathrm{M}}_{k,\mathbf{D}},\, x_d(x) \in (0,\alpha)\big\} \subset \Omega, \tag{138}$$

and
$$\Sigma_\alpha^{\mathrm{base}} = \big\{x \in \overline{\Omega},\, \mathsf{z}(x) \in \Gamma^{\mathrm{M}}_{k,\mathbf{D}},\, x_d(x) = \alpha\big\} \subset \Omega.$$

Let us now prove that there exists $\alpha_0 > 0$, such that for all $\alpha \in (0,\alpha_0)$, one has:

$$\nabla f \cdot \mathsf{n}_{\mathsf{C}_\alpha} > 0 \text{ on } \Sigma_\alpha^{\mathrm{lateral}}. \tag{139}$$

It holds $\Sigma_\alpha^{\mathrm{lateral}} = \big\{v \in \Omega,\, x_1(v) = 0,\, x_d(v) \in (0,\alpha)\big\}$ (from (131)–(133), (135), and (138)), and hence, one has for all $v \in \Sigma_\alpha^{\mathrm{lateral}}$:

$$\mathsf{n}_{\mathsf{C}_\alpha}(v) = -\frac{\nabla x_1(v)}{|\nabla x_1|(v)}. \tag{140}$$

Therefore, by a continuity argument, using (127) and (134), there exists $\alpha_0 > 0$ such that for all $\alpha \in (0,\alpha_0)$ and for all $v \in \Sigma_\alpha^{\mathrm{lateral}}$,

$$\nabla f(v) \cdot \mathsf{n}_{\mathsf{C}_\alpha}(v) > 0.$$

This concludes the proof of (139).

Step 1b: definition of Ω_k^M such that $\partial\Omega_k^M \cap \partial\Omega = \overline{\Gamma^M_{k,\mathbf{D}}}$. — Let us introduce (see Figure 4)

$$\Omega_k^{\mathrm{M}} := \mathsf{C}_\alpha \cup \Omega_{\mathsf{K}_{\alpha/2}}, \tag{141}$$

which is included in Ω. Let us mention that Ω_k^{M} depends on two parameters: the set $\Gamma^{\mathrm{M}}_{k,\mathbf{D}}$ (which can be chosen as large as needed in Γ_{z_k}), and the parameter $\alpha > 0$ (which can be chosen as small as needed). One obviously has $\overline{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}} \subset \partial\Omega_k^{\mathrm{M}}$. Let us define

$$\Gamma^{\mathrm{M}}_{k,\mathbf{N}} = \partial\Omega_k^{\mathrm{M}} \setminus \overline{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}}, \tag{142}$$

so that $\partial\Omega_k^{\mathrm{M}}$ is the disjoint union of $\overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}}$ and $\Gamma_{k,\mathbf{N}}^{\mathrm{M}}$. By definition, Ω_k^{M} is the union of two intersecting open connected subsets C_α and $\Omega_{\mathsf{K}_{\alpha/2}}$ of Ω, it is thus open and connected. Notice that one has:

$$\partial\Omega_k^{\mathrm{M}} \subset \partial\mathsf{C}_\alpha \cup \partial\Omega_{\mathsf{K}_{\alpha/2}} \tag{143}$$

and, since $\overline{\Sigma_\alpha^{\mathrm{base}}} \subset \mathsf{K}_{\alpha/2} \subset \Omega_{\mathsf{K}_{\alpha/2}} \subset \Omega_k^{\mathrm{M}}$ (see (137)), one has:

$$\partial\Omega_{\mathsf{K}_{\alpha/2}} \cap \overline{\Sigma_\alpha^{\mathrm{base}}} = \varnothing \quad \text{and} \quad \partial\Omega_k^{\mathrm{M}} \cap \overline{\Sigma_\alpha^{\mathrm{base}}} = \varnothing. \tag{144}$$

In addition, from the fact that $\partial\Omega_{\mathsf{K}_{\alpha/2}} \subset \Omega$ and $\overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}} \subset \partial\Omega$, it holds:

$$\partial\Omega_{\mathsf{K}_{\alpha/2}} \cap \overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}} = \varnothing. \tag{145}$$

Thus, from (143), (144), and (145) together with the definition of $\Gamma_{k,\mathbf{N}}^{\mathrm{M}}$, it holds: $\Gamma_{k,\mathbf{N}}^{\mathrm{M}} \subset (\partial\mathsf{C}_\alpha \cup \partial\Omega_{\mathsf{K}_{\alpha/2}}) \smallsetminus (\overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}} \cup \overline{\Sigma_\alpha^{\mathrm{base}}}) = \partial\mathsf{C}_\alpha \smallsetminus (\overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}} \cup \overline{\Sigma_\alpha^{\mathrm{base}}}) \cup \partial\Omega_{\mathsf{K}_{\alpha/2}}$ and thus, from (137),

$$\Gamma_{k,\mathbf{N}}^{\mathrm{M}} \subset \Sigma_\alpha^{\mathrm{lateral}} \cup \partial\Omega_{\mathsf{K}_{\alpha/2}} \subset \{v \in \Omega,\ \mathsf{d}_{\overline{\Omega}}(v, \partial\Omega) < \alpha\}, \tag{146}$$

where the last inclusion follows from the fact that

$$\partial\Omega_{\mathsf{K}_{\alpha/2}} \subset \{v \in \Omega,\ \mathsf{d}_{\overline{\Omega}}(v, \partial\Omega) \leqslant \alpha/2\}$$

and (138). In particular, this implies that, since $\overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}} \subset \partial\Omega$,

$$\partial\Omega_k^{\mathrm{M}} \cap \Omega = \Gamma_{k,\mathbf{N}}^{\mathrm{M}} \quad \text{and} \quad \partial\Omega_k^{\mathrm{M}} \cap \partial\Omega = \overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}}. \tag{147}$$

Step 2: Proofs of items 3 and 4 in Proposition 30

Step 2a. — Let us check that $\Gamma_{k,\mathbf{D}}^{\mathrm{M}}$ and $\Gamma_{k,\mathbf{N}}^{\mathrm{M}}$ meet at an angle strictly smaller than π in Ω_k^{M} (in the sense of Definition 31). To this end, let us prove that

$$\overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}} \cap \overline{\Gamma_{k,\mathbf{N}}^{\mathrm{M}}} = \overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}} \cap \overline{\Sigma_\alpha^{\mathrm{lateral}}}. \tag{148}$$

Notice that (148) implies that $\partial\Omega_k^{\mathrm{M}}$ is Lipschitz near $\overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}} \cap \overline{\Gamma_{k,\mathbf{N}}^{\mathrm{M}}}$ as the union of the closures of two disjoint open transverse $\mathcal{C}^\infty$ hypersurfaces $\Gamma_{k,\mathbf{D}}^{\mathrm{M}}$ and $\Sigma_\alpha^{\mathrm{lateral}}$ (this will be used in Step 3b below). Furthermore, (148) implies that $\Gamma_{k,\mathbf{D}}^{\mathrm{M}}$ and $\Gamma_{k,\mathbf{N}}^{\mathrm{M}}$ meet at an angle $\pi/2$ (see Figure 5), which thus yields item (3) in Proposition 30.

Let us thus prove (148). From (146) together with (145), it holds:

$$\overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}} \cap \overline{\Gamma_{k,\mathbf{N}}^{\mathrm{M}}} \subset \overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}} \cap \overline{\Sigma_\alpha^{\mathrm{lateral}}}.$$

Now, let us consider $x \in \overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}} \cap \overline{\Sigma_\alpha^{\mathrm{lateral}}}$. Then, there exists a sequence $(x_n)_{n\geqslant 0} \in \Sigma_\alpha^{\mathrm{lateral}}$ such that $x_n \to x$ as $n \to +\infty$. Let us prove that for all n large enough, $x_n \in \partial\Omega_k^{\mathrm{M}}$. For n large enough, x_n does not belong to $\overline{\Omega_{\mathsf{K}_{\alpha/2}}}$ because $\overline{\Omega_{\mathsf{K}_{\alpha/2}}} \subset \Omega$ and $x_n \to x \in \partial\Omega$. In addition $x_n \notin \mathsf{C}_\alpha$ (indeed $x_n \in \partial\mathsf{C}_\alpha$ since $x_n \in \Sigma_\alpha^{\mathrm{lateral}}$). Therefore, for n large enough, $x_n \notin \Omega_k^{\mathrm{M}}$. On the other hand, since $x_n \in \partial\mathsf{C}_\alpha$, $x_n \in \overline{\mathsf{C}_\alpha} \subset \overline{\Omega_k^{\mathrm{M}}}$. In conclusion, $x_n \in \Omega \cap \partial\Omega_k^{\mathrm{M}} = \Gamma_{k,\mathbf{N}}^{\mathrm{M}}$ (see (147)) and thus, $x \in \overline{\Gamma_{k,\mathbf{N}}^{\mathrm{M}}}$. This concludes the proof of (148).

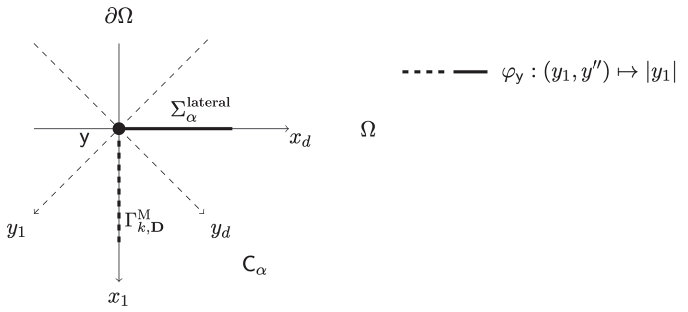

Figure 5. The sets $\Gamma^{\mathrm{M}}_{k,\mathbf{D}}$ and $\Sigma_\alpha^{\text{lateral}}$ meet at an angle $\pi/2$ in C_α (see Definition 31, (132), (133), and (137)). On the figure, $\mathsf{y}\in\overline{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}}\cap\overline{\Sigma_\alpha^{\text{lateral}}}$ and $\{x_d>0\}=\Omega$, $y_1=(-x_d+x_1)/2$, $y_d=(x_d+x_1)/2$, $y''=(x_2,\dots,x_{d-1})$ (which is, schematically, the coordinates perpendicular to the plane (x_1,x_d) centered at y), $\psi_{\mathsf{y}}(y'')=0$, and $\varphi_{\mathsf{y}}(y_1,y'')=|y_1|$ in Definition 31.

Step 2b. — Let us now prove item (4) in Proposition 30. To this end, let $\delta>0$. Let us choose $\Gamma^{\mathrm{M}}_{k,\mathbf{D}}$ such that the distance between $\overline{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}}$ and $\partial\Omega\smallsetminus\Gamma_{z_k}$ is smaller than $\delta/2$ (recall that $\overline{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}}\subset\Gamma_{z_k}$ can be chosen as large as needed in Γ_{z_k}, see Step 1a above), i.e.,

$$\mathsf{d}_{\overline{\Omega}}(\overline{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}},\partial\Omega\smallsetminus\Gamma_{z_k})\leqslant\delta/2. \tag{149}$$

Let us consider $x\in\Gamma^{\mathrm{M}}_{k,\mathbf{N}}$. According to (146), $x\in\Sigma_\alpha^{\text{lateral}}$ or $x\in\partial\Omega_{\mathsf{K}_{\alpha/2}}$. If $x\in\Sigma_\alpha^{\text{lateral}}$, then by the triangular inequality, it holds:

$$\mathsf{d}_{\overline{\Omega}}(x,\partial\Omega\smallsetminus\Gamma_{z_k})\leqslant\mathsf{d}_{\overline{\Omega}}(x,\overline{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}})+\mathsf{d}_{\overline{\Omega}}(\overline{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}},\partial\Omega\smallsetminus\Gamma_{z_k})\leqslant\alpha+\delta/2,$$

where we have used that according to (138), $\mathsf{d}_{\overline{\Omega}}(x,\overline{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}})\leqslant\mathsf{d}_{\overline{\Omega}}(x,\partial\Gamma^{\mathrm{M}}_{k,\mathbf{D}})\leqslant\alpha$, for all $x\in\Sigma_\alpha^{\text{lateral}}$. If $x\in\partial\Omega_{\mathsf{K}_{\alpha/2}}$, then $\mathsf{d}_{\overline{\Omega}}(x,\partial\Omega)\leqslant\alpha/2<\alpha$. Because $x\notin\mathsf{C}_\alpha$ (since $x\in\partial\Omega^{\mathrm{M}}_k$ and C_α is an open subset of Ω^{M}_k), one has $\mathsf{z}(x)\in\partial\Omega\smallsetminus\Gamma^{\mathrm{M}}_{k,\mathbf{D}}$. Therefore,

$$\mathsf{d}_{\overline{\Omega}}(x,\partial\Omega\smallsetminus\Gamma_{z_k})\leqslant\mathsf{d}_{\overline{\Omega}}(x,\mathsf{z}(x))+\mathsf{d}_{\overline{\Omega}}(\mathsf{z}(x),\partial\Omega\smallsetminus\Gamma_{z_k})\leqslant\alpha/2+\delta/2,$$

where we have used that either $\mathsf{z}(x)\in\partial\Omega\smallsetminus\Gamma_{z_k}$ (in which case $\mathsf{d}_{\overline{\Omega}}(\mathsf{z}(x),\partial\Omega\smallsetminus\Gamma_{z_k})=0$) or $\mathsf{z}(x)\in\Gamma_{z_k}\smallsetminus\Gamma^{\mathrm{M}}_{k,\mathbf{D}}$ (in which case $\mathsf{d}_{\overline{\Omega}}(\mathsf{z}(x),\partial\Omega\smallsetminus\Gamma_{z_k})\leqslant\delta/2$, see (149) together with the fact that $\mathsf{z}(x)\notin\Gamma^{\mathrm{M}}_{k,\mathbf{D}}$). In conclusion

$$\sup_{x\in\Gamma^{\mathrm{M}}_{k,\mathbf{N}}}\mathsf{d}_{\overline{\Omega}}(x,\partial\Omega\smallsetminus\Gamma_{z_k})\leqslant\alpha+\delta/2.$$

Choosing $\alpha\leqslant\delta/2$ concludes the proof of item (4) in Proposition 30.

Step 3: Proof that Ω_k^M is Lipschitz, and study of the sign of $\nabla f\cdot \mathsf{n}_{\Omega_k^M}$. — Let us first check that Ω_k^{M} is Lipschitz. Notice that the union of two Lipschitz (even smooth) subdomains of Ω is not necessarily a Lipschitz domain (the boundary is even not necessarily a manifold). In our setting, one has:

$$\partial\Omega_{\mathsf{K}_{\alpha/2}}\cap\partial\mathsf{C}_\alpha=\partial\Omega_{\mathsf{K}_{\alpha/2}}\cap\Sigma_\alpha^{\mathrm{lateral}}\quad\text{(see (137), (144), and (145))},$$

where (i) $\Sigma_\alpha^{\mathrm{lateral}}$ and $\partial\Omega_{\mathsf{K}_{\alpha/2}}$ are smooth, and (ii) the normal derivatives $\nabla f(v)\cdot\mathsf{n}_{\mathsf{C}_\alpha}(v)$ and $\nabla f(v)\cdot\mathsf{n}_{\Omega_{\mathsf{K}_{\alpha/2}}}(v)$ of f at $v\in\Sigma_\alpha^{\mathrm{lateral}}\cap\partial\Omega_{\mathsf{K}_{\alpha/2}}$ are positive (so that the two normal vectors cannot be opposite, a situation which could create cusps). These two points will be used to prove that the boundary of Ω_k^{M} is Lipschitz. One has:

$$\partial\Omega_k^{\mathrm{M}}\subset\partial\Omega_{\mathsf{K}_{\alpha/2}}\cup\partial\mathsf{C}_\alpha. \tag{150}$$

Define the two open subsets of $\partial\Omega_k^{\mathrm{M}}$

$$\mathsf{A}_1:=\partial\Omega_k^{\mathrm{M}}\cap(\partial\Omega_{\mathsf{K}_{\alpha/2}}\smallsetminus\partial\mathsf{C}_\alpha),\quad \mathsf{A}_2:=\partial\Omega_k^{\mathrm{M}}\cap(\partial\mathsf{C}_\alpha\smallsetminus\partial\Omega_{\mathsf{K}_{\alpha/2}}), \tag{151}$$

and the closed subset of $\partial\Omega_k^{\mathrm{M}}$ $\mathsf{A}_3:=\partial\Omega_k^{\mathrm{M}}\cap(\partial\Omega_{\mathsf{K}_{\alpha/2}}\cap\partial\mathsf{C}_\alpha)$, so that $\partial\Omega_k^{\mathrm{M}}$ is the disjoint union of A_1, A_2, and A_3. Let us now prove that, for $j\in\{1,2,3\}$, $\partial\Omega_k^{\mathrm{M}}$ is Lipschitz in a neighborhood of any point of A_j, and let us also study the sign of $\nabla f\cdot\mathsf{n}_{\Omega_k^{\mathrm{M}}}$ on A_j.

Step 3a: Study of A_1. — First notice that (because $\partial\Omega_{\mathsf{K}_{\alpha/2}}\subset\Omega$),

$$\mathsf{A}_1\subset\partial\Omega_{\mathsf{K}_{\alpha/2}}\smallsetminus\partial\mathsf{C}_\alpha\subset\Omega, \tag{152}$$

Let $z\in\mathsf{A}_1$. Then, there exists a neighborhood O_z of z in $\mathbb{R}^d$ such that $\mathsf{O}_z\cap\overline{\mathsf{C}_\alpha}=\varnothing$. Indeed, if not, z would belong to $\overline{\mathsf{C}_\alpha}=\partial\mathsf{C}_\alpha\cup\mathsf{C}_\alpha$, and z cannot belong to $\partial\mathsf{C}_\alpha$ (by definition of A_1) and z cannot belong to C_α (because $z\in\partial\Omega_k^{\mathrm{M}}$). Using (141), it then holds $\mathsf{O}_z\cap\overline{\Omega_k^{\mathrm{M}}}=\mathsf{O}_z\cap\overline{\Omega_{\mathsf{K}_{\alpha/2}}}$ (because $\overline{\Omega_k^{\mathrm{M}}}=\overline{\mathsf{C}_\alpha}\cup\overline{\Omega_{\mathsf{K}_{\alpha/2}}}$). Therefore, since in addition $\Omega_{\mathsf{K}_{\alpha/2}}$ is a smooth domain, A_1 is a smooth part of the boundary of Ω_k^{M} and $\mathsf{n}_{\Omega_k^{\mathrm{M}}}=\mathsf{n}_{\Omega_{\mathsf{K}_{\alpha/2}}}$ on A_1. Finally, using (136), it holds:

$$\partial_{\mathsf{n}_{\Omega_k^{\mathrm{M}}}}f>0\quad\text{on }\mathsf{A}_1. \tag{153}$$

Step 3b: Study of A_2. — It holds $\mathsf{A}_2\subset\partial\mathsf{C}_\alpha\smallsetminus\partial\Omega_{\mathsf{K}_{\alpha/2}}$. With the same arguments as in Step 3a (see the lines after (152)), $\mathsf{O}_z\cap\overline{\Omega_k^{\mathrm{M}}}=\mathsf{O}_z\cap\overline{\mathsf{C}_\alpha}$ for some neighborhood O_z at any point $z\in\mathsf{A}_2$. Moreover, from (137), $\partial\mathsf{C}_\alpha$ is $\mathcal{C}^\infty$ except on $\partial\Gamma_{k,\mathbf{D}}^{\mathrm{M}}\cup\partial\Sigma_\alpha^{\mathrm{base}}$, where it is Lipschitz since $\Gamma_{k,\mathbf{D}}^{\mathrm{M}}$ and $\Sigma_\alpha^{\mathrm{lateral}}$, and $\Sigma_\alpha^{\mathrm{base}}$ and $\Sigma_\alpha^{\mathrm{lateral}}$ are transverse (see Step 2a above). Thus, A_2 is a Lipschitz part of the boundary of Ω_k^{M} and

$$\mathsf{n}_{\Omega_k^{\mathrm{M}}}=\mathsf{n}_{\mathsf{C}_\alpha}\quad\text{on }\mathsf{A}_2\smallsetminus(\partial\Gamma_{k,\mathbf{D}}^{\mathrm{M}}\cup\partial\Sigma_\alpha^{\mathrm{base}}),\text{ i.e., a.e. on }\mathsf{A}_2. \tag{154}$$

Let us now study the sign of $\nabla f\cdot\mathsf{n}_{\Omega_k^{\mathrm{M}}}$ on A_2. Recall that $\partial\mathsf{C}_\alpha=\overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}}\cup\Sigma_\alpha^{\mathrm{lateral}}\cup\overline{\Sigma_\alpha^{\mathrm{base}}}$ (see (137)), $\overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}}\cap\partial\Omega_{\mathsf{K}_{\alpha/2}}=\varnothing$ (see indeed (145)), and $\partial\Omega_k^{\mathrm{M}}\cap\overline{\Sigma_\alpha^{\mathrm{base}}}=\varnothing$ (see (144)). Hence, it holds:

$$\mathsf{A}_2=\partial\Omega_k^{\mathrm{M}}\cap(\partial\mathsf{C}_\alpha\smallsetminus\partial\Omega_{\mathsf{K}_{\alpha/2}})=\underbrace{(\partial\Omega_k^{\mathrm{M}}\cap\overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}})}_{=\overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}}}\cup(\partial\Omega_k^{\mathrm{M}}\cap\Sigma_\alpha^{\mathrm{lateral}}\smallsetminus\partial\Omega_{\mathsf{K}_{\alpha/2}}). \tag{155}$$

Let $z \in \mathsf{A}_2$. If $z \in \Gamma^{\mathrm{M}}_{k,\mathbf{D}}$, then $\mathsf{n}_{\mathsf{C}_\alpha}(z) = \mathsf{n}_\Omega(z)$ and thus, using (154), it holds:

$$\nabla f \cdot \mathsf{n}_{\Omega^{\mathrm{M}}_k} = 0 \text{ on } \Gamma^{\mathrm{M}}_{k,\mathbf{D}}, \tag{156}$$

where we also used the fact that $\Gamma^{\mathrm{M}}_{k,\mathbf{D}} \subset \Gamma_{z_k}$ together with item (2) in (Ω-f). If $z \in \Sigma^{\mathrm{lateral}}_\alpha$, then from (139) and (154), it holds,

$$\nabla f \cdot \mathsf{n}_{\Omega^{\mathrm{M}}_k} > 0 \text{ on } \partial\Omega^{\mathrm{M}}_k \cap \Sigma^{\mathrm{lateral}}_\alpha \setminus \partial\Omega_{\mathsf{K}_{\alpha/2}}. \tag{157}$$

Step 3c: Study of A_3. — Notice that $\mathsf{A}_3 = \partial\Omega_{\mathsf{K}_{\alpha/2}} \cap \partial\mathsf{C}_\alpha$ (because $\partial\Omega_{\mathsf{K}_{\alpha/2}} \cap \partial\mathsf{C}_\alpha \subset \partial\Omega^{\mathrm{M}}_k$). Notice also that since $\partial\Omega_{\mathsf{K}_{\alpha/2}} \subset \Omega$,

$$\mathsf{A}_3 \subset \Omega. \tag{158}$$

Using (137), (144), and (145), it holds:

$$\mathsf{A}_3 = \partial\Omega_{\mathsf{K}_{\alpha/2}} \cap \partial\mathsf{C}_\alpha = \partial\Omega_{\mathsf{K}_{\alpha/2}} \cap \Sigma^{\mathrm{lateral}}_\alpha. \tag{159}$$

Thus, $\partial\Omega_{\mathsf{K}_{\alpha/2}}$ intersects $\partial\mathsf{C}_\alpha$ where $\partial\mathsf{C}_\alpha$ is smooth (i.e., on $\Sigma^{\mathrm{lateral}}_\alpha$). Let us consider $v \in \mathsf{A}_3$. Let us conclude the proof by considering successively the case when $\mathsf{n}_{\Omega_{\mathsf{K}_{\alpha/2}}}(v)$ is not collinear to $\mathsf{n}_{\mathsf{C}_\alpha}(v)$, and the case when $\mathsf{n}_{\Omega_{\mathsf{K}_{\alpha/2}}}(v) = \pm\mathsf{n}_{\mathsf{C}_\alpha}(v)$.

Let us first consider *the case when* $\mathsf{n}_{\Omega_{\mathsf{K}_{\alpha/2}}}(v)$ *is not collinear to* $\mathsf{n}_{\mathsf{C}_\alpha}(v)$. By a continuity argument, there exists a neighborhood O_v of v in Ω such that $\mathsf{O}_v \cap \partial\mathsf{C}_\alpha = \mathsf{O}_v \cap \Sigma^{\mathrm{lateral}}_\alpha$ (so that $\mathsf{n}_{\mathsf{C}_\alpha}$ is defined everywhere and continuous on $\mathsf{O}_v \cap \partial\mathsf{C}_\alpha$) and such that $\mathsf{n}_{\Omega_{\mathsf{K}_{\alpha/2}}}$ is not collinear to $\mathsf{n}_{\mathsf{C}_\alpha}$ on O_v. Consequently, $\partial\Omega_{\mathsf{K}_{\alpha/2}}$ and $\partial\mathsf{C}_\alpha$ are transverse on O_v (or equivalently, the natural immersion map $\mathsf{i} : \partial\Omega_{\mathsf{K}_{\alpha/2}} \to \mathbb{R}^d$ is transverse to $\partial\mathsf{C}_\alpha$ on O_v). Thus, $\mathsf{O}_v \cap \partial\Omega^{\mathrm{M}}_k$ is Lipschitz. In addition, as a consequence of the inverse image of a regular value Theorem [11, Th. (5.12)] and its proof (see also [87, 72, 37]) applied here to the smooth function i, one has, up to choosing O_v smaller, $\mathsf{O}_v \cap \mathsf{i}^{-1}(\partial\mathsf{C}_\alpha) = \mathsf{O}_v \cap (\partial\Omega_{\mathsf{K}_{\alpha/2}} \cap \partial\mathsf{C}_\alpha)$ (because $\mathsf{i}^{-1}(\partial\mathsf{C}_\alpha) = \partial\Omega_{\mathsf{K}_{\alpha/2}} \cap \partial\mathsf{C}_\alpha$) is a 1-codimensional smooth submanifold of $\partial\Omega_{\mathsf{K}_{\alpha/2}}$ (i.e., a 2-codimensional smooth submanifold of $\mathbb{R}^d$ included in $\partial\Omega^{\mathrm{M}}_k$). Therefore, for all $v \in \mathsf{A}_3$ such that $\mathsf{n}_{\Omega_{\mathsf{K}_{\alpha/2}}}(v)$ is not collinear to $\mathsf{n}_{\mathsf{C}_\alpha}(v)$, there exists a neighborhood O_v of v in Ω such that

$$\mathsf{O}_v \cap \mathsf{A}_3 \text{ is of measure 0 for the surface measure on } \mathsf{O}_v \cap \partial\Omega^{\mathrm{M}}_k. \tag{160}$$

Let us finally consider *the case when* $\mathsf{n}_{\Omega_{\mathsf{K}_{\alpha/2}}}(v) = \pm\mathsf{n}_{\mathsf{C}_\alpha}(v)$. Using (136) and (139), $\mathsf{n}_{\Omega_{\mathsf{K}_{\alpha/2}}}(v) = +\mathsf{n}_{\mathsf{C}_\alpha}(v)$. Moreover, from (135), (138), and (159) there exists a neighborhood O_v of v in Ω such that $\mathsf{O}_v \cap \partial\mathsf{C}_\alpha = \mathsf{O}_v \cap \Sigma^{\mathrm{lateral}}_\alpha$ and thus (see (132) and (133)),

$$\mathsf{O}_v \cap \mathsf{C}_\alpha = \mathsf{O}_v \cap \big\{w \in \overline{\Omega},\, x_1(w) > 0,\, x_d(w) \in (0,\alpha)\big\}$$

and (see (138))

$$\mathsf{O}_v \cap \partial\mathsf{C}_\alpha = \mathsf{O}_v \cap \big\{w \in \overline{\Omega},\, x_1(w) = 0,\, x_d(w) \in (0,\alpha)\big\} \ (= \mathsf{O}_v \cap \Sigma^{\mathrm{lateral}}_\alpha). \tag{161}$$

In the following, with a slight abuse of notation, we will denote by $x = (x_1, \widetilde{x})$ both a point in O_v and its coordinates in the local basis.

In addition, since $\mathsf{n}_{\Omega_{\mathsf{K}_{\alpha/2}}}(v) = +\mathsf{n}_{\mathsf{C}_\alpha}(v)$ and $\partial\Omega_{\mathsf{K}_\alpha}$ is smooth, up to choosing O_v smaller, there exists a smooth function $\Psi : \mathbb{R}^{d-1} \to \mathbb{R}$ such that $\Psi(\widetilde{x}(v)) = x_1(v) = 0$ and

$$\mathsf{O}_v \cap \partial\Omega_{\mathsf{K}_{\alpha/2}} = \{(\Psi(\widetilde{x}), \widetilde{x}),\ x = (x_1, \widetilde{x}) \in \mathsf{O}_v\} \tag{162}$$

is the graph[(4)] of Ψ in the $(x_1, \widetilde{x})$ coordinates, where we set $\widetilde{x} := (x_2, \dots, x_{d-1}, x_d)$. Moreover, one has

$$\mathsf{O}_v \cap \Omega_{\mathsf{K}_{\alpha/2}} = \{x = (x_1, \widetilde{x}) \in \mathsf{O}_v \text{ such that } x_1 > \Psi(\widetilde{x})\}.$$

Therefore, from (141), $\mathsf{O}_v \cap \Omega_k^{\mathrm{M}} = \{x = (x_1, \widetilde{x}) \in \mathsf{O}_v \text{ such that } x_1 > \min(\Psi(\widetilde{x}), 0)\}$ and thus,

$$\mathsf{O}_v \cap \partial\Omega_k^{\mathrm{M}} = \{x = (x_1, \widetilde{x}) \in \mathsf{O}_v \text{ such that } x_1 = \min(\Psi(\widetilde{x}), 0)\}$$

is Lipschitz (indeed $\Upsilon : \widetilde{x} \mapsto \min(\Psi(\widetilde{x}), 0)$ is a Lipschitz function). In addition, for a.e. $x = (x_1, \widetilde{x}) \in \mathsf{O}_v \cap \partial\Omega_k^{\mathrm{M}}$: $\mathsf{n}_{\Omega_k^{\mathrm{M}}}(x) \in \{\mathsf{n}_{\mathsf{C}_\alpha}(x), \mathsf{n}_{\Omega_{\mathsf{K}_\alpha}}(x)\}$. Indeed, in the $(x_1, \widetilde{x})$-coordinates, one has for a.e. $x = (x_1, \widetilde{x}) \in \mathsf{O}_v \cap \partial\Omega_k^{\mathrm{M}}$,

$$T_x\partial\Omega_k^{\mathrm{M}} = \Big\{\big(\widetilde{p} \cdot \nabla\Upsilon(\widetilde{x}), \widetilde{p}\big),\ \widetilde{p} \in \mathbb{R}^{d-1}\Big\} \quad \text{and} \quad \mathsf{n}_{\Omega_k^{\mathrm{M}}}(x) = \frac{(-1, \nabla\Upsilon(\widetilde{x}))}{\sqrt{1 + |\nabla\Upsilon(\widetilde{x})|^2}}.$$

Because for a.e. $\widetilde{x}$, $\nabla\Upsilon(\widetilde{x}) \in \{0, \nabla\Psi(\widetilde{x})\}$, it holds for a.e. $x = (x_1, \widetilde{x}) \in \mathsf{O}_v \cap \partial\Omega_k^{\mathrm{M}}$, $\mathsf{n}_{\Omega_k^{\mathrm{M}}}(x) \in \{\mathsf{n}_{\mathsf{C}_\alpha}(x), \mathsf{n}_{\Omega_{\mathsf{K}_\alpha}}(x)\}$. Moreover, using (136) and (139), it holds for a.e. $x = (x_1, \widetilde{x}) \in \mathsf{O}_v \cap \partial\Omega_k^{\mathrm{M}}$:

$$\nabla f(x) \cdot \mathsf{n}_{\Omega_k^{\mathrm{M}}}(x) > 0. \tag{163}$$

From (160) and (163), we thus conclude that for any point $v \in \mathsf{A}_3$, there exists a neighborhood O_v of v in Ω such that, for the surface measure on $\mathsf{O}_v \cap \partial\Omega_k^{\mathrm{M}}$, either $\mathsf{O}_v \cap \mathsf{A}_3$ is of measure 0 or $\nabla f \cdot \mathsf{n}_{\Omega_k^{\mathrm{M}}} > 0$ a.e. on $\mathsf{O}_v \cap \mathsf{A}_3$. This implies that, for the surface measure on $\partial\Omega_k^{\mathrm{M}}$,

$$\nabla f \cdot \mathsf{n}_{\Omega_k^{\mathrm{M}}} > 0 \quad \text{a.e. on } \mathsf{A}_3. \tag{164}$$

In conclusion, Ω_k^{M} is a Lipschitz subdomain of Ω. Furthermore, we have proved that:

$$\nabla f \cdot \mathsf{n}_{\Omega_k^{\mathrm{M}}} = 0 \quad \text{a.e. on } \overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}} = \partial\Omega_k^{\mathrm{M}} \cap \partial\Omega \ \text{ (see (156) and (147))}.$$

In addition, since (see (147), (152), (155), and (158))

$$\Gamma_{k,\mathbf{N}}^{\mathrm{M}} = \partial\Omega_k^{\mathrm{M}} \cap \Omega = \mathsf{A}_1 \cup (\mathsf{A}_2 \cap \Omega) \cup \mathsf{A}_3,$$

[(4)]The fact that $\mathsf{O}_v \cap \partial\Omega_{\mathsf{K}_{\alpha/2}}$ is the graph of a function of $\widetilde{x}$ is a consequence of the implicit function theorem, since $T_v\partial\Omega_{\mathsf{K}_\alpha} = \{\nabla x_1(v)\}^\perp$ ($\mathsf{n}_{\Omega_{\mathsf{K}_{\alpha/2}}}(v) = +\mathsf{n}_{\mathsf{C}_\alpha}(v)$ and (161)). Indeed, in a neighborhood of $y_0 := (x_1(v), \widetilde{x}(v)) = (0, \widetilde{x}(v))$ in $\mathbb{R}^d$, $\partial\Omega_{\mathsf{K}_\alpha}$ is the set of points $(x_1, \widetilde{x})$ such that $\phi(x_1, \widetilde{x}) = 0$ where $\phi : \mathbb{R}^d \to \mathbb{R}$ is smooth. In particular, $\nabla\phi(y_0) \neq 0$ is collinear to $\mathsf{n}_{\Omega_{\mathsf{K}_{\alpha/2}}}(v)$ and $\nabla_{\mathbf{T}}\phi(y_0) = 0$, where $\nabla_{\mathbf{T}}$ is the tangential gradient of ϕ along $\partial\Omega_{\mathsf{K}_{\alpha/2}}$). Since $T_v\partial\Omega_{\mathsf{K}_\alpha} = \{\nabla x_1(v)\}^\perp$ and $\nabla x_1(v) \perp \nabla\widetilde{x}_q(v)$ for $q = 2, \dots, d$ (we choose normal coordinates systems), one has $\nabla_{\widetilde{x}}\phi(y_0) = \nabla_{\mathbf{T}}\phi(y_0) = 0$ and thus, $\partial_{x_1}\phi(y_0) \neq 0$. Equation (162) then follows from the implicit function theorem.

and $\mathsf{A}_2 \cap \Omega = \partial\Omega_k^{\mathrm{M}} \cap \Sigma_\alpha^{\mathrm{lateral}} \setminus \partial\Omega_{\mathsf{K}_{\alpha/2}}$, one deduces from (153), (157), and (164), that

$$\nabla f \cdot \mathsf{n}_{\Omega_k^{\mathrm{M}}} > 0 \quad \text{a.e. on } \Gamma_{k,\mathbf{N}}^{\mathrm{M}} = \partial\Omega_k^{\mathrm{M}} \cap \Omega.$$

This concludes the proof of Proposition 30. □

3.3. Witten Laplacians with mixed Dirichlet-Neumann boundary conditions associated with $(z_k)_{k=1,\dots,n}$.

— In this section, we define a Witten Laplacian with mixed Dirichlet-Neumann boundary conditions associated with each saddle point z_k of f using the domain Ω_k^{M} constructed in the previous section. The idea is to define a Witten Laplacian in $\Lambda^q L^2(\Omega_k^{\mathrm{M}})$ with Dirichlet boundary conditions on $\Gamma_{k,\mathbf{D}}^{\mathrm{M}}$ (where $\nabla f \cdot \mathsf{n}_{\Omega_k^{\mathrm{M}}} = 0$) and Neumann boundary conditions on $\Gamma_{k,\mathbf{N}}^{\mathrm{M}}$ (where $\nabla f \cdot \mathsf{n}_{\Omega_k^{\mathrm{M}}} > 0$), see Proposition 30. Since $x_0 \in \Omega_k^{\mathrm{M}}$ is the only minimum of f in Ω_k^{M} and $z_k \in \partial\Omega_k^{\mathrm{M}}$ is the only saddle point of f in $\overline{\Omega_k^{\mathrm{M}}}$, we expect, in view of Theorem 4 and the results of [56], that such Witten Laplacians have only one eigenvalue smaller than $\mathsf{c}h$ when $q = 0$ and $q = 1$. Thanks to Witten's complex structure, this eigenvalue, already introduced as $\lambda(\Omega_k^{\mathrm{M}})$ at the beginning of Section 3, will be the same for $q = 0$ and $q = 1$. The quasi-mode $\mathsf{v}_k^{(1)}$ of $\Delta_{f,h}^{\mathsf{Di},(1)}(\Omega)$ associated with z_k will then be defined by multiplying by a cut-off function the principal 1-eigenform $\mathsf{u}_k^{(1)}$ of this Witten Laplacian with mixed Dirichlet-Neumann boundary conditions.

We first give the definition of Witten Laplacians with mixed Dirichlet- Neumann boundary conditions on Lipschitz domains in Section 3.3.1. We then study the spectral properties of these Witten Laplacians and derive some estimates on the principal eigenvalues and eigenforms in Sections 3.3.2, 3.3.3 and 3.3.4

3.3.1. *Witten Laplacians with mixed Dirichlet-Neumann boundary conditions on Lipschitz domains.*

— In this section, in order to ease the notation, we drop the subscript k in $(\Omega_k^{\mathrm{M}}, \Gamma_{k,\mathbf{D}}^{\mathrm{M}}, \Gamma_{k,\mathbf{N}}^{\mathrm{M}})$, since the results will then be applied to each of this triplet, for $k \in \{1, \dots, n\}$. Let thus Ω^{M} be a Lipschitz subdomain of Ω. Let $\Gamma_{\mathbf{D}}^{\mathrm{M}}$ and $\Gamma_{\mathbf{N}}^{\mathrm{M}}$ be two disjoint open subsets of $\partial\Omega^{\mathrm{M}}$ such that $\overline{\Gamma_{\mathbf{D}}^{\mathrm{M}}} \cup \overline{\Gamma_{\mathbf{N}}^{\mathrm{M}}} = \partial\Omega^{\mathrm{M}}$.

This section is organized as follows. We first recall the definition of weak traces for forms $w \in \Lambda^q H_{\mathsf{d}}(\Omega^{\mathrm{M}}) \cap \Lambda^q H_{\mathsf{d}^*}(\Omega^{\mathrm{M}})$ where for $q \in \{0, \dots, d\}$,

$$\Lambda^q H_{\mathsf{d}}(\Omega^{\mathrm{M}}) := \big\{w \in \Lambda^q L^2(\Omega^{\mathrm{M}}),\ \mathsf{d}w \in \Lambda^{q+1} L^2(\Omega^{\mathrm{M}})\big\} \tag{165}$$

and

$$\Lambda^q H_{\mathsf{d}^*}(\Omega^{\mathrm{M}}) := \big\{w \in \Lambda^q L^2(\Omega^{\mathrm{M}}),\ \mathsf{d}^* w \in \Lambda^{q-1} L^2(\Omega^{\mathrm{M}})\big\} \tag{166}$$

are equipped with their natural graph norms. Let us recall the convention $\Lambda^{-1} L^2 = \Lambda^{d+1} L^2 = \{0\}$. Secondly, we state trace estimates and regularity estimates for forms $w \in \Lambda^q H_{\mathsf{d}}(\Omega^{\mathrm{M}}) \cap \Lambda^q H_{\mathsf{d}^*}(\Omega^{\mathrm{M}})$ such that $\mathbf{t}w = 0$ on $\Gamma_{\mathbf{D}}^{\mathrm{M}}$ and $\mathbf{n}w = 0$ on $\Gamma_{\mathbf{N}}^{\mathrm{M}}$. Indeed (see [12, 49]), a trace in $\Lambda^q L^2(\partial\Omega^{\mathrm{M}})$ does not exist in general for such forms except if $\Gamma_{\mathbf{D}}^{\mathrm{M}}$ and $\Gamma_{\mathbf{N}}^{\mathrm{M}}$ meet at an angle strictly smaller than π (measured in Ω^{M}), in the sense of Definition 31. This explains the role of item (3) in Proposition 30. Finally, we introduce the Witten Laplacians of interest, together with an associated Green formula. This formula will be crucial to study the spectral properties of these operators in the next section.

Weak definitions of traces for elements in $\Lambda^q H_{\mathsf{d}}(\Omega^M)$ *or in* $\Lambda^q H_{\mathsf{d}^*}(\Omega^M)$. — Let us recall that for a differential form u in $\Lambda^q L^2(\partial\Omega^{\mathrm{M}})$, the tangential and normal components are defined as follows:

$$u = \mathbf{t}u + \mathbf{n}u \quad \text{with} \quad \mathbf{t}u = \mathbf{i}_{\mathsf{n}_{\Omega^{\mathrm{M}}}}(\mathsf{n}^\flat_{\Omega^{\mathrm{M}}} \wedge u) \quad \text{and} \quad \mathbf{n}u = \mathsf{n}^\flat_{\Omega^{\mathrm{M}}} \wedge (\mathbf{i}_{\mathsf{n}_{\Omega^{\mathrm{M}}}} u), \tag{167}$$

where the superscript $\flat$ stands for the usual musical isomorphism ($\mathsf{n}^\flat_{\Omega^{\mathrm{M}}}$ is the 1-form associated with $\mathsf{n}_{\Omega^{\mathrm{M}}}$, $\mathsf{n}_{\Omega^{\mathrm{M}}}$ being is the unit outward normal to Ω^{M}). Notice that $\mathbf{t}u$ is orthogonal to $\mathbf{n}u$ in $\Lambda^q L^2(\partial\Omega^{\mathrm{M}})$. Let us recall that the mapping

$$w \in \Lambda^q H^1(\Omega^{\mathrm{M}}) \longmapsto w|_{\partial\Omega^{\mathrm{M}}} \in \Lambda^q H^{1/2}(\partial\Omega^{\mathrm{M}}) \tag{168}$$

is well-defined, continuous, and surjective. We would like here to recall the procedure to extend the notion of traces to elements in the subspaces of $\Lambda^q H^1(\Omega^{\mathrm{M}})$: $\Lambda^q H_{\mathsf{d}}(\Omega^{\mathrm{M}})$ and $\Lambda^q H_{\mathsf{d}^*}(\Omega^{\mathrm{M}})$. This is achieved using a duality argument and the standard Green formula which reads for differential forms $(u,v) \in \Lambda^q H^1(\Omega^{\mathrm{M}}) \times \Lambda^{q+1} H^1(\Omega^{\mathrm{M}})$:

$$\begin{aligned}\langle \mathsf{d}u, v\rangle_{L^2(\Omega^{\mathrm{M}})} &- \langle u, \mathsf{d}^* v\rangle_{L^2(\Omega^{\mathrm{M}})} \\ &= \int_{\partial\Omega^{\mathrm{M}}} \langle \mathsf{n}^\flat_{\Omega^{\mathrm{M}}} \wedge u, v\rangle_{T^*_\sigma\Omega^{\mathrm{M}}} d\sigma = \int_{\partial\Omega^{\mathrm{M}}} \langle \mathsf{n}^\flat_{\Omega^{\mathrm{M}}} \wedge u, \mathbf{n}v\rangle_{T^*_\sigma\Omega^{\mathrm{M}}} d\sigma \\ &= \int_{\partial\Omega^{\mathrm{M}}} \langle u, \mathbf{i}_{\mathsf{n}_{\Omega^{\mathrm{M}}}} v\rangle_{T^*_\sigma\Omega^{\mathrm{M}}} d\sigma = \int_{\partial\Omega^{\mathrm{M}}} \langle \mathbf{t}u, \mathbf{i}_{\mathsf{n}_{\Omega^{\mathrm{M}}}} v\rangle_{T^*_\sigma\Omega^{\mathrm{M}}} d\sigma,\end{aligned} \tag{169}$$

where we used the fact that the adjoint of $\mathsf{n}^\flat_{\Omega^{\mathrm{M}}}\wedge$ in $\Lambda^q L^2(\partial\Omega^{\mathrm{M}})$ is $\mathbf{i}_{\mathsf{n}_{\Omega^{\mathrm{M}}}}$. Let us now consider $w \in \Lambda^q H_{\mathsf{d}}(\Omega^{\mathrm{M}})$. Then, $\mathsf{n}^\flat_{\Omega^{\mathrm{M}}} \wedge w$ is defined as an element in $\Lambda^{q+1} H^{-1/2}(\partial\Omega^{\mathrm{M}})$ by: $\forall \phi \in \Lambda^{q+1} H^{1/2}(\partial\Omega^{\mathrm{M}})$,

$$\langle \mathsf{n}^\flat_{\Omega^{\mathrm{M}}} \wedge w, \phi\rangle_{H^{-1/2}(\partial\Omega^{\mathrm{M}}), H^{1/2}(\partial\Omega^{\mathrm{M}})} = \langle \mathsf{d}w, \Phi\rangle_{L^2(\Omega^{\mathrm{M}})} - \langle w, \mathsf{d}^*\Phi\rangle_{L^2(\Omega^{\mathrm{M}})}, \tag{170}$$

where Φ is any form in $\Lambda^{q+1} H^1(\Omega^{\mathrm{M}})$ whose trace in $\Lambda^{q+1} H^{1/2}(\partial\Omega^{\mathrm{M}})$ is ϕ. Recall that this definition is independent of the chosen extension Φ of ϕ (this follows from (169) and the density of $\Lambda^q \mathcal{C}^\infty\big(\overline{\Omega^{\mathrm{M}}}\big)$ in $\Lambda^q H_{\mathsf{d}}(\Omega^{\mathrm{M}})$, see for example [49, Prop. 3.1]). Similarly, for any $w \in \Lambda^q H_{\mathsf{d}^*}(\Omega^{\mathrm{M}})$, $\mathbf{i}_{\mathsf{n}_{\Omega^{\mathrm{M}}}} w \in \Lambda^{q-1} H^{-1/2}(\partial\Omega^{\mathrm{M}})$ is defined by: $\forall \phi \in \Lambda^{q-1} H^{1/2}(\partial\Omega^{\mathrm{M}})$,

$$\langle \mathbf{i}_{\mathsf{n}_{\Omega^{\mathrm{M}}}} w, \phi\rangle_{H^{-1/2}(\partial\Omega^{\mathrm{M}}), H^{1/2}(\partial\Omega^{\mathrm{M}})} = \langle w, \mathsf{d}\Phi\rangle_{L^2(\Omega^{\mathrm{M}})} - \langle \mathsf{d}^* w, \Phi\rangle_{L^2(\Omega^{\mathrm{M}})}, \tag{171}$$

where Φ is any extension of ϕ in $\Lambda^{q-1} H^1(\Omega^{\mathrm{M}})$.

Let us now recover the decomposition (167) for forms $w \in \Lambda^q H_{\mathsf{d}}(\Omega^{\mathrm{M}}) \cap \Lambda^q H_{\mathsf{d}^*}(\Omega^{\mathrm{M}})$ such that, on a subset Γ of $\partial\Omega^{\mathrm{M}}$, the tangential trace or the normal trace are defined in a weak sense. Let $w \in \Lambda^q H_{\mathsf{d}}(\Omega^{\mathrm{M}})$. If $\mathsf{n}^\flat_{\Omega^{\mathrm{M}}} \wedge w \in \Lambda^{q+1} L^2(\Gamma)$, we define $\mathbf{t}w|_\Gamma$, the tangential trace of w on Γ, by

$$\mathbf{t}w|_\Gamma := \mathbf{i}_{\mathsf{n}_{\Omega^{\mathrm{M}}}}(\mathsf{n}^\flat_{\Omega^{\mathrm{M}}} \wedge w) \in \Lambda^q L^2(\Gamma), \quad \text{so that } \|\mathbf{t}w\|_{L^2(\Gamma)} = \|\mathsf{n}^\flat_{\Omega^{\mathrm{M}}} \wedge w\|_{L^2(\Gamma)}. \tag{172}$$

In particular $\mathbf{t}w|_\Gamma = 0$ if $\mathsf{n}^\flat_{\Omega^{\mathrm{M}}} \wedge w|_\Gamma = 0$. Let us now consider $w \in \Lambda^q H_{\mathsf{d}^*}(\Omega^{\mathrm{M}})$. When $\mathbf{i}_{\mathsf{n}_{\Omega^{\mathrm{M}}}} w \in \Lambda^{q-1}L^2(\Gamma)$, we define $\mathbf{n}w|_\Gamma$, the normal trace of w on Γ, by

$$\mathbf{n}u|_\Gamma := \mathsf{n}^\flat_{\Omega^{\mathrm{M}}} \wedge (\mathbf{i}_{\mathsf{n}_{\Omega^{\mathrm{M}}}} u) \in \Lambda^q L^2(\Gamma), \text{ so that } \|\mathbf{n}u\|_{L^2(\Gamma)} = \|\mathbf{i}_{\mathsf{n}_{\Omega^{\mathrm{M}}}} u\|_{L^2(\Gamma)}. \tag{173}$$

In particular, $\mathbf{n}u|_\Gamma = 0$ if $\mathbf{i}_{\mathsf{n}_{\Omega^{\mathrm{M}}}} w|_\Gamma = 0$. Lastly, if $w \in \Lambda^q H_{\mathsf{d}}(\Omega^{\mathrm{M}}) \cap \Lambda^q H_{\mathsf{d}^*}(\Omega^{\mathrm{M}})$ is such that $\mathsf{n}^\flat_{\Omega^{\mathrm{M}}} \wedge w|_\Gamma \in \Lambda^{q+1}L^2(\Gamma)$ and $\mathbf{i}_{\mathsf{n}_{\Omega^{\mathrm{M}}}} w \in \Lambda^{q-1}L^2(\Gamma)$ then w admits a trace $w|_\Gamma$ in $\Lambda^q L^2(\Gamma)$ defined by (see (172) and (173)),

$$w|_\Gamma := \mathbf{t}w|_\Gamma + \mathbf{n}w|_\Gamma. \tag{174}$$

In addition, one has for such w:

$$\|w|_\Gamma\|^2_{L^2(\Gamma)} = \|\mathbf{t}w|_\Gamma\|^2_{L^2(\Gamma)} + \|\mathbf{n}w|_\Gamma\|^2_{L^2(\Gamma)} = \|\mathsf{n}^\flat_{\Omega^{\mathrm{M}}} \wedge w\|^2_{L^2(\Gamma)} + \|\mathbf{i}_{\mathsf{n}_{\Omega^{\mathrm{M}}}} w\|^2_{L^2(\Gamma)}.$$

Let us mention that all the above definitions coincide with the usual ones when w belongs to $\Lambda^q H^1(\Omega^{\mathrm{M}})$. In particular, (174) can be seen as an extension of (167).

Trace estimates for forms $\Lambda^q H_{\mathsf{d}}(\Omega^M) \cap \Lambda^q H_{\mathsf{d}^*}(\Omega^M)$ satisfying mixed Dirichlet-Neumann boundary conditions and when Ω^M is not smooth. — Let Γ be any open Lipschitz subset of $\partial\Omega^{\mathrm{M}}$. According to [49, Prop. 3.1], the space

$$\big\{w \in \Lambda^q \mathcal{C}^\infty\big(\overline{\Omega^{\mathrm{M}}}\big),\ w = 0 \text{ in a neighborhood of } \partial\Omega^{\mathrm{M}} \smallsetminus \Gamma\big\}$$

is dense in

$$\Lambda^q H_{\mathsf{d},\Gamma}(\Omega^{\mathrm{M}}) := \big\{w \in \Lambda^q H_{\mathsf{d}}(\Omega^{\mathrm{M}}),\ \mathrm{supp}(\mathsf{n}^\flat_{\Omega^{\mathrm{M}}} \wedge w) \subset \overline{\Gamma}\big\}$$

and in

$$\Lambda^q H_{\mathsf{d}^*,\Gamma}(\Omega^{\mathrm{M}}) := \big\{w \in \Lambda^q H_{\mathsf{d}^*}(\Omega^{\mathrm{M}}),\ \mathrm{supp}(\mathbf{i}_{\mathsf{n}_{\Omega^{\mathrm{M}}}} w) \subset \overline{\Gamma}\big\}.$$

We are now in position to state the following result which is a consequence of [49, Th. 1.1 & 1.2] (see also [36, Th. 4.1 & 4.2]).

Proposition 32. — *Let us assume that $\Omega^M \subset \mathbb{R}^d$ is a Lipschitz domain. Let $\Gamma^M_{\mathbf{D}}$ and $\Gamma^M_{\mathbf{N}}$ be two disjoint Lipschitz open subsets of $\partial\Omega^M$ such that $\overline{\Gamma^M_{\mathbf{D}}} \cup \overline{\Gamma^M_{\mathbf{N}}} = \partial\Omega^M$ and such that $\Gamma^M_{\mathbf{D}}$ and $\Gamma^M_{\mathbf{N}}$ meet at an angle strictly smaller than π (in the sense of Definition* 31*). Then, the following results hold:*

(i) *Let w be a differential form such that (see* (165), (166), (172), *and* (173)*)*

$$w \in \Lambda^q H_{\mathsf{d}}(\Omega^M) \cap \Lambda^q H_{\mathsf{d}^*}(\Omega^M), \quad \mathbf{t}w|_{\Gamma^M_{\mathbf{D}}} = 0 \quad \textit{and} \quad \mathbf{n}w|_{\Gamma^M_{\mathbf{N}}} = 0.$$

Then w satisfies

$$w \in \Lambda^q H^{1/2}(\Omega^M) \quad \textit{and} \quad \mathbf{i}_{\mathsf{n}_{\Omega^M}} w,\ \mathsf{n}^\flat_{\Omega^M} \wedge w \in \Lambda L^2(\partial\Omega^M)$$

as well as the regularity estimate:

$$\|w\|_{H^{1/2}(\Omega^M)} + \|w|_{\partial\Omega^M}\|_{L^2(\partial\Omega^M)} \leqslant C\big(\|w\|_{L^2(\Omega^M)} + \|\mathsf{d}w\|_{L^2(\Omega^M)} + \|\mathsf{d}^*w\|_{L^2(\Omega^M)}\big), \tag{175}$$

where $w|_{\partial\Omega^M}$ is defined by (174) *and $C > 0$ is independent of w.*

(ii) *Assume that* $f\colon\overline{\Omega^M}\to\mathbb{R}$ *is a* $\mathcal{C}^\infty$ *function. The unbounded operators* $\mathsf{d}^{(q)}_{f,h,\mathbf{T}}(\Omega^M)$ *and* $\delta^{(q)}_{f,h,\mathbf{N}}(\Omega^M)$ *on* $\Lambda^q L^2(\Omega^M)$ *defined by*

$$\mathsf{d}^{(q)}_{f,h,\mathbf{T}}(\Omega^M) = \mathsf{d}^{(q)}_{f,h}$$

with domain

$$\mathcal{D}\big(\mathsf{d}^{(q)}_{f,h,\mathbf{T}}(\Omega^M)\big) = \big\{w\in\Lambda^q L^2(\Omega^M),\ \mathsf{d}_{f,h}w\in\Lambda^{q+1}L^2(\Omega^M),\ \mathbf{t}w|_{\Gamma^M_{\mathbf{D}}}=0\big\},$$

and

$$\delta^{(q)}_{f,h,\mathbf{N}}(\Omega^M) = \mathsf{d}^{(q)\,*}_{f,h}$$

with domain

$$\mathcal{D}\big(\delta^{(p)}_{f,h,\mathbf{N}}(\Omega^M)\big) = \big\{w\in\Lambda^q L^2(\Omega^M),\ \mathsf{d}^*_{f,h}w\in\Lambda^{q-1}L^2(\Omega^M),\ \mathbf{n}w|_{\Gamma^M_{\mathbf{N}}}=0\big\},$$

are closed, densely defined, and adjoint one of each other in $\Lambda^q L^2(\Omega^M)$*.*

On can check that (see [27, Eq. (130)])

$$\begin{cases}\overline{\operatorname{Im}\mathsf{d}_{f,h,\mathbf{T}}}\subset\operatorname{Ker}\mathsf{d}_{f,h,\mathbf{T}} \quad\text{and}\quad \mathsf{d}^2_{f,h,\mathbf{T}}=0,\\ \overline{\operatorname{Im}\delta_{f,h,\mathbf{N}}}\subset\operatorname{Ker}\delta_{f,h,\mathbf{N}} \quad\text{and}\quad \delta^2_{f,h,\mathbf{N}}=0.\end{cases}\tag{176}$$

Witten Laplacian with mixed Dirichlet-Neumann boundary conditions on $\partial\Omega^M$

We are now in position to define the Witten Laplacians with mixed Dirichlet-Neumann boundary conditions on $\partial\Omega^{\mathrm{M}}$ (see also [27, p. 89]).

Proposition 33. — *Let us assume that* Ω^M, $\Gamma^M_{\mathbf{D}}$, *and* $\Gamma^M_{\mathbf{N}}$ *satisfy the assumptions of Proposition* 32*. Let* $q=0,\dots,d$*. Let us define on* $\Lambda L^2(\Omega^M)$ *the operator*

$$\Delta^{M,(q)}_{f,h}(\Omega^M) := \mathsf{d}^{(q-1)}_{f,h,\mathbf{T}}(\Omega^M)\circ\delta^{(q)}_{f,h,\mathbf{N}}(\Omega^M) + \delta^{(q+1)}_{f,h,\mathbf{N}}(\Omega^M)\circ\mathsf{d}^{(q)}_{f,h,\mathbf{T}}(\Omega^M),\tag{177}$$

in the sense of composition of unbounded operators, see Proposition 32 *for the definitions of* $\mathsf{d}_{f,h,\mathbf{T}}(\Omega^M)$ *and* $\delta_{f,h,\mathbf{N}}(\Omega^M)$*. This operator is a densely defined nonnegative self-adjoint operator and its domain is given by*

$$\begin{aligned}\mathcal{D}\big(\Delta^{M,(q)}_{f,h}(\Omega^M)\big) &= \Big\{w\in\Lambda^q L^2(\Omega^M),\ \mathsf{d}_{f,h}w,\mathsf{d}^*_{f,h}w,\mathsf{d}^*_{f,h}\mathsf{d}_{f,h}w,\mathsf{d}_{f,h}\mathsf{d}^*_{f,h}w\in\Lambda L^2(\Omega^M),\\ &\qquad \mathbf{t}w|_{\Gamma^M_{\mathbf{D}}}=0,\ \mathbf{t}\mathsf{d}^*_{f,h}w|_{\Gamma^M_{\mathbf{D}}}=0,\ \mathbf{n}w|_{\Gamma^M_{\mathbf{N}}}=0,\ \mathbf{n}\mathsf{d}_{f,h}w|_{\Gamma^M_{\mathbf{N}}}=0\Big\}.\end{aligned}\tag{178}$$

In addition, the domain $\mathcal{D}\big(Q^{M,(q)}_{f,h}(\Omega^M)\big)$ *of the closed quadratic form* $Q^{M,(q)}_{f,h}(\Omega^M)$ *associated with* $\Delta^{M,(q)}_{f,h}(\Omega^M)$ *is given by*

$$\begin{aligned}\mathcal{D}\big(Q^{M,(q)}_{f,h}(\Omega^M)\big) &= \mathcal{D}\big(\mathsf{d}^{(q)}_{f,h,\mathbf{T}}(\Omega^M)\big)\cap\mathcal{D}\big(\delta^{(q)}_{f,h,\mathbf{N}}(\Omega^M)\big)\\ &= \Big\{w\in\Lambda^q H_{\mathsf{d}}(\Omega^M)\cap\Lambda^q H_{\mathsf{d}^*}(\Omega^M),\ \mathbf{t}w|_{\Gamma^M_{\mathbf{D}}}=0 \quad\textit{and}\quad \mathbf{n}w|_{\Gamma^M_{\mathbf{N}}}=0\Big\}\end{aligned}$$

and for any $u,w\in\mathcal{D}\big(Q^{M,(q)}_{f,h}(\Omega^M)\big)$,

$$Q^{M,(q)}_{f,h}(\Omega^M)(u,w) = \langle\mathsf{d}_{f,h,\mathbf{T}}u,\mathsf{d}_{f,h,\mathbf{T}}w\rangle_{L^2(\Omega^M)} + \langle\delta_{f,h,\mathbf{N}}u,\delta_{f,h,\mathbf{N}}w\rangle_{L^2(\Omega^M)}.$$

Let us mention an important consequence of Proposition 32. For $w\in\mathcal{D}\big(\Delta^{M,(q)}_{f,h}(\Omega^{\mathrm{M}})\big)$, the traces $\mathbf{t}\mathsf{d}^*_{f,h}w$ and $\mathbf{n}\mathsf{d}_{f,h}w$ are a priori defined in $\Lambda H^{-1/2}(\partial\Omega^{\mathrm{M}})$ but actually belong to $\Lambda L^2(\partial\Omega^{\mathrm{M}})$. Indeed, $\mathbf{n}\mathsf{d}_{f,h}u|_{\Gamma^{\mathrm{M}}_{\mathbf{N}}}=0$ by definition of $\mathcal{D}\big(\Delta^{\mathrm{M},(q)}_{f,h}(\Omega^{\mathrm{M}})\big)$ and $\mathbf{t}\mathsf{d}_{f,h}w|_{\Gamma^{\mathrm{M}}_{\mathbf{D}}}=0$ using (176). Therefore, $\mathsf{d}_{f,h}w$ is in $\mathcal{D}\big(Q^{\mathrm{M},(q+1)}_{f,h}(\Omega^{\mathrm{M}})\big)$ and therefore has a trace in $\Lambda L^2(\partial\Omega^{\mathrm{M}})$ according to Proposition 32. This argument also holds for $\mathsf{d}^*_{f,h}w\in\mathcal{D}\big(Q^{\mathrm{M},(q-1)}_{f,h}(\Omega^{\mathrm{M}})\big)$.

We end up this section with a Green formula which will be frequently used in the sequel (see [60, Lem. 2.10]).

Lemma 34. — *Let us assume that Ω^M, $\Gamma^M_{\mathbf{D}}$, and $\Gamma^M_{\mathbf{N}}$ satisfy the assumptions of Proposition 32. Let $q=0,\dots,d$. Let φ be a real-valued Lipschitz function on $\overline{\Omega^M}$. Then, for any $w\in\mathcal{D}\big(Q^{M,(q)}_{f,h}(\Omega^M)\big)$, one has:*

$$(179)\quad Q^{M,(q)}_{f,h}(\Omega^M)(w,e^{(2/h)\varphi}w)=h^2\big\|\mathsf{d}(e^{\varphi/h}w)\big\|^2_{L^2(\Omega^M)}+h^2\big\|\mathsf{d}^*(e^{\varphi/h}w)\big\|^2_{L^2(\Omega^M)}$$
$$+\big\langle(|\nabla f|^2-|\nabla\varphi|^2+h\mathcal{L}_{\nabla f}+h\mathcal{L}^*_{\nabla f})e^{\varphi/h}w,e^{\varphi/h}w\big\rangle_{L^2(\Omega^M)}$$
$$+h\bigg(\int_{\Gamma^M_{\mathbf{N}}}-\int_{\Gamma^M_{\mathbf{D}}}\bigg)\langle w,w\rangle_{T^*_\sigma\Omega^M}\,e^{(2/h)\varphi}\partial_{\mathsf{n}_{\Omega^M}}f\,d\sigma,$$

where we recall that $\mathcal{L}$ stands for the Lie derivative. Moreover, when w belongs to $\mathcal{D}\big(\Delta^{M,(q)}_{f,h}(\Omega^M)\big)$, the left-hand side of (179) *equals $\langle e^{(2/h)\varphi}\Delta^{M,(q)}_{f,h}(\Omega^M)w,w\rangle_{L^2(\Omega^M)}$.*

In the following, we will use this lemma several times with $(\Omega^{\mathrm{M}},\Gamma^{\mathrm{M}}_{\mathbf{D}},\Gamma^{\mathrm{M}}_{\mathbf{N}})=(\Omega^{\mathrm{M}}_k,\Gamma^{\mathrm{M}}_{k,\mathbf{D}},\Gamma^{\mathrm{M}}_{k,\mathbf{N}})$ (for $k\in\{1,\dots,n\}$), in which case $\partial_{\mathsf{n}_{\Omega^{\mathrm{M}}}}f=0$ on $\Gamma^{\mathrm{M}}_{\mathbf{D}}$ and $\partial_{\mathsf{n}_{\Omega^{\mathrm{M}}}}f>0$ on $\Gamma^{\mathrm{M}}_{\mathbf{N}}$ (see items (1b) and (2) in Proposition 30).

3.3.2. *Spectral properties of $\Delta^{M,(q)}_{f,h}(\Omega^M_k)$*

In view of Proposition 30, the results of Section 3.3.1 can be applied, for any $k\in\{1,\dots,n\}$, to $(\Omega^{\mathrm{M}},\Gamma^{\mathrm{M}}_{\mathbf{D}},\Gamma^{\mathrm{M}}_{\mathbf{N}})=(\Omega^{\mathrm{M}}_k,\Gamma^{\mathrm{M}}_{k,\mathbf{D}},\Gamma^{\mathrm{M}}_{k,\mathbf{N}})$. The main result of this section concerns the spectrum of the operator $\Delta^{\mathrm{M},(q)}_{f,h}(\Omega^{\mathrm{M}}_k)$, defined in Proposition 33.

Proposition 35. — *Let us assume that* $(\Omega\text{-}f)$ *is satisfied. Let $k\in\{1,\dots,n\}$ and Ω^M_k be the domain introduced in Proposition* 30. *For $q\in\{0,\dots,d\}$, let $\Delta^{M,(q)}_{f,h}(\Omega^M_k)$ be the unbounded nonnegative self-adjoint operator on $\Lambda^qL^2(\Omega^M_k)$ defined by* (177)–(178) *with $(\Omega^M,\Gamma^M_{\mathbf{D}},\Gamma^M_{\mathbf{N}})=(\Omega^M_k,\Gamma^M_{k,\mathbf{D}},\Gamma^M_{k,\mathbf{N}})$. Then, the following holds true:*

(i) *The operator $\Delta^{M,(q)}_{f,h}(\Omega^M_k)$ has compact resolvent.*

(ii) *For any eigenvalue λ of $\Delta^{M,(q)}_{f,h}(\Omega^M_k)$ and any associated eigenform $w^{(q)}$ in $\mathcal{D}\big(\Delta^{M,(q)}_{f,h}(\Omega^M_k)\big)$, one has*

$$\mathsf{d}_{f,h}w^{(q)}\in\mathcal{D}\big(\Delta^{M,(q+1)}_{f,h}(\Omega^M_k)\big)\quad\text{and}\quad\mathsf{d}^*_{f,h}w^{(q)}\in\mathcal{D}\big(\Delta^{M,(q-1)}_{f,h}(\Omega^M_k)\big),$$

with

$$\mathsf{d}_{f,h}\Delta^{M,(q)}_{f,h}(\Omega^M_k)w^{(q)}=\Delta^{M,(q+1)}_{f,h}(\Omega^M_k)\mathsf{d}_{f,h}w^{(q)}=\lambda\mathsf{d}_{f,h}w^{(q)}$$

and

$$\mathsf{d}^*_{f,h}\Delta^{M,(q)}_{f,h}(\Omega^M_k)w^{(q)}=\Delta^{M,(p-1)}_{f,h}(\Omega^M_k)\mathsf{d}^*_{f,h}w^{(q)}=\lambda\mathsf{d}^*_{f,h}w^{(q)}.$$

If in addition $\lambda\neq0$, either $\mathsf{d}_{f,h}w^{(q)}$ or $\mathsf{d}^*_{f,h}w^{(q)}$ is non-zero.

(iii) *There exist* $\mathsf{c}>0$ *and* $h_0>0$ *such that for any* $q\in\{0,\dots,d\}$ *and* $h\in(0,h_0)$,

$$\dim\mathrm{Ran}\ \pi_{[0,\mathsf{c}h]}\big(\Delta^{M,(q)}_{f,h}(\Omega^M_k)\big)=\begin{cases}1 & \text{if } q\in\{0,1\},\\ 0 & \text{if } q\in\{2,\dots,d\},\end{cases}$$

In addition, for all $h\in(0,h_0)$, *there exists* $\lambda(\Omega^M_k)\geqslant 0$ *such that for* $q\in\{0,1\}$,

$$\mathrm{Sp}\big(\Delta^{M,(q)}_{f,h}(\Omega^M_k)\big)\cap[0,\mathsf{c}h]=\{\lambda(\Omega^M_k)\}.$$

Finally, $\lambda(\Omega^M_k)$ *is non-zero and is exponentially small when* $h\to 0$.

Proof. — Item (i) is a consequence of the compactness of the embedding

$$\Lambda^q H^{1/2}(\Omega^{\mathrm{M}}_k)\longrightarrow\Lambda^q L^2(\Omega^{\mathrm{M}}_k)$$

and of the continuous inclusion $\mathcal{D}\big(\Delta^{\mathrm{M},(q)}_{f,h}(\Omega^{\mathrm{M}}_k)\big)\hookrightarrow\Lambda^q H^{1/2}(\Omega^{\mathrm{M}}_k)$ (see Proposition 32). Item (ii) is a straightforward consequence of the characterization of the domain of $\Delta^{\mathrm{M},(q)}_{f,h}(\Omega^{\mathrm{M}}_k)$ together with (176). Moreover, if $\lambda\neq 0$, then

$$\begin{aligned}0\neq\lambda\|w^{(q)}\|^2_{L^2(\Omega^{\mathrm{M}}_k)}&=\langle\Delta^{\mathrm{M},(q)}_{f,h}(\Omega^{\mathrm{M}}_k)w^{(q)},w^{(q)}\rangle_{L^2(\Omega^{\mathrm{M}}_k)}\\&=\langle\mathsf{d}_{f,h}w^{(q)},\mathsf{d}_{f,h}w^{(q)}\rangle_{L^2(\Omega^{\mathrm{M}}_k)}+\langle\mathsf{d}^*_{f,h}w^{(q)},\mathsf{d}^*_{f,h}w^{(q)}\rangle_{L^2(\Omega^{\mathrm{M}}_k)},\end{aligned}$$

which implies that either $\mathsf{d}_{f,h}w^{(q)}$ or $\mathsf{d}^*_{f,h}w^{(q)}$ is non-zero. Let us now prove item (iii) in Proposition 35. It is a consequence of Lemma 34 (with $\varphi=0$) and the fact that the normal derivative of f on $\Gamma^{\mathrm{M}}_{k,\mathbf{N}}$ is non negative (see item 2 in Proposition 30) together with arguments already used in Section 2.4. Let us be more precise on this. The function f is $\mathcal{C}^\infty$ on $\overline{\Omega^{\mathrm{M}}_k}$ and its critical points in $\overline{\Omega^{\mathrm{M}}_k}$ are exactly x_0 and z_k. Moreover, for $\varepsilon>0$ small enough,

$$\overline{\Omega^{\mathrm{M}}_k}\cap\{x\in\overline{\Omega},\,x_d(x)\in[0,\varepsilon]\}=\overline{\mathsf{C}_\alpha}\cap\{x\in\overline{\Omega},\,x_d(x)\in[0,\varepsilon]\}=\overline{\mathsf{C}_\varepsilon}.\tag{180}$$

In particular, Ω^{M}_k is smooth near z_k and

$$\mathsf{n}_{\Omega^{\mathrm{M}}_k}=\mathsf{n}_{\mathsf{C}_\alpha}=\mathsf{n}_\Omega\quad\text{on }\Gamma^{\mathrm{M}}_{k,\mathbf{D}}.\tag{181}$$

From assumption (Ω-f), it thus holds $\partial_{\mathsf{n}_{\Omega^{\mathrm{M}}_k}}f=0$ on $\Gamma^{\mathrm{M}}_{k,\mathbf{D}}$. Therefore, we can consider two neighborhoods V_{x_0} and V_{z_k} of respectively x_0 and z_k in $\overline{\Omega^{\mathrm{M}}_k}$ such that

– $\overline{\mathsf{V}_{x_0}}\subset\Omega^{\mathrm{M}}_k$ and x_0 is the only critical point of f in $\overline{\mathsf{V}_{x_0}}$,

– $\overline{\mathsf{V}_{z_k}}\cap\overline{\Gamma^{\mathrm{M}}_{k,\mathbf{N}}}=\varnothing$, $\partial_{\mathsf{n}_{\Omega^{\mathrm{M}}_k}}f=0$ on $\partial\overline{\Omega^{\mathrm{M}}_k}\cap\overline{\mathsf{V}_{z_k}}$ and, z_k is the only critical point of f in $\overline{\mathsf{V}_{z_k}}$,

– $\overline{\mathsf{V}_{x_0}}\cap\overline{\mathsf{V}_{z_k}}=\varnothing$.

For $y\in\{x_0,z_k\}$, let $\chi_y:\overline{\Omega^{\mathrm{M}}_k}\to[0,1]$ be a $\mathcal{C}^\infty$ supported in V_y and such that $\chi_y=1$ in a neighborhood of y in $\overline{\Omega^{\mathrm{M}}_k}$. Then, one defines:

$$\widetilde{\chi}:=\sqrt{1-\chi^2_{x_0}-\chi^2_{z_k}},$$

so that on $\overline{\Omega^{\mathrm{M}}_k}$, $\widetilde{\chi}^2+\chi^2_{x_0}+\chi^2_{z_k}=1$. Let $w\in\mathcal{D}(Q^{\mathrm{M},(q)}_{f,h}(\Omega^{\mathrm{M}}_k))$. The IMS formula [19, 42] yields:

$$\begin{aligned}Q^{\mathrm{M},(q)}_{f,h}(\Omega^{\mathrm{M}}_k)(w)&=Q^{\mathrm{M},(q)}_{f,h}(\widetilde{\chi}w)-h^2\,\|w\,\nabla\widetilde{\chi}\|^2_{L^2(\Omega^{\mathrm{M}}_k)}\\&\qquad+\sum_{y\in\{x_0,z_k\}}Q^{\mathrm{M},(q)}_{f,h}(\chi_y w)-h^2\,\big\|w\,\nabla\chi_y\big\|^2_{L^2(\Omega^{\mathrm{M}}_k)}.\end{aligned}$$

This formula easily follows from Lemma 34 (with $\varphi=0$) and the fact that $\widetilde{\chi}^2+\chi_{x_0}^2+\chi_{z_k}^2=1$ and $\chi w\in \mathcal{D}(Q^{\mathrm{M},(q)}_{f,h}(\Omega^{\mathrm{M}}_k))$ for any smooth function $\chi:\overline{\Omega^{\mathrm{M}}_k}\to\mathbb{R}$.

In the following $C>0$ and $c>0$ are constants independent of h and w, and which can change from one occurrence to another. Since $|\nabla f|^2\geqslant c$ on the support of $\widetilde{\chi}$ in $\overline{\Omega^{\mathrm{M}}_k}$, one deduces from Lemma 34 (applied to $\widetilde{\chi}w$ with $\varphi=0$), and the fact that $\partial_{\mathsf{n}_{\Omega^{\mathrm{M}}_k}}f>0$ on $\Gamma^{\mathrm{M}}_{k,\mathbf{N}}$ that for h small enough

$$Q^{\mathrm{M},(q)}_{f,h}(\Omega^{\mathrm{M}}_k)(\widetilde{\chi}w)\geqslant c\|w\,\widetilde{\chi}\|^2_{L^2(\Omega^{\mathrm{M}}_k)}.$$

Then, using the previous IMS formula, it holds for h small enough,

$$Q^{\mathrm{M},(q)}_{f,h}(\Omega^{\mathrm{M}}_k)(w)\geqslant c\|w\,\widetilde{\chi}\|^2_{L^2(\Omega^{\mathrm{M}}_k)}+\sum_{y\in\{x_0,z_k\}}Q^{\mathrm{M},(q)}_{f,h}(\Omega^{\mathrm{M}}_k)(\chi_y w)-Ch^2\|w\|^2_{L^2(\Omega^{\mathrm{M}}_k)}. \tag{182}$$

Let us assume that $q\geqslant 2$. Then, by the same analysis as in item (2) in Step 1b and item (2) in Step 3 in Section 2.4, one has (up to choosing V_{x_0} and V_{z_k} smaller), for all $y\in\{x_0,z_k\}$ and h small enough $Q^{\mathrm{M},(q)}_{f,h}(\Omega^{\mathrm{M}}_k)(\chi_y w)\geqslant Ch\|\chi_y w\|^2_{L^2(\Omega^{\mathrm{M}}_k)}$. Hence, using (182), it follows that, when $q\geqslant 2$,

$$Q^{\mathrm{M},(q)}_{f,h}(\Omega^{\mathrm{M}}_k)(w)\geqslant Ch\|w\|^2_{L^2(\Omega^{\mathrm{M}}_k)}.$$

This proves the first statement in item (iii) in Proposition 35 when $q\geqslant 2$.

Let us now consider $q\in\{0,1\}$. By the same analysis as in item (2) in Step 1b and item (1) in Step 3 in Section 2.4, one has that (up to choosing V_{x_0} and V_{z_k} smaller) for h small enough $Q^{\mathrm{M},(0)}_{f,h}(\Omega^{\mathrm{M}}_k)(\chi_{z_k}w)\geqslant Ch\|\chi_{z_k}w\|^2_{L^2(\Omega^{\mathrm{M}}_k)}$ and $Q^{\mathrm{M},(1)}_{f,h}(\Omega^{\mathrm{M}}_k)(\chi_{x_0}w)\geqslant Ch\|\chi_{x_0}w\|^2_{L^2(\Omega^{\mathrm{M}}_k)}$. Let us now assume that

$$Q^{\mathrm{M},(q)}_{f,h}(\Omega^{\mathrm{M}}_k)(w)\leqslant \mathsf{c}h\|w\|^2_{L^2(\Omega^{\mathrm{M}}_k)},$$

for some $\mathsf{c}>0$. Using the same arguments than those used in Step 4 in Section 2.4 (up to choosing V_{x_0} and V_{z_k} smaller), one obtains that, if $q=0$ (resp. $q=1$), w is at a distance $(\sqrt{\mathsf{c}}+o(1))\|w\|_{L^2(\Omega^{\mathrm{M}}_k)}$ of the one dimensional vector space spanned by $\Phi^{x_0}_h=\chi_{x_0}\Psi^{x_0}_h\,/\,\|\chi_{x_0}\Psi^{x_0}_h\|_{L^2(\Omega^{\mathrm{M}}_k)}$, see (102), (103), and (117) (resp. spanned by $\Phi^{z_k}_h=\chi_{z_k}\Psi^{z_k}_h\,/\,\|\chi_{z_k}\Psi^{z_k}_h\|_{L^2(\Omega^{\mathrm{M}}_k)}$, see (111), (112), and (117)). Hence, for $\mathsf{c}>0$ small enough and h small enough

$$\dim\operatorname{Ran}\ \pi_{[0,\mathsf{c}h]}\big(\Delta^{\mathrm{M},(q)}_{f,h}(\Omega^{\mathrm{M}}_k)\big)\leqslant 1.$$

Besides, using Proposition 33, $\Phi^{x_0}_h\in\mathcal{D}(Q^{\mathrm{M},(0)}_{f,h}(\Omega^{\mathrm{M}}_k))$ because the function $\Phi^{x_0}_h$ is smooth and is supported in $\overline{\mathsf{V}_{x_0}}\subset\Omega^{\mathrm{M}}_k$. It also holds $\Phi^{z_k}_h\in\mathcal{D}(Q^{\mathrm{M},(1)}_{f,h}(\Omega^{\mathrm{M}}_k))$. Indeed, the 1-form $\Phi^{z_k}_h$ is smooth, supported in $\overline{\mathsf{V}_{z_k}}\subset\overline{\Omega^{\mathrm{M}}_k}$ and $\overline{\mathsf{V}_{z_k}}\cap\overline{\Gamma^{\mathrm{M}}_{k,\mathbf{N}}}=\varnothing$, and therefore: $\mathbf{t}\Phi^{z_k}_h=0$ on $\Gamma^{\mathrm{M}}_{k,\mathbf{D}}$ and $\Phi^{z_k}_h=0$ on $\Gamma^{\mathrm{M}}_{k,\mathbf{N}}$. Using the Min-Max principle, Equations (103) (with $y=x_0$) and (112) (with $y=z_k$), one deduces that $\Delta^{\mathrm{M},(q)}_{f,h}(\Omega^{\mathrm{M}}_k)$ admits at least one eigenvalue $\lambda^{\mathrm{M},(q)}$ of order $O(h^2)$ when $h\to 0$. This shows that $\dim\operatorname{Ran}\ \pi_{[0,\mathsf{c}h]}\big(\Delta^{\mathrm{M},(q)}_{f,h}(\Omega^{\mathrm{M}}_k)\big)=1$ if $q\in\{0,1\}$.

Using the complex property (see (ii) in Proposition 35), it holds $\lambda^{\mathrm{M},(0)}=\lambda^{\mathrm{M},(1)}=:\lambda(\Omega^{\mathrm{M}}_k)$ for h small enough. In addition, $\lambda^{\mathrm{M},(0)}>0$ because $e^{-(1/h)f}$ does not belong to the domain of $\Delta^{\mathrm{M},(0)}_{f,h}(\Omega^{\mathrm{M}}_k)$. Finally, the fact that $\lambda^{\mathrm{M},(0)}$ is exponentially small when $h\to 0$ follows by standard arguments, using the test function $\chi_{x_0}e^{-(1/h)f}$ in the Min-Max principle for $\Delta^{\mathrm{M},(0)}_{f,h}(\Omega^{\mathrm{M}}_k)$ (see the end of the proof of Corollary 25 for a similar reasoning). The proof of Proposition 35 is complete. ☐

3.3.3. *Asymptotic equivalents of* $\lambda(\Omega^M_k)$ *and of* $\int_{\Gamma^M_{k,\mathbf{D}}}\mathsf{u}^{(1)}_k\cdot\mathsf{n}_{\Omega^M_k}\,e^{-(1/h)f}$. — Let us now provide asymptotic results on the principal eigenvalue and eigenform of $\Delta^{\mathrm{M},(1)}_{f,h}(\Omega^{\mathrm{M}}_k)$.

Proposition 36. — *Let us assume that assumption* (Ω-f) *is satisfied. Let* $k\in\{1,\dots,n\}$ *and* Ω^M_k *be the domain introduced in Proposition* 30. *For* $q\in\{0,1\}$, *let* $\Delta^{M,(q)}_{f,h}(\Omega^M_k)$ *be the unbounded nonnegative self-adjoint operator on* $\Lambda^qL^2(\Omega^M_k)$ *defined by* (177)–(178) *with* $(\Omega^M,\Gamma^M_{\mathbf{D}},\Gamma^M_{\mathbf{N}})=(\Omega^M_k,\Gamma^M_{k,\mathbf{D}},\Gamma^M_{k,\mathbf{N}})$.

Let $\lambda(\Omega^M_k)$ *be the principal eigenvalue of* $\Delta^{M,(q)}_{f,h}(\Omega^M_k)$ *(as introduced in item* (iii) *of Proposition* 35*). Then, it holds in the limit* $h\to 0$*:*

$$\lambda(\Omega^M_k)=\mathsf{A}_{x_0,z_k}h\,e^{-(2/h)(f(z_k)-f(x_0))}(1+O(\sqrt{h})) \tag{183}$$

with

$$\mathsf{A}_{x_0,z_k}:=\frac{2|\mu_{z_k}|\big(\det\operatorname{Hess}f(x_0)\big)^{1/2}}{\pi\big|\det\operatorname{Hess}f(z_k)\big|^{1/2}}, \tag{184}$$

where μ_{z_k} *is the negative eigenvalue of* $\operatorname{Hess}f(z_k)$.

Let $\mathsf{u}^{(1)}_k$ *be a* $L^2(\Omega^M_k)$*-normalized eigenform of* $\Delta^{M,(1)}_{f,h}(\Omega^M_k)$ *associated with the eigenvalue* $\lambda(\Omega^M_k)$. *The* 1*-form* $\mathsf{u}^{(1)}_k$ *is unique up to a multiplication by* ±1. *This multiplicative factor can be chosen such that: in the limit* $h\to 0$,

$$\int_{\Gamma^M_{k,\mathbf{D}}}\mathsf{u}^{(1)}_k\cdot\mathsf{n}_{\Omega^M_k}\,e^{-(1/h)f}=-\mathsf{b}_kh^{\mathsf{m}}\,e^{-(1/h)f(z_k)}(1+O(\sqrt{h})), \tag{185}$$

where

$$\mathsf{b}_k:=\sqrt{\mathsf{A}_{x_0,z_k}\kappa_{x_0}},\ \ \kappa_{x_0}:=\frac{\pi^{d/2}}{\sqrt{\det\operatorname{Hess}f(x_0)}},\quad \textit{and}\quad \mathsf{m}:=\frac{d}{4}-\frac{1}{2}. \tag{186}$$

Proof. — The proof of Proposition 36 is divided into three steps.

Step 1: Construction of the quasi-mode $\varphi^{M,(0)}_k$ *for* $\Delta^{M,(0)}_{f,h}(\Omega^M_k)$. — Let $\varepsilon>0$ be small enough such that $\overline{\Omega_{\mathsf{K}_{\alpha/2}}}\subset\{x_d>5\varepsilon\}$. Then it holds (see (180) and (135))

$$\overline{\Omega^{\mathrm{M}}_k}\cap\{x\in\overline{\Omega},\,x_d(x)\in[0,4\varepsilon]\}=\overline{\mathsf{C}_\alpha}\cap\{x\in\overline{\Omega},x_d(x)\in[0,4\varepsilon]\}=\overline{\mathsf{C}_{4\varepsilon}}. \tag{187}$$

Notice that since $x_0\in\Omega_{\mathsf{K}_{\alpha/2}}$, it then holds

$$x_0\in\Omega^{\mathrm{M}}_k\cap\{x\in\overline{\Omega},x_d(x)>4\varepsilon\}. \tag{188}$$

Since z_k belongs to the open set $\Gamma^{\mathrm{M}}_{k,\mathbf{D}}$, one can consider $r>0$ small enough such that $\overline{\mathsf{B}_{\partial\Omega}(z_k,r)}\subset\Gamma^{\mathrm{M}}_{k,\mathbf{D}}$ (where $\mathsf{B}_{\partial\Omega}(z_k,r)$ is the open ball of radius $r>0$ centered at z_k in $\partial\Omega$). Define

$$\mathsf{V}^r_{4\varepsilon}(z_k):=\{x\in\overline{\Omega},\,\mathsf{z}(x)\in\overline{\mathsf{B}_{\partial\Omega}(z_k,r)}\text{ and }x_d\in[0,4\varepsilon]\}\subset\overline{\mathsf{C}_{4\varepsilon}}. \tag{189}$$

A schematic representation of $\mathsf{V}^r_{4\varepsilon}(z_k)$ is given in Figure 6.

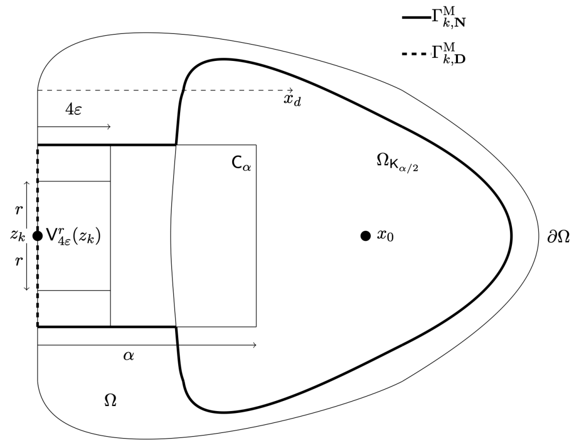

Figure 6. A schematic representation of $\mathsf{V}^r_{4\varepsilon}(z_k)$.

For each $z \in \overline{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}}$, recall that $x' = (x_1, \dots, x_{d-1})$ is a system of coordinates defined in a neighborhood of z in $\partial\Omega$ such that (131), (132), and (133) hold. Recall that $x \mapsto (\mathsf{z}(x), x_d(x))$ introduced in (105) and (129) defines a $\mathcal{C}^\infty$ diffeomorphism on $\{x \in \overline{\Omega},\ x_d(x) \in [0, 3\varepsilon)\}$. To ease the notation, from now on, we simply write $\{x_d \in \mathsf{O}\}$ for the set $\{x \in \overline{\Omega}, x_d(x) \in \mathsf{O}\}$ for $\mathsf{O} \subset \mathbb{R}_+$. Recall that by (106) and since $\mathsf{n}_{\mathsf{M}}(z_k)$ is an eigenvector of $\operatorname{Hess} f(z_k)$ for the eigenvalue $\mu_{z_k} < 0$, up to choosing $\varepsilon > 0$ and $r > 0$ smaller,

(190) $\forall x = (x', x_d) \in \mathsf{V}^r_{4\varepsilon}(z_k),$
$$f(x) \;=\; f(0) + \frac{1}{2} x' \cdot \operatorname{Hess} f|_{\partial\Omega}(z_k) x' - \frac{|\mu_{z_k}|}{2}\, x_d^2 + O(|x|^3).$$

Since $\operatorname{Hess} f|_{\partial\Omega}(z_k)$ is positive-definite, we may assume in the following that $r > 0$ and $\varepsilon > 0$ are small enough such that
$$\{z_k\} = \operatorname*{arg\,min}_{\mathsf{V}^r_{4\varepsilon}(z_k)} (f + |\mu_{z_k}| x_d^2). \tag{191}$$

Moreover, because
$$\overline{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}} \subset \Gamma_{z_k} \quad \text{and} \quad \Gamma_{z_k} \subset \mathsf{W}^+_{z_k}$$
(see (14)), one has $\{z_k\} = \operatorname{arg\,min}_{\overline{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}}} f$. With a slight abuse of notation, we still denote by f the function f in the (z, x_d) variable. Since $f(\mathsf{z}, x_d) = f(\mathsf{z}, 0) + o_\varepsilon(1)$ uniformly on $x = (\mathsf{z}, x_d) \in \overline{\mathsf{C}_{4\varepsilon}}$ as $\varepsilon \to 0$, it thus holds if in addition $\mathsf{z} \in \overline{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}} \smallsetminus \overline{\mathsf{B}_{\partial\Omega}(z_k, r)}$, $f(\mathsf{z}, x_d) \geqslant f(z_k) + c - o_\varepsilon(1)$ for some $c > 0$ independent of $x_d \in [0, 4\varepsilon]$. This implies that up to choosing $\varepsilon > 0$ smaller, it holds for some $c > 0$,

(192) $f > f(z_k) + c/2$
$$\text{on } \overline{\mathsf{C}_{4\varepsilon}} \smallsetminus \mathsf{V}^r_{4\varepsilon}(z_k) = \{x = (\mathsf{z}, x_d), \mathsf{z} \in \overline{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}} \smallsetminus \overline{\mathsf{B}_{\partial\Omega}(z_k, r)}, x_d \in [0, 4\varepsilon]\}.$$

Let us consider $\chi \in \mathcal{C}^\infty(\mathbb{R}_+, [0,1])$ such that supp $\chi \subset [0,\varepsilon]$ and $\chi = 1$ on $[0,\varepsilon/2]$. Inspired by [8] (see also [58, §4.2] and [25]), we build a quasi-mode for $\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})$ using the function $\phi_k^{\mathrm{M},(0)}$ defined on $\overline{\mathsf{C}_\alpha} \cap \{x_d \in [0,2\varepsilon]\} = \overline{\mathsf{C}_{2\varepsilon}}$ (see (135)) by:

$$\forall x = (\mathsf{z}, x_d) \in \overline{\mathsf{C}_{2\varepsilon}}, \quad \phi_k^{\mathrm{M},(0)}(\mathsf{z}, x_d) := \frac{\int_0^{x_d} \chi(t) e^{-(1/h)|\mu_{z_k}|\, t^2} dt}{\int_0^{2\varepsilon} \chi(t)\, e^{-(1/h)|\mu_{z_k}|\, t^2} dt}. \tag{193}$$

Notice that the function $\phi_k^{\mathrm{M},(0)}$ only depends on the variable x_d. Moreover, one has:

$$\phi_k^{\mathrm{M},(0)} \in \mathcal{C}^\infty\big(\overline{\mathsf{C}_{2\varepsilon}}\big) \quad \text{and} \quad \forall x = (\mathsf{z}, x_d) \in \overline{\mathsf{C}_{2\varepsilon}},\ \phi_k^{\mathrm{M},(0)}(x) = 1 \text{ if } x_d \in [\varepsilon, 2\varepsilon].$$

Let us set for $x = (\mathsf{z}, x_d) \in \overline{\mathsf{C}_{2\varepsilon}}$:

$$\psi_k^{\mathrm{M},(0)}(x) = \phi_k^{\mathrm{M},(0)}(\mathsf{z}, x_d). \tag{194}$$

We extend $\psi_k^{\mathrm{M},(0)}$ from $\overline{\mathsf{C}_{2\varepsilon}} = \overline{\Omega_k^{\mathrm{M}}} \cap \{x_d \in [0,2\varepsilon]\}$ (see (187)) to $\overline{\Omega_k^{\mathrm{M}}}$ by setting $\psi_k^{\mathrm{M},(0)} = 1$ on $\overline{\Omega_k^{\mathrm{M}}} \cap \{x_d > 2\varepsilon\} = \overline{\Omega_k^{\mathrm{M}}} \smallsetminus \overline{\mathsf{C}_{2\varepsilon}}$. One then has $\psi_k^{\mathrm{M},(0)} \in \mathcal{C}^\infty\big(\overline{\Omega_k^{\mathrm{M}}}\big)$. Notice that from (188),

$$\psi_k^{\mathrm{M},(0)} = 1 \quad \text{in a neighborhood of } x_0 \text{ in } \Omega_k^{\mathrm{M}}. \tag{195}$$

Then, define on $\overline{\Omega_k^{\mathrm{M}}}$:

$$\varphi_k^{\mathrm{M},(0)} = \frac{\psi_k^{\mathrm{M},(0)}\, e^{-(1/h) f}}{\|\psi_k^{\mathrm{M},(0)}\, e^{-(1/h) f}\|_{L^2(\Omega_k^{\mathrm{M}})}} \in \mathcal{C}^\infty\big(\overline{\Omega_k^{\mathrm{M}}}\big). \tag{196}$$

Let us check that $\varphi_k^{\mathrm{M},(0)}$ belongs to the domain of $\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})$, defined in (178). Because it is smooth on the bounded set $\overline{\Omega_k^{\mathrm{M}}}$, one just has to check that it satisfies the boundary conditions on $\partial\Omega_k^{\mathrm{M}}$. By definition of $\phi_k^{\mathrm{M},(0)}$ above, $\varphi_k^{\mathrm{M},(0)}(x) = 0$ for all $x = (\mathsf{z}, x_d) \in \overline{\mathsf{C}_{2\varepsilon}} \cap \{x_d = 0\} = \overline{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}}$ (see (135)). Let us now check that $\partial_{\mathsf{n}_{\Omega_k^{\mathrm{M}}}}(e^{f/h}\varphi_k^{\mathrm{M},(0)})(x) = 0$ for a.e. $x \in \Gamma_{k,\mathbf{N}}^{\mathrm{M}}$, i.e., that $\partial_{\mathsf{n}_{\Omega_k^{\mathrm{M}}}}\psi_k^{\mathrm{M},(0)}(x) = 0$ for a.e. $x \in \Gamma_{k,\mathbf{N}}^{\mathrm{M}}$. Recall that $\Gamma_{k,\mathbf{N}}^{\mathrm{M}} = \partial\Omega_k^{\mathrm{M}} \cap \Omega$ (see (147)). Let us first consider the case $x \in \Gamma_{k,\mathbf{N}}^{\mathrm{M}} \cap \{x_d \in (0,3\varepsilon)\}$. From (187) and (138), it holds:

$$\partial\Omega_k^{\mathrm{M}} \cap \{x_d \in (0,3\varepsilon)\} = \Sigma_{3\varepsilon}^{\mathrm{lateral}}. \tag{197}$$

Because $\overline{\Omega_{\mathsf{K}_{\alpha/2}}} \subset \{x_d > 5\varepsilon\}$ and $\Sigma_{3\varepsilon}^{\mathrm{lateral}} \subset \partial\mathsf{C}_\alpha$, one deduces that (see (150) and (151)),

$$\Sigma_{3\varepsilon}^{\mathrm{lateral}} = \Gamma_{k,\mathbf{N}}^{\mathrm{M}} \cap \{x_d \in (0,3\varepsilon)\} \subset \mathsf{A}_2.$$

Then using (154) and (140), $\mathsf{n}_{\Omega_k^{\mathrm{M}}} = -\nabla x_1/|\nabla x_1|$ on $\Sigma_{3\varepsilon}^{\mathrm{lateral}}$. Since $\nabla\psi_k^{\mathrm{M},(0)}$ is collinear to ∇x_d on $\overline{\mathsf{C}_{3\varepsilon}}$ which is, in view of (106), orthogonal to ∇x_1, it holds:

$$\partial_{\mathsf{n}_{\Omega_k^{\mathrm{M}}}}\psi_k^{\mathrm{M},(0)}(x) = 0 \quad \text{for } x \in \Gamma_{k,\mathbf{N}}^{\mathrm{M}} \cap \Sigma_{3\varepsilon}^{\mathrm{lateral}}.$$

Let us now consider the case $x \in \Gamma_{k,\mathbf{N}}^{\mathrm{M}} \cap \{x_d \geqslant 3\varepsilon\}$. Because $\psi_k^{\mathrm{M},(0)} = 1$ on $\overline{\Omega_k^{\mathrm{M}}} \smallsetminus \overline{\mathsf{C}_\varepsilon} = \overline{\Omega_k^{\mathrm{M}}} \cap \{x_d > \varepsilon\}$ (therefore $|\nabla\psi_k^{\mathrm{M},(0)}|(x) = 0$ on this set) and $\Gamma_{k,\mathbf{N}}^{\mathrm{M}} \cap \{x_d \geqslant 3\varepsilon\} = \partial\Omega_k^{\mathrm{M}} \cap \{x_d \geqslant 3\varepsilon\}$, it holds,

$$\partial_{\mathsf{n}_{\Omega_k^{\mathrm{M}}}}\psi_k^{\mathrm{M},(0)}(x) = 0 \quad \text{for a.e. } x \in \Gamma_{k,\mathbf{N}}^{\mathrm{M}} \cap \{x_d \geqslant 3\varepsilon\}.$$

In conclusion, one has

$$\varphi_k^{\mathrm{M},(0)} \in \mathcal{D}(\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})). \tag{198}$$

Step 2: Asymptotic estimates of

$$\langle \varphi_k^{\mathrm{M},(0)}, \Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\varphi_k^{\mathrm{M},(0)}\rangle_{L^2(\Omega_k^{\mathrm{M}})} \quad\text{and}\quad \|\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\varphi_k^{\mathrm{M},(0)}\|^2_{L^2(\Omega_k^{\mathrm{M}})} \quad \text{as } h \longrightarrow 0.$$

Let us first deal with $\mathsf{Z}_{z_k} := \|\psi_k^{\mathrm{M},(0)}\, e^{-(1/h)f}\|_{L^2(\Omega_k^{\mathrm{M}})}$. Because $|\psi_k^{\mathrm{M},(0)}| \leqslant 1$, $\{x_0\} = \arg\min_{\overline{\Omega_k^{\mathrm{M}}}} f$ (which follows from the fact that $x_0 \in \Omega_k^{\mathrm{M}} \subset \Omega$ and Lemma 4) and $\psi_k^{\mathrm{M},(0)} = 1$ near x_0 in Ω_k^{M} (see (195)) it holds, using Laplace's method, in the limit $h \to 0$:

$$\mathsf{Z}_{z_k} = \sqrt{\kappa_{x_0}}\, h^{d/4}\, e^{-(1/h)f(x_0)}\big(1 + O(h)\big), \tag{199}$$

where κ_{x_0} is defined in (186).

Let us now consider the term $\langle \varphi_k^{\mathrm{M},(0)}, \Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\varphi_k^{\mathrm{M},(0)}\rangle_{L^2(\Omega_k^{\mathrm{M}})}$. One has (see (198) and Proposition 33):

$$\langle \varphi_k^{\mathrm{M},(0)}, \Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\varphi_k^{\mathrm{M},(0)}\rangle_{L^2(\Omega_k^{\mathrm{M}})} = \int_{\Omega_k^{\mathrm{M}}} |\mathsf{d}_{f,h}\varphi_k^{\mathrm{M},(0)}|^2 = \frac{h^2 \int_{\mathsf{C}_{2\varepsilon}} |\nabla \psi_k^{\mathrm{M},(0)}|^2 e^{-(2/h)f}}{\mathsf{Z}_{z_k}^2},$$

where we also used the fact that $\psi_k^{\mathrm{M},(0)} = 1$ on $\overline{\Omega_k^{\mathrm{M}}} \smallsetminus \overline{\mathsf{C}_{2\varepsilon}}$. For $\eta \in [0, 2\varepsilon]$, set $\Gamma(\eta) = \{x \in \overline{\mathsf{C}_{2\varepsilon}},\ x_d(x) = \eta\}$. Note that $\Gamma(0) = \Gamma_{k,\mathbf{D}}^{\mathrm{M}}$ and that for any $\eta \in [0, 2\varepsilon]$, $\Gamma(\eta)$ is naturally parametrized by $\Gamma_{k,\mathbf{D}}^{\mathrm{M}}$ through the mapping $\mathsf{z} \in \Gamma_{k,\mathbf{D}}^{\mathrm{M}} \mapsto (\mathsf{z}, \eta)$ with Jacobian determinant $\mathsf{j}(\mathsf{z}, \eta)$ with $\mathsf{j}(\mathsf{z}, 0) = 1$. One has using (194), (193), the co-area formula [32] ($dx = d\sigma_{\Gamma(\eta)}|\nabla x_d|^{-1} d\eta$), and the fact that $|\nabla x_d| = 1$:

$$\begin{aligned} h^2 \int_{\mathsf{C}_{2\varepsilon}} |\nabla \psi_k^{\mathrm{M},(0)}|^2 e^{-(2/h)f} &= \frac{\int_{\eta=0}^{2\varepsilon} \chi^2(\eta) \int_{\Gamma(\eta)} |\nabla x_d|^2\, e^{-(2/h)(f + |\mu_{z_k}|\eta^2)} d\sigma_{\Gamma(\eta)} |\nabla x_d|^{-1} d\eta}{\big(\int_0^{2\varepsilon} \chi(t)\, e^{-(1/h)|\mu_{z_k}|\, t^2} dt\big)^2} \\ &= \frac{\int_{\eta=0}^{2\varepsilon} \chi^2(\eta) \int_{\mathsf{z}\in\Gamma_{k,\mathbf{D}}^{\mathrm{M}}} e^{-(2/h)(f(\mathsf{z},\eta) + |\mu_{z_k}|\eta^2)} \mathsf{j}(\mathsf{z},\eta) d\sigma_{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}} d\eta}{\big(\int_0^{2\varepsilon} \chi(t)\, e^{-(1/h)|\mu_{z_k}|\, t^2} dt\big)^2}. \end{aligned}$$

A straightforward computation implies that there exists $c > 0$ such that in the limit $h \to 0$,

$$\mathsf{N}_{z_k} := \int_0^{2\varepsilon} \chi(t)\, e^{-(1/h)|\mu_{z_k}|\, t^2} dt = \frac{\sqrt{\pi h}}{2\sqrt{|\mu_{z_k}|}}\big(1 + O(e^{-c/h})\big). \tag{200}$$

Using (192) and (189), one has for h small enough:

$$\begin{aligned} \int_{\eta=0}^{2\varepsilon} \chi^2(\eta) \int_{\mathsf{z}\in\Gamma_{k,\mathbf{D}}^{\mathrm{M}}} & e^{-(2/h)(f(\mathsf{z},\eta) + |\mu_{z_k}|\eta^2)} \mathsf{j}(\mathsf{z},\eta) d\sigma_{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}} d\eta \\ &= \int_{\eta=0}^{2\varepsilon} \chi^2(\eta) \int_{|\mathsf{z}|\leqslant r} e^{-(2/h)(f(\mathsf{z},\eta) + |\mu_{z_k}|\eta^2)} \mathsf{j}(\mathsf{z},\eta) d\sigma_{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}} d\eta \\ &\qquad + O(e^{-(2/h)(f(z_k)+c)}), \end{aligned}$$

for some $c>0$ independent of h. Using in addition (190), the same computations as in the proof of the step 1.b of [58, Prop. 24] imply that in the limit $h\to 0$:

$$\int_{\eta=0}^{2\varepsilon}\chi^2(\eta)\int_{|\mathsf{z}|\leqslant r} e^{-(2/h)(f(\mathsf{z},\eta)+|\mu_{z_k}|\eta^2)}\mathsf{j}(\mathsf{z},\eta)d\sigma_{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}}d\eta=\frac{(\pi h)^{d/2}e^{-(2/h)f(z_k)}}{2\sqrt{\mu_1\cdots\mu_{d-1}|\mu_{z_k}|}}\big(1+O(\sqrt{h})\big),$$

where the $O(\sqrt{h})$ is optimal in general. In conclusion, using also (199), one has as $h\to 0$:

$$\langle\varphi_k^{\mathrm{M},(0)},\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\varphi_k^{\mathrm{M},(0)}\rangle_{L^2(\Omega_k^{\mathrm{M}})}=\mathsf{A}_{x_0,z_k}h\;e^{-(2/h)(f(z_k)-f(x_0))}(1+O(\sqrt{h})).\tag{201}$$

Let us now consider the term $\|\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\varphi_k^{\mathrm{M},(0)}\|^2_{L^2(\Omega_k^{\mathrm{M}})}$. Using (118) and the definition of $\psi_k^{\mathrm{M},(0)}$, it holds on Ω_k^{M}:

$$\Delta_{f,h}^{(0)}\varphi_k^{\mathrm{M},(0)}=\frac{2he^{-(1/h)f}}{\|\psi_k^{\mathrm{M},(0)}\,e^{-(1/h)f}\|_{L^2(\Omega_k^{\mathrm{M}})}}\Big(\frac{h}{2}\Delta_{\mathbf{H}}^{(0)}+\nabla f\cdot\nabla\Big)\psi_k^{\mathrm{M},(0)}\tag{202}$$

is supported in $\overline{\mathsf{C}_{2\varepsilon}}$.

By (194), (200), and (193), for h small enough,

$$\|\Delta_{\mathbf{H}}^{(0)}\psi_k^{\mathrm{M},(0)}\|_{L^\infty(\mathsf{C}_{2\varepsilon})}\quad\text{and}\quad\|\nabla\psi_k^{\mathrm{M},(0)}\|_{L^\infty(\mathsf{C}_{2\varepsilon})}$$

are $O(h^\nu)$ for some $\nu\in\mathbb{R}$. Then, using (192) and (199), one has for h small enough (see (189)):

$$\begin{aligned}\|\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\varphi_k^{\mathrm{M},(0)}\|^2_{L^2(\Omega_k^{\mathrm{M}})}&=\|\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\varphi_k^{\mathrm{M},(0)}\|^2_{L^2(\mathsf{C}_{2\varepsilon})}\\&=\|\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\varphi_k^{\mathrm{M},(0)}\|^2_{L^2(\mathsf{V}^r_{2\varepsilon}(z_k))}+O(e^{-(2/h)(f(z_k)-f(x_0)+c)}),\end{aligned}\tag{203}$$

for some $c>0$ independent of h. Let us recall that $\mathbf{g}$ denotes the metric tensor in the (x',x_d) coordinates (see (106)). In the following, with a slight abuse of notation, we also denote by $\mathbf{g}$ the matrix $(\mathbf{G},0;0,1)$. In the (x',x_d)-coordinates, $\Delta_{\mathbf{H}}^{(0)}$ writes

$$\Delta_{\mathbf{H}}^{(0)}\phi_k^{\mathrm{M},(0)}=-\frac{1}{\sqrt{|\mathbf{g}|}}\sum_{i,j=1}^d\partial_{x_i}\big(\sqrt{|\mathbf{g}|}\,\mathbf{g}^{i,j}\partial_{x_j}\phi_k^{\mathrm{M},(0)}\big),$$

where $|\mathbf{g}|$ denotes the determinant of $\mathbf{g}$ and $\mathbf{g}^{i,j}$ the (i,j) entry of $\mathbf{g}^{-1}$. Then, from (202) and (193), one has on $\mathsf{V}^r_{2\varepsilon}(z_k)$,

$$\begin{aligned}\Delta_{f,h}\varphi_k^{\mathrm{M},(0)}&=\frac{2h\,e^{-f/h}}{\mathsf{Z}_{z_k}}\Big[-\frac{h}{2\sqrt{|\mathbf{g}|}}\sum_{i,j=1}^d\partial_{x_i}\big(\sqrt{|\mathbf{g}|}\,\mathbf{g}^{i,j}\partial_{x_j}\phi_k^{\mathrm{M},(0)}\big)+\sum_{i,j=1}^d\mathbf{g}^{i,j}\partial_{x_i}f\partial_{x_j}\phi_k^{\mathrm{M},(0)}\Big]\\&=\frac{2h\,e^{-(1/h)(f+|\mu_{z_k}|x_d^2)}}{\mathsf{Z}_{z_k}\mathsf{N}_{z_k}}\Big[-\frac{h}{2\sqrt{|\mathbf{g}|}}\sum_{i=1}^d\partial_{x_i}\big(\sqrt{|\mathbf{g}|}\,\mathbf{g}^{i,d}\big)\chi(x_d)+\mathbf{g}^{d,d}\chi(x_d)|\mu_{z_k}|x_d\\&\qquad+\chi(x_d)\sum_{i=1}^d\mathbf{g}^{i,d}\partial_{x_i}f-\frac{h}{2}\,\chi'(x_d)\,\mathbf{g}^{d,d}\Big]\\&=\frac{2h\,e^{-(1/h)(f+|\mu_{z_k}|x_d^2)}}{\mathsf{Z}_{z_k}\mathsf{N}_{z_k}}\big[O(h)+O(|x|^2)\big],\end{aligned}$$

where N_{z_k} is defined in (200), and where in the last inequality we have used that $\mathbf{g}^{i,d}=0$ for $i=1,\dots,d-1$ (see (106)), and $\partial_{x_d} f(x',x_d)=-|\mu_{z_k}|x_d+O(|x|^2)$ (see (190)). Notice the cancellation of the $O(x)$ terms in the previous computations due to the precise form of the quasi-mode $\varphi_k^{\mathrm{M},(0)}$. Thus, by (191), (199), (190), (200), and (201), one deduces using Laplace's method that as $h\to 0$,

$$\begin{aligned}\big\|\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\varphi_k^{\mathrm{M},(0)}\big\|^2_{L^2(\mathsf{V}_\varepsilon^r(z_k))}&=\frac{h^2h^{d/2}}{h^{d/2}h}\,O(h^2)\,e^{-(2/h)(f(z_k)-f(x_0))}\\&=O(h^2)\big|\langle\varphi_k^{\mathrm{M},(0)},\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\varphi_k^{\mathrm{M},(0)}\rangle_{L^2(\Omega_k^{\mathrm{M}})}\big|.\end{aligned}$$

Consequently, one deduces using (203), that

$$\|\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\varphi_k^{\mathrm{M},(0)}\|_{L^2(\Omega_k^{\mathrm{M}})}=O(h)\sqrt{\big|\langle\varphi_k^{\mathrm{M},(0)},\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\varphi_k^{\mathrm{M},(0)}\rangle_{L^2(\Omega_k^{\mathrm{M}})}\big|}.\tag{204}$$

Step 3: End of the proof of Proposition 36. — Let us introduce the constant $\mathsf{c}>0$ from item (iii) in Proposition 35. Because $\varphi_k^{\mathrm{M},(0)}\in\mathcal{D}(\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}}))$, see indeed (198), and since $\lambda(\Omega_k^{\mathrm{M}})$ is exponentially small when $h\to 0$ (actually $o(h)$ as $h\to 0$ would be enough), using the fact that (see the proof of [58, Prop. 27])

$$\big(1-\pi_{[0,\mathsf{c}h]}\big(\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\big)\big)\,\varphi_k^{\mathrm{M},(0)}=-\frac{1}{2\pi i}\int_{C(\mathsf{c}h/2)}z^{-1}(z-\Delta_{f,h}^{\mathrm{M},(0)})^{-1}\Delta_{f,h}^{\mathrm{M},(0)}\varphi_k^{\mathrm{M},(0)}dz,$$

where $C(\mathsf{c}h/2)\subset\mathbb{C}$ is the circle of radius $\mathsf{c}h/2$ centered at 0, it holds for h small enough

$$\big\|(1-\pi_{[0,\mathsf{c}h]}\big(\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\big))\,\varphi_k^{\mathrm{M},(0)}\big\|_{L^2(\Omega_k^{\mathrm{M}})}\leqslant Ch^{-1}\big\|\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\varphi_k^{\mathrm{M},(0)}\big\|_{L^2(\Omega_k^{\mathrm{M}})}.$$

Therefore, using (204), it holds:

$$\begin{aligned}\big\|(1-\pi_{[0,\mathsf{c}h]}\big(\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\big))\,\varphi_k^{\mathrm{M},(0)}\big\|_{L^2(\Omega_k^{\mathrm{M}})}&\\\leqslant C\sqrt{\big|\langle\varphi_k^{\mathrm{M},(0)},\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\varphi_k^{\mathrm{M},(0)}\rangle_{L^2(\Omega_k^{\mathrm{M}})}\big|}&.\end{aligned}\tag{205}$$

In particular, using (201) and the fact that $\|\varphi_k^{\mathrm{M},(0)}\|_{L^2(\Omega_k^{\mathrm{M}})}=1$, there exists $c>0$ (because $f(z_k)>f(x_0)$ see Lemma 4) such that, for $h>0$ small enough,

$$\big\|\pi_{[0,\mathsf{c}h]}\big(\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\big)\varphi_k^{\mathrm{M},(0)}\big\|_{L^2(\Omega_k^{\mathrm{M}})}=1+O(e^{-c/h}),\tag{206}$$

and the following function is therefore well-defined:

$$\mathsf{u}_k^{(0)}=\frac{\pi_{[0,\mathsf{c}h]}\big(\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\big)\varphi_k^{\mathrm{M},(0)}}{\big\|\pi_{[0,\mathsf{c}h]}\big(\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\big)\varphi_k^{\mathrm{M},(0)}\big\|_{L^2(\Omega_k^{\mathrm{M}})}}.\tag{207}$$

One has

$$\begin{aligned}\lambda(\Omega_k^{\mathrm{M}})&=\langle\mathsf{u}_k^{(0)},\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\mathsf{u}_k^{(0)}\rangle_{L^2(\Omega_k^{\mathrm{M}})}\\&=\langle\pi_{[0,\mathsf{c}h]}\big(\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\big)\varphi_k^{\mathrm{M},(0)},\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\varphi_k^{\mathrm{M},(0)}\rangle_{L^2(\Omega_k^{\mathrm{M}})}(1+O(e^{-c/h})),\end{aligned}\tag{208}$$

since the orthogonal projector $\pi_{[0,\mathsf{c}h]}\big(\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\big)$ and $\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})$ commute on $\mathcal{D}(\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}}))$ and $\varphi_k^{\mathrm{M},(0)} \in \mathcal{D}(\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}}))$. In addition, one has, using (205) and (204),

$$
\begin{aligned}
\big\langle \pi_{[0,\mathsf{c}h]}\big(\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\big)\varphi_k^{\mathrm{M},(0)}, \Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\varphi_k^{\mathrm{M},(0)}\big\rangle_{L^2(\Omega_k^{\mathrm{M}})}&\\
= \big\langle \varphi_k^{\mathrm{M},(0)}, \Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\varphi_k^{\mathrm{M},(0)}\big\rangle_{L^2(\Omega_k^{\mathrm{M}})}&\\
- \big\langle (1-\pi_{[0,\mathsf{c}h]}\big(\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\big))\varphi_k^{\mathrm{M},(0)}, \Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\varphi_k^{\mathrm{M},(0)}\big\rangle_{L^2(\Omega_k^{\mathrm{M}})}&\\
= \big\langle \varphi_k^{\mathrm{M},(0)}, \Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\varphi_k^{\mathrm{M},(0)}\big\rangle_{L^2(\Omega_k^{\mathrm{M}})}(1+O(h)),&\\
= \mathsf{A}_{x_0,z_k} h\, e^{-(2/h)(f(z_k)-f(x_0))}(1+O(\sqrt{h})),&
\end{aligned}
$$

where we used (201). This proves (183). It remains to prove Equation (185).

Let $\mathsf{u}_k^{(1)}$ be a $L^2(\Omega_k^{\mathrm{M}})$-normalized eigenform of $\Delta_{f,h}^{\mathrm{M},(1)}(\Omega_k^{\mathrm{M}})$ associated with the eigenvalue $\lambda(\Omega_k^{\mathrm{M}})$. In view of item (ii) and (iii) in Proposition 35 it holds ($\mathsf{u}_k^{(0)}$ is indeed a $L^2(\Omega_k^{\mathrm{M}})$-normalized principal eigenform of $\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})$, see (207)), $\mathsf{u}_k^{(1)} = \pm \mathsf{d}_{f,h}\mathsf{u}_k^{(0)}/\|\mathsf{d}_{f,h}\mathsf{u}_k^{(0)}\|_{L^2(\Omega_k^{\mathrm{M}})}$. Let us choose

$$
\mathsf{u}_k^{(1)} = \frac{\mathsf{d}_{f,h}\mathsf{u}_k^{(0)}}{\mathsf{N}_k^{(1)}} \quad \text{with } \mathsf{N}_k^{(1)} = \big\|\mathsf{d}_{f,h}\mathsf{u}_k^{(0)}\big\|_{L^2(\Omega_k^{\mathrm{M}})}. \tag{209}
$$

From (208), one has,

$$
\lambda(\Omega_k^{\mathrm{M}}) = \big\langle \mathsf{d}_{f,h}\mathsf{u}_k^{(0)}, \mathsf{d}_{f,h}\mathsf{u}_k^{(0)}\big\rangle_{L^2(\Omega_k^{\mathrm{M}})} = (\mathsf{N}_k^{(1)})^2,
$$

and thus, using (207) and the fact that

$$
\mathsf{d}_{f,h}\pi_{[0,\mathsf{c}h]}\big(\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\big) = \pi_{[0,\mathsf{c}h]}\big(\Delta_{f,h}^{\mathrm{M},(1)}(\Omega_k^{\mathrm{M}})\big)\mathsf{d}_{f,h}
$$

(see item (ii) in Proposition 35),

$$
\begin{aligned}
\lambda(\Omega_k^{\mathrm{M}}) &= \frac{\mathsf{N}_k^{(1)}\,\langle \mathsf{d}_{f,h}\varphi_k^{\mathrm{M},(0)}, \mathsf{u}_k^{(1)}\rangle_{L^2(\Omega_k^{\mathrm{M}})}}{\big\|\pi_{[0,\mathsf{c}h]}\big(\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\big)\varphi_k^{\mathrm{M},(0)}\big\|_{L^2(\Omega_k^{\mathrm{M}})}}\\
&= \frac{\mathsf{N}_k^{(1)}\,\langle \mathsf{d}\psi_k^{\mathrm{M},(0)}, he^{-(1/h)f}\mathsf{u}_k^{(1)}\rangle_{L^2(\Omega_k^{\mathrm{M}})}}{\big\|\pi_{[0,\mathsf{c}h]}\big(\Delta_{f,h}^{\mathrm{M},(0)}(\Omega_k^{\mathrm{M}})\big)\varphi_k^{\mathrm{M},(0)}\big\|_{L^2(\Omega_k^{\mathrm{M}})}\mathsf{Z}_{z_k}},
\end{aligned}
$$

where we also used (196) at the last line. Therefore, because $\mathsf{N}_k^{(1)} = \sqrt{\lambda(\Omega_k^{\mathrm{M}})}$, it follows from (183), (199) and (206), that, as $h \to 0$, it holds:

$$
\langle \mathsf{d}\psi_k^{\mathrm{M},(0)}, he^{-(1/h)f}\mathsf{u}_k^{(1)}\rangle_{L^2(\Omega_k^{\mathrm{M}})} = \sqrt{\mathsf{A}_{x_0,z_k}\, h\, \kappa_{x_0}\, h^{d/2}}\, e^{-(1/h)f(z_k)}(1+O(\sqrt{h})). \tag{210}
$$

Besides, using the fact that $\mathsf{u}_k^{(1)} \in \mathcal{D}(\Delta_{f,h}^{\mathrm{M},(1)}(\Omega_k^{\mathrm{M}}))$ (see item (ii) in Proposition 35) and the Green formula (171), one deduces that

$$(211)\quad \big\langle \mathsf{d}\psi_k^{\mathrm{M},(0)}, he^{-(1/h)f}\mathsf{u}_k^{(1)}\big\rangle_{L^2(\Omega_k^{\mathrm{M}})} = -\langle \mathsf{d}(1-\psi_k^{\mathrm{M},(0)}), he^{-(1/h)f}\mathsf{u}_k^{(1)}\big\rangle_{L^2(\Omega_k^{\mathrm{M}})}$$
$$= \big\langle (1-\psi_k^{\mathrm{M},(0)})e^{-(1/h)f}, \mathsf{d}_{f,h}^*\mathsf{u}_k^{(1)}\big\rangle_{L^2(\Omega_k^{\mathrm{M}})} - h\int_{\partial\Omega_k^{\mathrm{M}}}(1-\psi_k^{\mathrm{M},(0)})\mathsf{u}_k^{(1)}\cdot \mathsf{n}_{\Omega_k^{\mathrm{M}}}e^{-(1/h)f},$$

(where here and in the following, we use the notation $\mathsf{u}_k^{(1)}\cdot\mathsf{n}_{\Omega_k^{\mathrm{M}}} = \mathbf{i}_{\mathsf{n}_{\Omega_k^{\mathrm{M}}}}\mathsf{u}_k^{(1)}$) and

$$\mathsf{u}_k^{(1)}\cdot \mathsf{n}_{\Omega_k^{\mathrm{M}}} = 0 \text{ on } \Gamma_{k,\mathbf{N}}^{\mathrm{M}}.$$

Moreover, $\psi_k^{\mathrm{M},(0)}=0$ on $\Gamma_{k,\mathbf{D}}^{\mathrm{M}}$. Thus,

$$(212)\qquad \int_{\partial\Omega_k^{\mathrm{M}}}(1-\psi_k^{\mathrm{M},(0)})\mathsf{u}_k^{(1)}\cdot\mathsf{n}_{\Omega_k^{\mathrm{M}}}\,e^{-(1/h)f} = \int_{\Gamma_{k,\mathbf{D}}^{\mathrm{M}}}\mathsf{u}_k^{(1)}\cdot\mathsf{n}_{\Omega_k^{\mathrm{M}}}\,e^{-(1/h)f}.$$

Let us now deal with the term $\langle (1-\psi_k^{\mathrm{M},(0)})e^{-(1/h)f}, \mathsf{d}_{f,h}^*\mathsf{u}_k^{(1)}\big\rangle_{L^2(\Omega_k^{\mathrm{M}})}$. It holds,

$$\begin{aligned}\big|\langle (1-\psi_k^{\mathrm{M},(0)})e^{-(1/h)f}, \mathsf{d}_{f,h}^*\mathsf{u}_k^{(1)}\big\rangle_{L^2(\Omega_k^{\mathrm{M}})}\big| &\leqslant \big\|(1-\psi_k^{\mathrm{M},(0)})e^{-(1/h)f}\big\|_{L^2(\Omega_k^{\mathrm{M}})}\sqrt{\lambda(\Omega_k^{\mathrm{M}})}\\ &\leqslant Ce^{-(1/h)\min_{\mathrm{supp}(1-\psi_k^{\mathrm{M},(0)})}f}\sqrt{\lambda(\Omega_k^{\mathrm{M}})}\\ &\leqslant Ce^{-(1/h)(f(x_0)+\delta)}\sqrt{\lambda(\Omega_k^{\mathrm{M}})}\\ &\leqslant Ce^{-(1/h)(f(z_k)+\delta)},\end{aligned}$$

where we used the fact that, from (195) and since x_0 is the global minimum of f in $\overline{\Omega}$ (see Lemma 4), $\min_{\mathrm{supp}(1-\psi_k^{\mathrm{M},(0)})} f \geqslant f(x_0)+\delta$, for some $\delta>0$. Notice that we also used (183) at the last line of the previous computation. Equation (185) then follows from the previous inequality together with (210), (211), and (212). This concludes the proof of Proposition 36. □

3.3.4. *Agmon estimates on* $\mathsf{u}_k^{(1)}$. — The aim of this section is to prove that $\mathsf{u}_k^{(1)}$ (the principal eigenform of $\Delta_{f,h}^{\mathrm{M},(1)}(\Omega_k^{\mathrm{M}})$) decays exponentially fast away from z_k (see Proposition 38 below): these are so-called Agmon estimates.

Recall the Definition 3 of the Agmon distance. These are basic properties of the Agmon distance which follows from [44, App. 2], see also [65, Lem. 3.2]:

Proposition 37. — *Let us assume that $f:\overline{\Omega}\to\mathbb{R}$ is a $\mathcal{C}^\infty$ function. Then, the Agmon pseudo-distance $(x,y)\in\overline{\Omega}\times\overline{\Omega}\mapsto \mathsf{d}_a(x,y)$ (see Definition 3) is symmetric and satisfies the triangular inequality. In addition, it is a distance if f has a finite number of critical points in $\overline{\Omega}$. Moreover, for any fixed $y\in\overline{\Omega}$, $x\in\overline{\Omega}\mapsto \mathsf{d}_a(x,y)$ is Lipschitz (therefore, its gradient is well-defined almost everywhere). For all subset U of $\overline{\Omega}$ and for almost every $x\in\Omega$,*

$$(213)\qquad |\nabla_x \mathsf{d}_a(x,U)| \leqslant |\nabla f(x)|.$$

Moreover, for all $x,y\in\overline{\Omega}$, we have

$$(214)\qquad |f(x)-f(y)|\leqslant \mathsf{d}_a(x,y).$$

The main result of this section if the following:

Proposition 38

Let us assume that assumption (Ω-f) *is satisfied. Let* $k \in \{1,\dots,n\}$ *and* Ω_k^M *be the subdomain of* Ω *introduced in Proposition* 30. *Let* $\Delta_{f,h}^{M,(1)}(\Omega_k^M)$ *be the unbounded nonnegative self-adjoint operator on* $\Lambda^1 L^2(\Omega_k^M)$ *defined by* (177)–(178) *with* $(\Omega^M, \Gamma_{\mathbf{D}}^M, \Gamma_{\mathbf{N}}^M) = (\Omega_k^M, \Gamma_{k,\mathbf{D}}^M, \Gamma_{k,\mathbf{N}}^M)$. *Let* $\mathsf{u}_k^{(1)}$ *be a* $L^2(\Omega_k^M)$*-normalized eigenform of* $\Delta_{f,h}^{M,(1)}(\Omega_k^M)$ *associated with the eigenvalue* $\lambda(\Omega_k^M)$*, as introduced in Proposition* 35. *Then, for any* $\delta > 0$*, there exists* $h_\delta > 0$ *such that it holds for* $h \in (0, h_\delta)$*:*

$$\big\|e^{\Psi_k/h}\mathsf{u}_k^{(1)}\big\|_{L^2(\Omega_k^M)} + \big\|\mathsf{d}\big(e^{\Psi_k/h}\mathsf{u}_k^{(1)}\big)\big\|_{L^2(\Omega_k^M)} + \big\|\mathsf{d}^*\big(e^{\Psi_k/h}\mathsf{u}_k^{(1)}\big)\big\|_{L^2(\Omega_k^M)} \leqslant e^{\delta/h},$$

where $\Psi_k(x) := \mathsf{d}_a(x, z_k)$*.*

Proof. — Using Lemma 34 on Ω_k^{M} with $w = \mathsf{u}_k^{(1)}$ and since $\nabla f \cdot \mathsf{n}_{\Omega_k^{\mathrm{M}}} > 0$ a.e. $\Gamma_{k,\mathbf{N}}^{\mathrm{M}}$ (see item (2) in Proposition 30), it holds,

$$\lambda(\Omega_k^{\mathrm{M}})\|e^{\varphi/h}\mathsf{u}_k^{(1)}\|^2_{L^2(\Omega_k^{\mathrm{M}})} \geqslant h^2\big\|\mathsf{d}(e^{\varphi/h}\mathsf{u}_k^{(1)})\big\|^2_{L^2(\Omega_k^{\mathrm{M}})} + h^2\big\|\mathsf{d}^*(e^{\varphi/h}\mathsf{u}_k^{(1)})\big\|^2_{L^2(\Omega_k^{\mathrm{M}})} + \big\langle(|\nabla f|^2 - |\nabla\varphi|^2 + h\mathcal{L}_{\nabla f} + h\mathcal{L}^*_{\nabla f})e^{\varphi/h}\mathsf{u}_k^{(1)}, e^{\varphi/h}\mathsf{u}_k^{(1)}\big\rangle_{L^2(\Omega_k^{\mathrm{M}})}. \tag{215}$$

Using (215) and (213), it is then standard to get the estimate of Proposition 38 with $\mathsf{d}_a(\cdot, \{z_k\} \cup \{x_0\})$ instead of $\mathsf{d}_a(\cdot, z_k)$ using the same arguments as those used in the boundaryless case [39, Prop. 3.3.1]. Proving Proposition 38 requires a finer analysis. To this end, we follow the analysis of [43, §2.2] and [29, §6.c]. The proof is divided into two steps.

Step 1: A Witten Laplacian on 1*-forms with a spectrum bounded from below by ch*

Roughly speaking, recall that in view of the proof of item (iii) in Proposition 35, z_k is the only point which "creates" a small eigenvalue for $\Delta_{f,h}^{\mathrm{M},(1)}(\Omega_k^{\mathrm{M}})$, namely $\lambda(\Omega_k^{\mathrm{M}})$. Thus, if we "remove" z_k from $\overline{\Omega_k^{\mathrm{M}}}$, the spectrum of the Witten Laplacian $\Delta_{f,h}^{\mathrm{M},(1)}$ will be bounded from below by ch. To do so, we proceed as follows. Let us take $\eta > 0$ small enough such that $\overline{\mathsf{B}_a(z_k, 3\eta)} \cap \Omega \subset \Omega_k^{\mathrm{M}}$ and z_k is the only critical point of f in $\overline{\mathsf{B}_a(z_k, 3\eta)}$, where $\mathsf{B}_a(x, r)$ denotes the open ball of center x and radius r for the Agmon distance d_a (which is indeed a distance since f is a Morse function). Define

$$\mathsf{D}_{k,\eta} := \Omega_k^{\mathrm{M}} \smallsetminus \overline{\mathsf{B}_a(z_k, \eta)}.$$

We have $\partial\mathsf{D}_{k,\eta} = \overline{\Sigma_{k,\mathbf{N}}} \cup \Sigma_{k,\mathbf{D}} \cup \overline{\Sigma_{k,\mathbf{FD}}}$, where

$$\Sigma_{k,\mathbf{N}} := \Gamma_{k,\mathbf{N}}^{\mathrm{M}},\ \Sigma_{k,\mathbf{D}} := \Gamma_{k,\mathbf{D}}^{\mathrm{M}} \smallsetminus \overline{\mathsf{B}_a(z_k, \eta) \cap \partial\Omega_k^{\mathrm{M}}}, \quad \text{and} \quad \Sigma_{k,\mathbf{FD}} := \partial\mathsf{B}_a(z_k, \eta) \cap \Omega_k^{\mathrm{M}}.$$

We refer to Figure 7 for a schematic representation of $\mathsf{D}_{k,\eta}$ and its boundary. We use the subscript **FD** because we will consider a Witten Laplacian with full Dirichlet boundary conditions on $\Sigma_{k,\mathbf{FD}}$.

Following the procedure of Section 3.3.1, we can consider the Friedrichs extension $\Delta_{f,h}^{\mathcal{M},(1)}(\mathsf{D}_{k,\eta})$ (which has different boundary conditions from the mixed Laplacian $\Delta_{f,h}^{\mathrm{M},(1)}$ introduced in Proposition 33, hence the different notation) of the closed

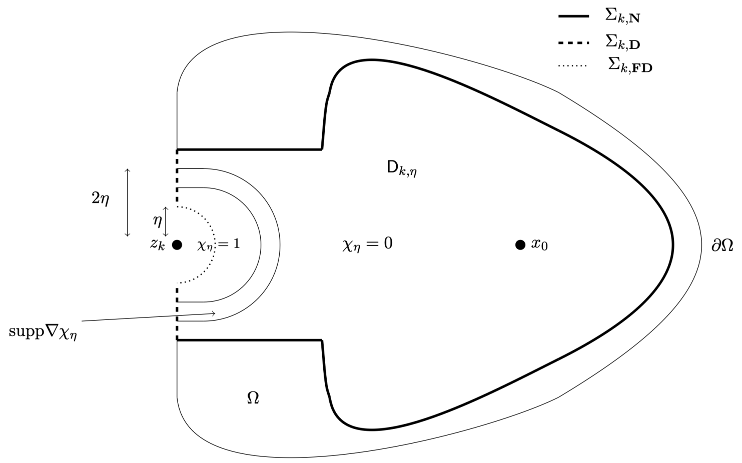

Figure 7. A schematic representation of $\mathsf{D}_{k,\eta}$.

quadratic form

$$Q^{\mathcal{M},(1)}_{f,h}(\mathsf{D}_{k,\eta})(u,w) = \langle \mathsf{d}_{f,h}u, \mathsf{d}_{f,h}w\rangle_{L^2(\mathsf{D}_{k,\eta})} + \langle \mathsf{d}^*_{f,h}u, \mathsf{d}^*_{f,h}w\rangle_{L^2(\mathsf{D}_{k,\eta})},$$

for all $u,w \in \mathcal{D}\big(Q^{\mathcal{M},(1)}_{f,h}(\mathsf{D}_{k,\eta})\big)$, where

$$\mathcal{D}\big(Q^{\mathcal{M},(1)}_{f,h}(\mathsf{D}_{k,\eta})\big) := \big\{w \in \Lambda^1 L^2(\mathsf{D}_{k,\eta}), \mathsf{d}_{f,h}w \text{ and } \mathsf{d}^*_{f,h}w \in \Lambda L^2(\mathsf{D}_{k,\eta}) \text{ with } \mathbf{n}w|_{\Sigma_{k,\mathbf{N}}} = 0, \mathbf{t}w|_{\Sigma_{k,\mathbf{D}}} = 0, \text{ and } w|_{\Sigma_{k,\mathbf{FD}}} = 0\big\}.$$

Let $w \in \mathcal{D}\big(Q^{\mathcal{M},(1)}_{f,h}(\mathsf{D}_{k,\eta})\big)$ and φ be a real-valued Lipschitz function on $\overline{\mathsf{D}_{k,\eta}}$. Since $w|_{\Sigma_{k,\mathbf{FD}}} = 0$ and $\nabla f \cdot \mathsf{n}_{\Omega^{\mathrm{M}}_k} = 0$ on $\Gamma^{\mathrm{M}}_{k,\mathbf{D}} \supset \Sigma_{k,\mathbf{D}}$, one has using the same arguments as those used to prove Lemma 34,

$$\begin{aligned}
Q^{\mathcal{M},(1)}_{f,h}&(\mathsf{D}_{k,\eta})(w, e^{(2/h)\varphi}w)\\
&= h^2\big\|\mathsf{d}(e^{\varphi/h}w)\big\|^2_{L^2(\mathsf{D}_{k,\eta})} + h^2\big\|\mathsf{d}^*(e^{\varphi/h}w)\big\|^2_{L^2(\mathsf{D}_{k,\eta})}\\
&\quad + \big\langle(|\nabla f|^2 - |\nabla\varphi|^2 + h\mathcal{L}_{\nabla f} + h\mathcal{L}^*_{\nabla f})e^{\varphi/h}w, e^{\varphi/h}w\big\rangle_{L^2(\mathsf{D}_{k,\eta})}\\
&\quad + h\int_{\Sigma_{k,\mathbf{N}}} \langle w,w\rangle_{T^*_\sigma \mathsf{D}_{k,\eta}}\, e^{(2/h)\varphi}\partial_{\mathsf{n}_{\Omega^{\mathrm{M}}_k}} f\, d\sigma\\
&\geqslant h^2\big\|\mathsf{d}(e^{\varphi/h}w)\big\|^2_{L^2(\mathsf{D}_{k,\eta})} + h^2\big\|\mathsf{d}^*(e^{\varphi/h}w)\big\|^2_{L^2(\mathsf{D}_{k,\eta})}\\
&\quad + \big\langle(|\nabla f|^2 - |\nabla\varphi|^2 + h\mathcal{L}_{\nabla f} + h\mathcal{L}^*_{\nabla f})e^{\varphi/h}w, e^{\varphi/h}w\big\rangle_{L^2(\mathsf{D}_{k,\eta})},
\end{aligned}\tag{216}$$

where we have used that $\partial_{\mathsf{n}_{\Omega^{\mathrm{M}}_k}} f \geqslant 0$ a.e. on $\Gamma^{\mathrm{M}}_{k,\mathbf{N}} = \Sigma_{k,\mathbf{N}}$. Thus, using (216) and the same analysis as the one made to prove item (iii) in Proposition 35, there exists $c > 0$ such that for h small enough:

$$\sigma\big(\Delta^{\mathcal{M},(1)}_{f,h}(\mathsf{D}_{k,\eta})\big) \geqslant ch. \tag{217}$$

Step 2: Resolvent estimates. — When D is a subdomain of Ω, and $w \in \Lambda^1 L^2(\mathsf{D})$ is such that $\mathsf{d}w$ and d^*w belong to $\Lambda L^2(\mathsf{D})$, we define

$$\|w\|^2_{\mathrm{W}^1(\mathsf{D})} := \|w\|^2_{L^2(\mathsf{D})} + \|\mathsf{d}w\|^2_{L^2(\mathsf{D})} + \|\mathsf{d}^*w\|^2_{L^2(\mathsf{D})}. \tag{218}$$

Notice that by (215) (with $\varphi = 0$), it holds

$$\|\mathsf{u}_k^{(1)}\|_{\mathrm{W}^1(\Omega_k^{\mathrm{M}})} \leqslant Ch^{-1/2}. \tag{219}$$

By (217) and since $\lambda(\Omega_k^{\mathrm{M}})$ is exponentially small as h goes to 0 (see (183)), the distance of $\lambda(\Omega_k^{\mathrm{M}})$ to $\sigma\big(\Delta_{f,h}^{\mathcal{M},(1)}(\mathsf{D}_{k,\eta})\big)$ is bounded from below by $ch/2$, as $h \to 0$. Then, adopting the notation of [29, p. 56], and using (213) and (216), we obtain using resolvent estimates as in the proof of [29, Prop. 6.5] (with, in our context, $K(h) = \{\lambda(\Omega_k^{\mathrm{M}})\}$),

$$\big(\Delta_{f,h}^{\mathcal{M},(1)}(\mathsf{D}_{k,\eta}) - \lambda(\Omega_k^{\mathrm{M}})\big)^{-1}(x,y) = \widehat{O}\big(e^{-(1/h)\mathsf{d}_a(x,y)}\big) \quad \text{for all } x,y \in \mathsf{D}_{k,\eta}. \tag{220}$$

The $\widehat{O}$ in (220) means that for any $x, y \in \mathsf{D}_{k,\eta}$ and $\varepsilon > 0$, there exist neighborhoods V_x and V_y in $\mathsf{D}_{k,\eta}$ of x and y respectively such that for h small enough,

$$\big\|\big(\Delta_{f,h}^{\mathcal{M},(1)}(\mathsf{D}_{k,\eta}) - \lambda(\Omega_k^{\mathrm{M}})\big)^{-1} w\|_{\mathrm{W}^1(V_x)} \leqslant e^{-(1/h)(\mathsf{d}_a(x,y)-\varepsilon)}\|w\|_{L^2(V_y)},$$

for all $w \in \Lambda^1 L^2(\mathsf{D}_{k,\eta})$ supported in V_y. We are now in position to prove Proposition 38.

Step 3: Proof of the Agmon estimate. — Let χ_η be a smooth cut-off function supported in $\mathsf{B}_a(z_k, 2\eta)$ which equals 1 on $\mathsf{B}_a(z_k, 3\eta/2)$ and such that $\nabla\chi_\eta \cdot \mathsf{n}_{\Omega_k^{\mathrm{M}}} = 0$. We claim that

$$\begin{aligned} &(1-\chi_\eta)\mathsf{u}_k^{(1)} \in \mathcal{D}(\Delta_{f,h}^{\mathcal{M},(1)}(\mathsf{D}_{k,\eta})),\\ &\Delta_{f,h}^{\mathcal{M},(1)}(\mathsf{D}_{k,\eta})((1-\chi_\eta)\mathsf{u}_k^{(1)}) = \Delta_{f,h}^{(1)}((1-\chi_\eta)\mathsf{u}_k^{(1)}). \end{aligned} \tag{221}$$

To prove (221), we use the integration by parts formula [27, Eq. (120)] on $\mathsf{D}_{k,\eta}$ with, using the notation there, $u = (1-\chi_\eta)\mathsf{u}_k^{(1)}$ and an arbitrary $v \in \mathcal{D}\big(Q_{f,h}^{\mathcal{M},(1)}(\mathsf{D}_{k,\eta})\big)$ and we observe that all the boundary terms vanish. To do so, we check that $u = (1-\chi_\eta)\mathsf{u}_k^{(1)}$ satisfies the required regularity, and that the boundary terms are zero. This shows that $Q_{f,h}^{\mathcal{M},(1)}(\mathsf{D}_{k,\eta})(u,v) = \langle \Delta_{f,h}^{(1)}(u), v\rangle_{L^2(\mathsf{D}_{k,\eta})}$ is bounded by $C(u)\|v\|_{L^2(\mathsf{D}_{k,\eta})}$. Thus $u \in \mathcal{D}(\Delta_{f,h}^{\mathcal{M},(1)}(\mathsf{D}_{k,\eta}))$, and $\Delta_{f,h}^{\mathcal{M},(1)}(\mathsf{D}_{k,\eta})u = \Delta_{f,h}^{(1)}u$.

Let us give some more details on the regularity and trace of $u = (1-\chi_\eta)\mathsf{u}_k^{(1)}$. It is easy to check that $u \in \mathcal{D}\big(Q_{f,h}^{\mathcal{M},(1)}(\mathsf{D}_{k,\eta})\big)$. Moreover, $\mathbf{n}\mathsf{d}_{f,h}u = 0$ on $\Sigma_{k,\mathbf{N}}$ and $\mathsf{d}^*_{f,h}u = 0$ on $\Sigma_{k,\mathbf{FD}} \cup \Sigma_{k,\mathbf{D}}$ are consequences of the fact that $\mathsf{u}_k^{(1)} \in \mathcal{D}(\Delta_{f,h}^{\mathrm{M},(1)}(\Omega_k^{\mathrm{M}}))$ and $u = 0$ in a neighborhood of $\overline{\Sigma_{k,\mathbf{FD}}}$ in $\overline{\mathsf{D}_{k,\eta}}$. In particular, $\mathsf{d}^*_{f,h}u = 0$ on $\Sigma_{k,\mathbf{D}}$, since, $\mathsf{d}^*_{f,h}u = -\nabla\chi_\eta \cdot \mathsf{u}_k^{(1)} = 0$ on $\Sigma_{k,\mathbf{D}}$ (because $\mathsf{d}^*_{f,h}\mathsf{u}_k^{(1)} = 0$ and $\mathbf{t}\mathsf{u}_k^{(1)} = 0$ on $\Gamma_{k,\mathbf{D}}^{\mathrm{M}} \supset \Sigma_{k,\mathbf{D}}$). This yields $Q_{f,h}^{\mathcal{M},(1)}(\mathsf{D}_{k,\eta})(u,v) = \langle \Delta_{f,h}^{(1)}u, v\rangle_{L^2(\mathsf{D}_{k,\eta})}$, using [27, Eq. (120)], since $v \in \mathcal{D}\big(Q_{f,h}^{\mathcal{M},(1)}(\mathsf{D}_{k,\eta})\big)$, $\mathbf{n}\mathsf{d}_{f,h}u = 0$ on $\Sigma_{k,\mathbf{N}}$ and $\mathsf{d}^*_{f,h}u = 0$ on $\Sigma_{k,\mathbf{FD}} \cup \Sigma_{k,\mathbf{D}}$, and thus concludes the proof of 221.

We have, using (221), and since $\mathsf{D}_{k,\eta} \subset \Omega_k^{\mathrm{M}}$,

$$\big(\Delta_{f,h}^{\mathrm{M},(1)}(\mathsf{D}_{k,\eta}) - \lambda(\Omega_k^{\mathrm{M}})\big)((1-\chi_\eta)\mathsf{u}_k^{(1)}) = \big[\Delta_{f,h}^{(1)}, (1-\chi_\eta)\big]\mathsf{u}_k^{(1)}$$

is supported in $\overline{\mathsf{B}_a(z_k,2\eta)}\setminus\mathsf{B}_a(z_k,3\eta/2)$ (we used here the commutator brackets notation). Using (219) and (220), and the fact that $\big[\Delta^{(1)}_{f,h},(1-\chi_\eta)\big]$ is a bounded linear operator from $\Lambda^1\mathrm{W}^1(\mathsf{D}_{k,\eta})$ to $\Lambda^1L^2(\mathsf{D}_{k,\eta})$, for all $x\in\mathsf{D}_{k,\eta}$ and $\varepsilon>0$, there exists a neighborhood V_x of x in $\mathsf{D}_{k,\eta}$ such that for h small enough:

$$\|(1-\chi_\eta)\mathsf{u}^{(1)}_k\|_{\mathrm{W}^1(V_x)}\leqslant e^{\varepsilon/h}e^{-(1/h)(\mathsf{d}_a(x,z_k)-2\eta)}\|\mathsf{u}^{(1)}_k\|_{\mathrm{W}^1(\mathsf{D}_{k,\eta})}\leqslant e^{\varepsilon/h}e^{-(1/h)(\mathsf{d}_a(x,z_k)-3\eta)}.$$

Proposition 38 is a consequence of the previous estimate, a compactness argument, and the fact that $\mathsf{u}^{(1)}_k=\chi_\eta\mathsf{u}^{(1)}_k+(1-\chi_\eta)\mathsf{u}^{(1)}_k$ and $\|e^{(1/h)\mathsf{d}_a(x,z_k)}\chi_\eta\mathsf{u}^{(1)}_k\|_{\mathrm{W}^1(\Omega^{\mathrm{M}}_k)}\leqslant e^{3\eta/h}$ (by (219) and the continuity of the Agmon distance $\mathsf{d}_a(\cdot,z_k)$). ☐

3.4. Quasi-modes associated with $(z_k)_{k=1,\dots,n}$. — The principal eigenform $\mathsf{u}^{(1)}_k$ of $\Delta^{\mathrm{M},(1)}_{f,h}(\Omega^{\mathrm{M}}_k)$ introduced in Proposition 36 (see (209)) will be used as a quasi-mode for $\Delta^{\mathsf{Di},(1)}_{f,h}(\Omega)$. To do so, we multiply it by a smooth cut-off function χ^{M}_k whose gradient is supported as close as needed to $\Gamma^{\mathrm{M}}_{k,\mathbf{N}}$ and so that $\chi^{\mathrm{M}}_k\mathsf{u}^{(1)}_k$ belongs to the form domain of $\Delta^{\mathsf{Di},(1)}_{f,h}(\Omega)$, namely $\Lambda^1H^1_{\mathbf{T}}(\Omega)$ (as required by item (1) in Proposition 26, see also (119)). More precisely, we have the following result.

Proposition 39. — *Let us assume that the assumptions of Proposition 38 hold. Let $\mathsf{u}^{(1)}_k$ be defined by (209). Let $\beta>0$ and $\chi^M_k(\beta):\overline{\Omega^M_k}\to[0,1]$ be a $\mathcal{C}^\infty$ function such that*

$$\chi^M_k(\beta)=1\ \text{on}\ \big\{x\in\overline{\Omega^M_k},\ \mathsf{d}_{\overline{\Omega}}(x,\overline{\Gamma^M_{k,\mathbf{N}}})>2\beta\big\},\tag{222}$$

and,

$$\chi^M_k(\beta)=0\ \text{on}\ \big\{x\in\overline{\Omega^M_k},\ \mathsf{d}_{\overline{\Omega}}(x,\overline{\Gamma^M_{k,\mathbf{N}}})\leqslant\beta\big\},\tag{223}$$

where we recall that $\mathsf{d}_{\overline{\Omega}}$ denotes the geodesic distance in $\overline{\Omega}$. We extend $\chi^M_k(\beta)$ by 0 on $\overline{\Omega}\setminus\overline{\Omega^M_k}$, and thus $\chi^M_k(\beta)\in\mathcal{C}^\infty(\overline{\Omega})$ (see Figure 8 for a schematic representation of the support of χ^M_k). Then, one defines

$$\mathsf{v}^{(1)}_k:=\frac{\chi^M_k(\beta)\mathsf{u}^{(1)}_k}{\|\chi^M_k(\beta)\mathsf{u}^{(1)}_k\|_{L^2(\Omega)}},\tag{224}$$

for any $\beta\in(0,\beta_0)$ with $\beta_0>0$ small enough so that $\chi^M_k(\beta)\neq0$. For ease of notation, we do not refer to β when writing $\mathsf{v}^{(1)}_k$. Then

$$\mathsf{v}^{(1)}_k\in\Lambda^1H^1_{\mathbf{T}}(\Omega)\cap\Lambda^1\mathcal{C}^\infty_c(\overline{\Omega}).$$

Finally, for any $\delta>0$, there exists $h_\delta>0$ such that for all $h\in(0,h_\delta)$ and $\beta\in(0,\beta_0)$:

$$\big\|\mathsf{d}_{f,h}\mathsf{v}^{(1)}_k\big\|^2_{L^2(\Omega)}+\big\|\mathsf{d}^*_{f,h}\mathsf{v}^{(1)}_k\big\|^2_{L^2(\Omega)}\leqslant C\lambda(\Omega^M_k)+e^{\delta/h}e^{-(2/h)\inf_{\operatorname{supp}\nabla\chi^M_k(\beta)}\mathsf{d}_a(\cdot,z_k)},$$

where $C>0$ is independent of h, β, and δ.

Notice that since $\overline{\Sigma_{z_k}}$ is included in the open subset $\Gamma^{\mathrm{M}}_{k,\mathbf{D}}$ of $\partial\Omega^{\mathrm{M}}_k=\Gamma^{\mathrm{M}}_{k,\mathbf{D}}\cup\overline{\Gamma^{\mathrm{M}}_{k,\mathbf{N}}}$ (see item (1) in Proposition 30), from (222), for $\beta>0$ small enough,

$$\chi^{\mathrm{M}}_k(\beta)=1\ \text{in a neighborhood of}\ \overline{\Sigma_{z_k}}\ \text{in}\ \overline{\Omega^{\mathrm{M}}_k},\tag{225}$$

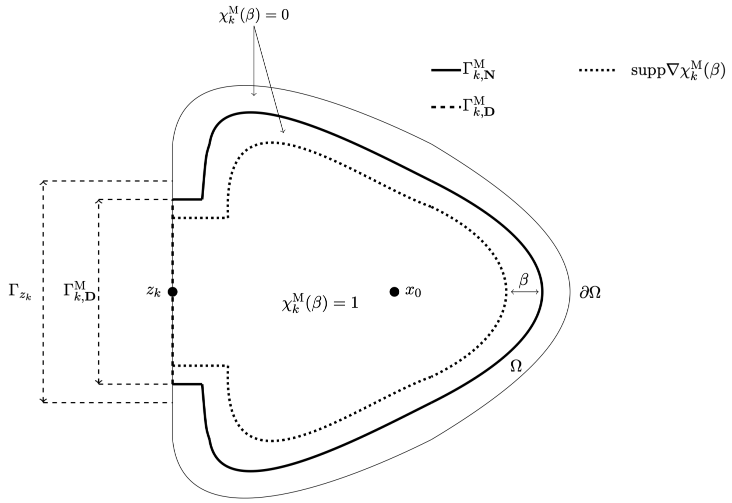

Figure 8. Schematic representation of the cut-off function $\chi_k^{\rm M}(\beta)$, see Proposition 39. The support of $\nabla\chi_k^{\rm M}(\beta)$ is as close as needed to $\overline{\Gamma^{\rm M}_{k,\mathbf{N}}}$, and $\overline{\Gamma^{\rm M}_{k,\mathbf{N}}}$ can be as closed as needed to $\partial\Omega\smallsetminus\Gamma_{z_k}$.

or equivalently, in a neighborhood of $\overline{\Sigma_{z_k}}$ in $\overline{\Omega}$, by (180)–(135)). In addition, one also has that, since $x_0\in\Omega_k^{\rm M}$, for $\beta>0$ small enough,

$$\chi_k^{\rm M}(\beta)=1 \text{ in a neighborhood of } x_0 \text{ in } \Omega_k^{\rm M} \text{ (or equivalently, in } \Omega). \tag{226}$$

In the following, we assume that $\beta>0$ is small enough such that (225) and (226) hold.

Proof. — From (178), $\mathsf{u}_k^{(1)},\mathsf{d}\mathsf{u}_k^{(1)},\mathsf{d}^*\mathsf{u}_k^{(1)}\in\Lambda^1L^2(\Omega_k^{\rm M})$ and $\mathbf{t}\mathsf{u}_k^{(1)}|_{\Gamma^{\rm M}_{k,\mathbf{D}}}=0$. Since $\chi_k^{\rm M}(\beta)=0$ on $\overline{\Omega}\smallsetminus\overline{\Omega_k^{\rm M}}$,

$$\mathsf{v}_k^{(1)},\mathsf{d}\mathsf{v}_k^{(1)},\mathsf{d}^*\mathsf{v}_k^{(1)}\in\Lambda^1L^2(\Omega).$$

Since $\chi_k^{\rm M}(\beta)=0$ on $\partial\Omega\smallsetminus\partial\Omega_k^{\rm M}$ and $\mathbf{t}\mathsf{u}_k^{(1)}|_{\mathrm{int}\,(\partial\Omega\cap\partial\Omega_k^{\rm M})}=0$ (because int $(\partial\Omega_k^{\rm M}\cap\partial\Omega)=\Gamma^{\rm M}_{k,\mathbf{D}}$, see item (1) in Proposition 30), it holds: $\mathbf{t}\mathsf{v}_k^{(1)}=0$ on $\partial\Omega$. Then, by [27, Lem. 73],

$$\mathsf{v}_k^{(1)}\in\Lambda^1H^1_{\mathbf{T}}(\Omega).$$

In addition, since $\Delta^{(1)}_{f,h}\mathsf{u}_k^{(1)}=\lambda(\Omega_k^{\rm M})\mathsf{u}_k^{(1)}\in\Lambda^1L^2(\Omega_k^{\rm M})$ with, on the smooth open subset $\Gamma^{\rm M}_{k,\mathbf{D}}$ of $\Omega_k^{\rm M}$, $\mathbf{t}\mathsf{u}_k^{(1)}=0$ and $\mathbf{t}\mathsf{d}^*_{f,h}\mathsf{u}_k^{(1)}=0$, it holds, by local elliptic regularity (see for example [17]), $\mathsf{u}_k^{(1)}\in\Lambda^1\mathcal{C}^\infty(\Omega_k^{\rm M}\cup\Gamma^{\rm M}_{k,\mathbf{D}})$. Therefore,

$$\mathsf{v}_k^{(1)}\in\Lambda^1\mathcal{C}^\infty_c(\overline{\Omega}).$$

Let us now compute the energy of $\mathsf{v}_k^{(1)}$ in Ω. Let us first deal with $\|\chi_k^{\rm M}(\beta)\mathsf{u}_k^{(1)}\|_{L^2(\Omega)}$. First of all, $\|\chi_k^{\rm M}(\beta)\mathsf{u}_k^{(1)}\|_{L^2(\Omega)}=\|\chi_k^{\rm M}(\beta)\mathsf{u}_k^{(1)}\|_{L^2(\Omega_k^{\rm M})}\leqslant 1$ (we have used that

$\|\mathsf{u}_k^{(1)}\|_{L^2(\Omega)} = 1$, $\chi_k^{\mathrm{M}}(\beta) = 0$ on $\overline{\Omega} \setminus \overline{\Omega_k^{\mathrm{M}}}$, and $\chi_k^{\mathrm{M}} \in [0,1]$). On the other hand, it holds

$$\|\chi_k^{\mathrm{M}}(\beta)\mathsf{u}_k^{(1)}\|_{L^2(\Omega_k^{\mathrm{M}})} \geqslant 1 - \big\|[1-\chi_k^{\mathrm{M}}(\beta)]\mathsf{u}_k^{(1)}\big\|_{L^2(\Omega_k^{\mathrm{M}})}$$

and

$$\big\|[1-\chi_k^{\mathrm{M}}(\beta)]\mathsf{u}_k^{(1)}\big\|_{L^2(\Omega_k^{\mathrm{M}})} = \big\|[1-\chi_k^{\mathrm{M}}(\beta)]e^{-\Psi_k/h}\,\mathsf{u}_k^{(1)}e^{\Psi_k/h}\big\|_{L^2(\Omega_k^{\mathrm{M}})},$$

where we introduced the function $\Psi_k(x) = \mathsf{d}_a(x, z_k)$. Furthermore, $\chi_k^{\mathrm{M}}(\beta) = 1$ in a neighborhood of z_k in $\overline{\Omega}$ (by (225) together with the fact that $z_k \in \Sigma_{z_k}$). Thus, there exists $c > 0$ such that

$$\inf_{\operatorname{supp}(1-\chi_k^{\mathrm{M}}(\beta))} \Psi_k > c.$$

Then, using Proposition 38, one deduces that $\big\|[1-\chi_k^{\mathrm{M}}(\beta)]\mathsf{u}_k^{(1)}\big\|_{L^2(\Omega_k^{\mathrm{M}})} = O(e^{-c/h})$, for some $c > 0$ and as $h \to 0$. Consequently,

$$\|\chi_k^{\mathrm{M}}(\beta)\mathsf{u}_k^{(1)}\|_{L^2(\Omega)} = 1 + O(e^{-c/h}). \tag{227}$$

In addition one has, using again Proposition 38,

$$\begin{aligned}\big\|\mathsf{d}_{f,h}(\chi_k^{\mathrm{M}}(\beta)\mathsf{u}_k^{(1)})\big\|_{L^2(\Omega)} &\leqslant \|\chi_k^{\mathrm{M}}(\beta)\mathsf{d}_{f,h}\mathsf{u}_k^{(1)}\|_{L^2(\Omega_k^{\mathrm{M}})} + h\big\|\nabla\chi_k^{\mathrm{M}}(\beta)\wedge \mathsf{u}_k^{(1)}\big\|_{L^2(\Omega_k^{\mathrm{M}})}\\ &\leqslant \sqrt{\lambda(\Omega_k^{\mathrm{M}})} + e^{\delta/h}e^{-(1/h)\inf_{\operatorname{supp}\nabla\chi_k^{\mathrm{M}}(\beta)}\Psi_k}.\end{aligned}$$

The same inequality holds for $\big\|\mathsf{d}^*_{f,h}(\chi_k^{\mathrm{M}}(\beta)\mathsf{u}_k^{(1)})\big\|_{L^2(\Omega)}$ because

$$\big\|\mathsf{d}^*_{f,h}(\chi_k^{\mathrm{M}}(\beta)\mathsf{u}_k^{(1)})\big\|_{L^2(\Omega)} \leqslant \|\chi_k^{\mathrm{M}}(\beta)\mathsf{d}^*_{f,h}\mathsf{u}_k^{(1)}\|_{L^2(\Omega_k^{\mathrm{M}})} + h\big\|\nabla\chi_k^{\mathrm{M}}(\beta)\cdot \mathsf{u}_k^{(1)}\big\|_{L^2(\Omega_k^{\mathrm{M}})}.$$

The proof of Proposition 39 is complete using (227) and (224). □

According to (126), (222), and (223), for any $\gamma > 0$, one can choose Ω_k^{M} in Proposition 30 and $\beta > 0$ small enough in Proposition 39 (see Figure 8) such that:

$$\sup_{x\in\operatorname{supp}\nabla\chi_k^{\mathrm{M}}(\beta)} \mathsf{d}_{\overline{\Omega}}(x, \partial\Omega\setminus\Gamma_{z_k}) \leqslant \gamma.$$

Hence, for any $\delta > 0$, one can choose $\beta > 0$ and Ω_k^{M} such that:

$$\inf_{\operatorname{supp}\nabla\chi_k^{\mathrm{M}}(\beta)} \mathsf{d}_a(\cdot, z_k) \geqslant \inf_{\partial\Omega\setminus\Gamma_{z_k}} \mathsf{d}_a(\cdot, z_k) - \delta/4. \tag{228}$$

Then, once (228) is satisfied, one can use (183) and Proposition 39 with such $\beta > 0$ and Ω_k^{M} fixed as a function δ, to obtain the following result.

Corollary 40. — *Let us assume that the assumptions of Proposition 38 hold. For any $\delta > 0$, there exists a domain Ω_k^{M}, $\beta > 0$, and $h_\delta > 0$ such that for $h \in (0, h_\delta)$:*

$$\big\|\mathsf{d}_{f,h}\mathsf{v}_k^{(1)}\big\|^2_{L^2(\Omega)} + \big\|\mathsf{d}^*_{f,h}\mathsf{v}_k^{(1)}\big\|^2_{L^2(\Omega)} \leqslant Che^{-(2/h)(f(z_k)-f(x_0))} + e^{\delta/h}e^{-(2/h)\inf_{\partial\Omega\setminus\Gamma_{z_k}}\mathsf{d}_a(\cdot,z_k)},$$

where $C > 0$ is independent of $h > 0$ and $\delta > 0$.

By Corollary 40, and because $\inf_{z\in\partial\Omega\setminus\Gamma_{z_k}} \mathsf{d}_a(z,z_k)>0$ and $f(z_k)>f(x_0)$, there exists $c>0$ such that for h small enough:

$$\big\|\mathsf{d}_{f,h}\mathsf{v}_k^{(1)}\big\|^2_{L^2(\Omega)}+\big\|\mathsf{d}^*_{f,h}\mathsf{v}_k^{(1)}\big\|^2_{L^2(\Omega)}\leqslant Ce^{-c/h}.$$

This implies that $\mathsf{v}_k^{(1)}$ is a quasi-mode associated with the spectrum in $[0,ch]$ of $\Delta^{\mathrm{M},(1)}_{f,h}(\Omega_k^{\mathrm{M}})$ because, using in addition Lemma 11 and the fact that, by Proposition 39, $\mathsf{v}_k^{(1)}\in\Lambda^1H^1_{\mathbf{T}}(\Omega)=\mathcal{D}(Q^{\mathsf{Di},(1)}_{f,h}(\Omega))$, it holds:

$$\big\|\big[1-\pi_{[0,ch]}(\Delta^{\mathsf{Di},(1)}_{f,h}(\Omega))\big]\mathsf{v}_k^{(1)}\big\|^2_{L^2(\Omega)}\leqslant Ce^{-c/h}. \tag{229}$$

4. Proofs of the main results

In this section, we give the proofs of the main results stated in Section 1.2.4.

4.1. Proofs of Theorem 1, Proposition 7, Theorem 2, and Corollary 8

The quasi-modes for $\mathsf{L}^{\mathsf{Di},(0)}_{f,h}(\Omega)$ and $\mathsf{L}^{\mathsf{Di},(1)}_{f,h}(\Omega)$ are defined as follows.

Definition 41. — Let us assume that (Ω-f) is satisfied. Then, one defines for $k\in\{1,\dots,n\}$ (see (209) and (224)):

$$\mathsf{f}_k^{(1)}:=e^{(1/h)f}\mathsf{v}_k^{(1)}\in\Lambda^1H^1_{w,\mathbf{T}}(\Omega).$$

For $r\in(0,\min_{\partial\Omega}f-f(x_0))$, consider $\chi_r\in\mathcal{C}^\infty_c(\Omega)$ such that $\chi_r=1$ on the set $\{f<\min_{\partial\Omega}f-r\}$. Then, one defines:

$$\mathsf{u}^{(0)}:=\frac{\chi_r}{\|\chi_r\|_{L^2_w(\Omega)}}\in\mathcal{C}^\infty_c(\Omega).$$

For ease of notation, we do not refer to $r>0$ in the notation of $\mathsf{u}^{(0)}$. Recall that the family $\{\mathsf{f}_1^{(1)},\dots,\mathsf{f}_n^{(1)}\}$ depends on the parameter $\delta>0$ introduced in Corollary 40. Let us now check that there exist $r>0$ and $\delta>0$ such that the family of quasi-modes $\{\mathsf{f}_1^{(1)},\dots,\mathsf{f}_n^{(1)}\}\cup\{\mathsf{u}^{(0)}\}$ introduced in Definition 41 satisfies the assumptions of Propositions 26 and 27. As explained at the end of this section, Theorem 1, Proposition 7, Theorem 2, and Corollary 8 are then consequences of the results of Propositions 26 and 27.

Let us start with the following lemma.

Lemma 42. — *Let us assume that (Ω-f) is satisfied. Let $\{\mathsf{f}_1^{(1)},\dots,\mathsf{f}_n^{(1)}\}$ and $\mathsf{u}^{(0)}$ be as introduced in Definition 41. Then, item (1) in Proposition 26 is satisfied as well as item (2b). Furthermore, there exists $C>0$ such that for all h small enough:*

$$\big\|u_h-\mathsf{u}^{(0)}\big\|_{L^2_w(\Omega)}\leqslant C\,h^{-d/4+1/2}e^{-(1/h)(f(z_1)-f(x_0)-r)}, \tag{230}$$

where we recall that $r\in(0,f(z_1)-f(x_0))$. Finally, (28) is satisfied.

Proof. — Item (1) in Proposition 26 is satisfied by Definition 41. First of all, because $\{x_0\}=\arg\min_{\overline{\Omega}}f$ (see Lemma 4) and since $\chi_r=1$ near x_0 in Ω (see Definition 41), it holds, using Laplace's method, in the limit $h\to 0$:

$$\|\chi_r\|^2_{L^2_w(\Omega)}=\kappa_{x_0}h^{d/2}e^{-(2/h)f(x_0)}\big(1+O(h)\big), \tag{231}$$

where κ_{x_0} is defined in (186). Recall that from Corollary 25 (see also (122) for the definition of $\pi_h^{(0)}$), the $L^2_w(\Omega)$-orthogonal projector $\pi_h^{(0)}$ associated with $\mathsf{L}^{\mathsf{Di},(0)}_{f,h}(\Omega)$ has rank 1. Because $\mathsf{u}^{(0)} \in \mathcal{D}(Q^{\mathsf{Di},(0)}_{f,h}(\Omega))$ (see Proposition 24 and Section 1.2.3), it holds thanks to Lemma 11:

$$\big\|(1-\pi_h^{(0)})\mathsf{u}^{(0)}\big\|^2_{L^2_w(\Omega)} \leqslant \frac{1}{\mathsf{c}} Q^{\mathsf{Di},(0)}_{f,h}(\Omega)(\mathsf{u}^{(0)}) = \frac{h}{2\mathsf{c}}\|\nabla \mathsf{u}^{(0)}\|^2_{L^2_w(\Omega)}.$$

Using (231) and because $\chi_r \in \mathcal{C}^\infty_c(\Omega)$ such that $\chi_r = 1$ on $\{f < \min_{\partial\Omega} f - r\}$, one has for h small enough:

$$\frac{h}{2}\|\nabla \mathsf{u}^{(0)}\|^2_{L^2_w(\Omega)} = \frac{h}{2}\frac{\|\nabla\chi_r\|^2_{L^2_w(\Omega)}}{\|\chi_r\|^2_{L^2_w(\Omega)}} \leqslant C\|\nabla\chi_r\|^2_{L^\infty(\Omega)}\, h^{-d/2+1}\, e^{-(2/h)(\min_{\partial\Omega} f - f(x_0) - r)}.$$

Hence, because $f(z_1) = \min_{\partial\Omega} f$ (see Lemma 4 and (15)), $\mathsf{u}^{(0)}$ satisfies item (2b) in Proposition 26. In addition, one has:

$$\big\|(1-\pi_h^{(0)})\mathsf{u}^{(0)}\big\|^2_{L^2_w(\Omega)} \leqslant C\|\nabla\chi_r\|^2_{L^\infty(\Omega)}\, h^{-d/2+1}\, e^{-(2/h)(f(z_1)-f(x_0)-r)}.$$

Choosing $r>0$ small enough, it hence holds for h small enough:

$$\|\pi_h^{(0)}\mathsf{u}^{(0)}\|_{L^2_w(\Omega)} = 1 + O(e^{-c/h}) \neq 0,$$

and then (using in addition the fact that u_h and $\mathsf{u}^{(0)}$ are non negative),

$$u_h = \frac{\pi_h^{(0)}\mathsf{u}^{(0)}}{\|\pi_h^{(0)}\mathsf{u}^{(0)}\|_{L^2_w(\Omega)}} = \frac{\mathsf{u}^{(0)}}{\|\pi_h^{(0)}\mathsf{u}^{(0)}\|_{L^2_w(\Omega)}} + \frac{(\pi_h^{(0)}-1)\mathsf{u}^{(0)}}{\|\pi_h^{(0)}\mathsf{u}^{(0)}\|_{L^2_w(\Omega)}} \text{ in } L^2_w(\Omega).$$

Equation (230) is a direct consequence of the three last equations. Moreover, the latter equation implies

$$\int_\Omega u_h\, e^{-(2/h)f} = (1+O(e^{-c/h}))\Big[\int_\Omega \mathsf{u}^{(0)}\, e^{-(2/h)f} + e_h\Big],$$

where

$$|e_h| \leqslant \big\|(1-\pi_h^{(0)})\mathsf{u}^{(0)}\big\|_{L^2_w(\Omega)}\big\|1\big\|_{L^2_w(\Omega)} \leqslant Ce^{-(1/h)(f(x_0)+c_r)},$$

where $c_r = f(z_1) - f(x_0) - r > 0$ (since $r \in (0, f(z_1) - f(x_0))$). On the other hand, from (231) together with the fact that $\int_\Omega \chi\, e^{-(2/h)f}$ has the same asymptotic equivalent as $\int_\Omega \chi^2\, e^{-(2/h)f}$ when $h\to 0$,

$$\int_\Omega \mathsf{u}^{(0)}\, e^{-(2/h)f} = h^{d/4}\sqrt{\kappa_{x_0}}e^{-(1/h)f(x_0)}\big(1+O(h)\big).$$

This proves (28) and concludes the proof of Lemma 42. □

Let us now check that $\{\mathsf{f}_1^{(1)},\dots,\mathsf{f}_n^{(1)}\}$ satisfies item (2a) and item (3) in Proposition 26.

Lemma 43. — *Assume that* (Ω-f) *is satisfied. Let* $\{\mathsf{f}_1^{(1)},\dots,\mathsf{f}_n^{(1)}\}$ *be the family of* 1*-forms introduced in Definition 41. Let* $k\in\{1,\dots,n\}$*. Then, for any* $\delta>0$*, there exists* $h_\delta>0$ *such that for* $h\in(0,h_\delta)$*:*

$$(232)\quad \big\|(1-\pi_h^{(1)})\mathsf{f}_k^{(1)}\big\|^2_{H^1_w(\Omega)} \leqslant Ch^{-2}e^{-(2/h)(f(z_k)-f(x_0))} + e^{\delta/h}e^{-(2/h)(\inf_{\partial\Omega\setminus\Gamma_{z_k}}\mathsf{d}_a(\cdot,z_k))},$$

and for all $\ell \in \{1, \dots, n\}$, $\ell \neq k$,

$$\big|\big\langle \mathsf{f}_k^{(1)}, \mathsf{f}_\ell^{(1)} \big\rangle_{L^2_w(\Omega)}\big| \leqslant e^{\delta/h} e^{-(1/h)\mathsf{d}_a(z_k, z_\ell)}. \tag{233}$$

In particular, choosing $\delta > 0$ small enough, $\{\mathsf{f}_1^{(1)}, \dots, \mathsf{f}_n^{(1)}\}$ satisfies items (2a) *and* (3) *in Proposition* 26, *and if* (25) *and* (26) *hold, then $\{\mathsf{f}_1^{(1)}, \dots, \mathsf{f}_n^{(1)}\}$ satisfies items* (1) *and* (2) *in Proposition* 27.

Proof. — Using Lemma 11 and Proposition 10,

$$\big\|\big[1 - \pi_{[0,\mathsf{c}h]}(\Delta_{f,h}^{\mathsf{Di},(1)}(\Omega))\big]\mathsf{v}_k^{(1)}\big\|^2_{L^2(\Omega)} \leqslant \frac{\big\|\mathsf{d}_{f,h}\mathsf{v}_k^{(1)}\big\|^2_{L^2(\Omega)} + \big\|\mathsf{d}^*_{f,h}\mathsf{v}_k^{(1)}\big\|^2_{L^2(\Omega)}}{\mathsf{c}h}.$$

Therefore, using Corollary 40, for any $\delta > 0$, there exists $h_\delta > 0$ such that for $h \in (0, h_\delta)$:

$$\begin{aligned}\big\|\big[1 - \pi_{[0,\mathsf{c}h]}(\Delta_{f,h}^{\mathsf{Di},(1)}(\Omega))\big]\mathsf{v}_k^{(1)}\big\|^2_{L^2(\Omega)}&\\ &\leqslant Ce^{-(2/h)(f(z_k)-f(x_0))} + e^{\delta/h}e^{-(2/h)(\inf_{\partial\Omega\smallsetminus\Gamma_{z_k}}\mathsf{d}_a(\cdot,z_k))}.\end{aligned}$$

Let us prove that this inequality also holds in $\Lambda^1 H^1(\Omega)$. Set

$$\mathsf{v}_{k,\pi}^{(1)} = \big[1 - \pi_{[0,\mathsf{c}h]}(\Delta_{f,h}^{\mathsf{Di},(1)}(\Omega))\big]\mathsf{v}_k^{(1)}.$$

It holds, using Proposition 10,

$$\big[1 - \pi_{[0,\mathsf{c}h]}(\Delta_{f,h}^{\mathsf{Di},(2)}(\Omega))\big]\mathsf{d}_{f,h}\mathsf{v}_k^{(1)} = \mathsf{d}_{f,h}\mathsf{v}_{k,\pi}^{(1)} = h\mathsf{d}\mathsf{v}_{k,\pi}^{(1)} + \nabla f \wedge \mathsf{v}_{k,\pi}^{(1)}.$$

Therefore,

$$h\|\mathsf{d}\mathsf{v}_{k,\pi}^{(1)}\|_{L^2(\Omega)} \leqslant \|\mathsf{d}_{f,h}\mathsf{v}_k^{(1)}\|_{L^2(\Omega)} + C\|\mathsf{v}_{k,\pi}^{(1)}\|_{L^2(\Omega)}.$$

Similarly, one has $h\|\mathsf{d}^*\mathsf{v}_{k,\pi}^{(1)}\|_{L^2(\Omega)} \leqslant \|\mathsf{d}^*_{f,h}\mathsf{v}_k^{(1)}\|_{L^2(\Omega)} + C\|\mathsf{v}_{k,\pi}^{(1)}\|_{L^2(\Omega)}$. Hence, using also the standard Gaffney inequality in Ω (see [81]), since $\mathsf{v}_{k,\pi}^{(1)} \in \Lambda^1 H^1_{\mathbf{T}}(\Omega)$ (by Proposition 39), it holds:

$$\begin{aligned}C_{\text{Gaffney}}\big\|\mathsf{v}_{k,\pi}^{(1)}\big\|^2_{H^1(\Omega)} &\leqslant \big\|\mathsf{v}_{k,\pi}^{(1)}\big\|^2_{L^2(\Omega)} + \big\|\mathsf{d}\mathsf{v}_{k,\pi}^{(1)}\big\|^2_{L^2(\Omega)} + \big\|\mathsf{d}^*\mathsf{v}_{k,\pi}^{(1)}\big\|^2_{L^2(\Omega)}\\ &\leqslant Ch^{-2}\big(\|\mathsf{d}_{f,h}\mathsf{v}_k^{(1)}\|^2_{L^2(\Omega)} + \|\mathsf{d}^*_{f,h}\mathsf{v}_k^{(1)}\|^2_{L^2(\Omega)} + \|\mathsf{v}_{k,\pi}^{(1)}\|^2_{L^2(\Omega)}\big).\end{aligned} \tag{234}$$

This implies that for $h \in (0, h_\delta)$:

$$\big\|\mathsf{v}_{k,\pi}^{(1)}\big\|^2_{H^1(\Omega)} \leqslant Ch^{-2}\big[e^{-(2/h)(f(z_k)-f(x_0))} + e^{\delta/h}e^{-(2/h)(\inf_{\partial\Omega\smallsetminus\Gamma_{z_k}}\mathsf{d}_a(\cdot,z_k))}\big]. \tag{235}$$

From (119), it holds:

$$\pi_{[0,\mathsf{c}h]}(\Delta_{f,h}^{\mathsf{Di},(1)}(\Omega)) = e^{-(1/h)f}\pi_h^{(1)}e^{(1/h)f}.$$

Therefore, by definition of $\mathsf{f}_k^{(1)}$ (see Definition 41) and from (235),

$$\big\|(1 - \pi_h^{(1)})\mathsf{f}_k^{(1)}\big\|^2_{H^1_w(\Omega)} \leqslant Ch^{-2}e^{-(2/h)(f(z_k)-f(x_0))} + e^{\delta/h}e^{-(2/h)(\inf_{\partial\Omega\smallsetminus\Gamma_{z_k}}\mathsf{d}_a(\cdot,z_k))}.$$

This proves Equation (232).

Let us now prove (233). One has (see Definition 41) using the triangular inequality for d_a,

$$\big|\langle \mathsf{f}_k^{(1)}, \mathsf{f}_\ell^{(1)}\rangle_{L^2_w(\Omega)}\big| = \big|\langle \mathsf{v}_k^{(1)}, \mathsf{v}_\ell^{(1)}\rangle_{L^2(\Omega)}\big| \\ \leqslant e^{-(1/h)\mathsf{d}_a(z_\ell,z_k)}\big\|\mathsf{v}_k^{(1)} e^{(1/h)\mathsf{d}_a(\cdot,z_k)}\big\|_{L^2(\Omega)}\big\|\mathsf{v}_\ell^{(1)} e^{(1/h)\mathsf{d}_a(\cdot,z_\ell)}\big\|_{L^2(\Omega)}.$$

Equation (233) is thus a consequence of the previous inequality together with Proposition 38 and (227) (see also (224)).

Since $f(z_k)-f(x_0)>0$, $\mathsf{d}_a(z_k,z_\ell)>0$, and $\inf_{z\in\partial\Omega\smallsetminus\Gamma_{z_k}}\mathsf{d}_a(z_k,z)>0$ (because d_a is a distance), $\{\mathsf{f}_1^{(1)},\dots,\mathsf{f}_n^{(1)}\}$ satisfies items 2(a) and 3 in Proposition 26 hold choosing $\delta>0$ small enough in (232) and (233). Finally, since $z_\ell\in\partial\Omega\smallsetminus\Gamma_{z_k}$ (because $z_\ell\notin\mathsf{W}^+_{z_k}$ and $\Gamma_{z_k}\subset\mathsf{W}^+_{z_k}$, see (14))

$$\mathsf{d}_a(z_k,z_\ell)\geqslant\inf_{z\in\partial\Omega\smallsetminus\Gamma_{z_k}}\mathsf{d}_a(z_k,z).$$

In addition, $f(z_k)-f(x_0)\geqslant f(z_1)-f(x_0)$ and if $k>\ell$, $f(z_k)-f(z_1)\geqslant f(z_k)-f(z_\ell)$. Thus, if (25) and (26) hold, then $\{\mathsf{f}_1^{(1)},\dots,\mathsf{f}_n^{(1)}\}$ satisfies items 1 and 2 in Proposition 27. ☐

Lemma 44. — *Let us assume that* $(\Omega\text{-}f)$ *is satisfied. Let* $\{\mathsf{f}_1^{(1)},\dots,\mathsf{f}_n^{(1)}\}$ *be the family of* 1*-forms introduced in Definition* 41*. Let* $k,\ell\in\{1,\dots,n\}$*. Then, it holds,*

$$\int_{\Sigma_{z_\ell}}\mathsf{f}_k^{(1)}\cdot\mathsf{n}_\Omega\, e^{-(2/h)f}d\sigma=\begin{cases}0 & \text{if } k\neq\ell,\\ -\mathsf{b}_k\, h^{\mathsf{m}}\, e^{-(1/h)f(z_k)}\,(1+O(\sqrt{h})) & \text{if } k=\ell,\end{cases}$$

where b_k *and* m *are defined in* (186)*. Let* $\mathsf{u}^{(0)}$ *be as introduced in Definition* 41*. Then, for all* $k\in\{1,\dots,n\}$*, there exists* $c>0$ *such that as* $h\to0$*:*

$$\big\langle\nabla\mathsf{u}^{(0)},\mathsf{f}_k^{(1)}\big\rangle_{L^2_w(\Omega)}=\begin{cases}\mathsf{K}_k h^{\mathsf{p}}\, e^{-(1/h)(f(z_1)-f(x_0))}(1+O(\sqrt{h})) & \text{if } k\in\{1,\dots,n_0\},\\ O(e^{-(1/h)(f(z_1)-f(x_0)+c)}) & \text{if } k>n_0,\end{cases}$$

where K_k *and* p *are defined in* (237) *below. In particular,* $\{\mathsf{f}_1^{(1)},\dots,\mathsf{f}_n^{(1)}\}$ *and* $\mathsf{u}^{(0)}$ *satisfy item* (4) *in Proposition* 26*. If moreover* (25) *and* (26) *hold, one has as* $h\to0$*,*

$$\big\langle\nabla\mathsf{u}^{(0)},\mathsf{f}_k^{(1)}\big\rangle_{L^2_w(\Omega)}=\mathsf{K}_k h^{\mathsf{p}}\, e^{-(1/h)(f(z_k)-f(x_0))}(1+O(\sqrt{h})).$$

Hence, if (25) *and* (26) *hold,* $\{\mathsf{f}_1^{(1)},\dots,\mathsf{f}_n^{(1)}\}$ *and* $\mathsf{u}^{(0)}$ *satisfy items* (3) *and* (4) *in Proposition* 27*.*

Proof. — Recall the definitions of $\mathsf{u}^{(0)}$ and $\{\mathsf{f}_1^{(1)},\dots,\mathsf{f}_n^{(1)}\}$ in Definition 41. The proof is divided into several steps.

Step 1. — Let us first compute $\int_{\Sigma_{z_k}}\mathsf{u}_k^{(1)}\cdot\mathsf{n}_\Omega\, e^{-(1/h)f}$. One has since $\overline{\Sigma_{z_k}}\subset\Gamma^{\mathrm{M}}_{k,\mathbf{D}}$ (see item (1) in Proposition 30),

$$\int_{\Sigma_{z_k}}\mathsf{u}_k^{(1)}\cdot\mathsf{n}_\Omega\, e^{-(1/h)f}=\int_{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}}\mathsf{u}_k^{(1)}\cdot\mathsf{n}_\Omega\, e^{-(1/h)f}d\sigma-\int_{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}\smallsetminus\Sigma_{z_k}}\mathsf{u}_k^{(1)}\cdot\mathsf{n}_\Omega\, e^{-(1/h)f}.$$

It holds, using the trace estimate (175) and Proposition 38, for any $\delta>0$, there exists $h_\delta>0$ such that for $h\in(0,h_\delta)$:

$$\Big|\int_{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}\setminus\Sigma_{z_k}}\mathsf{u}^{(1)}_k\cdot\mathsf{n}_\Omega\ e^{-(1/h)f}\Big|\leqslant e^{-(1/h)\inf_{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}\setminus\Sigma_{z_k}}(\mathsf{d}_a(\cdot,z_k)+f(z_k))}e^{\delta/h}.$$

Notice that we have used that $f\geqslant f(z_k)$ on $\Gamma^{\mathrm{M}}_{k,\mathbf{D}}$ (because $\Gamma^{\mathrm{M}}_{k,\mathbf{D}}\subset\Gamma_{z_k}\subset\mathsf{W}^+_{z_k}$, see Lemma 14). Thus, since $\inf_{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}\setminus\Sigma_{z_k}}\mathsf{d}_a(\cdot,z_k)>0$, for $\delta>0$ small enough, one has for h small enough

$$\Big|\int_{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}\setminus\Sigma_{z_k}}\mathsf{u}^{(1)}_k\cdot\mathsf{n}_\Omega\ e^{-(1/h)f}\Big|\leqslant e^{-(1/h)(f(z_k)+c)}. \tag{236}$$

Using (185), it then holds as $h\to 0$:

$$\int_{\Sigma_{z_k}}\mathsf{u}^{(1)}_k\cdot\mathsf{n}_{\Omega^{\mathrm{M}}_k}\ e^{-(1/h)f}=-\mathsf{b}_k h^{\mathsf{m}}\,e^{-(1/h)f(z_k)}(1+O(\sqrt{h})),$$

where b_k and m are defined in (186).

Step 2. — Let us deal with the terms $\int_{\Sigma_{z_\ell}}\mathsf{f}^{(1)}_k\cdot\mathsf{n}_\Omega\,e^{-(1/h)f}$. One has $\chi^{\mathrm{M}}_k(\beta)=0$ on $\partial\Omega\setminus\overline{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}}$. Indeed, $\chi^{\mathrm{M}}_k(\beta)$ is supported in $\overline{\Omega^{\mathrm{M}}_k}$ (see (222), and (223)) and

$$\overline{\Omega^{\mathrm{M}}_k}\cap\partial\Omega=\partial\Omega^{\mathrm{M}}_k\cap\partial\Omega=\overline{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}}$$

(see item (1) Proposition 30). In particular, because $\overline{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}}\subset\Gamma_{z_k}$, and $\Gamma_{z_k}\cap\Sigma_\ell\subset\Gamma_{z_k}\cap\Gamma_{z_\ell}=\varnothing$ when $k\neq\ell$ (see the line after the proof of Lemma 4 and (16)), $\chi^{\mathrm{M}}_k(\beta)=0$ on Σ_{z_ℓ} when $k\neq\ell$. Then, one has using (224), (225) and (227),

$$\begin{aligned}\int_{\Sigma_{z_\ell}}\mathsf{f}^{(1)}_k\cdot\mathsf{n}_\Omega\ e^{-(2/h)f}&=\int_{\Sigma_{z_\ell}}\mathsf{v}^{(1)}_k\cdot\mathsf{n}_\Omega\ e^{-(1/h)f}d\sigma\\&=\frac{1}{\|\chi^{\mathrm{M}}_k(\beta)\mathsf{u}^{(1)}_k\|_{L^2(\Omega)}}\int_{\Sigma_{z_\ell}}\chi^{\mathrm{M}}_k(\beta)\mathsf{u}^{(1)}_k\cdot\mathsf{n}_\Omega\ e^{-(1/h)f}\\&=(1+O(e^{-c/h}))\times\begin{cases}0&\text{if }k\neq\ell,\\\int_{\Sigma_{z_k}}\mathsf{u}^{(1)}_k\cdot\mathsf{n}_\Omega\ e^{-(1/h)f}&\text{if }k=\ell,\end{cases}\\&=\begin{cases}0&\text{if }k\neq\ell,\\-\mathsf{b}_k\ h^{\mathsf{m}}\ e^{-(1/h)f(z_k)}\ (1+O(\sqrt{h}))&\text{if }k=\ell.\end{cases}\end{aligned}$$

This proves the first statement in Lemma 44. In particular, $\{\mathsf{f}^{(1)}_1,\dots,\mathsf{f}^{(1)}_n\}$ satisfies item (4b) in Proposition 26 and item (4) in Proposition 27.

Step 3. — Let us finally deal with the terms $\big\langle \nabla \mathsf{u}^{(0)}, \mathsf{f}_k^{(1)}\big\rangle_{L^2_w(\Omega)}$. One has, since $\chi_r = 0$ on $\partial\Omega$, from (224),

$$\begin{aligned}
&\big\langle \nabla \mathsf{u}^{(0)}, \mathsf{f}_k^{(1)}\big\rangle_{L^2_w(\Omega)} = \frac{1}{\|\chi_r\|_{L^2_w(\Omega)}}\big\langle \nabla \chi_r, e^{-(1/h)f}\mathsf{v}_k^{(1)}\big\rangle_{L^2(\Omega)}\\
&= -\frac{1}{\|\chi_r\|_{L^2_w(\Omega)}}\big\langle \nabla (1-\chi_r), e^{-(1/h)f}\mathsf{v}_k^{(1)}\big\rangle_{L^2(\Omega)}\\
&= \frac{1}{\|\chi_r\|_{L^2_w(\Omega)}}\Big[h^{-1}\big\langle (1-\chi_r), e^{-(1/h)f}\mathsf{d}^*_{f,h}\mathsf{v}_k^{(1)}\big\rangle_{L^2(\Omega)} - \int_{\partial\Omega} e^{-(1/h)f}\mathsf{v}_k^{(1)}\cdot \mathsf{n}_\Omega\Big]\\
&= \frac{1}{\|\chi_r\|_{L^2_w(\Omega)}}\Big[h^{-1}\big\langle (1-\chi_r)e^{-(1/h)f}, \mathsf{d}^*_{f,h}\mathsf{v}_k^{(1)}\big\rangle_{L^2(\Omega)} - \int_{\partial\Omega\cap \operatorname{supp}\chi_k^{\mathrm{M}}(\beta)} e^{-(1/h)f}\mathsf{v}_k^{(1)}\cdot \mathsf{n}_\Omega\Big].
\end{aligned}$$

Let us first deal with the boundary term in the previous equality. Because $\chi_k^{\mathrm{M}}(\beta) = 0$ on $\partial\Omega \smallsetminus \overline{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}}$, from (224) and (227), it holds:

$$\begin{aligned}
\int_{\partial\Omega\cap \operatorname{supp}\chi_k^{\mathrm{M}}(\beta)} e^{-(1/h)f}\mathsf{v}_k^{(1)}\cdot \mathsf{n}_\Omega &= (1+O(e^{-c/h}))\int_{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}} \chi_k^{\mathrm{M}}(\beta) e^{-(1/h)f}\mathsf{u}_k^{(1)}\cdot \mathsf{n}_\Omega\\
&= (1+O(e^{-c/h}))\Big[\int_{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}} (\chi_k^{\mathrm{M}}(\beta)-1) e^{-(1/h)f}\mathsf{u}_k^{(1)}\cdot \mathsf{n}_\Omega + \int_{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}} e^{-(1/h)f}\mathsf{u}_k^{(1)}\cdot \mathsf{n}_\Omega\Big].
\end{aligned}$$

It holds, from (225),

$$\begin{aligned}
\Big|\int_{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}} (\chi_k^{\mathrm{M}}(\beta)-1) e^{-(1/h)f}\mathsf{u}_k^{(1)}\cdot \mathsf{n}_\Omega\Big| &= \Big|\int_{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}\smallsetminus \Sigma_{z_k}} (\chi_k^{\mathrm{M}}(\beta)-1) e^{-(1/h)f}\mathsf{u}_k^{(1)}\cdot \mathsf{n}_\Omega\Big|\\
&\leqslant C\Big|\int_{\Gamma^{\mathrm{M}}_{k,\mathbf{D}}\smallsetminus \Sigma_{z_k}} e^{-(1/h)f}\mathsf{u}_k^{(1)}\cdot \mathsf{n}_\Omega\Big|.
\end{aligned}$$

Thus from (236) and (185), it then holds as $h\to 0$:

$$\int_{\partial\Omega\cap \operatorname{supp}\chi_k^{\mathrm{M}}(\beta)} e^{-(1/h)f}\mathsf{v}_k^{(1)}\cdot \mathsf{n}_\Omega = -\mathsf{b}_k h^{\mathsf{m}}\, e^{-(1/h)f(z_k)}(1+O(\sqrt{h})).$$

Hence, as $h\to 0$, one has using (231) (see also (186)):

$$-\frac{1}{\|\chi_r\|_{L^2_w(\Omega)}}\int_{\partial\Omega\cap \operatorname{supp}\chi_k^{\mathrm{M}}(\beta)} e^{-(1/h)f}\mathsf{v}_k^{(1)}\cdot \mathsf{n}_\Omega = \mathsf{K}_k h^{\mathsf{p}}\, e^{-(1/h)(f(z_k)-f(x_0))}(1+O(\sqrt{h})),$$

with

$$\mathsf{K}_k = \frac{\mathsf{b}_k}{\sqrt{\kappa_{x_0}}} = \sqrt{\mathsf{A}_{x_0,z_k}} \quad\text{and}\quad \mathsf{p} = \mathsf{m} - \frac{d}{4} = -\frac{1}{2}, \tag{237}$$

where A_{x_0,z_k} is defined in (184).

Let us now deal with the error term $\big\langle (1-\chi_r)e^{-(1/h)f}, \mathsf{d}^*_{f,h}\mathsf{v}_k^{(1)}\big\rangle_{L^2(\Omega)}$. Using Proposition 39 and Corollary 40, for any $\delta>0$, there exists $h_\delta>0$ such that for $h\in(0,h_\delta)$:

$$\begin{aligned}
\big|\big\langle (1-\chi_r), e^{-(1/h)f}\mathsf{d}^*_{f,h}\mathsf{v}_k^{(1)}\big\rangle_{L^2(\Omega)}\big| &\leqslant C e^{-(1/h)\min_{\operatorname{supp}(1-\chi_r)} f}\|\mathsf{d}^*_{f,h}\mathsf{v}_k^{(1)}\|_{L^2(\Omega)}\\
&\leqslant C e^{-(1/h)(f(z_1)-r)}\big[e^{-(1/h)(f(z_k)-f(x_0))} + e^{\delta/h} e^{-(1/h)(\inf_{z\in\partial\Omega\smallsetminus\Gamma_{z_k}} \mathsf{d}_a(z_k,z))}\big].
\end{aligned}$$

Therefore, using (231),

$$\frac{\big|\big\langle(1-\chi_r)e^{-(1/h)f},\mathsf{d}^*_{f,h}\mathsf{v}^{(1)}_k\big\rangle_{L^2(\Omega)}\big|}{\|\chi_r\|_{L^2_w(\Omega)}} \leqslant C\big[h^{-d/4}e^{-(1/h)(f(z_k)-f(x_0))}e^{-(1/h)(f(z_1)-f(x_0)-r)} + e^{\delta/h}e^{-(1/h)(\inf_{z\in\partial\Omega\smallsetminus\Gamma_{z_k}}\mathsf{d}_a(z_k,z))}e^{-(1/h)(f(z_1)-f(x_0)-r)}\big] \leqslant e^{-(1/h)\mathsf{E}_k(r,\delta)},$$

where, for $r>0$ and $\delta>0$ small enough, one can choose $\mathsf{E}_k(r,\delta)>f(z_1)-f(x_0)$. Moreover, if (25) and (26) hold, then $\inf_{z\in\partial\Omega\smallsetminus\Gamma_{z_k}}\mathsf{d}_a(z_k,z)>f(z_k)-f(z_1)$ and $f(z_1)-f(x_0)>f(z_k)-f(z_1)$. Thus, for $r>0$ and $\delta>0$ small enough, one can choose $\mathsf{E}_k(r,\delta)>f(z_k)-f(x_0)$. The proof of Lemma 44 is complete. □

In this section, we proved (see Lemmas 42, 43, and 44) that the quasi-modes $\{\mathsf{f}^{(1)}_1,\dots,\mathsf{f}^{(1)}_n\}\cup\{\mathsf{u}^{(0)}\}$ satisfy all the assumptions of Propositions 26 and 27. We can now conclude the proofs of Theorem 1, Proposition 7, Theorem 2, and Corollary 8, using the results of Propositions 26 and 27. Theorem 1 is a consequence of Propositions 26 and 27 together with the formulas (186) and (237) for the constants b_k, m, K_k, and p. Proposition 7 is a consequence of Lemma 42 and Proposition 26 (notice that using Lemma 4, Proposition 7 is also a consequence of the results of [58]: we thus here provide a new proof using 1-forms). Theorem 2 is a consequence of Theorem 1 and Proposition 7 together with (21). Corollary 8 is a consequence of Theorem 1, Proposition 7, and (22). It remains to prove Theorem 3.

4.2. Generalization to deterministic initial conditions: proof of Theorem 3

The proof of Theorem 3 relies on so-called leveling results (see Corollary 47 below) which only requires that $f:\overline{\Omega}\to\mathbb{R}$ is a $\mathcal{C}^\infty$ function which satisfies item (1) in (Ω-f). For $F\in\mathcal{C}^\infty(\partial\Omega,\mathbb{R})$, let us define

$$\forall x\in\overline{\Omega},\quad w_h(x)=\mathbb{E}_x[F(X_\tau)], \tag{238}$$

where τ is defined by (2).

4.2.1. *Leveling result on w_h.* — For any closed subset $\mathsf{F}\subset\mathbb{R}^d$, one denotes by

$$\tau_{\mathsf{F}}=\inf\{t\geqslant 0,\ X_t\in\mathsf{F}\}$$

the first time the process (1) hits F (in particular, $\tau=\tau_{\Omega^c}$). Let x_0 be a local minimum of f in Ω. Let us recall that $\mathsf{B}(x_0,h)$ is the open ball centered at x_0 of radius h. Let us assume that h is small enough so that $\overline{\mathsf{B}}(x_0,h)\subset\Omega$, where $\overline{\mathsf{B}}(x_0,h)$ is the closure of $\mathsf{B}(x_0,h)$. The function

$$\mathsf{p}_{x_0}:x\longmapsto\mathbb{P}_x\big[\tau_{\Omega^c}<\tau_{\overline{\mathsf{B}}(x_0,h)}\big]$$

is called the *committor function* (or the *equilibrium potential*) between Ω^c and $\overline{\mathsf{B}}(x_0,h)$. We have the following precise leveling result on $\mathsf{p}_{x_0}:\overline{\Omega}\to\mathbb{R}$.

Proposition 45. — *Let us assume that* $f:\overline{\Omega}\to\mathbb{R}$ *is a* $\mathcal{C}^\infty$ *Morse function which satisfies item* (1) *in* (Ω-f)*. Let* K *be a compact subset of* $\{f<\min_{\partial\Omega} f\}$*. Then, there exist* $C_{\mathsf{K}}>0$ *and* $h_0>0$ *such that for all* $h\in(0,h_0)$ *and* $x\in\mathsf{K}$*:*

$$\mathsf{p}_{x_0}(x)\leqslant C_{\mathsf{K}}\, h^{-d}e^{-(2/h)(\min_{\partial\Omega} f-f(x))}. \tag{239}$$

We refer to Figure 9 for a schematic representation of $\{f<\min_{\partial\Omega} f\}$ and $\mathsf{B}(x_0,h)$ (recall that since item (1) in (Ω-f) holds, f satisfies item (1) in Lemma 4).

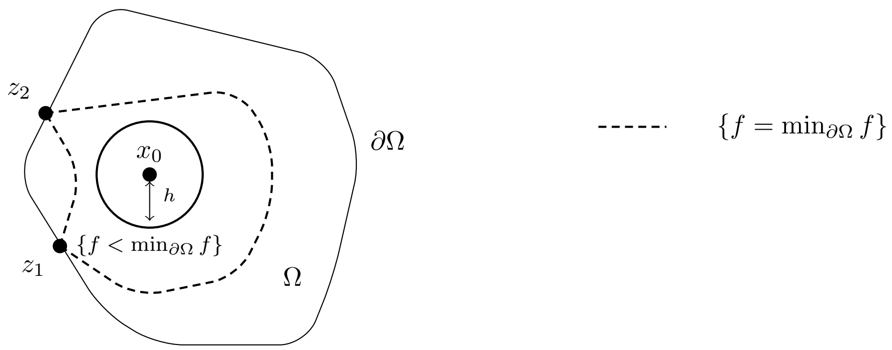

Figure 9. Schematic representation of $\{f<\min_{\partial\Omega} f\}$ and $\mathsf{B}(x_0,h)$. On the figure, it holds $\partial\{f<\min_{\partial\Omega} f\}\cap\partial\Omega=\{z_1,z_2\}$.

Proof. — The proof of this result is inspired by the proofs of [8, Lem. 4.6] and [53, Prop. 7.9]. Let $x\in\Omega$. If $x\in\overline{\mathsf{B}}(x_0,h)$, then $\mathsf{p}_{x_0}=0$. Let us thus deal with the case when $x\in\Omega\smallsetminus\overline{\mathsf{B}}(x_0,h)$.

Step 1. First inequality for $\mathsf{p}_{x_0}(x)$ *using capacities*. — In this step, we prove Equation (242) below. Let us denote by $\mathsf{d}_{\mathbb{R}^d}$ the standard Euclidean distance in $\mathbb{R}^d$. Let G_h be the Green function of $\mathsf{L}^{\mathsf{Di},(0)}_{f,h}(\Omega\smallsetminus\overline{\mathsf{B}}(x_0,h))$, see [8, Eq. (2.3)]. Set for $x\in\Omega\smallsetminus\overline{\mathsf{B}}(x_0,h)$,

$$c=\mathsf{d}_{\mathbb{R}^d}(x,\Omega^c\cup\overline{\mathsf{B}}(x_0,h))/2. \tag{240}$$

Define

$$\rho=ch>0 \text{ and } R=\rho/3.$$

On the one hand, using this pair (ρ,R) in the proof of [8, Lem. 4.6], one deduces that there exists $C_H>0$ such that for all $x\in\Omega\smallsetminus\overline{\mathsf{B}}(x_0,h)$, $h\in(0,1]$,

$$\sup_{z\in\partial\mathsf{B}(x,\rho)} G_h(x,z)\leqslant C_H^{\pi\rho/R}\inf_{z\in\partial\mathsf{B}(x,\rho)} G_h(x,z). \tag{241}$$

Notice that c depends on h and x (which was *a priori* not the case in [8, Lem. 4.6]). Let us explain more precisely why (241) remains valid in our setting. To get Equation (241), one uses k times the Harnack inequality [35] (see also [8, Lem. 4.1]) on k balls $\mathsf{B}(x_i,\rho)$ where $x_i\in\partial\mathsf{B}(x,\rho)$ with $\mathsf{B}(x_i,R)\cap\mathsf{B}(x_{i+1},R)\neq\varnothing$ ($i=1,\dots,k$, $x_{k+1}=x_1$), and where $k\leqslant\pi\rho/R$. The constant C_H in (241) is the one from the Harnack inequality used on each $\mathsf{B}(x_i,R)$. In addition, this constant C_H depends on $h^{-2}R^2$ and thus can be chosen independently of h since for all $x \in \Omega \setminus \overline{\mathsf{B}}(x_0, h)$ and $h > 0$,

$$h^{-2}R^2 \leqslant \mathsf{d}^2_{\mathbb{R}^d}(x, \Omega^c \cup \{x_0\})/6^2 \leqslant \mathsf{M}_0^2/36,$$

where $\mathsf{M}_0 := \max_{y\in\overline{\Omega}} \mathsf{d}_{\mathbb{R}^d}(y, \Omega^c \cup \{x_0\})$. The condition $h \leqslant 1$ in (241) ensures that we can use the Harnack inequality, since for all $x \in \Omega \setminus \overline{\mathsf{B}}(x_0, h)$ and all $i = 1, \ldots, k$,

$$\mathsf{B}(x_i, 2R) \subset \Omega \setminus \overline{\mathsf{B}}(x_0, h),$$

which follows from the fact that, if $h \leqslant 1$, $\rho + 2R = 5\mathsf{d}_{\mathbb{R}^d}(x, \Omega^c \cup \overline{\mathsf{B}}(x_0, h))h/6 < \mathsf{d}_{\mathbb{R}^d}(x, \Omega^c \cup \overline{\mathsf{B}}(x_0, h))$. Finally notice that we have that

$$C_H^{\pi\rho/R} = C_H^{\pi/3}.$$

On the other hand, using the arguments of the proof of [53, Prop. 7.9] with $\mathcal{C} = \mathsf{B}(x, \rho)$ there, together with (241), one deduces that there exists $C > 0$ such that for all $x \in \Omega \setminus \overline{\mathsf{B}}(x_0, h)$ and h small enough:

$$\mathsf{p}_{x_0}(x) \leqslant C \frac{\mathrm{cap}(\mathsf{B}(x, \rho), \Omega^c)}{\mathrm{cap}(\mathsf{B}(x, \rho), \mathsf{B}(x_0, h) \cup \Omega^c)}, \tag{242}$$

where we recall that (see [8, §2]) for two subsets C and D of $\mathbb{R}^d$ such that $\overline{\mathsf{C}} \cap \overline{\mathsf{D}} = \varnothing$,

$$\mathrm{cap}(\mathsf{C}, \mathsf{D}) = \frac{h}{2} \inf_{\varphi \in H_{\mathsf{C},\mathsf{D}}} \int_{\mathbb{R}^d \setminus (\mathsf{D}\cup\mathsf{C})} \big|\nabla\varphi(x)\big|^2 e^{-(2/h)f(x)} dx, \tag{243}$$

where

$$H_{\mathsf{C},\mathsf{D}} = \big\{\varphi \in H^1(\mathbb{R}^d),\ \varphi(x) = 1 \text{ for } x \in \mathsf{C},\ \varphi(x) = 0 \text{ for } x \in \mathsf{D}\big\}.$$

Step 2. Upper bound on $\mathrm{cap}(\mathsf{B}(x, \rho), \Omega^c)$ *and lower bound on* $\mathrm{cap}(\mathsf{B}(x, \rho), \mathsf{B}(x_0, h) \cup \Omega^c)$

Let us first obtain a lower bound on $\mathrm{cap}(\mathsf{B}(x, \rho), \mathsf{B}(x_0, h) \cup \Omega^c)$. By the variational principle for capacities (243), it holds:

$$\mathrm{cap}(\mathsf{B}(x, \rho), \mathsf{B}(x_0, h) \cup \Omega^c) \geqslant \mathrm{cap}(\mathsf{B}(x, \rho), \mathsf{B}(x_0, h)).$$

Let K be a compact subset of Ω. Following the proof of [53, Lem. 7.10] (see also [8, Prop. 4.7]) with here $\rho : [0, 1] \to \Omega$ a smooth path connecting x to x_0 and such that $t \in [0, 1] \mapsto f(\rho(t))$ is decreasing, there exists $C > 0$ such that for all $x \in \mathsf{K}$ and $h > 0$ (recall x_0 is the global minimum of f in $\overline{\Omega}$),

$$\mathrm{cap}(\mathsf{B}(x, \rho), \mathsf{B}(x_0, h)) \geqslant C h^d e^{-(2/h)f(x)}. \tag{244}$$

Let us now deal with $\mathrm{cap}(\mathsf{B}(x, \rho), \Omega^c)$. Let U_h be the subdomain of $\{f < \min_{\partial\Omega} f\}$ such that $\overline{\mathsf{U}_h} \subset \{f < \min_{\partial\Omega} f\}$ and for all $x \in \partial\mathsf{U}_h$, $\mathsf{d}_{\mathbb{R}^d}(x, \{f < \min_{\partial\Omega} f\}^c) = h$. It then follows that for h small enough,

$$\min_{\{f<\min_{\partial\Omega} f\}\setminus \mathsf{U}_h} f \geqslant \min_{\partial\Omega} f - \varepsilon h, \tag{245}$$

for some $\varepsilon > 0$ independent of h. Let ϕ_h be a smooth function on $\mathbb{R}^d$ such that $\phi_h = 0$ on $\{f < \min_{\partial\Omega} f\}^c$, $\phi_h = 1$ on U_h, and for some $C > 0$ independent of h,

$$\|\nabla\phi_h\|_{L^\infty(\Omega)} \leqslant C h^{-1}. \tag{246}$$

Assume now that K is a compact subset of $\{f < \min_{\partial\Omega} f\}$. Then, for h small enough, it holds for all $x \in \mathsf{K}$:

$$\mathsf{B}(x,\rho) \subset \mathsf{U}_h,$$

where we recall $\rho = ch > 0$ where c is defined by (240) and satisfies $c \leqslant \mathsf{M}_0/2$. Hence, using the variational formula (243), it holds, for h small enough and all $x \in \mathsf{K}$,

$$\operatorname{cap}(\mathsf{B}(x,\rho),\Omega^c) \leqslant \frac{h}{2}\int_{\mathbb{R}^d} |\nabla\phi_h|^2 e^{-(2/h)f} = \frac{h}{2}\int_{\{f<\min_{\partial\Omega} f\}\smallsetminus \mathsf{U}_h} |\nabla\phi_h|^2 e^{-(2/h)f}.$$

Using in addition (245) and (246), one deduces that for h small enough and all $x \in \mathsf{K}$,

$$\operatorname{cap}(\mathsf{B}(x,\rho),\Omega^c) \leqslant Ce^{-(2/h)(\min_{\partial\Omega} f - ch)} \tag{247}$$

where $C > 0$ is a constant independent of $x \in \mathsf{K}$ and h. In conclusion, Equations (242), (244), and (247) imply (239). This concludes the proof of Proposition 45. $\square$

Let us recall that $w_h(x) = \mathbb{E}_x[F(X_{\tau_{\Omega^c}})]$ (see (238)). We will need the following leveling result on w_h in $\mathsf{B}(x_0,h)$ (see [52, Lem. 1] or [75, Lem. 3] for a proof).

Lemma 46. — *Let us assume that $f : \overline{\Omega} \to \mathbb{R}$ is a $\mathcal{C}^\infty$ Morse function. Let x_0 be a local minimum of f in Ω. Then, it holds for h small enough*

$$\sup_{x\in\mathsf{B}(x_0,h)} |w_h(x) - w_h(x_0)| \leqslant C\sqrt{h}\, w_h(x_0).$$

The two previous results have the following consequence on w_h.

Corollary 47. — *Let us assume that $f : \overline{\Omega} \to \mathbb{R}$ is a $\mathcal{C}^\infty$ Morse function which satisfies item (1) in (Ω-f). Let K be a compact subset of $\{f < \min_{\partial\Omega} f\}$. Then, for h small enough and uniformly in $x \in \mathsf{K}$, one has,*

$$w_h(x) = w_h(x_0)(1 + O(\sqrt{h})) + O(h^{-d}e^{-(2/h)(\min_{\partial\Omega} f - \max_{\mathsf{K}} f)}).$$

Let us mention that a similar result was proved in [27, §5.1.4] using [30, Th. 1] when f has no critical point on the boundary of Ω. When this is no longer the case, [30, Th. 1] does not apply and we prove this result using the strong Markov property together with Proposition 45 and Lemma 46.

Proof. — Let K be a compact subset of $\{f < \min_{\partial\Omega} f\}$ and $x \in \mathsf{K}$. Then write:

$$\mathbb{E}_x[F(X_{\tau_{\Omega^c}})] = \mathbb{E}_x\big[F(X_{\tau_{\Omega^c}})\,\mathbf{1}_{\tau_{\mathsf{B}(x_0,h)}<\tau_{\Omega^c}}\big] + \mathbb{E}_x\big[F(X_{\tau_{\Omega^c}})\mathbf{1}_{\tau_{\mathsf{B}(x_0,h)}\geqslant\tau_{\Omega^c}}\big]. \tag{248}$$

By the strong Markov property,

$$\mathbb{E}_x\big[F(X_{\tau_{\Omega^c}})\mathbf{1}_{\tau_{\mathsf{B}(x_0,h)}<\tau_{\Omega^c}}\big] = \mathbb{E}_x\big[\mathbf{1}_{\tau_{\mathsf{B}(x_0,h)}<\tau_{\Omega^c}}\mathbb{E}_{X_{\tau_{\mathsf{B}(x_0,h)}}}[F(X_{\tau_{\Omega^c}})]\big].$$

Using Proposition 45 and Lemma 46, for all h small enough and $x \in \mathsf{K}$, it holds:

$$\begin{aligned}&\mathbb{E}_x\big[F(X_{\tau_{\Omega^c}})\,\mathbf{1}_{\tau_{\mathsf{B}(x_0,h)}<\tau_{\Omega^c}}\big] = \big(1 + O(e^{-c/h})\big)\big(1 + O(\sqrt{h})\big)w_h(x_0),\\ &\text{uniformly in } x \in \mathsf{K},\end{aligned} \tag{249}$$

where $c > 0$ is any constant such that $c < 2(\min_{\partial\Omega} f - \max_{\mathsf{K}} f)$. Let us now deal with the last term in (248). For $x \in \mathsf{K}$, it holds:

$$\mathbb{E}_x\big[F(X_{\tau_{\Omega^c}})\mathbf{1}_{\tau_{\mathsf{B}(x_0,h)}\geqslant\tau_{\Omega^c}}\big] \leqslant \|F\|_{L^\infty(\partial\Omega)}\mathbb{P}_x[\tau_{\mathsf{B}(x_0,h)} \geqslant \tau_{\Omega^c}].$$

Using Proposition 45, it thus holds for h small enough:

$$\max_{x\in \mathsf{K}} \mathbb{E}_x\big[F(X_{\tau_{\Omega^c}})\mathbf{1}_{\tau_{\mathsf{B}(x_0,h)}\geqslant \tau_{\Omega^c}}\big] \leqslant Ch^{-d}e^{-(2/h)(\min_{\partial\Omega} f-\max_{\mathsf{K}} f)}.$$

Together with (249) and (248), this concludes the proof of Corollary 47. □

4.2.2. *Proof of Theorem* 3. — We are now in position to prove Theorem 3.

Proof of Theorem 3. — Let us assume that Assumption (Ω-f) is satisfied. Let us define for $\alpha \in \mathbb{R}$,

$$\mathsf{K}_\alpha := \{f \leqslant \alpha\}.$$

In the following we consider $f(x_0) < \alpha < \min_{\partial\Omega} f$ so that

$$\mathsf{K}_\alpha \text{ is a non empty compact subset of } \{f < \min_{\partial\Omega} f\}.$$

Write

$$\mathbb{E}_{\nu_h}[F(X_{\tau_\Omega})] = \mathsf{Z}_h^{-1}\int_{\Omega\smallsetminus \mathsf{K}_\alpha} w_h\, u_h\, e^{-(2/h)f} + \mathsf{Z}_h^{-1}\int_{\mathsf{K}_\alpha} w_h\, u_h\, e^{-(2/h)f}, \tag{250}$$

where we have defined $\mathsf{Z}_h := \int_\Omega u_h\, e^{-(2/h)f}$. Let us deal with the first term in the right-hand side of (250). It holds:

$$\mathsf{Z}_h^{-1}\int_{\Omega\smallsetminus \mathsf{K}_\alpha} w_h\, u_h\, e^{-(2/h)f} \leqslant \|F\|_{L^\infty(\partial\Omega)}\ \mathsf{Z}_h^{-1}\int_{\Omega\smallsetminus \mathsf{K}_\alpha} u_h\, e^{-(2/h)f}.$$

Moreover, using Lemma 42, it holds (see Definition 41)

$$\int_{\Omega\smallsetminus \mathsf{K}_\alpha} u_h\, e^{-(2/h)f} = \frac{\int_{\Omega\smallsetminus \mathsf{K}_\alpha}\chi_r e^{-(2/h)f}}{\|\chi_r\|_{L^2_w}} + O\big(h^{-d/4+1/2}e^{-(1/h)(f(z_1)-f(x_0)-r)}\big)\sqrt{\int_{\Omega\smallsetminus \mathsf{K}_\alpha} e^{-(2/h)f}}.$$

Recall that when $h\to 0$ (see Proposition 7, (231), and (186)),
$\mathsf{Z}_h = \sqrt{\kappa_0}\, h^{d/4}\, e^{-(1/h)f(x_0)}(1+O(h))$ and $\|\chi_r\|_{L^2_w} = \sqrt{\kappa_0}\, h^{d/4}\, e^{-(1/h)f(x_0)}(1+O(h))$.
Then, since $f\geqslant \alpha$ on $\Omega\smallsetminus \mathsf{K}_\alpha$, there exists $\beta>0$ such that:

$$\mathsf{Z}_h^{-1}\int_{\Omega\smallsetminus \mathsf{K}_\alpha} u_h\, e^{-(2/h)f} \leqslant Ch^{-\beta}\big[e^{-(2/h)(\alpha-f(x_0))} + e^{-(1/h)(f(z_1)+\alpha-2f(x_0)-r)}\big].$$

Therefore, because $\min_{\partial\Omega} f = f(z_1)\geqslant \alpha$, for any $r>0$, it holds for h small enough:

$$\mathsf{Z}_h^{-1}\int_{\Omega\smallsetminus \mathsf{K}_\alpha} u_h\, e^{-(2/h)f} \leqslant e^{-(2/h)(\alpha-f(x_0)-r)}. \tag{251}$$

In conclusion, the first term in the right-hand side of (250) satisfies the following upper bound: for any $r>0$, it holds for h small enough:

$$\mathsf{Z}_h^{-1}\int_{\Omega\smallsetminus \mathsf{K}_\alpha} w_h\, u_h\, e^{-(2/h)f} \leqslant e^{-(2/h)(\alpha-f(x_0)-r)}. \tag{252}$$

Let us now deal with the second term in the right-hand side of (250). Using Corollary 47 with $\mathsf{K}=\mathsf{K}_\alpha$ there, it holds:

$$\mathsf{Z}_h^{-1}\int_{\mathsf{K}_\alpha} w_h\, u_h\, e^{-(2/h)f} = \Big[w_h(x_0)(1+O(\sqrt{h})) + O(h^{-d}e^{-(2/h)(\min_{\partial\Omega} f-\max_{\mathsf{K}_\alpha} f)})\Big] \times \frac{\int_{\mathsf{K}_\alpha} u_h\, e^{-(2/h)f}}{\int_\Omega u_h\, e^{-(2/h)f}}.$$

In addition, by (251),

$$\frac{\int_{\mathsf{K}_\alpha} u_h\, e^{-(2/h)f}}{\int_\Omega u_h\, e^{-(2/h)f}} = 1 - \mathsf{Z}_h^{-1}\int_{\Omega\smallsetminus\mathsf{K}_\alpha} u_h\, e^{-(2/h)f} = 1 + O(e^{-c/h}).$$

Thus, the second term in the right-hand side of (250) satisfies the equivalent in the limit $h\to 0$:

$$\mathsf{Z}_h^{-1}\int_{\mathsf{K}_\alpha} w_h\, u_h\, e^{-(2/h)f} = \Big[w_h(x_0)(1+O(\sqrt{h})) + O(h^{-d}e^{-(2/h)(\min_{\partial\Omega} f-\alpha)})\Big](1+O(e^{-c/h})). \tag{253}$$

Choosing $r>0$ small enough, Equations (35) and (36) when $x=x_0$ are then consequences of (252), (253), (250) together with (30) and (31) in Theorem 2, and the fact that $f(x_0)<\alpha<\min_{\partial\Omega} f$. The asymptotic result on $\mathbb{P}_{x_0}(X_\tau\in\Sigma_{z_k})$ is obtained as a consequence of the asymptotic result on $\mathbb{E}_{x_0}(F(X_\tau))$ for smooth test functions F by writing $F\leqslant 1_{\Sigma_{z_k}}\leqslant G$ for two smooth test functions $F,G:\partial\Omega\to[0,1]$ supported in Γ_{z_k} such that $G\equiv 1$ and $F\equiv 1$ around z_k. For more details, see the analysis led just after Equation (268) in [27].

To obtain (35) and (36) uniformly on all x in any compact subset K of $\{f<\min_{\partial\Omega} f\}$, one uses in addition Corollary 47 with K_α where K is such that $\mathsf{K}\subset\mathsf{K}_\alpha$ (with $f(x_0)<\alpha<\min_{\partial\Omega} f$). Using the procedure of step 2 of the proof of [64, Prop. 14] and since the domain of attraction $\mathcal{A}(\{f<\min_{\partial\Omega} f\})$ of $\{f<\min_{\partial\Omega} f\}$ for the dynamics (12) (see [64, §1.2.2] for the definition of $\mathcal{A}(\{f<\min_{\partial\Omega} f\})$) is equal to Ω (by item (1) of (Ω-f)), (35) and (36) extends to all $x\in\mathsf{K}$, K a compact set of Ω.

It remains to prove (38). To this end, assume that (25) and (26) are satisfied. Assume in addition there exists $\ell_0\in\{n_0+1,\dots,n\}$ such that (see (37))

$$2(f(z_{\ell_0})-f(z_1)) < f(z_1)-f(x_0).$$

Let $k_0\in\{n_0+1,\dots,\ell_0\}$ and $\alpha_*\in\mathbb{R}$ be such that $f(x_0)<\alpha_*<2f(z_1)-f(z_{k_0})$. Notice that we can assume without loss of generality (up to increasing α_* if α_* is smaller than $f(x_0)+f(z_{k_0})-f(z_1)$, see (37)) that

$$f(x_0)+f(z_{k_0})-f(z_1) < \alpha_* < 2f(z_1)-f(z_{k_0}). \tag{254}$$

Let us consider $x\in\mathsf{K}_{\alpha^*}$ and $k\in\{n_0+1,\dots,k_0\}$. Thanks to (254) and the fact that $f(z_k)\leqslant f(z_{k_0})$

$$\min_{\partial\Omega} f-\alpha_* = f(z_1)-\alpha_* > f(z_{k_0})-f(z_1) \geqslant f(z_k)-f(z_1),$$

and

$$\alpha_*-f(x_0) > f(z_{k_0})-f(z_1) \geqslant f(z_k)-f(z_1).$$

Choosing $r>0$ small enough in (252), and using (253) and (250) together with (32) in Theorem 2, one then deduces Equation (38) when $x=x_0$. Using Corollary 47, one proves that (38) holds uniformly on $x\in\mathsf{K}_{\alpha^*}$. The proof of Theorem 3 is complete. □

Appendix. Proofs of some technical results and additional comments

A.1. Proof of Lemma 4

Proof of Lemma 4. — The proof is divided into two steps.

Step 1: Proof of item (1) *in Lemma* 4. — Let us prove that $\partial_{\mathsf{n}_\Omega} f \geqslant 0$ on $\partial\Omega$. Let us assume that there exists $z \in \partial\Omega$ such that $\partial_{\mathsf{n}_\Omega} f(z) < 0$. Then, there exists $s_z > 0$ such that $\varphi_z(t) \notin \overline{\Omega}$ for all $t \in (0, s_z]$. Let $\varepsilon > 0$ be such that $\overline{\mathsf{B}(\varphi_z(s_z), \varepsilon)} \subset \mathbb{R}^d \smallsetminus \overline{\Omega}$. Since $(s, x) \mapsto \varphi_x(s)$ is continuous, there exists $\alpha > 0$ such that if $|s - s_z| \leqslant \alpha$ and $|x - z| \leqslant \alpha$, then $\varphi_x(s) \in \mathsf{B}(\varphi_z(s_z), \varepsilon)$. Therefore, for all $x \in \Omega$ such that $|x - z| \leqslant \alpha$, $\varphi_x(s) \notin \Omega$, which contradicts item (1) in (Ω-f). Therefore $\partial_{\mathsf{n}_\Omega} f \geqslant 0$ on $\partial\Omega$.

The fact that x_0 is the only critical point of the function f in Ω is also a direct consequence of item (1) in (Ω-f). In addition, there is no local minimum $x \in \partial\Omega$ of f in $\overline{\Omega}$. Indeed, assume the existence of such a point $x \in \partial\Omega$. Necessarily $\partial_{\mathsf{n}_\Omega} f(x) \leqslant 0$, and by the previous discussion, $\partial_{\mathsf{n}_\Omega} f(x) = 0$. Then, x is a critical point of f and a local minimum of f in $\mathbb{R}^d$. Since $\operatorname{Hess} f(x) > 0$, x is (positively) asymptotically stable for the flow (12). This contradicts item (1) in (Ω-f).

Let us now prove that $f(x_0) = \min_{\overline{\Omega}} f < \min_{\partial\Omega} f$. For $\beta > 0$, set $\mathsf{V}_\beta = f|_{\Omega}^{-1}((-\infty, f(x_0) + \beta))$. Since $\operatorname{Hess} f(x_0) > 0$, for $\beta > 0$ small enough, V_β is a nonempty open neighborhood of x_0 in Ω such that x_0 is the unique global minimum of f on $\overline{\mathsf{V}_\beta}$. Let $x \in \Omega \smallsetminus \mathsf{V}_\beta$. Let $t_x := \inf\{t \geqslant 0, \varphi_x(t_x) \in \overline{\mathsf{V}_\beta}\}$. By item (1) in ($\Omega$-$f$), $t_x < +\infty$. In addition, by continuity of $t \mapsto \varphi_x(t)$, $\varphi_x(t_x) \in \partial\mathsf{V}_\beta \subset \{f = f(x_0) + \beta\}$. Thus,

$$f(x) = f(\varphi_x(t_x)) + \int_0^{t_x} |\nabla f(\varphi_x(s))|^2 ds \geqslant f(x_0) + \beta.$$

Let us now consider $x \in \partial\Omega$. Let $x_n \in \Omega$ be such that $x_n \to x$ as $n \to +\infty$. Since for n large enough $f(x_n) \geqslant f(x_0) + \beta$, it follows that $f(x) \geqslant f(x_0) + \beta$. In conclusion

$$f(x_0) = \min_{\overline{\Omega}} f < \min_{\partial\Omega} f.$$

It remains to prove that $\{f < \min_{\partial\Omega} f\}$ is connected and $\partial\{f < \min_{\partial\Omega} f\} \cap \partial\Omega = \arg\min_{\partial\Omega} f$. The fact that $\{f < \min_{\partial\Omega} f\}$ is connected follows from the facts that $\{f < \min_{\partial\Omega} f\}$ is actually an open subset of Ω and that there is only one local minimum of f in Ω (namely x_0). Let us now prove that $\partial\{f < \min_{\partial\Omega} f\} \cap \partial\Omega = \arg\min_{\partial\Omega} f$. It is clear that $\partial\{f < \min_{\partial\Omega} f\} \cap \partial\Omega \subset \arg\min_{\partial\Omega} f$. Let $z \in \arg\min_{\partial\Omega} f$. If $z \notin \partial\{f < \min_{\partial\Omega} f\}$, then there exists $\varepsilon > 0$ such that for all $x \in \overline{\mathsf{B}(z, \varepsilon)} \cap \overline{\Omega}$, $f(x) \geqslant \min_{\partial\Omega} f = f(z)$. Thus, z is a local minimum of f in $\overline{\Omega}$, which is not possible. Consequently $z \in \partial\{f < \min_{\partial\Omega} f\}$. Therefore, $\partial\{f < \min_{\partial\Omega} f\} \cap \partial\Omega = \arg\min_{\partial\Omega} f$. This ends the proof of item (1) in Lemma 4.

Step 2: Proof of item (2) *in Lemma* 4. — Let $z \in \partial\Omega$ be such that $|\nabla f|(z) = 0$. Let $(e_1, , \ldots, e_d)$ be an orthonormal basis such that (i) $\operatorname{Span}(e_1, \ldots, e_{d-1}) = T_z\partial\Omega$ and (ii) $e_d = \mathsf{n}_\Omega(z)$. Let us introduce the affine change of variables:

$$\varphi : (y_1, \ldots, y_d) \mapsto z + \textstyle\sum_{i=1}^d y_i e_i.$$

The Hessian of f at point z is unitarily equivalent to the matrix with (i,j)-component $\frac{\partial^2 f}{\partial y_i \partial y_j}(0)$ for $1 \leqslant i,j \leqslant d$ (where with a slight abuse of notation, $f(y)$ refers to $f(\varphi(y))$). Let us prove that $\frac{\partial^2 f}{\partial y_i \partial y_d}(0)=0$ for all $i\in\{1,\dots,d-1\}$. For any such i, let $t\in(-1,1)\mapsto\gamma(t)\in\partial\Omega$ be a curve such that $\gamma(0)=z$ and $\gamma'(0)=e_i$. By item (2) in (Ω-f), one has $\frac{d}{dt}\nabla f(\gamma(t))\cdot \mathsf{n}_\Omega(\gamma(t))\big|_{t=0}=0$ (since $\nabla f(\gamma(t))\cdot\mathsf{n}_\Omega(\gamma(t))=0$ on a neighborhood of $t=0$). This writes: $\frac{\partial^2 f}{\partial y_i \partial y_d}(0)=0$. This implies that $(0,\dots,0,1)^T$ is an eigenvector of $\Big(\frac{\partial^2 f}{\partial y_i\partial y_j}(0)\Big)_{1\leqslant i,j\leqslant d}$ associated with the eigenvalue $\frac{\partial^2 f}{\partial y_d^2}(0)$. Since f is a Morse function in $\overline{\Omega}$, one has $\frac{\partial^2 f}{\partial y_d^2}(0)\neq 0$. Finally, item (1) in ($\Omega$-$f$) then implies that necessarily $\frac{\partial^2 f}{\partial y_d^2}(0)<0$. This proves that $\mathsf{n}_\Omega(z)$ is an eigenvector of the Hessian of f at z associated with a negative eigenvalue. □

A.2. On WKB-approximation for $\mathsf{v}_k^{(1)}$. — As explained in Section 3, the quasi-modes $\mathsf{f}_k^{(1)}$ for $\mathsf{L}_{f,h}^{\mathsf{Di},(1)}(\Omega)$ are built using the principal 1-eigenform $\mathsf{v}_k^{(1)}$ of a Witten Laplacian on Ω_k^{M} with mixed Dirichlet-Neumann boundary conditions. Since $|\nabla f(z_k)|=0$, the constructions of the domain Ω_k^{M} and of the quasi-mode $\mathsf{v}_k^{(1)}$ are very different from the ones done in [27] and require to overcome a major technical issue.

Indeed, we do not have a satisfactory WKB-approximation of $\mathsf{v}_k^{(1)}$ near Σ_{z_k} in $\overline{\Omega_k^{\mathrm{M}}}$. An accurate WKB-approximation, constructed in [42], was used in [27] (see also [28] for similar computations) to estimate (in the limit $h\to 0$), the quantities

$$\int_{\Sigma_{z_k}} \mathsf{v}_k^{(1)}\cdot \mathsf{n}_\Omega e^{-(1/h)f},\quad k=1,\dots,n, \tag{255}$$

which were in turn used to compute asymptotically $\int_{\Sigma_{z_k}}\partial_{\mathsf{n}_\Omega}u_h e^{-(1/h)f}$, since (see Corollary 25, (40) and (119))

$$\int_{\Sigma_{z_k}}\partial_{\mathsf{n}_\Omega}u_h e^{-(1/h)f}\sim\sum_{k=1}^n\int_\Omega \nabla u_h\cdot \mathsf{v}_k^{(1)}\, e^{-(1/h)f}\ \int_{\Sigma_{z_k}}\mathsf{v}_k^{(1)}\cdot\mathsf{n}_\Omega\, e^{-(1/h)f}.$$

In our context (see [58, §1.4] for more details), the only possible candidate is the WKB ansatz constructed in [44, §2] on $\mathsf{B}(z_k,\rho)$ (for some $\rho>0$). However, only its first term $\omega_0 e^{-(1/h)\mathsf{d}_a(.,z_k)}|_\Omega$ belongs to the form domain of $\Delta_{f,h}^{\mathsf{Di},(1)}(\Omega)$ in general, i.e., satisfies $\mathbf{t}a_0=0$ on $\partial\Omega\cap\mathsf{B}(z_k,\rho)$. Thus, only this first term can be used to approximate $\mathsf{v}_k^{(1)}$ with the help of Lemma 11, but this approximation is not accurate enough. Let us briefly explain why, by showing that for a smooth function ξ supported in $\mathsf{B}(z_k,\rho/2)$ which equals 1 in $\mathsf{B}(z_k,\rho/3)$, the 1-form

$$\mathsf{u}_{wkb,0}=\frac{\xi\omega_0 e^{-(1/h)\mathsf{d}_a(.,z_k)}|_\Omega}{\|\xi\omega_0 e^{-(1/h)\mathsf{d}_a(.,z_k)}|_\Omega\|_{L^2(\Omega)}}$$

is in general not close enough to $\mathsf{v}_k^{(1)}$ in $\Lambda^1H^1(\Omega)$ (recall that we are looking for an equivalent of (255)). Using (14), by construction of ω_0 in [44, Th. 2.5] and using an integration by parts, it holds, for h small enough:

$$\begin{aligned}\|\xi\omega_0 e^{-(1/h)\mathsf{d}_a(.,z_k)}|_\Omega\|^2_{L^2(\Omega)}&\Big(\|\mathsf{d}_{f,h}\mathsf{u}_{wkb,0}\|^2_{L^2(\Omega)}+\|\mathsf{d}^*_{f,h}\mathsf{u}_{wkb,0}\|^2_{L^2(\Omega)}\Big)\\&=\langle\Delta^{(1)}_{f,h}\mathsf{u}_{wkb,0},\mathsf{u}_{wkb,0}\rangle_{L^2(\Omega)}-h\int_{\partial\Omega\cap\mathsf{B}(z_k,\rho)}\mathbf{t}\mathsf{d}^*_{f,h}\mathsf{u}_{wkb,0}\,\mathsf{u}_{wkb,0}\cdot\mathsf{n}_\Omega\\&=O(h^2)\|e^{-(2/h)\mathsf{d}_a(.,z_k)}\xi\omega_0\Delta_{\mathbf{H}}\omega_0\|^2_{L^2(\Omega)}+O(e^{-c/h})\\&\quad-h\int_{\partial\Omega\cap\mathsf{B}(z_k,\rho)}\xi^2e^{-(2/h)\mathsf{d}_a(.,z_k)}\mathbf{t}\big[h\mathsf{d}^*\omega_0+\underbrace{\mathbf{i}_{\nabla(\mathsf{d}_a(\cdot,z_k)+f)}(\omega_0)}_{=0}\big]\,\omega_0\cdot\mathsf{n}_\Omega.\end{aligned}$$

Therefore, using Laplace's method and [44, Th. 2.5], one cannot expect in general a better estimate when $h\to 0$ than

$$\|\mathsf{d}_{f,h}\mathsf{u}_{wkb,0}\|^2_{L^2(\Omega)}+\|\mathsf{d}^*_{f,h}\mathsf{u}_{wkb,0}\|^2_{L^2(\Omega)}\leqslant Ch^{3/2},$$

which only implies, using Lemma 11, that $\mathsf{u}_{wkb,0}$ is at a distance of the order $O(h^{1/4})$ from $\mathsf{v}_k^{(1)}$ in $\Lambda^1L^2(\Omega)$. In view of the computations made in the proof of [27, Prop. 90] (which is very similar to the proof of Lemma 43, see in particular (234)), this is not sufficient to prove that the distance between $\mathsf{u}_{wkb,0}$ and $\mathsf{v}_k^{(1)}$ converges to 0 in $\Lambda^1H^1(\Omega)$ as $h\to 0$. One would indeed at least need that $\|\mathsf{d}_{f,h}\mathsf{u}_{wkb,0}\|^2_{L^2(\Omega)}+\|\mathsf{d}^*_{f,h}\mathsf{u}_{wkb,0}\|^2_{L^2(\Omega)}=o(h^3)$ as $h\to 0$.

A.3. Proofs of Propositions 28 and 29

Proof of Proposition 28. — Let $k\in\{1,\dots,n\}$. The proof of Proposition 28 is divided into several steps.

Step 1: Properties of Γ_{z_k} *and preliminary definitions.* — Let us recall that since $\Gamma_{z_k}\subset\mathsf{W}^+_{z_k}$ (see (14) in (Ω-f)), it holds

$$\text{for all } x\in\Gamma_{z_k},\quad \nabla f(x)=\nabla_{\mathbf{T}}f(x)\in T_x\partial\Omega.$$

Moreover, for all $y\in\Gamma_{z_k}$, since $\varphi_y(s)\in\Gamma_{z_k}$ for all $s\geqslant 0$ (see (12)), it holds: $\lim_{s\to+\infty}\varphi_y(s)=z_k$. Let $r>0$ and define:

$$\mathsf{C}_{z_k}=(f|_{\Gamma_{z_k}})^{-1}\big((-\infty,f(z_k)+r)\big).$$

For $r>0$ small, $|\nabla f|\neq 0$ on $\partial\mathsf{C}_{z_k}$ and thus, C_{z_k} is a smooth open neighborhood of z_k and $\nabla f\cdot\mathsf{n}_{\mathsf{C}_{z_k}}>0$ on $\partial\mathsf{C}_{z_k}$. For $y\in\Gamma_{z_k}\smallsetminus\overline{\mathsf{C}_{z_k}}$, let:

$$t_{\mathsf{C}_{z_k}}(y)=\inf\{\,s\geqslant 0,\ \varphi_y(s)\in\overline{\mathsf{C}_{z_k}}\,\},\tag{256}$$

which is finite since $\lim_{s\to+\infty}\varphi_y(s)=z_k$. By continuity of $s\geqslant 0\mapsto\varphi_y(s)$, for $y\in\Gamma_{z_k}\smallsetminus\overline{\mathsf{C}_{z_k}}$, $\varphi_y(t_{\mathsf{C}_{z_k}}(y))\in\partial\mathsf{C}_{z_k}$ and for all $s>t_{\mathsf{C}_{z_k}}(y)$, $\varphi_y(s)\in\mathsf{C}_{z_k}$. Moreover, $t_{\mathsf{C}_{z_k}}(y)$ is defined by

$$\int_0^{t_{\mathsf{C}_{z_k}}(y)}|\nabla f(\varphi_y(s))|^2ds=f(y)-(f(z_k)+r),$$

and thus since $|\nabla f|\neq 0$ on $\partial\mathsf{C}_{z_k}$, by the implicit functions theorem,

$$y\in\Gamma_{z_k}\smallsetminus\overline{\mathsf{C}_{z_k}}\longmapsto t_{\mathsf{C}_{z_k}}(y)\text{ is }\mathcal{C}^\infty.\tag{257}$$

For all $x \in \partial \mathsf{C}_{z_k}$ and $s \in \mathbb{R}$, let $\gamma_x(s) := \varphi_x(-s)$ (see (12)) which satisfy for all $s \in \mathbb{R}$

$$\frac{d}{ds}\gamma_x(s) = \nabla f(\gamma_x(s)) \text{ with } \gamma_x(0) = x. \tag{258}$$

Let us define for all $x \in \partial \mathsf{C}_{z_k}$,

$$s_{\Gamma_{z_k}}(x) := \inf\{s \geqslant 0,\ \gamma_x(s) \notin \Gamma_{z_k}\}. \tag{259}$$

Let us prove that

$$s_{\Gamma_{z_k}} : \partial \mathsf{C}_{z_k} \longrightarrow \mathbb{R}_+ \text{ is lower semicontinuous.} \tag{260}$$

Let us first prove that for all $x \in \partial \mathsf{C}_{z_k}$, $s_{\Gamma_{z_k}}(x) < +\infty$. It it is not the case, there exists $y \in \partial \mathsf{C}_{z_k}$ such that $\gamma_y(s) \in \Gamma_{z_k}$ for all $s \geqslant 0$. Thus, the curve γ_y converges to a critical point of f in $\overline{\Gamma_{z_k}}$, the only one being z_k (by (14)), which is impossible because $\gamma_y(s) \notin \mathsf{C}_{z_k}$ for all $s \geqslant 0$. Let us now prove that $s_{\Gamma_{z_k}}$ is lower semicontinuous. To this end, let $(x_n)_{n\geqslant 0}$ be a sequence in $\partial \mathsf{C}_{z_k}$ converging to $x_\infty \in \partial \mathsf{C}_{z_k}$ and a limit s_* of a subsequence of $(s_{\Gamma_{z_k}}(x_n))_{n\geqslant 0}$. If $s_* = +\infty$, then, $s_{\Gamma_{z_k}}(x_\infty) \leqslant s_*$. Let us then consider the case when $s_* < +\infty$. Up to extracting a subsequence, we assume that $s_{\Gamma_{z_k}}(x_n) \to s_*$ when $n \to \infty$. Notice that for all $n \geqslant 0$, since $s_{\Gamma_{z_k}}(x_n) < +\infty$ and $s \mapsto \gamma_{x_n}(s)$ is continuous, $\gamma_{x_n}(s_{\Gamma_{z_k}}(x_n)) \in \partial\Gamma_{z_k}$. In addition, since $s_* < +\infty$, $\partial\Gamma_{z_k}$ is a closed set, and by continuity of $(x,t) \mapsto \gamma_x(t)$, it holds

$$\gamma_{x_n}(s_{\Gamma_{z_k}}(x_n)) \longrightarrow \gamma_{x_\infty}(s_*) \in \partial\Gamma_{z_k} \quad \text{when } n \longrightarrow \infty.$$

This implies that $s_{\Gamma_{z_k}}(x_\infty) \leqslant s_*$ by definition of $s_{\Gamma_{z_k}}$. This implies that $s_{\Gamma_{z_k}}$ is lower semicontinuous and concludes the proof of (260).

Finally, since Γ_{z_k} is open, one can consider an open subset O_F of Γ_{z_k} such that

$$\overline{\mathsf{C}_{z_k}} \cup \mathsf{F} \subset \mathsf{O}_\mathsf{F} \quad \text{and} \quad \overline{\mathsf{O}_\mathsf{F}} \subset \Gamma_{z_k}.$$

Step 2: Construction of a set $\mathsf{V}_\mathsf{F} \subset \Gamma_{z_k}$ *containing* O_F *which is stable for* (12). — Define for all $x \in \partial \mathsf{C}_{z_k}$, $s_{\mathsf{O}_\mathsf{F}}(x) := \sup\{s \geqslant 0,\ \gamma_x(s) \in \overline{\mathsf{O}_\mathsf{F}}\}$. Let us prove that

$$s_{\mathsf{O}_\mathsf{F}} < +\infty \quad \text{and} \quad s_{\mathsf{O}_\mathsf{F}} < s_{\Gamma_{z_k}}. \tag{261}$$

To prove the first statement in (261), we argue by contradiction: assume that there exists $x \in \partial \mathsf{C}_{z_k}$ such that $s_{\mathsf{O}_\mathsf{F}}(x) = +\infty$. Then, there exists a sequence $s_n \in (\mathbb{R}_+)^\mathbb{N}$ such that $s_n \to +\infty$ when $n \to +\infty$ and for all n, $\gamma_x(s_n) \in \overline{\mathsf{O}_\mathsf{F}}$. Thus, $\gamma_x(s_n)$ converges when $n \to +\infty$ to a critical point of f in $\overline{\mathsf{O}_\mathsf{F}}$, the only one being z_k, which is not possible because $\gamma_x(s_n) \notin \mathsf{C}_{z_k}$ for all n. This proves the first statement in (261). To prove the second statement in (261), let us consider $x \in \partial \mathsf{C}_{z_k}$. Notice that since $s_{\mathsf{O}_\mathsf{F}}(x)$ is finite and the trajectories of (258) are continuous in time, $\gamma_x(s_{\mathsf{O}_\mathsf{F}}(x)) \in \overline{\mathsf{O}_\mathsf{F}} \subset \Gamma_{z_k}$. Since Γ_{z_k} is stable for the dynamics (12), $\gamma_x(s) = \varphi_{\gamma_x(s_{\mathsf{O}_\mathsf{F}}(x))}(s_{\mathsf{O}_\mathsf{F}}(x) - s) \in \Gamma_{z_k}$ for all $s \in [0, s_{\mathsf{O}_\mathsf{F}}(x)]$ (see (12) and (258)). Moreover, since Γ_{z_k} is open, and the trajectories of (258) are continuous, there exists $\varepsilon_x > 0$ such that:

$$\big\{\gamma_x(s),\ x \in \partial \mathsf{C}_{z_k} \text{ and } s \in [0, s_{\mathsf{O}_\mathsf{F}}(x) + \varepsilon_x]\big\} \subset \Gamma_{z_k}. \tag{262}$$

Therefore, $s_{\Gamma_{z_k}}(x) \geqslant s_{\mathsf{O}_\mathsf{F}}(x) + \varepsilon_x$. This concludes the proof of (261).

Let us now define:

$$\mathsf{V_F} := \mathsf{C}_{z_k} \cup \big\{\gamma_x(s),\ x\in \partial \mathsf{C}_{z_k} \text{ and } s\in [0, s_{\mathsf{O_F}}(x)]\big\}. \tag{263}$$

By construction, the set $\mathsf{V_F}$ is stable for the dynamics (12). From (262) and since $\overline{\mathsf{C}_{z_k}}\subset \Gamma_{z_k}$, one has $\mathsf{V_F}\subset \Gamma_{z_k}$. We now claim that

$$s_{\mathsf{O_F}}: \partial \mathsf{C}_{z_k} \longrightarrow \mathbb{R}_+ \text{ is upper semicontinuous and } \mathsf{V_F} \text{ is a closed set.} \tag{264}$$

Let us first prove the first statement in (264). To this end, let $(x_n)_{n\geqslant 0}$ be a sequence in $\partial \mathsf{C}_{z_k}$ converging to $x_\infty\in \partial \mathsf{C}_{z_k}$ and s_* a limit of a subsequence of $(s_{\mathsf{O_F}}(x_n))_{n\geqslant 0}$. Up to extracting a subsequence, we assume that $s_{\mathsf{O_F}}(x_n)\to s_*$ when $n\to\infty$. Notice that for all $n\geqslant 0$, $\gamma_{x_n}(s_{\mathsf{O_F}}(x_n))\in \overline{\mathsf{O_F}}$. Let us prove that s_* is finite. Assume that it is not the case, i.e., that $s_{\mathsf{O_F}}(x_n)\to +\infty$. From (261), for all $t\in [0, s_{\mathsf{O_F}}(x_n)]$, $\gamma_{x_n}(t)\in \Gamma_{z_k}$. Let $T>0$ and consider $N\geqslant 1$ such that $s_{\mathsf{O_F}}(x_n)\geqslant T$ for all $n\geqslant N$. Then, for all $t\in[0,T]$ and $n\geqslant N$, $\gamma_{x_n}(t)\in \overline{\Gamma_{z_k}}$. Passing to the limit, one obtains that $\gamma_x(t)\in\overline{\Gamma_{z_k}}$ for all $t\in[0,T]$. Since $T>0$ is arbitrary, one deduces that $\gamma_x(t)\in \overline{\Gamma_{z_k}}$ for all $t>0$. This is not possible because, as already explained, the limit points of the curve γ_x are outside $\overline{\Gamma_{z_k}}$. Thus s_* is finite. Since $\overline{\mathsf{O_F}}$ is a closed set, by continuity of $(x,t)\mapsto \gamma_x(t)$, it holds $\gamma_{x_n}(s_{\mathsf{O_F}}(x_n))\to \gamma_{x_\infty}(s_*)\in \overline{\mathsf{O_F}}$ when $n\to\infty$. Therefore, $s_{\mathsf{O_F}}(x_\infty)\geqslant s_*$, and thus, $s_{\mathsf{O_F}}(x_\infty)\geqslant \limsup_{n\to+\infty} s_{\mathsf{V_F}}(x_n)$. This proves that $s_{\mathsf{O_F}}$ is upper semicontinuous. This proves the first statement in (264).

Let us now prove the second statement in (264). To prove that $\mathsf{V_F}$ is a closed set it is sufficient to show that $A=\big\{\gamma_x(s),\ x\in\partial \mathsf{C}_{z_k} \text{ and } s\in[0,s_{\mathsf{O_F}}(x)]\big\}$ is a closed set. To this end, let $(y_n)_{n\geqslant 0}$ be a sequence in A converging to y_*. Let us show that $y_*\in A$. Write $y_n=\gamma_{x_n}(s_n)$ where $x_n\in\partial \mathsf{C}_{z_k}$ and $0\leqslant s_n\leqslant s_{\mathsf{O_F}}(x_n)$. By compactness and up to extracting a subsequence, let $x_\infty\in \partial\mathsf{C}_{z_k}$ such that $x_n\to x_\infty$ when $n\to+\infty$. Since $s_{\mathsf{O_F}}<+\infty$ is upper semicontinuous on the compact set $\partial \mathsf{C}_{z_k}$, $s_{\mathsf{O_F}}$ is bounded on $\partial\mathsf{C}_{z_k}$. Therefore, $(s_n)_{n\geqslant 0}$ and $(s_{\mathsf{O_F}}(x_n))_{n\geqslant 0}$ are bounded. Denote by s_* a limit of a subsequence of $(s_n)_{n\geqslant 0}$. Then, it holds

$$s_*\leqslant \limsup_{n\to+\infty} s_n\leqslant \limsup_{n\to+\infty} s_{\mathsf{O_F}}(x_n)\leqslant s_{\mathsf{O_F}}(x_\infty),$$

where the last inequality follows from the fact that $s_{\mathsf{O_F}}$ is upper semicontinuous. Since $y_n=\gamma_{x_n}(s_n)\to\gamma_{x_\infty}(s_*)=y_*$ when $n\to+\infty$, and $s_*\leqslant s_{\mathsf{O_F}}(x_\infty)$, this implies that $y_*\in \big\{\gamma_x(s),\ x\in\partial\mathsf{C}_{z_k} \text{ and } s\in[0,s_{\mathsf{O_F}}(x)]\big\}$. The set A is therefore closed and thus, so is $\mathsf{V_F}$.

Finally, let us prove that,

$$\mathsf{O_F}\subset \mathsf{V_F}. \tag{265}$$

To prove (265), we consider $y\in\mathsf{O_F}$. The curve

$$s\in[0,t_{\mathsf{C}_{z_k}}(y)]\longmapsto \gamma_{\varphi_y(t_{\mathsf{C}_{z_k}}(y))}(s)=\varphi_y(t_{\mathsf{C}_{z_k}}(y)-s)$$

passes through $y\in\mathsf{O_F}$ at time $s=t_{\mathsf{C}_{z_k}}(y)$ (see (12), (258), and (256)). Thus, by definition of $s_{\mathsf{O_F}}$, it holds $t_{\mathsf{C}_{z_k}}(y)\leqslant s_{\mathsf{O_F}}(\varphi_y(t_{\mathsf{C}_{z_k}}(y)))$ and thus, by definition of $\mathsf{V_F}$,

$y = \gamma_{\varphi_y(t_{\mathsf{C}_{z_k}}(y))}(t_{\mathsf{C}_{z_k}}(y)) \in \{\gamma_{\varphi_y(t_{\mathsf{C}_{z_k}}(y))}(s),\, s \in [0, s_{\mathsf{O}_\mathsf{F}}(x))\} = \mathsf{V}_\mathsf{F}$. This proves (265) and in particular $\mathsf{F} \subset \mathsf{V}_\mathsf{F}$.

The interior of V_F might be a good candidate to be Γ_F but this set is not necessarily smooth or does not satisfy (125). This is due to the fact that the function $s_{\mathsf{O}_\mathsf{F}}$ is not necessarily smooth. For this reason, we approximate $s_{\mathsf{O}_\mathsf{F}}$ from above by a smooth function: this is made in the next step, see (268).

Step 3: Construction of Γ_F

Step 3a: Approximation of $s_{\mathsf{O}_\mathsf{F}}$ *from above by a smooth function and definition of* Γ_F

Since $s_{\mathsf{O}_\mathsf{F}}$ is upper semicontinuous (see (264)), from [89, Th. 3], there exists a decreasing sequence of continuous functions $\widetilde{s}_n : \partial \mathsf{C}_{z_k} \to \mathbb{R}$, $n \geqslant 1$, such that for all $n \geqslant 1$, $\widetilde{s}_n \geqslant s_{\mathsf{O}_\mathsf{F}}$ and for all $x \in \partial \mathsf{C}_{z_k}$, $\widetilde{s}_n(x) \to s_{\mathsf{O}_\mathsf{F}}(x)$ when $n \to +\infty$. Let us prove that there exists $n_0 \geqslant 1$ such that:

$$\text{for all } x \in \partial \mathsf{C}_{z_k}, \quad s_{\mathsf{O}_\mathsf{F}}(x) \leqslant \widetilde{s}_{n_0}(x) < s_{\Gamma_{z_k}}(x). \tag{266}$$

We just have to prove the second inequality in (266). For that purpose, we argue by contradiction: assume that

$$\text{for all } n \geqslant 1, \text{ there exists } x_n \in \partial \mathsf{C}_{z_k} \text{ such that } \widetilde{s}_n(x_n) \geqslant s_{\Gamma_{z_k}}(x_n). \tag{267}$$

By compactness and up to extracting a subsequence, let $x_\infty \in \partial \mathsf{C}_{z_k}$ such that $x_n \to x_\infty$ when $n \to +\infty$. Let $\varepsilon > 0$. There exists $N_0 \geqslant 1$ such that for all $n \geqslant N_0$, $\widetilde{s}_n(x_\infty) - s_{\mathsf{O}_\mathsf{F}}(x_\infty) \leqslant \varepsilon/2$. One then has for all $n \geqslant N_0$, using that $\widetilde{s}_n \leqslant \widetilde{s}_{N_0}$,

$$\begin{aligned} \widetilde{s}_n(x_n) - s_{\mathsf{O}_\mathsf{F}}(x_\infty) &= (\widetilde{s}_n(x_n) - \widetilde{s}_{N_0}(x_\infty)) + (\widetilde{s}_{N_0}(x_\infty) - s_{\mathsf{O}_\mathsf{F}}(x_\infty)) \\ &\leqslant \widetilde{s}_{N_0}(x_n) - \widetilde{s}_{N_0}(x_\infty) + \varepsilon/2. \end{aligned}$$

Moreover, because $\widetilde{s}_{N_0}$ is a continuous function, there exists $N_1 \geqslant 1$ such that for all $n \geqslant N_1$, $|\widetilde{s}_{N_0}(x_n) - \widetilde{s}_{N_0}(x_\infty)| \leqslant \varepsilon/2$. Thus, for $n \geqslant \max(N_0, N_1)$, $\widetilde{s}_n(x_n) - s_{\mathsf{O}_\mathsf{F}}(x_\infty) \leqslant \varepsilon$, i.e., $\limsup_{n\to+\infty} \widetilde{s}_n(x_n) - s_{\mathsf{O}_\mathsf{F}}(x_\infty) \leqslant 0$. Now, since $s_{\Gamma_{z_k}}$ is lower semicontinuous (see (260)) and from (267), it holds:

$$s_{\mathsf{O}_\mathsf{F}}(x_\infty) \geqslant \limsup_{n\to+\infty} \widetilde{s}_n(x_n) \geqslant \liminf_{n\to+\infty} s_{\Gamma_{z_k}}(x_n) \geqslant s_{\Gamma_{z_k}}(x_\infty).$$

This contradicts the second statement in (261), and thus concludes the proof of (266). Since the function $s_{\Gamma_{z_k}} - \widetilde{s}_{n_0}$ is lower semicontinuous and $\partial \mathsf{C}_{z_k}$ is compact, $s_{\Gamma_{z_k}} - \widetilde{s}_{n_0}$ attains its infimum on $\partial \mathsf{C}_{z_k}$ and since $s_{\Gamma_{z_k}} > \widetilde{s}_{n_0}$ (see (266)), this minimum is positive. Let us then consider $0 < \varepsilon < \min_{\partial \mathsf{C}_{z_k}} (s_{\Gamma_{z_k}} - \widetilde{s}_{n_0})$ so that

$$\widetilde{s}_{n_0} + \varepsilon < s_{\Gamma_{z_k}} \quad \text{on } \partial \mathsf{C}_{z_k}. \tag{268}$$

Since $\partial \mathsf{C}_{z_k}$ is compact and $\widetilde{s}_{n_0} + \varepsilon$ is continuous on $\partial \mathsf{C}_{z_k}$, there exists $\beta \in \mathcal{C}^\infty(\partial \mathsf{C}_{z_k}, \mathbb{R})$ such that $\widetilde{s}_{n_0} + \varepsilon/2 \leqslant \beta \leqslant \widetilde{s}_{n_0} + 3\varepsilon/4$, so that in view of (266) and (268),

$$s_{\mathsf{O}_\mathsf{F}} < \beta < s_{\Gamma_{z_k}} \quad \text{on } \partial \mathsf{C}_{z_k}. \tag{269}$$

We now define

$$\Gamma_\mathsf{F} := \mathsf{C}_{z_k} \cup \big\{ \gamma_x(s),\, x \in \partial \mathsf{C}_{z_k} \text{ and } s \in [0, \beta(x)) \big\}. \tag{270}$$

Step 3b: Properties of Γ_{F}. — Let us finally prove that Γ_{F} satisfies all the properties listed in Proposition 28. First notice that by construction, $\overline{\Gamma_{\mathsf{F}}}$ is included in Γ_{z_k}, this indeed follows from (270) together with the second inequality in (269). Moreover, Γ_{F} contains V_{F} (since $s_{\mathsf{O}_{\mathsf{F}}} < \beta$, see (269) and (263)) and thus, $\mathsf{F} \subset \Gamma_{\mathsf{F}}$. Furthermore, by construction, Γ_{F} is simply connected. Let us now prove that Γ_{F} is open and satisfies (125).

(1) *Proof of the fact that* Γ_{F} *is open.* To this end, let us first show that $\Gamma_{\mathsf{F}} \setminus \overline{\mathsf{C}_{z_k}}$ is open. Let us denote by $\mathsf{d}_{\partial\Omega}$ the geodesic distance in $\partial\Omega$. Let $y_1 \in \Gamma_{\mathsf{F}} \setminus \overline{\mathsf{C}_{z_k}}$ and write $y_1 = \gamma_{x_1}(s_1)$ where $x_1 \in \partial \mathsf{C}_{z_k}$ and $s_1 \in (0, \beta(x_1))$. Then, there exists $t_1 \in (s_1, \beta(x_1))$ such that $\gamma_{y_1}(-t_1) \in \mathsf{C}_{z_k}$. Since the mapping $x \mapsto \beta(x)$ is continuous and $t_1 < \beta(x_1)$, there exists $\varepsilon_1 > 0$ such that for all $x \in \partial\mathsf{C}_{z_k}$,

$$\mathsf{d}_{\partial\Omega}(x, x_1) \leqslant \varepsilon_1 \implies t_1 < \beta(x). \tag{271}$$

Let $\varepsilon_0 = \mathsf{d}_{\partial\Omega}(\gamma_{y_1}(-t_1), \partial\mathsf{C}_{z_k}) > 0$. Since the mapping $y \mapsto \gamma_y(-t_1)$ is continuous, there exists $\varepsilon_2 > 0$ such that if $\mathsf{d}_{\partial\Omega}(y, y_1) \leqslant \varepsilon_2$ then

$$\mathsf{d}_{\partial\Omega}(\gamma_y(-t_1), \gamma_{y_1}(-t_1)) \leqslant \varepsilon_0/2,$$

and thus $\gamma_y(-t_1) \in \mathsf{C}_{z_k}$. Let $y \in \Gamma_{z_k}$. Write $y = \gamma_x(t_{\mathsf{C}_{z_k}}(y))$ where $x = \varphi_y(t_{\mathsf{C}_{z_k}}(y)) \in \partial\mathsf{C}_{z_k}$, see (256). Since when $\mathsf{d}_{\partial\Omega}(y, y_1) \leqslant \varepsilon_2$ one has $\varphi_y(t_1) = \gamma_y(-t_1) \in \mathsf{C}_{z_k}$, it holds:

$$\text{for all } y \in \Gamma_{z_k},\ \mathsf{d}_{\partial\Omega}(y, y_1) \leqslant \varepsilon_2 \implies t_{\mathsf{C}_{z_k}}(y) < t_1. \tag{272}$$

Since $y \in \Gamma_{z_k} \setminus \overline{\mathsf{C}_{z_k}} \mapsto \varphi_y(t_{\mathsf{C}_{z_k}}(y)) \in \partial\mathsf{C}_{z_k}$ is smooth (see indeed (257)), there exists $\varepsilon_3 > 0$ such that if $\mathsf{d}_{\partial\Omega}(y, y_1) \leqslant \varepsilon_3$, then $y \in \Gamma_{z_k} \setminus \overline{\mathsf{C}_{z_k}}$ and $\mathsf{d}_{\partial\Omega}(x, x_1) \leqslant \varepsilon_1$ with $x = \varphi_y(t_{\mathsf{C}_{z_k}}(y))$ and $x_1 = \varphi_{y_1}(t_{\mathsf{C}_{z_k}}(y_1))$. In conclusion, from (271) and (272), if $\mathsf{d}_{\partial\Omega}(y, y_1) \leqslant \min(\varepsilon_2, \varepsilon_3)$, then $t_{\mathsf{C}_{z_k}}(y) < t_1 < \beta(x)$, where $x = \varphi_y(t_{\mathsf{C}_{z_k}}(y))$ and $y = \gamma_x(t_{\mathsf{C}_{z_k}}(y))$. Thus, from (270), if $\mathsf{d}_{\partial\Omega}(y, y_1) \leqslant \min(\varepsilon_2, \varepsilon_3)$, then $y \in \Gamma_{\mathsf{F}} \setminus \overline{\mathsf{C}_{z_k}}$. The set $\Gamma_{\mathsf{F}} \setminus \overline{\mathsf{C}_{z_k}}$ is therefore open. In addition, since $\overline{\mathsf{C}_{z_k}} \subset \mathsf{O}_{\mathsf{F}} \subset \Gamma_{\mathsf{F}}$ and O_{F} is open, $\Gamma_{\mathsf{F}} = (\Gamma_{\mathsf{F}} \setminus \overline{\mathsf{C}_{z_k}}) \cup \overline{\mathsf{C}_{z_k}} \subset \operatorname{int}(\Gamma_{\mathsf{F}})$. Therefore the set Γ_{F} is open.

Moreover, using the same arguments as those used to prove the second statement of (264), it holds:

$$\overline{\Gamma_{\mathsf{F}}} = \mathsf{C}_{z_k} \cup \big\{\gamma_x(s),\ x \in \partial\mathsf{C}_{z_k} \text{ and } s \in [0, \beta(x)]\big\}. \tag{273}$$

Consequently, since $\beta < s_{\Gamma_{z_k}}$ and the trajectories of (258) are continuous (see also (259)), one has:

$$\overline{\Gamma_{\mathsf{F}}} \subset \Gamma_{z_k}.$$

In addition, from (273) and (270), one has:

$$\partial\Gamma_{\mathsf{F}} = \big\{\gamma_x(\beta(x)),\ x \in \partial\mathsf{C}_{z_k}\big\}. \tag{274}$$

(2) Proof of the fact that the set Γ_{F} satisfies (125), i.e., that $\nabla f \cdot \mathsf{n}_{\Gamma_{\mathsf{F}}} > 0$ on $\partial\Gamma_{\mathsf{F}}$, where we recall that $\mathsf{n}_{\Gamma_{\mathsf{F}}} \in T\partial\Omega$ is the unit outward normal to Γ_{F}. Notice that by construction, the set Γ_{F} is a stable set for the dynamics (12) and thus $\nabla f \cdot \mathsf{n}_{\Gamma_{\mathsf{F}}} \geqslant 0$

on $\partial\Gamma_{\mathsf{F}}$. Let us prove that this inequality is actually a strict inequality. Let us define the function

$$\Upsilon : y \in \Gamma_{z_k} \smallsetminus \overline{\mathsf{C}_{z_k}} \longmapsto (x,t) \in \partial\mathsf{C}_{z_k} \times \mathbb{R}_+^* \quad \text{such that } \gamma_x(t) = y.$$

Notice that if $\Upsilon(y) = (x,t)$, then $t = t_{\mathsf{C}_{z_k}}(y)$ (see (256)) and $x = \varphi_y(t_{\mathsf{C}_{z_k}}(y))$. The mapping Υ is a $\mathcal{C}^\infty$ diffeomorphism from $\Gamma_{z_k} \smallsetminus \overline{\mathsf{C}_{z_k}}$ into its range. Let us denote by $F := \Upsilon^{-1}$ its inverse function, i.e.,

$$F(x,t) = \gamma_x(t). \tag{275}$$

Thus, for all $x \in \partial\mathsf{C}_{z_k}$, $(\operatorname{Jac} F)(x,\beta(x))$ is a bijection between $T_x\partial\mathsf{C}_{z_k} \times \mathbb{R}$ and $T_{\gamma_x(\beta(x))}\Gamma_{z_k}$. For all $x \in \partial\mathsf{C}_{z_k}$ and $v = (v_1,v_2) \in T_x\partial\mathsf{C}_{z_k} \times \mathbb{R}$, one has:

$$(\operatorname{Jac} F)(x,\beta(x))v = (\partial_x F)(x,\beta(x))v_1 + (\partial_t F)(x,\beta(x)) \times v_2 \in T_{\gamma_x(\beta(x))}\Gamma_{z_k}, \tag{276}$$

where $(\partial_t F)(x,\beta(x)) = \nabla f(\gamma_x(\beta(x))$ (see (275) and (258)). Using the chain rule, one has:

$$\begin{aligned} \operatorname{Jac}_x\big(F(x,\beta(x))\big)v_1 &= (\partial_x F)(x,\beta(x))v_1 + (\partial_t F)(x,\beta(x)))\big(\nabla\beta(x)\cdot v_1\big) \\ &= (\partial_x F)(x,\beta(x))v_1 + \nabla f(\gamma_x(\beta(x))\big(\nabla\beta(x)\cdot v_1\big), \end{aligned} \tag{277}$$

where $\operatorname{Jac}_x\big(F(x,\beta(x))\big)v_1 \in T_{\gamma_x(\beta(x))}\Gamma_{\mathsf{F}}$ and $\nabla\beta(x) \in T_x\partial\mathsf{C}_{z_k}$. To prove (125) we argue by contradiction: assume that there exists $x \in \partial\mathsf{C}_{z_k}$ such that

$$\nabla f(\gamma_x(\beta(x))) \cdot \mathsf{n}_{\Gamma_{\mathsf{F}}}(\gamma_x(\beta(x))) = 0$$

(see (274)) which is equivalent to $\nabla f(\gamma_x(\beta(x))) \in T_{\gamma_x(\beta(x))}\partial\Gamma_{\mathsf{F}}$. This implies, in view of (276) and (277) that $\operatorname{Ran}(\operatorname{Jac} F)(x,\beta(x)) \subset T_{\gamma_x(\beta(x))}\partial\Gamma_{\mathsf{F}}$, which contradicts the fact that F is a diffeomorphism. This concludes the proof of (125).

The proof of Proposition 28 is complete. □

Proof of Proposition 29. — For all $y \in \Omega$, recall that $\varphi_y(s) \in \Omega$ for all $s \geqslant 0$ (see (12)) and $\lim_{s\to+\infty} \varphi_y(s) = x_0$. Define for $r > 0$:

$$\mathsf{C}_{x_0} = (f|_\Omega)^{-1}\big((-\infty, f(x_0)+r)\big).$$

For $r > 0$ small enough, $\overline{\mathsf{C}_{x_0}} \subset \Omega$ and $|\nabla f| \neq 0$ on $\partial\mathsf{C}_{x_0}$. Thus, C_{x_0} is a smooth open neighborhood of x_0 and $\nabla f \cdot \mathsf{n}_{\mathsf{C}_{x_0}} > 0$ on $\partial\mathsf{C}_{x_0}$. For all $x \in \partial\mathsf{C}_{x_0}$ and $s \in \mathbb{R}$, let $\gamma_x(s) := \varphi_x(-s)$ (see (12)) which satisfy for all $s \in \mathbb{R}$

$$\frac{d}{dt}\gamma_x(s) = \nabla f(\varphi_x(s)) \text{ with } \gamma_x(0) = x.$$

Let us define for all $x \in \partial\mathsf{C}_{x_0}$,

$$s_\Omega(x) := \inf\{s \geqslant 0,\ \gamma_x(s) \notin \Omega\}.$$

The proof of Proposition 29 follows exactly the same lines as the proof of Proposition 28 if one shows that s_Ω is lower semicontinuous. The difference here, comparing $s_{\Gamma_{z_k}}$ (see (259)) and s_Ω, is that s_Ω can be infinite due to the existence of critical points of f on $\partial\Omega$. Let us thus prove that $s_\Omega : \partial\mathsf{C}_{x_0} \to \mathbb{R}_+ \cup \{+\infty\}$ is lower semicontinuous. To this end, let $(x_n)_{n\geqslant 0}$ be a sequence in $\partial\mathsf{C}_{x_0}$ converging to $x_\infty \in \partial\mathsf{C}_{x_0}$ and $s_* \in \mathbb{R}_+ \cup \{+\infty\}$ a limit of a subsequence of $(s_\Omega(x_n))_{n\geqslant 0}$. For ease of notation, up to extracting a subsequence, we assume that $s_\Omega(x_n) \to s_*$ when $n \to +\infty$. If $s_* = +\infty$ then, $s^* \geqslant s_\Omega(x_\infty)$. Let us now consider the case when $s^* < +\infty$. In particular, $s_\Omega(x_n)$ is finite for n large enough. In this case, $s_\Omega(x_\infty) \leqslant s_*$ by the same proof as the one made to show (260). In conclusion s_Ω is lower semicontinuous. Then, the same arguments as those used to prove Proposition 28 allows us to conclude the proof of Proposition 29. □

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